



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:35 AM UTC

PDB ID : 6CUL / pdb_00006cul
Title : PvdF of pyoverdinin biosynthesis is a structurally unique N10-formyltetrahydrofolate-dependent formyltransferase
Authors : Kenjic, N.; Hoag, M.R.; Moraski, G.C.; Caperelli, C.A.; Moran, G.R.; Lamb, A.L.
Deposited on : 2018-03-26
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

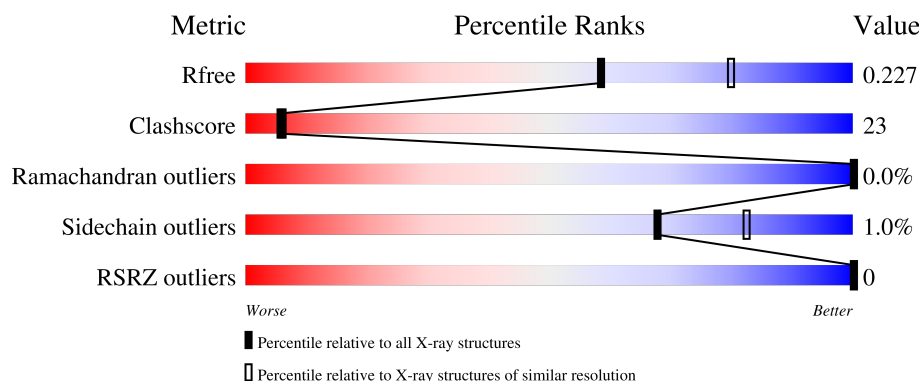
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



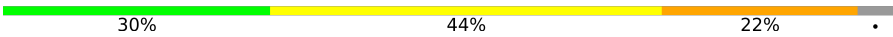
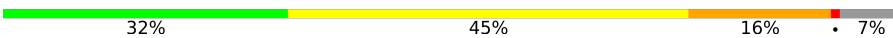
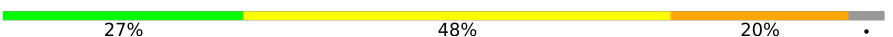
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	29% 48% 19% ••
1	B	275	32% 45% 19% •
1	C	275	37% 43% 17% •
1	D	275	23% 52% 21% •

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Mol	Chain	Length	Quality of chain
1	E	275	
1	F	275	
1	G	275	
1	H	275	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FGD	C	301	-	X	-	-
2	FGD	E	301	-	X	X	-
3	CIT	F	302	-	X	-	-
3	CIT	G	302	-	-	X	-

2 Entry composition

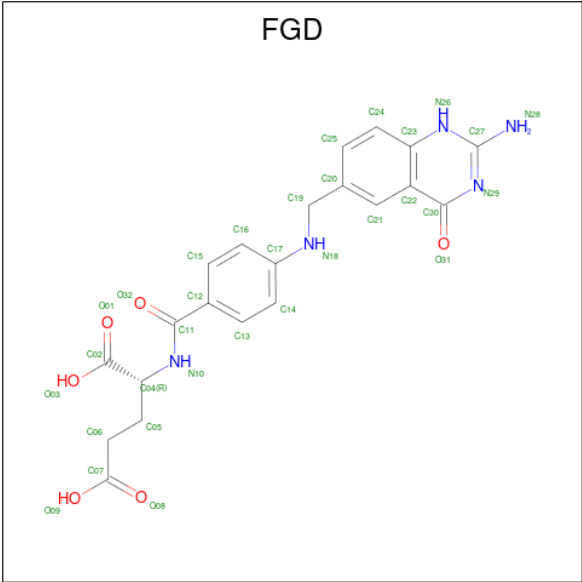
There are 4 unique types of molecules in this entry. The entry contains 34394 atoms, of which 16779 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyoverdine synthetase F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	H	N	O	Se	0	0	0
			4231	1368	2093	367	400	3			
1	B	263	Total	C	H	N	O	Se	0	0	0
			4167	1346	2059	362	397	3			
1	C	267	Total	C	H	N	O	Se	0	1	0
			4253	1374	2104	371	401	3			
1	D	267	Total	C	H	N	O	Se	0	0	0
			4239	1370	2098	367	401	3			
1	E	264	Total	C	H	N	O	Se	0	0	0
			4183	1353	2071	363	393	3			
1	F	257	Total	C	H	N	O	Se	0	0	0
			4075	1322	2016	351	383	3			
1	G	265	Total	C	H	N	O	Se	0	0	0
			4197	1358	2075	362	399	3			
1	H	267	Total	C	H	N	O	Se	0	0	0
			4224	1367	2090	363	401	3			

- Molecule 2 is N-(4-[(2-amino-4-oxo-1,4-dihydroquinazolin-6-yl)methyl]amino)benzene-1-carbonyl)-D-glutamic acid (CCD ID: FGD) (formula: C₂₁H₂₁N₅O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			51	21	19	5	6		
2	C	1	Total	C	H	N	O	0	0
			51	21	19	5	6		
2	D	1	Total	C	H	N	O	0	0
			51	21	19	5	6		
2	E	1	Total	C	H	N	O	0	0
			51	21	19	5	6		
2	F	1	Total	C	H	N	O	0	0
			51	21	19	5	6		
2	G	1	Total	C	H	N	O	0	0
			51	21	19	5	6		
2	H	1	Total	C	H	N	O	0	0
			51	21	19	5	6		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			18	6	5	7		
3	B	1	Total	C	H	O	0	0
			18	6	5	7		
3	C	1	Total	C	H	O	0	0
			18	6	5	7		
3	D	1	Total	C	H	O	0	0
			18	6	5	7		
3	E	1	Total	C	H	O	0	0
			18	6	5	7		
3	F	1	Total	C	H	O	0	0
			18	6	5	7		
3	G	1	Total	C	H	O	0	0
			18	6	5	7		
3	H	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	51	Total	O	0	0
			51	51		
4	C	32	Total	O	0	0
			32	32		
4	D	37	Total	O	0	0
			37	37		

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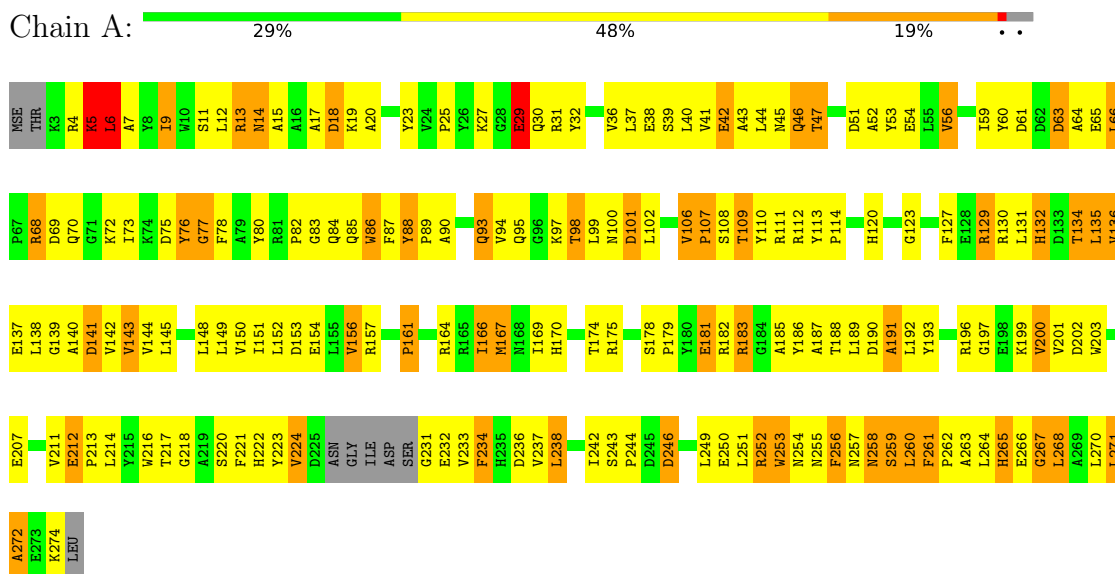
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	36	Total 36	O 36	0	0
4	F	33	Total 33	O 33	0	0
4	G	47	Total 47	O 47	0	0
4	H	45	Total 45	O 45	0	0

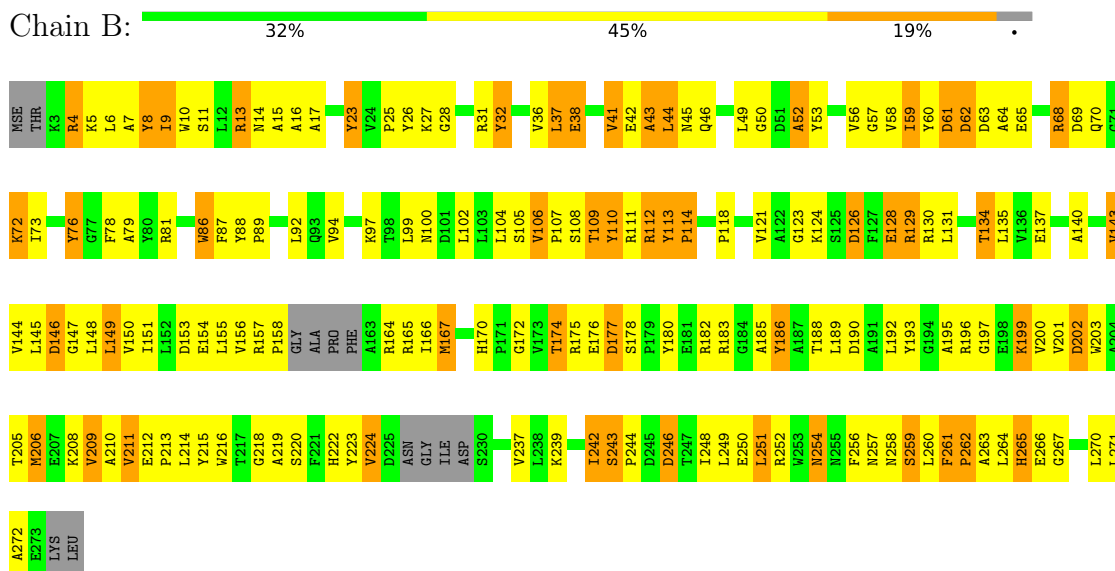
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyoverdine synthetase F

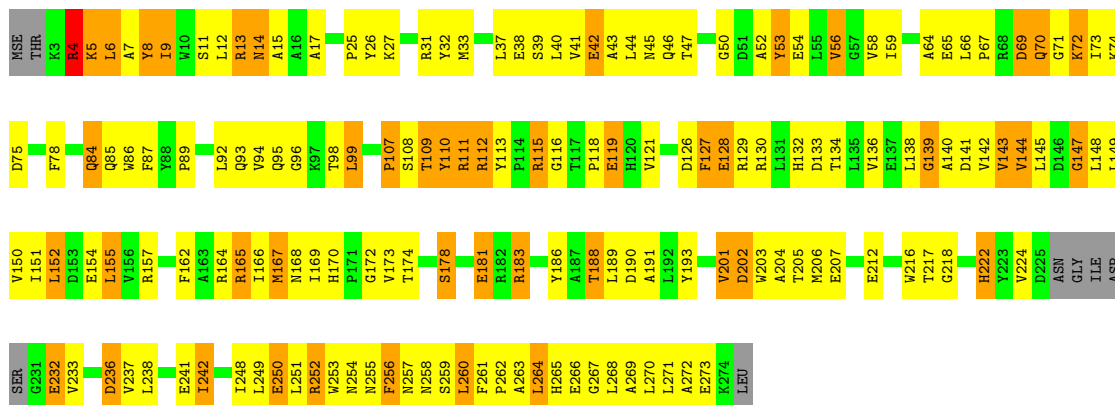


• Molecule 1: Pyoverdine synthetase F

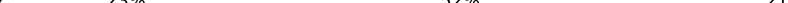


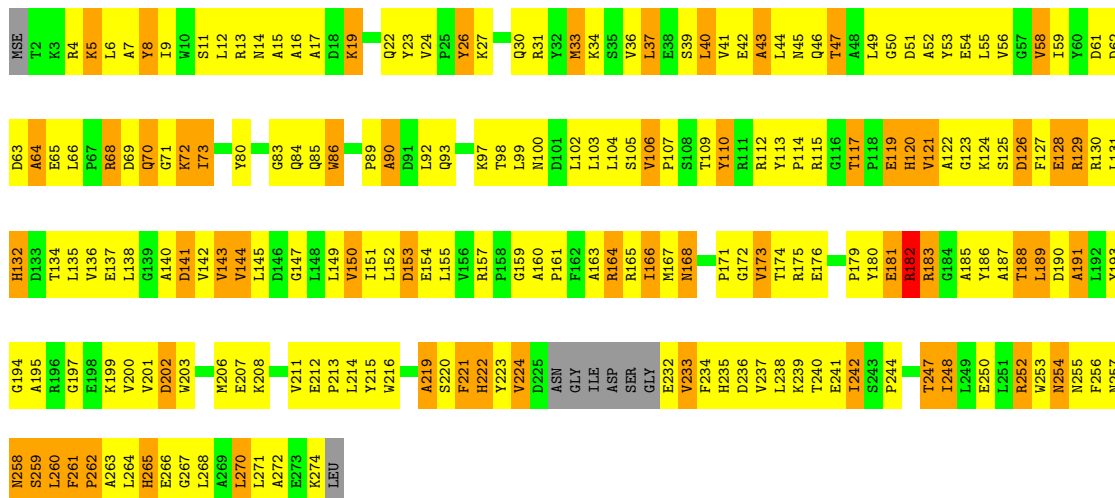
- Molecule 1: Pyoverdine synthetase F

Chain C:  37% 43% 17% .

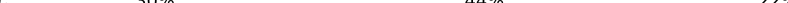


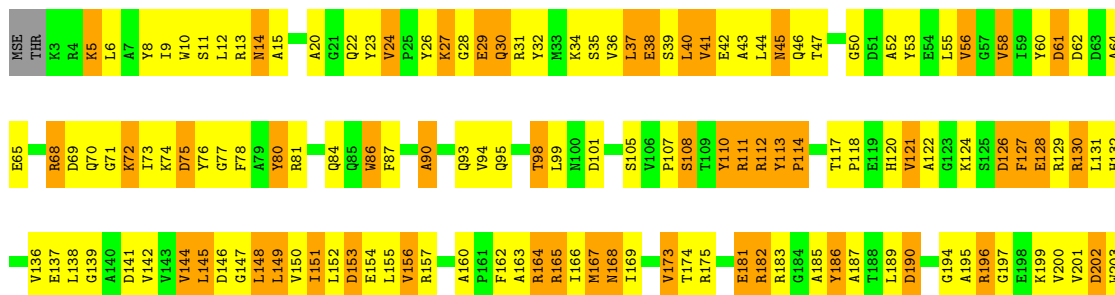
- Molecule 1: Pyoverdine synthetase F

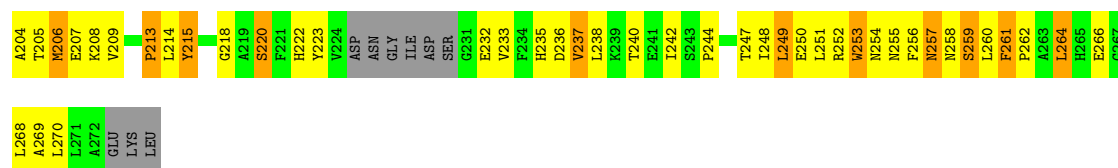
Chain D:  23% 52% 21% .



- Molecule 1: Pyoverdine synthetase F

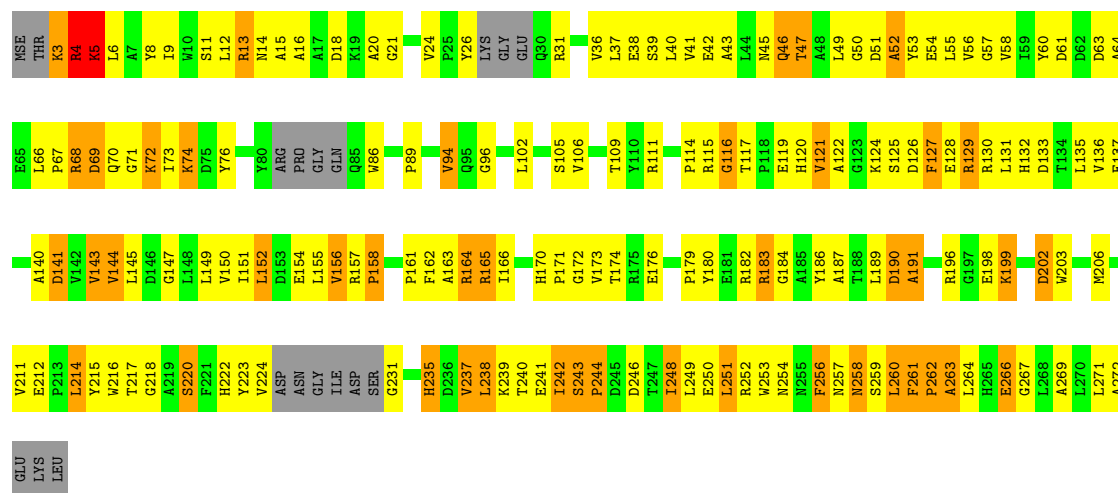
Chain E:  30% 44% 22% .





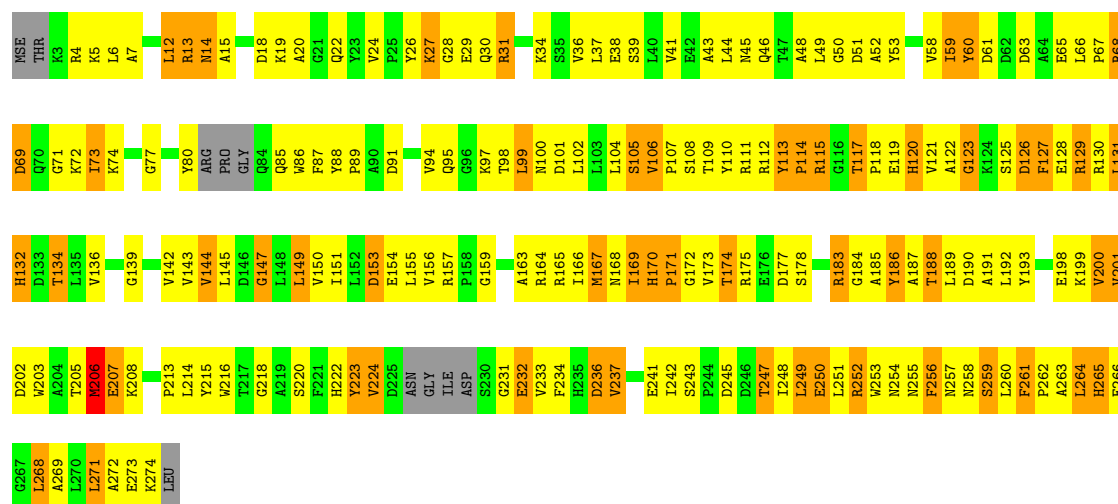
• Molecule 1: Pyoverdine synthetase F

Chain F: 32% 45% 16% 7%



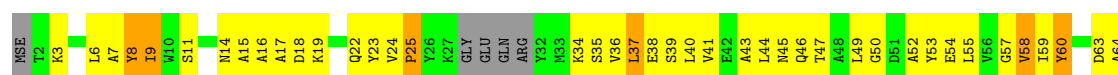
• Molecule 1: Pyoverdine synthetase F

Chain G: 27% 48% 20%



• Molecule 1: Pyoverdine synthetase F

Chain H: 29% 51% 17%



P262	A263	L264	L268	A269	L270	L271	A272	E273	K274	L275	G194	A195	R196	G197	E198	K199	V200	V201	D202	W203	A204	T205	M206	E207	K208	V209	P213	L214	Y215	W216	T217	G218	A219	S220	F221	H222	Y223	V224	D225	ASN	GLY	ILE	D229	S230	D236	V237	L238	E241	I242	S243	P244	D245	D246	L249	E250	L251	R252	W253	N254	N255	F256	N257	N258	S259	L260	F261	R129	R130	L131	H132	D133	T134	L135	V136	E137	L138	G139	A140	V143	V144	L145	D146	G147	L148	L149	V150	I151	L152	D153	E154	L155	V156	R157	F162	A163	R164	R165	I166	M167	N168	I169	H170	P171	G172	V173	T174	R175	E176	P179	Y180	E181	R182	R183	G184	A185	Y186	A187	T188	L189	D190	A191	L192	Y193	E128	F127	D126	S125	K124	L123	A122	V121	H120	E119	P118	T117	G116	R115	P114	Y113	R112	Y110	T109	S108	P107	V106	S105	L104	L103	L102	D101	N100	L99	V94	R93	L92	D91	A90	P89	Y88	F87	W86	Q85	Q84	G83	P82	R81	Y80	A79	F78	G77	Y76	I73	K72	G71	Q70	D69	R68	P67	L66	E65
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.99Å 92.77Å 127.58Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	38.76 – 2.30 38.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.8 (38.76-2.30) 91.0 (38.76-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.227 , 0.249 0.207 , 0.227	Depositor DCC
R_{free} test set	6150 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.317 for -l,k,h 0.389 for -h,-k,l 0.299 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34394	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7216e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FGD, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.40	115/2187 (5.3%)	1.49	35/2967 (1.2%)
1	B	2.49	124/2154 (5.8%)	1.53	31/2921 (1.1%)
1	C	2.47	130/2198 (5.9%)	1.45	21/2981 (0.7%)
1	D	2.56	153/2190 (7.0%)	1.46	31/2972 (1.0%)
1	E	2.46	124/2161 (5.7%)	1.51	24/2933 (0.8%)
1	F	2.37	107/2105 (5.1%)	1.44	28/2856 (1.0%)
1	G	2.50	134/2169 (6.2%)	1.56	30/2941 (1.0%)
1	H	2.60	148/2182 (6.8%)	1.51	24/2961 (0.8%)
All	All	2.48	1035/17346 (6.0%)	1.49	224/23532 (1.0%)

All (1035) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	PRO	N-CD	-14.23	1.27	1.47
1	B	114	PRO	N-CD	-14.19	1.27	1.47
1	G	218	GLY	C-O	-11.97	1.15	1.23
1	H	67	PRO	N-CD	-11.83	1.31	1.47
1	B	158	PRO	N-CD	-11.47	1.31	1.47
1	C	237	VAL	C-O	-11.30	1.12	1.24
1	H	261	PHE	C-O	-10.89	1.14	1.24
1	D	219	ALA	N-CA	-10.79	1.32	1.45
1	D	220	SER	C-O	-10.65	1.12	1.24
1	H	36	VAL	C-O	-10.15	1.12	1.24
1	H	114	PRO	C-O	-10.10	1.12	1.23
1	B	106	VAL	N-CA	-9.72	1.39	1.46
1	A	237	VAL	C-O	-9.56	1.14	1.24
1	H	256	PHE	C-O	-9.48	1.13	1.24
1	D	150	VAL	C-O	-9.36	1.14	1.24
1	C	15	ALA	C-O	-9.35	1.13	1.24
1	B	107	PRO	C-O	-9.30	1.14	1.23
1	H	82	PRO	N-CD	-9.19	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	69	ASP	C-O	-9.07	1.13	1.24
1	B	150	VAL	C-O	-9.03	1.13	1.24
1	E	258	ASN	C-O	-9.03	1.13	1.24
1	E	261	PHE	C-O	-8.92	1.15	1.24
1	A	253	TRP	C-O	-8.87	1.14	1.24
1	G	119	GLU	C-O	-8.80	1.14	1.24
1	F	94	VAL	C-O	-8.80	1.14	1.24
1	H	242	ILE	C-O	-8.75	1.15	1.24
1	H	259	SER	C-O	-8.71	1.12	1.24
1	H	220	SER	C-O	-8.67	1.13	1.24
1	C	218	GLY	C-O	-8.65	1.17	1.23
1	H	129	ARG	C-O	-8.61	1.13	1.24
1	H	121	VAL	C-O	-8.56	1.14	1.24
1	D	69	ASP	C-O	-8.51	1.14	1.24
1	F	186	TYR	N-CA	-8.49	1.36	1.46
1	H	41	VAL	C-O	-8.49	1.14	1.24
1	D	36	VAL	C-O	-8.46	1.14	1.24
1	H	150	VAL	C-O	-8.46	1.14	1.24
1	F	242	ILE	C-O	-8.46	1.15	1.24
1	B	261	PHE	N-CA	-8.46	1.39	1.46
1	A	72	LYS	C-O	-8.45	1.13	1.24
1	G	134	THR	C-O	-8.41	1.14	1.24
1	G	200	VAL	C-O	-8.40	1.15	1.24
1	D	219	ALA	CA-C	-8.36	1.42	1.52
1	C	201	VAL	C-O	-8.35	1.16	1.24
1	G	172	GLY	C-O	-8.34	1.15	1.23
1	B	60	TYR	C-O	-8.29	1.13	1.23
1	H	255	ASN	C-O	-8.28	1.14	1.24
1	F	12	LEU	C-O	-8.28	1.13	1.24
1	D	171	PRO	CA-CB	-8.25	1.48	1.53
1	D	143	VAL	C-O	-8.24	1.15	1.24
1	A	166	ILE	C-O	-8.22	1.15	1.24
1	C	256	PHE	C-O	-8.22	1.14	1.24
1	G	254	ASN	C-O	-8.20	1.14	1.24
1	H	237	VAL	C-O	-8.18	1.15	1.24
1	H	172	GLY	C-O	-8.15	1.15	1.24
1	D	220	SER	CB-OG	-8.09	1.25	1.42
1	H	263	ALA	C-O	-8.08	1.14	1.24
1	D	168	ASN	C-O	-8.06	1.13	1.24
1	G	190	ASP	C-O	-8.05	1.14	1.24
1	A	242	ILE	C-O	-8.03	1.15	1.24
1	F	256	PHE	C-O	-7.99	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	C-O	-7.99	1.14	1.24
1	F	45	ASN	C-O	-7.99	1.14	1.24
1	H	126	ASP	C-O	-7.97	1.14	1.24
1	C	262	PRO	C-O	-7.96	1.14	1.24
1	H	253	TRP	C-O	-7.95	1.14	1.24
1	G	261	PHE	C-O	-7.90	1.17	1.24
1	A	259	SER	C-O	-7.90	1.14	1.24
1	C	111	ARG	C-O	-7.89	1.14	1.24
1	B	59	ILE	C-O	-7.86	1.15	1.24
1	C	252[A]	ARG	C-O	-7.85	1.14	1.24
1	C	252[B]	ARG	C-O	-7.85	1.14	1.24
1	D	207	GLU	C-O	-7.84	1.14	1.23
1	A	139	GLY	C-O	-7.84	1.13	1.24
1	C	193	TYR	C-O	-7.83	1.15	1.24
1	D	190	ASP	C-O	-7.82	1.15	1.24
1	F	60	TYR	C-O	-7.82	1.14	1.23
1	F	267	GLY	C-O	-7.80	1.14	1.23
1	D	43	ALA	C-O	-7.77	1.14	1.24
1	E	255	ASN	C-O	-7.77	1.14	1.24
1	E	37	LEU	C-O	-7.75	1.15	1.24
1	C	37	LEU	C-O	-7.71	1.15	1.24
1	C	45	ASN	C-O	-7.71	1.14	1.24
1	H	43	ALA	C-O	-7.69	1.15	1.24
1	E	70	GLN	C-O	-7.68	1.15	1.24
1	A	152	LEU	C-O	-7.68	1.14	1.24
1	G	269	ALA	C-O	-7.68	1.15	1.24
1	D	105	SER	C-O	-7.67	1.14	1.24
1	A	112	ARG	C-O	-7.67	1.15	1.24
1	H	40	LEU	C-O	-7.66	1.15	1.24
1	E	173	VAL	C-O	-7.66	1.16	1.24
1	G	69	ASP	C-O	-7.62	1.15	1.24
1	C	154	GLU	C-O	-7.61	1.15	1.24
1	D	149	LEU	C-O	-7.61	1.12	1.24
1	G	151	ILE	C-O	-7.61	1.16	1.24
1	H	128	GLU	C-O	-7.61	1.15	1.24
1	D	220	SER	CA-C	7.61	1.61	1.52
1	A	252	ARG	C-O	-7.60	1.15	1.24
1	H	164	ARG	C-O	-7.60	1.14	1.24
1	E	253	TRP	C-O	-7.60	1.15	1.24
1	B	144	VAL	C-O	-7.59	1.15	1.24
1	G	37	LEU	C-O	-7.59	1.15	1.24
1	D	161	PRO	C-O	-7.58	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	186	TYR	C-O	-7.58	1.14	1.24
1	F	172	GLY	C-O	-7.58	1.15	1.24
1	B	106	VAL	C-O	-7.57	1.15	1.24
1	B	109	THR	C-O	-7.55	1.14	1.24
1	B	37	LEU	C-O	-7.54	1.15	1.24
1	H	8	TYR	C-O	-7.53	1.14	1.23
1	D	98	THR	C-O	-7.53	1.14	1.24
1	A	101	ASP	C-O	-7.52	1.14	1.24
1	C	172	GLY	C-O	-7.51	1.15	1.24
1	C	254	ASN	C-O	-7.50	1.15	1.24
1	E	220	SER	C-O	-7.49	1.15	1.24
1	D	11	SER	C-O	-7.48	1.15	1.24
1	G	125	SER	C-O	-7.47	1.15	1.24
1	G	73	ILE	C-O	-7.46	1.15	1.24
1	G	188	THR	C-O	-7.45	1.15	1.24
1	H	254	ASN	C-O	-7.42	1.15	1.24
1	E	53	TYR	C-O	-7.41	1.14	1.24
1	D	63	ASP	C-O	-7.40	1.15	1.24
1	D	44	LEU	C-O	-7.39	1.15	1.24
1	H	251	LEU	C-O	-7.38	1.15	1.24
1	C	25	PRO	C-O	-7.37	1.15	1.23
1	E	122	ALA	C-O	-7.37	1.15	1.24
1	F	13	ARG	C-O	-7.36	1.15	1.24
1	B	69	ASP	C-O	-7.36	1.15	1.24
1	F	237	VAL	C-O	-7.36	1.16	1.24
1	G	12	LEU	C-O	-7.34	1.15	1.24
1	A	14	ASN	C-O	-7.33	1.15	1.24
1	G	264	LEU	C-O	-7.32	1.15	1.24
1	E	72	LYS	C-O	-7.32	1.15	1.24
1	E	42	GLU	C-O	-7.31	1.15	1.24
1	G	249	LEU	C-O	-7.30	1.15	1.24
1	F	264	LEU	C-O	-7.30	1.15	1.24
1	F	105	SER	C-O	-7.29	1.15	1.24
1	C	74	LYS	C-O	-7.28	1.15	1.24
1	D	151	ILE	C-O	-7.28	1.15	1.24
1	D	135	LEU	C-O	-7.28	1.15	1.24
1	H	58	VAL	C-O	-7.27	1.16	1.24
1	H	151	ILE	C-O	-7.27	1.15	1.24
1	B	72	LYS	C-O	-7.27	1.15	1.24
1	D	248	ILE	C-O	-7.26	1.15	1.24
1	F	248	ILE	C-O	-7.26	1.15	1.24
1	D	233	VAL	C-O	-7.26	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	260	LEU	C-O	-7.26	1.15	1.24
1	B	86	TRP	C-O	-7.26	1.14	1.23
1	A	76	TYR	C-O	-7.25	1.15	1.23
1	D	144	VAL	C-O	-7.25	1.16	1.24
1	B	129	ARG	C-O	-7.25	1.15	1.24
1	C	40	LEU	C-O	-7.24	1.15	1.24
1	D	185	ALA	C-O	-7.23	1.15	1.24
1	H	132	HIS	C-O	-7.23	1.15	1.24
1	E	202	ASP	C-O	-7.23	1.15	1.23
1	B	186	TYR	C-O	-7.21	1.14	1.24
1	C	147	GLY	C-O	-7.21	1.14	1.24
1	H	182	ARG	C-O	-7.20	1.14	1.23
1	C	32	TYR	C-O	-7.19	1.15	1.24
1	D	102	LEU	C-O	-7.18	1.14	1.24
1	H	186	TYR	C-O	-7.15	1.14	1.24
1	C	134	THR	C-O	-7.15	1.15	1.24
1	D	124	LYS	C-O	-7.14	1.15	1.24
1	D	262	PRO	C-O	-7.14	1.15	1.24
1	C	47	THR	C-O	-7.14	1.16	1.23
1	A	47	THR	C-O	-7.14	1.14	1.23
1	B	123	GLY	C-O	-7.13	1.15	1.23
1	H	122	ALA	C-O	-7.13	1.15	1.24
1	D	126	ASP	C-O	-7.12	1.15	1.24
1	B	13	ARG	C-O	-7.10	1.15	1.24
1	C	249	LEU	C-O	-7.09	1.15	1.24
1	E	44	LEU	C-O	-7.09	1.16	1.24
1	F	15	ALA	C-O	-7.09	1.16	1.24
1	F	218	GLY	C-O	-7.09	1.16	1.23
1	G	15	ALA	C-O	-7.08	1.15	1.24
1	H	94	VAL	C-O	-7.07	1.16	1.24
1	D	92	LEU	C-O	-7.05	1.15	1.23
1	D	257	ASN	C-O	-7.05	1.16	1.24
1	B	8	TYR	C-O	-7.05	1.15	1.24
1	H	15	ALA	C-O	-7.05	1.15	1.24
1	G	191	ALA	C-O	-7.04	1.16	1.24
1	H	23	TYR	C-O	-7.04	1.15	1.23
1	C	253	TRP	C-O	-7.03	1.15	1.24
1	F	129	ARG	C-O	-7.03	1.16	1.24
1	C	167	MSE	C-O	-7.02	1.14	1.23
1	H	272	ALA	C-O	-7.01	1.16	1.24
1	G	108	SER	C-O	-6.99	1.16	1.23
1	B	267	GLY	C-O	-6.99	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219	ALA	C-O	-6.99	1.15	1.23
1	G	13	ARG	C-O	-6.99	1.16	1.24
1	E	114	PRO	CA-C	-6.99	1.44	1.52
1	A	249	LEU	C-O	-6.98	1.16	1.24
1	B	62	ASP	C-O	-6.97	1.15	1.23
1	H	174	THR	C-O	-6.97	1.14	1.24
1	D	253	TRP	C-O	-6.97	1.16	1.24
1	F	257	ASN	C-O	-6.97	1.16	1.24
1	G	149	LEU	C-O	-6.96	1.14	1.24
1	A	40	LEU	C-O	-6.96	1.16	1.24
1	E	111	ARG	C-O	-6.96	1.15	1.24
1	G	131	LEU	C-O	-6.96	1.16	1.24
1	G	22	GLN	C-O	-6.95	1.15	1.23
1	G	252	ARG	C-O	-6.95	1.16	1.24
1	B	11	SER	C-O	-6.95	1.16	1.24
1	D	219	ALA	C-N	-6.94	1.24	1.33
1	D	17	ALA	C-O	-6.94	1.16	1.24
1	H	77	GLY	C-O	-6.94	1.15	1.23
1	D	153	ASP	C-O	-6.94	1.15	1.24
1	F	122	ALA	C-O	-6.93	1.16	1.24
1	H	181	GLU	C-O	-6.93	1.15	1.24
1	E	58	VAL	C-O	-6.93	1.16	1.24
1	G	241	GLU	C-O	-6.93	1.15	1.23
1	A	261	PHE	C-O	-6.92	1.18	1.24
1	B	68	ARG	C-O	-6.92	1.16	1.24
1	C	250	GLU	C-O	-6.91	1.16	1.24
1	A	68	ARG	C-O	-6.91	1.15	1.24
1	G	253	TRP	C-O	-6.91	1.16	1.24
1	D	71	GLY	C-O	-6.90	1.15	1.23
1	B	6	LEU	C-O	-6.90	1.15	1.24
1	C	270	LEU	C-O	-6.90	1.15	1.24
1	G	186	TYR	C-O	-6.90	1.15	1.24
1	F	250	GLU	C-O	-6.89	1.16	1.24
1	C	139	GLY	C-O	-6.89	1.16	1.24
1	G	248	ILE	C-O	-6.89	1.16	1.24
1	A	181	GLU	C-O	-6.87	1.15	1.23
1	H	134	THR	C-O	-6.87	1.16	1.24
1	D	265	HIS	C-O	-6.87	1.16	1.24
1	D	40	LEU	C-O	-6.87	1.16	1.24
1	G	243	SER	C-O	-6.87	1.16	1.23
1	H	145	LEU	C-O	-6.86	1.15	1.24
1	C	233	VAL	C-O	-6.85	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	TYR	C-O	-6.85	1.14	1.24
1	G	129	ARG	C-O	-6.84	1.16	1.24
1	A	191	ALA	C-O	-6.84	1.16	1.24
1	B	257	ASN	C-O	-6.83	1.16	1.24
1	G	201	VAL	C-O	-6.83	1.16	1.24
1	G	222	HIS	C-O	-6.83	1.15	1.23
1	E	189	LEU	C-O	-6.82	1.16	1.24
1	H	100	ASN	C-O	-6.82	1.15	1.24
1	A	189	LEU	C-O	-6.81	1.16	1.24
1	C	170	HIS	C-O	-6.81	1.16	1.24
1	C	152	LEU	C-O	-6.81	1.15	1.23
1	D	89	PRO	C-O	-6.81	1.15	1.23
1	B	112	ARG	C-O	-6.81	1.16	1.24
1	F	16	ALA	C-O	-6.81	1.16	1.24
1	H	244	PRO	C-O	-6.81	1.15	1.24
1	G	89	PRO	C-O	-6.81	1.14	1.23
1	C	115	ARG	C-O	-6.80	1.15	1.23
1	D	13	ARG	C-O	-6.80	1.16	1.24
1	F	144	VAL	C-O	-6.80	1.16	1.24
1	A	144	VAL	C-O	-6.79	1.16	1.24
1	A	192	LEU	C-O	-6.79	1.16	1.24
1	A	39	SER	C-O	-6.79	1.16	1.24
1	D	59	ILE	C-O	-6.78	1.16	1.24
1	H	99	LEU	C-O	-6.78	1.16	1.24
1	B	213	PRO	C-O	-6.77	1.16	1.23
1	F	64	ALA	C-O	-6.77	1.15	1.24
1	C	265	HIS	C-O	-6.77	1.16	1.24
1	F	127	PHE	C-O	-6.76	1.16	1.24
1	F	51	ASP	C-O	-6.76	1.16	1.24
1	E	105	SER	C-O	-6.75	1.15	1.24
1	E	41	VAL	C-O	-6.75	1.16	1.24
1	E	132	HIS	C-O	-6.75	1.16	1.24
1	C	258	ASN	C-O	-6.74	1.16	1.24
1	C	269	ALA	C-O	-6.74	1.16	1.24
1	G	132	HIS	C-O	-6.73	1.16	1.24
1	B	108	SER	C-O	-6.73	1.15	1.23
1	C	54	GLU	C-O	-6.72	1.16	1.24
1	C	150	VAL	C-O	-6.72	1.16	1.24
1	H	190	ASP	C-O	-6.72	1.16	1.24
1	B	249	LEU	C-O	-6.70	1.16	1.24
1	D	234	PHE	C-O	-6.70	1.16	1.24
1	A	264	LEU	C-O	-6.69	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	60	TYR	C-O	-6.69	1.15	1.23
1	E	149	LEU	C-O	-6.69	1.16	1.24
1	G	113	TYR	C-O	-6.69	1.15	1.23
1	A	41	VAL	C-O	-6.68	1.16	1.24
1	G	251	LEU	C-O	-6.68	1.16	1.24
1	C	272	ALA	C-O	-6.68	1.16	1.24
1	F	4	ARG	C-O	-6.67	1.15	1.24
1	A	69	ASP	C-O	-6.67	1.15	1.24
1	G	126	ASP	C-O	-6.67	1.16	1.24
1	G	101	ASP	C-O	-6.66	1.15	1.24
1	D	66	LEU	C-O	-6.65	1.15	1.24
1	F	243	SER	C-O	-6.65	1.15	1.24
1	F	252	ARG	C-O	-6.65	1.16	1.24
1	D	129	ARG	C-O	-6.64	1.16	1.24
1	H	92	LEU	C-O	-6.64	1.16	1.23
1	D	42	GLU	C-O	-6.63	1.15	1.24
1	G	60	TYR	C-O	-6.63	1.15	1.23
1	E	45	ASN	C-O	-6.62	1.16	1.24
1	A	45	ASN	C-O	-6.59	1.16	1.24
1	B	70	GLN	C-O	-6.59	1.16	1.24
1	B	149	LEU	C-O	-6.59	1.15	1.24
1	A	266	GLU	C-O	-6.59	1.16	1.24
1	B	197	GLY	C-O	-6.58	1.15	1.24
1	G	233	VAL	C-O	-6.58	1.16	1.24
1	C	89	PRO	C-O	-6.58	1.15	1.23
1	G	170	HIS	C-O	-6.58	1.16	1.23
1	H	14	ASN	C-O	-6.58	1.16	1.24
1	A	256	PHE	C-O	-6.57	1.16	1.24
1	F	147	GLY	C-O	-6.57	1.14	1.23
1	C	257	ASN	C-O	-6.57	1.16	1.24
1	G	36	VAL	C-O	-6.56	1.16	1.24
1	C	242	ILE	C-O	-6.56	1.16	1.24
1	A	250	GLU	C-O	-6.55	1.16	1.24
1	E	128	GLU	C-O	-6.55	1.16	1.24
1	H	25	PRO	C-O	-6.55	1.16	1.23
1	A	136	VAL	C-O	-6.55	1.16	1.24
1	A	258	ASN	C-O	-6.55	1.16	1.24
1	D	256	PHE	C-O	-6.55	1.16	1.24
1	F	41	VAL	C-O	-6.54	1.16	1.24
1	F	238	LEU	C-O	-6.54	1.14	1.23
1	G	39	SER	C-O	-6.54	1.16	1.24
1	B	153	ASP	C-O	-6.54	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	123	GLY	C-O	-6.53	1.16	1.24
1	F	191	ALA	C-O	-6.53	1.16	1.24
1	G	220	SER	C-O	-6.53	1.16	1.24
1	A	59	ILE	C-O	-6.52	1.16	1.24
1	H	249	LEU	C-O	-6.52	1.16	1.24
1	F	187	ALA	C-O	-6.51	1.16	1.24
1	D	107	PRO	C-O	-6.51	1.16	1.23
1	H	140	ALA	C-O	-6.51	1.16	1.24
1	B	53	TYR	C-O	-6.51	1.15	1.23
1	C	96	GLY	C-O	-6.50	1.15	1.24
1	A	238	LEU	CA-C	-6.50	1.46	1.53
1	C	190	ASP	C-O	-6.50	1.16	1.24
1	C	8	TYR	C-O	-6.50	1.16	1.24
1	G	173	VAL	C-O	-6.50	1.16	1.24
1	D	53	TYR	C-O	-6.49	1.16	1.23
1	D	7	ALA	C-O	-6.48	1.16	1.24
1	H	59	ILE	C-O	-6.48	1.15	1.24
1	A	37	LEU	C-O	-6.48	1.16	1.24
1	H	120	HIS	C-O	-6.47	1.16	1.24
1	B	146	ASP	C-O	-6.47	1.16	1.23
1	D	93	GLN	C-O	-6.47	1.16	1.24
1	A	141	ASP	C-O	-6.46	1.16	1.24
1	E	165	ARG	C-O	-6.46	1.15	1.24
1	G	45	ASN	C-O	-6.46	1.16	1.24
1	G	100	ASN	C-O	-6.46	1.16	1.24
1	A	77	GLY	C-O	-6.45	1.15	1.23
1	H	124	LYS	C-O	-6.45	1.16	1.24
1	D	182	ARG	C-O	-6.45	1.15	1.23
1	E	256	PHE	C-O	-6.45	1.16	1.24
1	A	13	ARG	C-O	-6.43	1.16	1.24
1	H	200	VAL	C-O	-6.43	1.17	1.24
1	E	15	ALA	C-O	-6.42	1.16	1.24
1	D	122	ALA	C-O	-6.42	1.16	1.24
1	D	117	THR	C-O	-6.42	1.15	1.23
1	H	270	LEU	C-O	-6.42	1.16	1.24
1	A	170	HIS	C-O	-6.42	1.16	1.24
1	H	17	ALA	C-O	-6.41	1.16	1.24
1	D	247	THR	C-O	-6.41	1.15	1.23
1	D	39	SER	C-O	-6.41	1.16	1.24
1	A	102	LEU	C-O	-6.41	1.15	1.24
1	C	32	TYR	CA-C	-6.41	1.45	1.52
1	A	15	ALA	C-O	-6.41	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	18	ASP	C-O	-6.40	1.15	1.24
1	B	15	ALA	C-O	-6.40	1.16	1.24
1	E	22	GLN	C-O	-6.40	1.15	1.23
1	C	189	LEU	C-O	-6.39	1.16	1.24
1	F	50	GLY	C-O	-6.38	1.15	1.23
1	B	113	TYR	C-O	-6.38	1.15	1.24
1	D	120	HIS	C-O	-6.38	1.16	1.24
1	C	202	ASP	C-O	-6.38	1.16	1.23
1	E	62	ASP	C-O	-6.38	1.16	1.23
1	D	260	LEU	C-O	-6.37	1.16	1.24
1	H	84	GLN	C-O	-6.37	1.16	1.23
1	G	115	ARG	C-O	-6.36	1.16	1.23
1	H	46	GLN	C-O	-6.36	1.15	1.24
1	E	98	THR	C-O	-6.36	1.16	1.24
1	G	271	LEU	C-O	-6.35	1.15	1.24
1	H	264	LEU	N-CA	-6.35	1.38	1.46
1	C	132	HIS	C-O	-6.34	1.16	1.24
1	G	163	ALA	C-O	-6.34	1.16	1.24
1	E	197	GLY	C-O	-6.33	1.15	1.23
1	D	237	VAL	C-O	-6.33	1.17	1.23
1	D	15	ALA	C-O	-6.31	1.16	1.24
1	F	253	TRP	C-O	-6.31	1.16	1.24
1	G	188	THR	N-CA	-6.31	1.38	1.46
1	C	224	VAL	C-O	-6.31	1.17	1.24
1	G	41	VAL	C-O	-6.30	1.16	1.24
1	D	221	PHE	C-O	-6.30	1.16	1.24
1	B	134	THR	C-O	-6.30	1.16	1.24
1	C	64	ALA	C-O	-6.30	1.16	1.24
1	D	271	LEU	C-O	-6.30	1.15	1.24
1	G	106	VAL	C-O	-6.30	1.16	1.24
1	G	272	ALA	C-O	-6.30	1.16	1.24
1	B	246	ASP	C-O	-6.29	1.16	1.23
1	B	126	ASP	C-O	-6.29	1.16	1.24
1	H	268	LEU	C-O	-6.29	1.16	1.24
1	A	218	GLY	C-O	-6.28	1.15	1.23
1	D	188	THR	C-O	-6.28	1.16	1.24
1	G	145	LEU	C-O	-6.28	1.16	1.24
1	G	165	ARG	C-O	-6.28	1.15	1.24
1	C	39	SER	C-O	-6.28	1.16	1.24
1	F	47	THR	C-O	-6.28	1.15	1.23
1	D	47	THR	C-O	-6.27	1.16	1.23
1	E	71	GLY	C-O	-6.27	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	141	ASP	C-O	-6.27	1.15	1.24
1	F	189	LEU	C-O	-6.27	1.16	1.24
1	G	139	GLY	C-O	-6.26	1.17	1.24
1	G	171	PRO	C-O	-6.25	1.15	1.24
1	E	264	LEU	C-O	-6.25	1.16	1.24
1	E	47	THR	C-O	-6.24	1.15	1.23
1	E	99	LEU	C-O	-6.24	1.16	1.24
1	H	262	PRO	C-O	-6.24	1.16	1.24
1	F	161	PRO	C-O	-6.24	1.16	1.24
1	H	188	THR	C-O	-6.24	1.16	1.24
1	D	134	THR	C-O	-6.20	1.17	1.24
1	E	38	GLU	C-O	-6.20	1.16	1.24
1	C	98	THR	C-O	-6.19	1.16	1.24
1	H	152	LEU	C-O	-6.19	1.16	1.23
1	C	92	LEU	C-O	-6.19	1.16	1.23
1	A	222	HIS	C-O	-6.18	1.16	1.23
1	H	137	GLU	C-O	-6.18	1.16	1.24
1	G	247	THR	C-O	-6.17	1.15	1.23
1	B	43	ALA	C-O	-6.17	1.17	1.24
1	C	87	PHE	C-O	-6.16	1.16	1.24
1	C	69	ASP	C-O	-6.16	1.17	1.24
1	G	59	ILE	C-O	-6.15	1.17	1.24
1	A	261	PHE	N-CA	-6.15	1.40	1.46
1	G	178	SER	C-O	-6.15	1.17	1.24
1	C	71	GLY	C-O	-6.14	1.16	1.23
1	C	164	ARG	C-O	-6.14	1.15	1.24
1	G	72	LYS	C-O	-6.13	1.17	1.24
1	G	156	VAL	C-O	-6.13	1.17	1.24
1	A	151	ILE	C-O	-6.13	1.17	1.24
1	H	250	GLU	C-O	-6.12	1.17	1.24
1	F	24	VAL	C-O	-6.12	1.16	1.24
1	C	166	ILE	C-O	-6.11	1.17	1.24
1	F	56	VAL	C-O	-6.11	1.16	1.24
1	G	63	ASP	C-O	-6.11	1.16	1.24
1	D	51	ASP	C-O	-6.11	1.16	1.24
1	C	173	VAL	C-O	-6.10	1.16	1.24
1	E	148	LEU	C-O	-6.10	1.16	1.24
1	G	97	LYS	C-O	-6.10	1.16	1.24
1	C	188	THR	C-O	-6.10	1.17	1.24
1	E	114	PRO	C-O	-6.10	1.16	1.23
1	G	144	VAL	C-O	-6.10	1.17	1.24
1	E	153	ASP	C-O	-6.09	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	238	LEU	C-O	-6.08	1.15	1.23
1	B	64	ALA	C-O	-6.08	1.16	1.24
1	B	110	TYR	N-CA	-6.08	1.38	1.46
1	G	26	TYR	C-O	-6.08	1.17	1.24
1	G	169	ILE	C-O	-6.08	1.17	1.24
1	C	168	ASN	C-O	-6.07	1.16	1.23
1	H	38	GLU	C-O	-6.06	1.17	1.24
1	G	102	LEU	C-O	-6.06	1.15	1.24
1	B	272	ALA	C-O	-6.06	1.16	1.24
1	D	97	LYS	C-O	-6.05	1.16	1.23
1	B	41	VAL	N-CA	-6.05	1.39	1.46
1	E	56	VAL	C-O	-6.05	1.18	1.24
1	A	265	HIS	C-O	-6.04	1.17	1.24
1	H	162	PHE	C-O	-6.04	1.16	1.24
1	E	260	LEU	C-O	-6.04	1.17	1.24
1	H	112	ARG	C-O	-6.04	1.16	1.24
1	B	271	LEU	C-O	-6.04	1.16	1.24
1	A	107	PRO	C-O	-6.03	1.16	1.23
1	F	212	GLU	CA-C	-6.03	1.46	1.52
1	G	242	ILE	C-O	-6.03	1.17	1.24
1	H	111	ARG	C-O	-6.02	1.16	1.24
1	H	101	ASP	C-O	-6.02	1.16	1.24
1	D	45	ASN	C-O	-6.02	1.17	1.24
1	B	25	PRO	C-O	-6.01	1.18	1.23
1	A	185	ALA	C-O	-6.01	1.16	1.24
1	E	168	ASN	C-O	-6.01	1.16	1.24
1	H	125	SER	N-CA	-6.01	1.39	1.46
1	E	27	LYS	CA-C	-6.00	1.46	1.53
1	H	63	ASP	C-O	-6.00	1.17	1.23
1	F	249	LEU	C-O	-6.00	1.17	1.24
1	C	268	LEU	C-O	-5.99	1.16	1.24
1	C	126	ASP	C-O	-5.99	1.16	1.24
1	C	127	PHE	C-O	-5.99	1.17	1.24
1	F	120	HIS	C-O	-5.99	1.17	1.24
1	E	136	VAL	C-O	-5.99	1.17	1.24
1	D	125	SER	C-O	-5.98	1.17	1.24
1	G	52	ALA	C-O	-5.97	1.16	1.24
1	H	173	VAL	C-O	-5.97	1.17	1.24
1	H	105	SER	C-O	-5.97	1.16	1.24
1	D	173	VAL	C-O	-5.97	1.17	1.24
1	E	14	ASN	C-O	-5.96	1.17	1.24
1	G	114	PRO	C-O	-5.96	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	39	SER	C-O	-5.95	1.17	1.24
1	D	27	LYS	C-O	-5.95	1.17	1.24
1	D	61	ASP	C-O	-5.95	1.15	1.24
1	D	132	HIS	C-O	-5.95	1.17	1.24
1	F	131	LEU	C-O	-5.95	1.17	1.24
1	D	8	TYR	C-O	-5.95	1.16	1.24
1	B	130	ARG	C-O	-5.94	1.16	1.24
1	C	72	LYS	C-O	-5.94	1.17	1.24
1	B	218	GLY	C-O	-5.93	1.16	1.23
1	E	190	ASP	C-O	-5.93	1.16	1.24
1	C	267	GLY	C-O	-5.92	1.16	1.23
1	G	232	GLU	C-O	-5.92	1.16	1.24
1	H	115	ARG	C-O	-5.92	1.16	1.23
1	F	86	TRP	C-O	-5.92	1.16	1.23
1	F	215	TYR	C-O	-5.92	1.16	1.24
1	C	99	LEU	C-O	-5.92	1.17	1.24
1	E	182	ARG	C-O	-5.92	1.15	1.23
1	C	264	LEU	C-O	-5.91	1.17	1.24
1	F	261	PHE	C-O	-5.90	1.18	1.24
1	C	9	ILE	C-O	-5.90	1.18	1.24
1	B	262	PRO	C-O	-5.90	1.16	1.24
1	H	47	THR	C-O	-5.89	1.16	1.23
1	H	264	LEU	C-O	-5.89	1.17	1.24
1	H	49	LEU	C-O	-5.88	1.16	1.24
1	H	203	TRP	C-O	-5.88	1.16	1.24
1	D	240	THR	N-CA	-5.88	1.39	1.46
1	H	198	GLU	C-O	-5.87	1.16	1.23
1	E	13	ARG	C-O	-5.87	1.16	1.24
1	A	111	ARG	C-O	-5.87	1.16	1.24
1	A	236	ASP	C-O	-5.87	1.17	1.23
1	D	100	ASN	C-O	-5.86	1.16	1.24
1	B	87	PHE	C-O	-5.86	1.16	1.24
1	F	63	ASP	C-O	-5.86	1.17	1.24
1	A	36	VAL	C-O	-5.86	1.17	1.24
1	B	121	VAL	C-O	-5.86	1.17	1.24
1	E	144	VAL	C-O	-5.86	1.18	1.24
1	E	147	GLY	C-O	-5.86	1.17	1.24
1	E	52	ALA	C-O	-5.86	1.17	1.24
1	F	72	LYS	C-O	-5.85	1.16	1.24
1	C	255	ASN	C-O	-5.85	1.17	1.24
1	D	110	TYR	C-O	-5.84	1.16	1.24
1	B	105	SER	C-O	-5.84	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	PHE	C-O	-5.84	1.17	1.24
1	C	238	LEU	C-O	-5.84	1.16	1.23
1	F	140	ALA	C-O	-5.84	1.17	1.24
1	H	87	PHE	C-O	-5.84	1.16	1.24
1	B	203	TRP	C-O	-5.84	1.16	1.24
1	C	58	VAL	C-O	-5.84	1.17	1.24
1	A	66	LEU	C-O	-5.84	1.17	1.24
1	H	39	SER	C-O	-5.83	1.17	1.24
1	B	16	ALA	C-O	-5.83	1.17	1.24
1	B	265	HIS	C-O	-5.83	1.17	1.24
1	F	89	PRO	C-O	-5.83	1.16	1.23
1	G	147	GLY	C-O	-5.83	1.17	1.24
1	H	202	ASP	C-O	-5.82	1.17	1.23
1	E	93	GLN	C-O	-5.82	1.16	1.23
1	G	98	THR	C-O	-5.82	1.17	1.24
1	G	192	LEU	N-CA	-5.82	1.39	1.46
1	B	199	LYS	C-O	-5.82	1.17	1.24
1	G	167	MSE	C-O	-5.82	1.16	1.24
1	C	261	PHE	N-CA	-5.81	1.41	1.46
1	H	7	ALA	C-O	-5.81	1.16	1.24
1	G	185	ALA	C-O	-5.81	1.16	1.24
1	B	266	GLU	C-O	-5.81	1.17	1.24
1	F	171	PRO	CA-CB	-5.81	1.50	1.53
1	A	263	ALA	C-O	-5.81	1.17	1.24
1	G	214	LEU	C-O	-5.80	1.16	1.24
1	G	236	ASP	C-O	-5.80	1.16	1.23
1	C	129	ARG	C-O	-5.80	1.17	1.24
1	C	263	ALA	C-O	-5.80	1.17	1.24
1	G	153	ASP	C-O	-5.80	1.16	1.24
1	G	187	ALA	C-O	-5.80	1.17	1.24
1	B	260	LEU	C-O	-5.79	1.17	1.24
1	C	138	LEU	C-O	-5.79	1.16	1.24
1	H	86	TRP	C-O	-5.79	1.16	1.23
1	A	169	ILE	C-O	-5.79	1.17	1.24
1	E	108	SER	C-O	-5.79	1.16	1.23
1	E	214	LEU	C-O	-5.79	1.17	1.24
1	E	162	PHE	C-O	-5.78	1.15	1.23
1	H	68	ARG	C-O	-5.78	1.17	1.24
1	E	68	ARG	C-O	-5.78	1.17	1.24
1	H	53	TYR	C-O	-5.78	1.16	1.23
1	B	263	ALA	C-O	-5.78	1.17	1.24
1	C	157	ARG	CA-C	-5.78	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	LEU	CA-C	5.78	1.60	1.52
1	C	149	LEU	C-O	-5.77	1.15	1.24
1	C	212	GLU	CA-C	-5.77	1.47	1.53
1	D	41	VAL	C-O	-5.77	1.17	1.24
1	E	261	PHE	N-CA	-5.77	1.41	1.46
1	B	222	HIS	C-O	-5.76	1.16	1.23
1	G	68	ARG	C-O	-5.76	1.17	1.24
1	A	246	ASP	CG-OD1	-5.76	1.14	1.25
1	A	251	LEU	C-O	-5.75	1.17	1.24
1	A	255	ASN	C-O	-5.75	1.17	1.24
1	G	87	PHE	C-O	-5.75	1.16	1.24
1	G	224	VAL	C-O	-5.75	1.16	1.24
1	H	109	THR	C-O	-5.75	1.17	1.24
1	F	158	PRO	C-O	-5.75	1.17	1.23
1	A	17	ALA	C-O	-5.75	1.17	1.24
1	H	44	LEU	C-O	-5.75	1.17	1.24
1	E	150	VAL	C-O	-5.75	1.17	1.24
1	E	236	ASP	C-O	-5.75	1.16	1.23
1	G	255	ASN	C-O	-5.74	1.17	1.24
1	F	46	GLN	C-O	-5.74	1.16	1.24
1	G	44	LEU	N-CA	-5.74	1.39	1.46
1	E	164	ARG	C-O	-5.74	1.16	1.24
1	H	139	GLY	C-O	-5.73	1.17	1.24
1	D	70	GLN	C-O	-5.72	1.17	1.24
1	E	10	TRP	C-O	-5.72	1.16	1.24
1	H	260	LEU	C-O	-5.72	1.17	1.24
1	C	136	VAL	C-O	-5.72	1.17	1.24
1	D	172	GLY	C-O	-5.72	1.18	1.23
1	D	254	ASN	C-O	-5.71	1.17	1.24
1	B	237	VAL	C-O	-5.71	1.18	1.24
1	B	68	ARG	CZ-NH2	-5.71	1.26	1.33
1	B	209	VAL	C-O	-5.71	1.18	1.24
1	H	88	TYR	C-O	-5.71	1.17	1.24
1	H	156	VAL	C-O	-5.71	1.18	1.24
1	C	95	GLN	C-O	-5.71	1.15	1.23
1	E	20	ALA	C-O	-5.71	1.17	1.23
1	D	159	GLY	C-O	-5.70	1.16	1.24
1	H	37	LEU	C-O	-5.70	1.17	1.24
1	H	69	ASP	C-O	-5.70	1.17	1.24
1	A	63	ASP	C-O	-5.70	1.17	1.24
1	B	118	PRO	C-O	-5.70	1.16	1.24
1	H	271	LEU	C-O	-5.70	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	271	LEU	C-O	-5.70	1.16	1.24
1	D	267	GLY	C-O	-5.69	1.17	1.23
1	D	34	LYS	C-O	-5.69	1.17	1.23
1	G	120	HIS	C-O	-5.69	1.17	1.24
1	D	14	ASN	C-O	-5.69	1.17	1.24
1	A	267	GLY	C-O	-5.68	1.17	1.23
1	B	167	MSE	C-O	-5.68	1.16	1.23
1	G	268	LEU	C-O	-5.68	1.17	1.24
1	E	5	LYS	C-O	-5.67	1.17	1.24
1	G	73	ILE	N-CA	-5.67	1.39	1.46
1	C	7	ALA	C-O	-5.67	1.17	1.24
1	C	43	ALA	C-O	-5.67	1.17	1.24
1	B	264	LEU	C-O	-5.67	1.17	1.24
1	H	127	PHE	C-O	-5.67	1.17	1.24
1	C	31	ARG	C-O	-5.66	1.16	1.23
1	B	105	SER	C-N	-5.66	1.28	1.33
1	B	252	ARG	C-O	-5.66	1.17	1.24
1	E	130	ARG	C-O	-5.66	1.17	1.24
1	D	84	GLN	C-O	-5.66	1.17	1.23
1	D	109	THR	C-O	-5.66	1.16	1.24
1	F	14	ASN	C-O	-5.66	1.17	1.24
1	C	94	VAL	C-O	-5.65	1.17	1.24
1	B	270	LEU	C-O	-5.65	1.17	1.24
1	F	162	PHE	C-O	-5.65	1.16	1.24
1	G	121	VAL	C-O	-5.65	1.17	1.24
1	G	256	PHE	C-O	-5.65	1.17	1.24
1	D	220	SER	N-CA	-5.64	1.39	1.46
1	F	11	SER	C-O	-5.64	1.17	1.24
1	E	155	LEU	C-O	-5.64	1.17	1.24
1	H	9	ILE	C-O	-5.64	1.17	1.24
1	H	110	TYR	C-O	-5.63	1.16	1.24
1	H	16	ALA	C-O	-5.63	1.17	1.24
1	H	135	LEU	C-O	-5.63	1.17	1.24
1	H	199	LYS	C-O	-5.63	1.17	1.23
1	G	258	ASN	C-O	-5.63	1.16	1.24
1	D	212	GLU	CA-C	-5.63	1.47	1.53
1	E	213	PRO	C-O	-5.62	1.16	1.23
1	G	107	PRO	C-O	-5.62	1.17	1.23
1	A	268	LEU	C-O	-5.62	1.17	1.24
1	D	258	ASN	C-O	-5.62	1.17	1.24
1	E	186	TYR	N-CA	-5.62	1.39	1.46
1	A	89	PRO	C-O	-5.62	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	TYR	C-O	-5.62	1.17	1.24
1	F	21	GLY	C-O	-5.62	1.16	1.23
1	C	121	VAL	C-O	-5.61	1.17	1.24
1	C	110	TYR	C-O	-5.61	1.17	1.24
1	E	27	LYS	C-O	-5.61	1.17	1.23
1	A	179	PRO	C-O	-5.60	1.17	1.24
1	E	165	ARG	N-CA	-5.60	1.39	1.46
1	A	56	VAL	C-O	-5.60	1.17	1.23
1	D	37	LEU	C-O	-5.60	1.17	1.24
1	B	7	ALA	C-O	-5.60	1.17	1.23
1	F	251	LEU	C-O	-5.60	1.17	1.24
1	E	36	VAL	C-O	-5.59	1.17	1.24
1	A	113	TYR	C-O	-5.59	1.16	1.23
1	D	252	ARG	C-O	-5.59	1.17	1.24
1	G	265	HIS	C-O	-5.59	1.17	1.24
1	A	11	SER	C-O	-5.59	1.17	1.24
1	B	17	ALA	C-O	-5.59	1.17	1.24
1	F	202	ASP	C-O	-5.58	1.17	1.23
1	D	242	ILE	C-O	-5.58	1.18	1.24
1	H	50	GLY	C-O	-5.58	1.16	1.23
1	H	218	GLY	C-O	-5.57	1.16	1.23
1	B	14	ASN	C-O	-5.57	1.17	1.24
1	D	261	PHE	C-O	-5.57	1.19	1.24
1	B	254	ASN	C-O	-5.57	1.17	1.24
1	G	215	TYR	C-O	-5.57	1.16	1.24
1	F	115	ARG	C-O	-5.56	1.17	1.23
1	H	93	GLN	C-O	-5.56	1.16	1.23
1	D	166	ILE	C-O	-5.55	1.18	1.24
1	H	140	ALA	N-CA	-5.55	1.39	1.46
1	F	133	ASP	C-O	-5.55	1.17	1.24
1	H	123	GLY	C-O	-5.55	1.17	1.23
1	D	64	ALA	C-O	-5.55	1.17	1.24
1	D	72	LYS	C-O	-5.55	1.17	1.24
1	E	127	PHE	C-O	-5.54	1.17	1.24
1	E	151	ILE	C-O	-5.54	1.18	1.24
1	C	17	ALA	C-O	-5.54	1.17	1.24
1	F	220	SER	C-O	-5.54	1.17	1.24
1	C	232	GLU	C-O	-5.54	1.17	1.23
1	C	39	SER	N-CA	-5.53	1.39	1.46
1	E	35	SER	C-O	-5.53	1.16	1.23
1	A	86	TRP	C-O	-5.53	1.17	1.23
1	D	119	GLU	C-O	-5.53	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	THR	C-O	-5.53	1.16	1.24
1	G	189	LEU	C-O	-5.53	1.17	1.24
1	A	132	HIS	C-O	-5.53	1.17	1.24
1	H	131	LEU	C-O	-5.53	1.17	1.24
1	B	219	ALA	C-O	-5.52	1.17	1.23
1	C	4	ARG	C-O	-5.52	1.18	1.23
1	F	58	VAL	C-O	-5.52	1.18	1.24
1	D	73	ILE	N-CA	-5.52	1.40	1.46
1	D	136	VAL	C-O	-5.52	1.17	1.24
1	E	118	PRO	C-O	-5.51	1.17	1.24
1	D	164	ARG	C-O	-5.51	1.16	1.24
1	G	39	SER	N-CA	-5.51	1.39	1.46
1	F	140	ALA	N-CA	-5.50	1.39	1.46
1	A	60	TYR	C-O	-5.50	1.17	1.23
1	B	46	GLN	C-O	-5.50	1.16	1.24
1	G	20	ALA	C-O	-5.50	1.17	1.23
1	A	98	THR	C-O	-5.50	1.17	1.23
1	B	190	ASP	C-O	-5.50	1.17	1.24
1	D	187	ALA	C-O	-5.50	1.17	1.24
1	G	207	GLU	C-O	-5.50	1.17	1.24
1	F	190	ASP	C-O	-5.49	1.17	1.24
1	B	147	GLY	C-O	-5.49	1.18	1.24
1	H	24	VAL	N-CA	-5.49	1.41	1.46
1	G	178	SER	CA-C	-5.49	1.47	1.53
1	H	52	ALA	C-O	-5.49	1.17	1.24
1	D	137	GLU	C-O	-5.48	1.17	1.24
1	F	109	THR	C-O	-5.48	1.17	1.24
1	A	39	SER	N-CA	-5.48	1.39	1.46
1	A	42	GLU	C-O	-5.48	1.17	1.24
1	H	189	LEU	C-O	-5.47	1.17	1.24
1	H	194	GLY	C-O	-5.47	1.16	1.23
1	D	5	LYS	C-O	-5.47	1.17	1.24
1	H	258	ASN	C-O	-5.47	1.16	1.23
1	G	125	SER	CA-C	-5.46	1.45	1.52
1	G	257	ASN	C-O	-5.46	1.17	1.24
1	H	72	LYS	C-O	-5.46	1.17	1.24
1	A	143	VAL	C-O	-5.46	1.18	1.24
1	E	110	TYR	C-O	-5.46	1.17	1.24
1	G	77	GLY	C-O	-5.46	1.16	1.23
1	C	133	ASP	C-O	-5.46	1.17	1.24
1	E	181	GLU	C-O	-5.46	1.17	1.24
1	C	56	VAL	C-O	-5.45	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	GLY	C-O	-5.45	1.17	1.23
1	B	128	GLU	C-O	-5.45	1.17	1.24
1	D	126	ASP	CG-OD2	-5.45	1.15	1.25
1	B	170	HIS	C-O	-5.45	1.18	1.24
1	C	70	GLN	C-O	-5.45	1.17	1.24
1	D	268	LEU	C-O	-5.45	1.17	1.24
1	B	57	GLY	C-O	-5.45	1.18	1.24
1	A	5	LYS	C-O	-5.44	1.17	1.24
1	D	189	LEU	C-O	-5.44	1.17	1.24
1	B	205	THR	C-O	-5.43	1.16	1.24
1	B	78	PHE	C-O	-5.43	1.17	1.24
1	C	183	ARG	C-O	-5.43	1.16	1.23
1	A	233	VAL	C-O	-5.43	1.18	1.24
1	A	260	LEU	C-O	-5.42	1.17	1.24
1	E	12	LEU	C-O	-5.42	1.17	1.24
1	E	240	THR	C-O	-5.42	1.17	1.24
1	H	179	PRO	C-O	-5.42	1.18	1.23
1	A	109	THR	C-O	-5.42	1.17	1.24
1	D	68	ARG	C-O	-5.41	1.17	1.24
1	E	113	TYR	C-O	-5.41	1.18	1.24
1	A	70	GLN	C-O	-5.41	1.17	1.24
1	E	55	LEU	C-O	-5.41	1.17	1.24
1	B	9	ILE	C-O	-5.41	1.18	1.24
1	E	60	TYR	C-O	-5.41	1.17	1.23
1	C	130	ARG	CZ-NH2	-5.41	1.26	1.33
1	C	66	LEU	C-O	-5.40	1.17	1.24
1	C	261	PHE	C-O	-5.40	1.19	1.24
1	E	126	ASP	C-O	-5.40	1.17	1.24
1	G	118	PRO	C-O	-5.40	1.17	1.24
1	C	11	SER	C-O	-5.39	1.17	1.24
1	A	110	TYR	C-O	-5.39	1.17	1.24
1	C	93	GLN	C-O	-5.39	1.17	1.24
1	A	183	ARG	C-O	-5.39	1.16	1.23
1	A	234	PHE	C-O	-5.38	1.17	1.24
1	D	121	VAL	C-O	-5.38	1.17	1.24
1	A	272	ALA	N-CA	-5.38	1.39	1.46
1	F	266	GLU	C-O	-5.37	1.18	1.24
1	D	147	GLY	C-O	-5.37	1.18	1.24
1	G	122	ALA	C-O	-5.37	1.17	1.24
1	C	144	VAL	C-O	-5.37	1.18	1.24
1	D	179	PRO	C-O	-5.36	1.17	1.24
1	C	143	VAL	C-O	-5.36	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	54	GLU	C-O	-5.36	1.18	1.24
1	C	12	LEU	C-O	-5.36	1.17	1.24
1	B	188	THR	CB-CG2	-5.36	1.34	1.52
1	E	218	GLY	C-O	-5.36	1.17	1.24
1	F	222	HIS	C-O	-5.36	1.17	1.23
1	H	125	SER	C-O	-5.35	1.18	1.24
1	E	249	LEU	C-O	-5.34	1.17	1.24
1	C	14	ASN	C-O	-5.34	1.17	1.24
1	A	9	ILE	C-O	-5.34	1.18	1.24
1	B	100	ASN	C-O	-5.34	1.17	1.24
1	A	38	GLU	C-O	-5.34	1.17	1.24
1	B	28	GLY	C-O	-5.34	1.16	1.24
1	D	23	TYR	C-O	-5.34	1.17	1.24
1	H	126	ASP	CG-OD2	-5.34	1.15	1.25
1	F	66	LEU	C-O	-5.33	1.17	1.24
1	E	145	LEU	C-O	-5.33	1.17	1.24
1	H	66	LEU	C-O	-5.33	1.17	1.24
1	B	216	TRP	CB-CG	-5.33	1.33	1.50
1	F	8	TYR	C-O	-5.33	1.17	1.24
1	F	269	ALA	C-O	-5.33	1.17	1.24
1	G	18	ASP	C-O	-5.33	1.17	1.24
1	B	143	VAL	C-O	-5.32	1.18	1.24
1	B	165	ARG	C-O	-5.32	1.17	1.24
1	E	203	TRP	C-O	-5.32	1.17	1.24
1	E	80	TYR	N-CA	-5.32	1.39	1.46
1	A	212	GLU	C-O	-5.32	1.17	1.24
1	F	69	ASP	C-O	-5.32	1.17	1.24
1	F	135	LEU	C-O	-5.32	1.18	1.24
1	C	236	ASP	C-O	-5.31	1.17	1.23
1	D	167	MSE	N-CA	-5.31	1.39	1.45
1	D	138	LEU	C-O	-5.31	1.16	1.24
1	E	237	VAL	C-O	-5.31	1.18	1.24
1	D	106	VAL	C-O	-5.30	1.17	1.24
1	B	200	VAL	C-O	-5.30	1.18	1.24
1	E	87	PHE	C-O	-5.30	1.17	1.24
1	G	65	GLU	C-O	-5.30	1.17	1.24
1	E	187	ALA	C-O	-5.30	1.18	1.24
1	G	61	ASP	C-O	-5.30	1.16	1.23
1	B	44	LEU	C-O	-5.30	1.18	1.24
1	D	132	HIS	N-CA	-5.30	1.40	1.46
1	A	123	GLY	C-O	-5.30	1.17	1.23
1	H	35	SER	C-O	-5.29	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	ARG	C-O	-5.29	1.17	1.24
1	A	140	ALA	C-O	-5.29	1.17	1.24
1	C	53	TYR	C-O	-5.29	1.17	1.23
1	H	272	ALA	CA-C	-5.29	1.45	1.52
1	C	165	ARG	C-O	-5.29	1.16	1.24
1	F	246	ASP	CA-C	-5.29	1.45	1.52
1	A	85	GLN	C-O	-5.29	1.17	1.23
1	A	7	ALA	C-O	-5.29	1.17	1.24
1	A	216	TRP	C-O	-5.29	1.17	1.23
1	B	259	SER	C-O	-5.29	1.17	1.24
1	G	250	GLU	C-O	-5.28	1.18	1.24
1	C	86	TRP	C-O	-5.28	1.17	1.23
1	E	129	ARG	C-O	-5.28	1.17	1.24
1	B	248	ILE	C-O	-5.27	1.18	1.24
1	F	235	HIS	C-O	-5.27	1.17	1.23
1	C	42	GLU	C-O	-5.27	1.18	1.24
1	C	142	VAL	C-O	-5.27	1.18	1.23
1	F	143	VAL	C-O	-5.27	1.18	1.24
1	C	181	GLU	C-O	-5.27	1.17	1.24
1	B	58	VAL	C-O	-5.26	1.17	1.23
1	E	39	SER	N-CA	-5.26	1.40	1.46
1	D	30	GLN	C-O	-5.26	1.17	1.23
1	D	127	PHE	C-O	-5.26	1.18	1.24
1	A	187	ALA	C-O	-5.26	1.18	1.24
1	B	185	ALA	C-O	-5.26	1.17	1.24
1	E	121	VAL	C-O	-5.26	1.18	1.24
1	H	183	ARG	N-CA	-5.26	1.39	1.45
1	H	184	GLY	C-O	-5.26	1.16	1.24
1	H	259	SER	N-CA	-5.26	1.40	1.46
1	A	187	ALA	N-CA	-5.25	1.40	1.46
1	B	32	TYR	C-O	-5.25	1.17	1.24
1	B	201	VAL	C-O	-5.25	1.19	1.24
1	E	137	GLU	C-O	-5.25	1.18	1.24
1	H	197	GLY	C-O	-5.25	1.17	1.24
1	C	67	PRO	C-O	-5.24	1.17	1.24
1	D	255	ASN	C-O	-5.24	1.18	1.24
1	F	244	PRO	C-O	-5.24	1.17	1.24
1	C	155	LEU	C-O	-5.24	1.17	1.24
1	E	95	GLN	C-O	-5.24	1.17	1.23
1	A	23	TYR	C-O	-5.24	1.17	1.23
1	G	156	VAL	N-CA	-5.24	1.39	1.46
1	D	55	LEU	C-O	-5.24	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	40	LEU	C-O	-5.23	1.18	1.24
1	D	33	MSE	CA-C	-5.23	1.47	1.53
1	D	112	ARG	C-O	-5.23	1.18	1.24
1	B	178	SER	N-CA	-5.23	1.39	1.45
1	E	248	ILE	C-O	-5.23	1.18	1.24
1	D	191	ALA	C-O	-5.22	1.18	1.24
1	F	262	PRO	C-O	-5.22	1.18	1.24
1	H	236	ASP	C-O	-5.22	1.17	1.23
1	C	13	ARG	C-O	-5.22	1.17	1.24
1	D	90	ALA	C-O	-5.22	1.18	1.24
1	C	216	TRP	C-O	-5.22	1.17	1.23
1	D	86	TRP	C-O	-5.21	1.17	1.23
1	G	123	GLY	C-O	-5.21	1.17	1.23
1	D	16	ALA	C-O	-5.21	1.18	1.24
1	G	203	TRP	C-O	-5.21	1.18	1.24
1	E	24	VAL	C-N	-5.21	1.29	1.33
1	G	199	LYS	C-O	-5.21	1.18	1.24
1	H	45	ASN	C-O	-5.21	1.17	1.24
1	A	44	LEU	C-O	-5.21	1.18	1.24
1	G	136	VAL	C-O	-5.20	1.18	1.24
1	G	177	ASP	N-CA	-5.20	1.40	1.46
1	F	36	VAL	C-O	-5.20	1.18	1.24
1	F	173	VAL	C-O	-5.19	1.18	1.24
1	A	51	ASP	C-O	-5.19	1.17	1.24
1	B	89	PRO	C-O	-5.19	1.16	1.23
1	H	243	SER	C-O	-5.19	1.18	1.24
1	B	23	TYR	C-O	-5.18	1.17	1.24
1	B	178	SER	C-O	-5.18	1.18	1.24
1	G	216	TRP	C-O	-5.18	1.17	1.23
1	F	37	LEU	C-O	-5.18	1.18	1.24
1	C	266	GLU	C-O	-5.18	1.18	1.24
1	F	187	ALA	CA-C	-5.17	1.46	1.52
1	C	251	LEU	C-O	-5.17	1.18	1.24
1	H	208	LYS	C-O	-5.17	1.17	1.24
1	F	68	ARG	C-O	-5.17	1.18	1.24
1	F	212	GLU	C-O	-5.17	1.17	1.24
1	G	112	ARG	C-O	-5.17	1.18	1.24
1	A	271	LEU	C-O	-5.17	1.17	1.24
1	H	224	VAL	C-O	-5.17	1.18	1.24
1	F	74	LYS	C-O	-5.17	1.18	1.24
1	C	109	THR	C-O	-5.16	1.17	1.24
1	D	270	LEU	N-CA	-5.16	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	77	GLY	C-O	-5.16	1.17	1.23
1	E	131	LEU	C-O	-5.16	1.18	1.24
1	H	34	LYS	N-CA	-5.16	1.39	1.46
1	A	270	LEU	C-O	-5.16	1.18	1.24
1	D	263	ALA	C-O	-5.16	1.18	1.24
1	E	112	ARG	CZ-NH2	-5.16	1.26	1.33
1	H	64	ALA	C-O	-5.16	1.17	1.24
1	C	85	GLN	C-O	-5.16	1.17	1.23
1	C	178	SER	C-O	-5.16	1.17	1.23
1	G	67	PRO	C-O	-5.15	1.17	1.24
1	E	183	ARG	C-O	-5.15	1.17	1.23
1	A	264	LEU	N-CA	-5.15	1.40	1.46
1	E	43	ALA	C-O	-5.15	1.18	1.24
1	H	151	ILE	CA-C	-5.15	1.46	1.52
1	H	169	ILE	C-O	-5.15	1.17	1.23
1	A	257	ASN	C-O	-5.15	1.17	1.24
1	A	151	ILE	CA-C	-5.14	1.46	1.52
1	D	201	VAL	C-O	-5.14	1.18	1.24
1	D	220	SER	CA-CB	-5.14	1.45	1.53
1	G	237	VAL	C-O	-5.14	1.18	1.24
1	C	119	GLU	C-O	-5.14	1.18	1.24
1	A	200	VAL	C-O	-5.14	1.18	1.24
1	A	12	LEU	C-O	-5.14	1.17	1.24
1	A	221	PHE	C-O	-5.14	1.17	1.23
1	F	52	ALA	C-O	-5.14	1.18	1.24
1	B	36	VAL	C-O	-5.13	1.18	1.24
1	E	257	ASN	N-CA	-5.13	1.40	1.46
1	B	102	LEU	N-CA	-5.13	1.39	1.46
1	D	256	PHE	N-CA	-5.13	1.40	1.46
1	H	202	ASP	N-CA	-5.12	1.40	1.46
1	B	10	TRP	C-O	-5.12	1.17	1.23
1	A	190	ASP	CG-OD2	-5.12	1.15	1.25
1	E	107	PRO	C-O	-5.12	1.18	1.23
1	F	39	SER	C-O	-5.12	1.18	1.24
1	E	258	ASN	CG-OD1	-5.12	1.13	1.23
1	H	192	LEU	C-O	-5.12	1.18	1.24
1	A	43	ALA	C-O	-5.11	1.18	1.24
1	B	150	VAL	N-CA	-5.11	1.40	1.46
1	B	211	VAL	C-O	-5.11	1.17	1.23
1	B	88	TYR	C-O	-5.11	1.17	1.24
1	F	263	ALA	C-O	-5.11	1.18	1.24
1	E	185	ALA	C-O	-5.11	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	140	ALA	C-O	-5.11	1.17	1.23
1	E	236	ASP	CG-OD2	-5.11	1.15	1.25
1	E	235	HIS	C-O	-5.11	1.17	1.23
1	D	39	SER	N-CA	-5.11	1.40	1.46
1	F	165	ARG	C-O	-5.11	1.17	1.24
1	A	129	ARG	C-O	-5.10	1.18	1.24
1	D	83	GLY	C-O	-5.10	1.16	1.24
1	D	104	LEU	N-CA	-5.10	1.39	1.46
1	D	219	ALA	CA-CB	-5.10	1.41	1.54
1	D	183	ARG	C-O	-5.10	1.17	1.23
1	D	128	GLU	C-O	-5.10	1.18	1.24
1	A	32	TYR	C-O	-5.10	1.17	1.24
1	B	114	PRO	CA-CB	-5.10	1.46	1.53
1	D	202	ASP	C-O	-5.10	1.18	1.23
1	H	54	GLU	C-O	-5.10	1.18	1.24
1	E	269	ALA	C-O	-5.09	1.18	1.24
1	A	224	VAL	C-O	-5.09	1.18	1.24
1	D	52	ALA	C-O	-5.09	1.18	1.24
1	F	96	GLY	C-O	-5.09	1.17	1.23
1	G	99	LEU	C-O	-5.09	1.18	1.24
1	A	191	ALA	N-CA	-5.09	1.40	1.46
1	B	126	ASP	CG-OD2	-5.09	1.15	1.25
1	B	202	ASP	C-O	-5.09	1.17	1.23
1	D	129	ARG	N-CA	-5.09	1.40	1.46
1	D	152	LEU	C-O	-5.08	1.17	1.23
1	B	110	TYR	C-O	-5.08	1.17	1.24
1	D	141	ASP	C-O	-5.08	1.17	1.24
1	G	49	LEU	C-O	-5.08	1.17	1.24
1	G	91	ASP	C-O	-5.08	1.16	1.24
1	H	34	LYS	C-O	-5.08	1.17	1.23
1	G	159	GLY	C-O	-5.08	1.16	1.24
1	B	137	GLU	C-O	-5.08	1.18	1.24
1	D	26	TYR	C-O	-5.08	1.17	1.23
1	E	195	ALA	C-O	-5.08	1.17	1.24
1	E	111	ARG	CZ-NH2	-5.08	1.26	1.33
1	G	14	ASN	C-O	-5.08	1.18	1.24
1	A	188	THR	C-O	-5.08	1.18	1.24
1	B	172	GLY	C-O	-5.07	1.18	1.23
1	F	164	ARG	C-O	-5.07	1.17	1.24
1	B	220	SER	C-O	-5.07	1.18	1.24
1	E	9	ILE	C-O	-5.07	1.18	1.24
1	E	242	ILE	CA-C	-5.07	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	247	THR	C-O	-5.07	1.17	1.23
1	D	58	VAL	C-O	-5.07	1.18	1.24
1	E	11	SER	C-O	-5.07	1.18	1.24
1	G	266	GLU	C-O	-5.07	1.18	1.24
1	C	128	GLU	C-O	-5.06	1.18	1.24
1	H	118	PRO	C-O	-5.06	1.17	1.24
1	E	196	ARG	C-O	-5.06	1.17	1.24
1	A	18	ASP	C-O	-5.06	1.16	1.24
1	G	127	PHE	C-O	-5.06	1.18	1.24
1	H	164	ARG	N-CA	-5.06	1.39	1.46
1	F	67	PRO	C-O	-5.06	1.17	1.24
1	F	38	GLU	C-O	-5.05	1.18	1.24
1	F	40	LEU	C-O	-5.05	1.18	1.24
1	B	242	ILE	C-O	-5.05	1.18	1.24
1	H	175	ARG	C-O	-5.05	1.17	1.23
1	F	246	ASP	N-CA	-5.05	1.39	1.46
1	H	195	ALA	C-O	-5.04	1.17	1.24
1	C	112	ARG	C-O	-5.04	1.17	1.24
1	H	39	SER	N-CA	-5.04	1.40	1.46
1	F	156	VAL	C-O	-5.04	1.18	1.24
1	G	95	GLN	C-O	-5.04	1.17	1.23
1	C	191	ALA	C-O	-5.04	1.18	1.24
1	B	102	LEU	C-O	-5.04	1.17	1.24
1	E	75	ASP	C-O	-5.04	1.17	1.24
1	A	174	THR	C-O	-5.03	1.16	1.23
1	G	4	ARG	C-O	-5.03	1.17	1.24
1	G	105	SER	C-O	-5.03	1.17	1.23
1	E	86	TRP	C-O	-5.03	1.17	1.23
1	F	125	SER	C-O	-5.03	1.18	1.24
1	B	189	LEU	N-CA	-5.03	1.40	1.46
1	D	193	TYR	C-O	-5.03	1.18	1.24
1	E	50	GLY	C-O	-5.03	1.17	1.23
1	F	150	VAL	C-O	-5.02	1.18	1.24
1	E	215	TYR	C-O	-5.02	1.17	1.23
1	G	259	SER	C-O	-5.02	1.16	1.23
1	H	138	LEU	C-O	-5.02	1.17	1.24
1	H	146	ASP	C-O	-5.02	1.17	1.23
1	B	251	LEU	C-O	-5.02	1.18	1.24
1	D	190	ASP	CG-OD1	-5.02	1.15	1.25
1	H	18	ASP	C-O	-5.01	1.17	1.24
1	C	250	GLU	CD-OE2	-5.01	1.15	1.25
1	E	257	ASN	C-O	-5.01	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	5	LYS	C-O	-5.01	1.17	1.24
1	F	199	LYS	C-O	-5.01	1.18	1.24
1	G	50	GLY	C-O	-5.01	1.17	1.23
1	H	11	SER	C-O	-5.01	1.18	1.24
1	C	259	SER	C-O	-5.01	1.16	1.23
1	F	137	GLU	C-O	-5.01	1.18	1.24
1	F	183	ARG	C-O	-5.01	1.17	1.23
1	H	70	GLN	C-O	-5.00	1.18	1.24
1	F	203	TRP	C-O	-5.00	1.17	1.24

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3	LYS	N-CA-C	11.92	127.99	109.52
1	D	224	VAL	N-CA-C	11.28	124.55	109.21
1	E	29	GLU	N-CA-C	11.10	134.45	110.80
1	B	106	VAL	N-CA-C	-10.91	96.75	107.55
1	E	30	GLN	N-CA-C	9.99	125.80	108.02
1	G	224	VAL	N-CA-C	9.91	124.72	111.44
1	E	28	GLY	N-CA-C	-9.67	90.26	113.18
1	H	260	LEU	N-CA-C	9.50	121.40	111.14
1	G	28	GLY	N-CA-C	-9.47	90.74	113.18
1	H	209	VAL	CB-CA-C	-9.11	98.44	110.84
1	B	4	ARG	N-CA-C	8.76	124.28	113.50
1	B	258	ASN	N-CA-C	8.58	120.72	111.36
1	B	215	TYR	N-CA-C	8.54	126.42	113.61
1	H	151	ILE	CB-CA-C	-8.42	100.21	111.15
1	B	177	ASP	N-CA-C	8.37	120.18	111.14
1	A	135	LEU	N-CA-C	-8.27	102.21	111.14
1	C	206	MSE	CG-SE-CE	-8.00	81.33	98.92
1	E	207	GLU	N-CA-C	7.94	121.91	110.24
1	A	260	LEU	N-CA-C	7.86	119.62	111.14
1	D	220	SER	N-CA-C	7.82	121.16	108.34
1	C	203	TRP	N-CA-C	7.76	119.82	111.36
1	F	46	GLN	N-CA-C	7.76	121.56	112.72
1	A	88	TYR	CA-C-N	-7.60	111.92	119.90
1	A	88	TYR	C-N-CA	-7.60	111.92	119.90
1	C	222	HIS	N-CA-C	7.55	120.55	109.07
1	C	258	ASN	N-CA-C	7.53	119.56	111.36
1	B	140	ALA	N-CA-C	7.51	121.28	107.99
1	F	267	GLY	N-CA-C	-7.50	103.73	112.73
1	G	259	SER	N-CA-C	7.49	123.15	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	273	GLU	CA-C-N	7.45	135.12	121.70
1	G	273	GLU	C-N-CA	7.45	135.12	121.70
1	E	260	LEU	N-CA-C	7.44	119.18	111.14
1	B	78	PHE	N-CA-C	-7.42	102.88	112.23
1	H	156	VAL	N-CA-C	7.40	122.32	113.22
1	D	272	ALA	N-CA-C	7.38	121.73	112.87
1	B	224	VAL	N-CA-C	7.36	120.08	108.89
1	H	73	ILE	CB-CA-C	-7.34	103.75	112.19
1	B	164	ARG	N-CA-C	-7.33	101.89	111.71
1	H	222	HIS	N-CA-C	7.31	120.28	109.24
1	G	178	SER	N-CA-C	7.29	117.98	109.60
1	B	206	MSE	N-CA-C	7.25	121.52	111.74
1	F	260	LEU	N-CA-C	7.19	118.90	111.14
1	C	224	VAL	N-CA-C	7.10	118.71	108.48
1	E	257	ASN	N-CA-CB	-7.07	99.77	110.01
1	E	257	ASN	N-CA-C	7.05	118.62	111.07
1	F	258	ASN	N-CA-C	7.05	119.04	111.36
1	C	74	LYS	N-CA-C	6.91	118.81	111.28
1	H	116	GLY	N-CA-C	6.91	124.55	115.36
1	D	46	GLN	N-CA-C	6.86	121.36	112.92
1	D	259	SER	N-CA-C	6.86	121.50	112.72
1	G	206	MSE	CG-SE-CE	-6.85	83.85	98.92
1	D	248	ILE	N-CA-C	6.84	117.63	110.72
1	H	73	ILE	N-CA-C	6.79	117.96	111.91
1	C	259	SER	N-CA-C	6.77	122.18	113.18
1	F	187	ALA	N-CA-C	6.75	118.29	111.07
1	A	167	MSE	N-CA-C	6.72	120.13	109.50
1	E	61	ASP	N-CA-C	6.72	121.50	113.16
1	C	46	GLN	N-CA-C	6.69	121.51	112.88
1	G	260	LEU	N-CA-C	6.67	119.54	111.40
1	E	215	TYR	N-CA-C	6.66	121.56	113.17
1	A	143	VAL	N-CA-C	6.66	117.70	108.12
1	G	85	GLN	N-CA-C	6.65	119.93	109.96
1	G	184	GLY	N-CA-C	6.64	126.52	112.17
1	E	81	ARG	N-CA-C	-6.64	99.60	109.42
1	E	111	ARG	N-CA-C	6.62	120.95	112.34
1	E	30	GLN	N-CA-CB	-6.62	100.78	110.84
1	A	161	PRO	N-CA-C	6.62	122.52	113.98
1	D	258	ASN	N-CA-C	6.61	118.57	111.36
1	D	61	ASP	N-CA-C	6.57	121.36	112.88
1	E	156	VAL	N-CA-C	6.57	118.46	112.29
1	B	52	ALA	N-CA-C	6.56	118.52	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	TYR	CA-C-N	6.54	127.24	119.98
1	D	193	TYR	C-N-CA	6.54	127.24	119.98
1	F	106	VAL	CA-C-N	-6.51	113.24	120.14
1	F	106	VAL	C-N-CA	-6.51	113.24	120.14
1	H	52	ALA	N-CA-C	6.50	121.50	113.50
1	G	46	GLN	N-CA-C	6.49	121.28	113.23
1	G	187	ALA	N-CA-C	6.47	117.99	111.07
1	E	136	VAL	CB-CA-C	-6.46	103.42	112.14
1	F	52	ALA	N-CA-C	6.45	118.39	111.36
1	H	230	SER	N-CA-C	6.41	120.93	113.18
1	A	220	SER	N-CA-C	6.34	119.28	109.07
1	G	193	TYR	CA-C-N	6.34	127.02	119.98
1	G	193	TYR	C-N-CA	6.34	127.02	119.98
1	G	29	GLU	N-CA-C	6.32	124.25	110.80
1	G	45	ASN	N-CA-C	6.31	117.96	111.14
1	G	245	ASP	N-CA-C	6.31	120.98	113.16
1	G	177	ASP	N-CA-C	6.29	118.01	111.03
1	F	184	GLY	N-CA-C	6.28	123.51	112.83
1	G	183	ARG	N-CA-C	6.24	119.30	110.50
1	B	46	GLN	N-CA-C	6.23	120.89	113.16
1	D	234	PHE	N-CA-C	6.21	117.85	111.14
1	C	271	LEU	N-CA-C	6.20	120.10	112.54
1	G	109	THR	N-CA-C	6.19	118.83	111.71
1	B	242	ILE	N-CA-C	6.17	116.91	107.77
1	C	257	ASN	N-CA-C	6.17	117.81	111.14
1	A	61	ASP	N-CA-C	6.16	120.93	113.17
1	D	9	ILE	N-CA-C	6.14	116.71	107.75
1	G	261	PHE	N-CA-C	-6.12	104.47	113.16
1	D	53	TYR	N-CA-C	6.12	118.72	109.23
1	D	45	ASN	N-CA-C	6.12	118.03	111.36
1	H	154	GLU	N-CA-C	6.12	118.74	111.71
1	B	224	VAL	CA-C-N	6.09	132.67	121.70
1	B	224	VAL	C-N-CA	6.09	132.67	121.70
1	C	116	GLY	N-CA-C	6.05	123.08	115.21
1	D	222	HIS	N-CA-C	6.04	119.04	109.50
1	F	61	ASP	N-CA-C	6.01	120.61	113.28
1	H	163	ALA	N-CA-C	6.01	117.52	110.97
1	H	157	ARG	CA-C-N	5.99	126.34	119.93
1	H	157	ARG	C-N-CA	5.99	126.34	119.93
1	C	5	LYS	N-CA-C	5.96	119.13	110.42
1	F	239	LYS	N-CA-C	5.95	120.39	112.30
1	B	61	ASP	N-CA-C	5.94	120.53	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	CB-CA-C	-5.92	102.87	110.98
1	C	149	LEU	N-CA-C	5.92	120.19	113.15
1	F	116	GLY	N-CA-C	5.89	123.18	115.40
1	H	257	ASN	N-CA-C	5.88	120.52	113.23
1	C	178	SER	N-CA-C	5.84	118.77	110.24
1	F	49	LEU	CA-C-N	5.83	127.43	120.14
1	F	49	LEU	C-N-CA	5.83	127.43	120.14
1	A	256	PHE	CB-CA-C	-5.83	101.73	110.88
1	C	151	ILE	CB-CA-C	-5.80	104.29	111.08
1	C	107	PRO	N-CA-C	5.77	119.92	111.03
1	A	87	PHE	N-CA-C	5.77	119.42	112.38
1	D	224	VAL	CB-CA-C	-5.74	103.19	111.34
1	B	70	GLN	CA-C-N	5.72	126.33	119.98
1	B	70	GLN	C-N-CA	5.72	126.33	119.98
1	C	250	GLU	N-CA-C	5.71	117.31	111.14
1	A	156	VAL	CA-C-N	5.71	130.17	121.03
1	A	156	VAL	C-N-CA	5.71	130.17	121.03
1	H	155	LEU	N-CA-C	5.70	117.49	111.28
1	F	163	ALA	N-CA-C	5.69	117.16	111.07
1	A	46	GLN	N-CA-C	5.65	120.17	113.16
1	A	108	SER	CA-C-N	5.65	128.41	120.28
1	A	108	SER	C-N-CA	5.65	128.41	120.28
1	A	27	LYS	CB-CA-C	-5.64	103.57	111.80
1	G	213	PRO	N-CA-C	5.62	119.71	110.55
1	D	224	VAL	CA-C-N	5.61	131.79	121.70
1	D	224	VAL	C-N-CA	5.61	131.79	121.70
1	A	107	PRO	N-CA-C	5.58	119.63	111.03
1	A	272	ALA	CA-C-N	-5.57	113.59	122.66
1	A	272	ALA	C-N-CA	-5.57	113.59	122.66
1	G	174	THR	N-CA-C	5.57	120.23	113.38
1	H	107	PRO	N-CA-C	5.56	119.92	111.19
1	B	148	LEU	N-CA-C	-5.54	101.44	109.59
1	D	24	VAL	CA-C-N	-5.54	114.05	119.76
1	D	24	VAL	C-N-CA	-5.54	114.05	119.76
1	D	59	ILE	N-CA-C	5.53	116.69	108.23
1	H	271	LEU	N-CA-C	5.50	118.19	111.82
1	B	38	GLU	N-CA-C	5.49	117.34	111.36
1	D	220	SER	N-CA-CB	-5.47	102.18	110.77
1	E	206	MSE	CA-C-O	-5.47	113.67	119.97
1	F	121	VAL	CB-CA-C	-5.47	104.85	112.02
1	B	260	LEU	N-CA-C	5.47	117.33	111.36
1	A	52	ALA	N-CA-C	5.47	120.01	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	184	GLY	N-CA-C	5.47	122.66	112.77
1	A	6	LEU	N-CA-C	5.46	117.87	109.07
1	F	267	GLY	CA-C-O	-5.46	115.12	120.75
1	B	174	THR	N-CA-C	5.46	120.09	113.38
1	E	167	MSE	N-CA-CB	-5.45	101.46	111.37
1	F	5	LYS	N-CA-C	5.45	122.40	110.80
1	B	263	ALA	N-CA-C	5.44	116.89	111.07
1	E	52	ALA	N-CA-C	5.43	117.01	111.14
1	G	242	ILE	N-CA-C	5.43	115.94	108.12
1	H	213	PRO	N-CA-C	5.43	118.99	110.80
1	D	185	ALA	N-CA-C	5.42	118.11	111.82
1	H	167	MSE	N-CA-C	5.41	118.30	109.59
1	B	243	SER	CA-C-N	5.39	125.21	119.28
1	B	243	SER	C-N-CA	5.39	125.21	119.28
1	B	76	TYR	CA-C-N	-5.37	113.99	121.67
1	B	76	TYR	C-N-CA	-5.37	113.99	121.67
1	F	170	HIS	CA-C-N	-5.36	116.24	121.65
1	F	170	HIS	C-N-CA	-5.36	116.24	121.65
1	G	215	TYR	N-CA-C	5.35	118.82	112.72
1	D	56	VAL	N-CA-C	5.34	117.24	111.58
1	B	239	LYS	N-CA-C	5.34	118.86	111.71
1	D	107	PRO	N-CA-C	5.33	120.44	111.32
1	C	85	GLN	N-CA-C	5.33	117.59	110.35
1	A	201	VAL	N-CA-C	5.33	115.54	110.53
1	G	27	LYS	CA-C-N	5.32	131.84	121.41
1	G	27	LYS	C-N-CA	5.32	131.84	121.41
1	C	52	ALA	N-CA-C	5.31	117.98	111.82
1	F	70	GLN	N-CA-C	5.31	116.87	111.14
1	A	87	PHE	CA-C-N	5.30	129.74	122.06
1	A	87	PHE	C-N-CA	5.30	129.74	122.06
1	B	45	ASN	CB-CA-C	-5.29	102.58	110.88
1	E	90	ALA	N-CA-C	5.27	117.02	111.28
1	E	46	GLN	N-CA-C	5.26	119.80	113.17
1	A	45	ASN	N-CA-C	5.25	116.85	111.03
1	C	33	MSE	N-CA-CB	-5.24	103.02	110.46
1	A	106	VAL	N-CA-C	-5.24	97.57	108.88
1	D	257	ASN	N-CA-C	5.24	116.80	111.14
1	D	19	LYS	N-CA-C	5.22	118.79	111.74
1	A	9	ILE	N-CA-C	5.22	115.63	108.12
1	B	210	ALA	N-CA-C	5.20	117.58	110.24
1	E	203	TRP	CA-C-N	5.20	127.70	120.63
1	E	203	TRP	C-N-CA	5.20	127.70	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ALA	N-CA-C	5.19	116.93	111.28
1	A	30	GLN	N-CA-C	5.18	117.07	109.24
1	G	61	ASP	N-CA-C	5.18	119.70	113.17
1	F	152	LEU	N-CA-C	5.17	118.65	109.96
1	F	257	ASN	N-CA-C	5.17	116.72	111.14
1	A	56	VAL	N-CA-C	5.16	116.25	111.81
1	D	239	LYS	N-CA-C	5.15	119.10	112.41
1	H	213	PRO	CA-C-O	-5.14	115.17	121.03
1	F	198	GLU	N-CA-C	5.13	117.43	108.76
1	E	53	TYR	N-CA-C	5.12	117.84	109.59
1	C	148	LEU	N-CA-C	-5.12	102.27	109.96
1	F	271	LEU	N-CA-C	5.12	117.59	111.71
1	G	117	THR	N-CA-C	-5.11	103.21	109.65
1	A	193	TYR	CA-C-N	5.11	125.65	119.98
1	A	193	TYR	C-N-CA	5.11	125.65	119.98
1	F	176	GLU	N-CA-C	5.11	116.84	111.28
1	G	223	TYR	N-CA-C	-5.11	101.64	109.76
1	D	191	ALA	N-CA-C	5.10	116.53	111.07
1	D	11	SER	N-CA-C	-5.09	100.23	108.52
1	A	236	ASP	N-CA-C	5.08	117.69	109.06
1	F	136	VAL	CB-CA-C	-5.08	105.28	112.14
1	F	214	LEU	N-CA-C	-5.08	100.63	108.90
1	E	84	GLN	N-CA-C	5.05	117.32	110.35
1	D	224	VAL	O-C-N	5.04	128.67	122.72
1	E	259	SER	N-CA-C	5.04	119.17	112.72
1	B	59	ILE	N-CA-C	5.02	115.52	108.89
1	H	82	PRO	CA-C-O	-5.01	115.70	121.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2138	2093	2093	124	0
1	B	2108	2059	2061	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2149	2104	2102	81	0
1	D	2141	2098	2098	101	0
1	E	2112	2071	2071	123	0
1	F	2059	2016	2015	95	0
1	G	2122	2075	2075	111	0
1	H	2134	2090	2090	76	0
2	A	32	19	0	3	0
2	C	32	19	0	3	0
2	D	32	19	0	0	0
2	E	32	19	0	9	0
2	F	32	19	0	3	0
2	G	32	19	0	0	0
2	H	32	19	0	1	0
3	A	13	5	5	1	0
3	B	13	5	5	3	0
3	C	13	5	5	2	0
3	D	13	5	5	0	0
3	E	13	5	5	1	0
3	F	13	5	5	0	0
3	G	13	5	5	9	0
3	H	13	5	5	0	0
4	A	43	0	0	1	0
4	B	51	0	0	10	0
4	C	32	0	0	4	0
4	D	37	0	0	3	1
4	E	36	0	0	4	0
4	F	33	0	0	2	0
4	G	47	0	0	2	1
4	H	45	0	0	3	0
All	All	17615	16779	16645	786	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (786) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD12	1:A:142:VAL:CG1	1.29	1.55
1:F:174:THR:O	1:F:183:ARG:NH2	1.60	1.35
1:A:196:ARG:NH1	1:A:244:PRO:O	1.64	1.29
1:B:154:GLU:O	1:B:157:ARG:CG	1.82	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:HD3	1:C:250:GLU:OE2	1.34	1.25
1:G:68:ARG:NH2	3:G:302:CIT:O4	1.70	1.23
1:H:19:LYS:HD2	1:H:22:GLN:OE1	1.40	1.19
1:B:176:GLU:OE1	4:B:401:HOH:O	1.59	1.18
1:A:6:LEU:CD1	1:A:142:VAL:CG1	2.25	1.14
1:E:223:TYR:HB2	1:E:232:GLU:OE2	1.48	1.14
1:C:6:LEU:HD13	1:C:53:TYR:CD1	1.83	1.13
1:A:164:ARG:NH2	1:A:232:GLU:OE2	1.81	1.13
1:A:6:LEU:HD12	1:A:142:VAL:HG11	1.26	1.11
1:E:157:ARG:NH1	1:F:196:ARG:HH21	1.45	1.11
1:B:154:GLU:O	1:B:157:ARG:HG2	1.43	1.11
1:G:13:ARG:NE	3:G:302:CIT:O6	1.84	1.11
1:C:6:LEU:CD1	1:C:53:TYR:CD1	2.32	1.10
1:A:164:ARG:NH1	1:A:232:GLU:OE2	1.83	1.09
1:B:134:THR:OG1	4:B:402:HOH:O	1.69	1.09
1:A:6:LEU:CD1	1:A:142:VAL:HG13	1.80	1.08
1:H:107:PRO:O	1:H:130:ARG:NH2	1.87	1.07
1:A:223:TYR:O	1:A:231:GLY:HA3	1.54	1.06
1:G:68:ARG:CZ	3:G:302:CIT:O4	2.05	1.04
1:G:68:ARG:NE	3:G:302:CIT:O4	1.92	1.02
1:A:164:ARG:CZ	1:A:232:GLU:OE2	2.08	1.02
1:G:27:LYS:HB2	1:G:250:GLU:OE2	1.60	1.02
1:F:199:LYS:HG2	1:F:211:VAL:HG21	1.40	1.01
1:C:14:ASN:ND2	1:C:147:GLY:O	1.94	1.01
1:A:143:VAL:HG13	1:A:166:ILE:HG13	1.39	1.00
1:A:164:ARG:HH12	1:A:232:GLU:CD	1.71	0.99
1:B:27:LYS:NZ	1:B:246:ASP:OD1	1.93	0.98
1:A:181:GLU:OE2	1:A:183:ARG:CD	2.11	0.98
1:B:167:MSE:HE1	1:B:223:TYR:CE1	2.02	0.95
1:E:128:GLU:OE1	1:E:154:GLU:N	1.99	0.95
1:F:235:HIS:NE2	1:F:266:GLU:OE1	1.99	0.95
1:A:6:LEU:HD12	1:A:142:VAL:HG13	0.96	0.94
1:B:154:GLU:O	1:B:157:ARG:HG3	1.68	0.92
1:F:26:TYR:CB	1:F:31:ARG:HD3	2.00	0.92
1:G:113:TYR:HB2	1:G:120:HIS:HB2	1.53	0.91
1:F:26:TYR:CD2	1:F:31:ARG:NE	2.39	0.91
1:E:174:THR:OG1	4:E:401:HOH:O	1.88	0.90
1:G:234:PHE:CE2	1:G:271:LEU:HB2	2.07	0.90
1:F:26:TYR:HB3	1:F:31:ARG:HD3	1.50	0.90
1:A:143:VAL:CG1	1:A:166:ILE:HG13	2.01	0.89
1:G:247:THR:OG1	1:G:250:GLU:HG3	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:GLU:O	1:E:270:LEU:HD12	1.74	0.88
1:F:116:GLY:O	1:G:186:TYR:OH	1.90	0.88
1:C:27:LYS:CD	1:C:250:GLU:OE2	2.22	0.88
1:D:106:VAL:HG11	1:D:131:LEU:HD23	1.54	0.88
1:D:222:HIS:NE2	1:D:224:VAL:HG12	1.91	0.86
1:G:43:ALA:HB2	1:G:265:HIS:CD2	2.10	0.86
1:B:8:TYR:OH	1:B:146:ASP:OD2	1.94	0.85
1:F:119:GLU:OE1	1:F:119:GLU:N	2.08	0.85
1:E:173:VAL:HG21	1:E:238:LEU:HD13	1.59	0.85
1:A:202:ASP:HB3	1:A:207:GLU:OE1	1.77	0.85
1:B:126:ASP:O	1:B:129:ARG:HB3	1.77	0.84
1:E:223:TYR:CB	1:E:232:GLU:OE2	2.24	0.84
1:B:4:ARG:NH2	4:B:403:HOH:O	1.92	0.83
1:A:6:LEU:CD1	1:A:142:VAL:HG11	1.97	0.83
1:H:73:ILE:O	1:H:76:TYR:O	1.95	0.83
1:A:4:ARG:NH1	1:A:274:LYS:O	2.12	0.82
1:G:164:ARG:NH1	1:G:232:GLU:OE1	2.12	0.82
1:F:4:ARG:HB2	1:F:52:ALA:O	1.80	0.82
1:H:81:ARG:O	1:H:84:GLN:HB3	1.78	0.82
1:C:174:THR:HG22	1:C:183:ARG:HG3	1.62	0.81
1:C:174:THR:HA	1:C:183:ARG:HD2	1.61	0.81
1:F:202:ASP:OD2	4:F:401:HOH:O	1.98	0.81
1:A:164:ARG:HD2	1:A:223:TYR:CD1	2.17	0.80
1:D:180:TYR:HE1	1:D:216:TRP:H	1.30	0.80
1:A:181:GLU:OE2	1:A:183:ARG:HG3	1.80	0.80
1:F:164:ARG:HD2	1:F:223:TYR:CE1	2.16	0.80
1:F:26:TYR:HB3	1:F:31:ARG:CD	2.12	0.80
1:C:41:VAL:HG21	1:C:99:LEU:HD22	1.63	0.79
1:G:126:ASP:OD1	1:G:129:ARG:NH1	2.15	0.79
1:E:186:TYR:OH	1:H:116:GLY:O	1.99	0.79
1:A:181:GLU:OE2	1:A:183:ARG:CG	2.31	0.79
1:E:61:ASP:HB2	1:E:108:SER:HB3	1.65	0.78
1:D:222:HIS:CD2	1:D:224:VAL:HG12	2.18	0.78
1:D:259:SER:C	1:D:262:PRO:HD2	2.08	0.78
1:G:68:ARG:HE	3:G:302:CIT:C5	1.96	0.77
1:B:192:LEU:O	4:B:404:HOH:O	2.01	0.77
1:B:143:VAL:CG1	1:B:166:ILE:HG12	2.13	0.77
1:C:5:LYS:HB3	1:C:56:VAL:HG21	1.67	0.77
1:C:241:GLU:O	4:C:401:HOH:O	2.01	0.77
1:E:232:GLU:OE1	1:E:232:GLU:N	2.17	0.77
1:D:168:ASN:OD1	4:D:401:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:MSE:HE1	1:B:223:TYR:CD1	2.20	0.76
1:H:73:ILE:HD11	1:H:78:PHE:CD1	2.20	0.76
1:C:9:ILE:HG13	1:C:59:ILE:HB	1.66	0.76
1:C:188:THR:HG22	1:C:248:ILE:HD11	1.66	0.76
1:F:26:TYR:CG	1:F:31:ARG:HD3	2.20	0.76
1:B:65:GLU:OE2	4:B:405:HOH:O	2.03	0.76
1:E:157:ARG:HH12	1:F:196:ARG:HH21	1.33	0.76
1:B:94:VAL:HG13	1:B:94:VAL:O	1.86	0.75
1:C:38:GLU:O	1:C:42:GLU:HG3	1.87	0.75
1:F:164:ARG:HD2	1:F:223:TYR:HE1	1.50	0.75
1:F:4:ARG:HB3	1:F:53:TYR:CD1	2.22	0.75
1:A:196:ARG:NH2	1:B:154:GLU:OE2	2.20	0.74
1:E:68:ARG:O	1:E:72:LYS:HD2	1.86	0.74
1:D:4:ARG:NH1	1:D:274:LYS:HG2	2.02	0.74
1:G:27:LYS:CB	1:G:250:GLU:OE2	2.35	0.74
1:D:188:THR:HG21	1:D:252:ARG:HE	1.53	0.73
1:H:72:LYS:O	4:H:401:HOH:O	2.06	0.73
1:E:249:LEU:C	1:E:249:LEU:HD23	2.13	0.73
1:G:175:ARG:NE	1:G:236:ASP:OD2	2.20	0.73
1:E:6:LEU:HD13	1:E:142:VAL:HG13	1.71	0.73
1:G:175:ARG:CZ	1:G:236:ASP:OD2	2.37	0.73
1:G:261:PHE:O	1:G:265:HIS:ND1	2.21	0.72
1:B:182:ARG:NH2	4:B:407:HOH:O	2.22	0.72
1:C:6:LEU:CD1	1:C:53:TYR:CE1	2.71	0.72
1:B:13:ARG:NH2	1:B:61:ASP:OD2	2.16	0.72
1:D:180:TYR:HD1	1:D:216:TRP:O	1.73	0.72
1:A:88:TYR:CE1	1:A:99:LEU:HD23	2.25	0.72
1:F:20:ALA:O	1:F:76:TYR:OH	2.05	0.72
1:H:130:ARG:O	1:H:134:THR:OG1	2.06	0.72
1:D:43:ALA:HB2	1:D:265:HIS:CD2	2.25	0.72
1:D:180:TYR:CD1	1:D:216:TRP:O	2.43	0.72
1:D:4:ARG:HH11	1:D:274:LYS:HG2	1.55	0.72
1:E:72:LYS:HZ1	2:E:301:FGD:C05	2.03	0.71
1:G:106:VAL:HG11	1:G:131:LEU:HD23	1.72	0.71
1:H:202:ASP:OD2	1:H:205:THR:OG1	2.08	0.71
1:B:27:LYS:CE	1:B:246:ASP:OD1	2.39	0.71
1:F:128:GLU:OE1	1:F:154:GLU:HG2	1.92	0.70
1:H:68:ARG:O	1:H:72:LYS:HG3	1.91	0.70
1:G:174:THR:O	1:G:183:ARG:NH2	2.24	0.70
1:G:53:TYR:OH	1:G:268:LEU:O	2.07	0.70
1:B:26:TYR:OH	1:B:254:ASN:OD1	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:242:ILE:HD13	1:H:251:LEU:HD13	1.73	0.70
1:E:160:ALA:O	1:E:163:ALA:HB2	1.92	0.70
1:F:164:ARG:NH1	1:F:223:TYR:OH	2.22	0.69
1:C:6:LEU:HD13	1:C:53:TYR:CG	2.28	0.69
1:C:9:ILE:HD13	1:C:143:VAL:HG13	1.73	0.69
1:A:181:GLU:OE2	1:A:183:ARG:HD2	1.91	0.69
1:E:8:TYR:OH	1:E:146:ASP:OD2	2.11	0.69
1:F:143:VAL:HG13	1:F:166:ILE:HG13	1.75	0.69
1:B:154:GLU:HG3	1:B:157:ARG:HE	1.57	0.69
1:A:13:ARG:NH2	3:A:302:CIT:O3	2.22	0.69
1:B:154:GLU:C	1:B:157:ARG:HG2	2.17	0.68
1:A:80:TYR:CD2	1:F:74:LYS:HE3	2.28	0.68
1:D:5:LYS:HD3	1:D:54:GLU:OE2	1.94	0.68
1:E:94:VAL:O	1:E:94:VAL:HG13	1.92	0.68
1:A:5:LYS:HB3	1:A:141:ASP:H	1.57	0.68
1:F:26:TYR:HD2	1:F:31:ARG:NE	1.87	0.68
1:A:164:ARG:HD2	1:A:223:TYR:CE1	2.28	0.68
1:B:143:VAL:HG11	1:B:166:ILE:HG12	1.75	0.68
1:C:5:LYS:HB3	1:C:56:VAL:CG2	2.24	0.68
1:D:216:TRP:CZ2	1:D:241:GLU:HG3	2.28	0.68
1:C:69:ASP:OD2	1:C:111:ARG:NH2	2.27	0.68
1:C:145:LEU:HD11	1:C:152:LEU:HD11	1.74	0.68
1:H:19:LYS:HD2	1:H:22:GLN:CD	2.14	0.68
1:A:4:ARG:O	1:A:53:TYR:HD1	1.76	0.67
1:B:97:LYS:HE3	4:B:408:HOH:O	1.94	0.67
1:E:157:ARG:NH1	1:F:196:ARG:NH2	2.31	0.67
1:E:215:TYR:HE1	1:E:244:PRO:HD3	1.60	0.67
1:A:75:ASP:OD2	2:A:301:FGD:N26	2.28	0.67
1:E:6:LEU:CD1	1:E:142:VAL:HG13	2.23	0.67
1:A:127:PHE:HE2	1:A:150:VAL:HG11	1.59	0.67
1:E:98:THR:HB	1:E:101:ASP:OD2	1.94	0.67
1:D:182:ARG:HH22	1:D:214:LEU:HD12	1.59	0.67
1:A:80:TYR:HD2	1:F:74:LYS:HE3	1.59	0.67
1:B:180:TYR:CE1	1:B:214:LEU:HD22	2.30	0.67
1:H:25:PRO:O	4:H:402:HOH:O	2.11	0.67
1:A:181:GLU:OE2	1:A:183:ARG:NE	2.27	0.66
1:A:197:GLY:C	1:A:211:VAL:HG12	2.20	0.66
1:C:8:TYR:C	1:C:9:ILE:HD12	2.20	0.66
1:C:73:ILE:HD12	1:C:73:ILE:O	1.96	0.66
1:A:95:GLN:O	1:A:95:GLN:OE1	2.14	0.66
1:C:9:ILE:HB	1:C:145:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:TYR:O	1:G:231:GLY:HA3	1.95	0.66
1:G:71:GLY:O	1:G:74:LYS:HB2	1.95	0.66
1:D:6:LEU:HD13	1:D:142:VAL:HG13	1.78	0.66
1:E:128:GLU:OE1	1:E:153:ASP:N	2.28	0.66
1:C:73:ILE:HD12	1:C:73:ILE:C	2.20	0.66
1:F:156:VAL:HG11	1:F:224:VAL:HG12	1.76	0.66
2:C:301:FGD:C05	1:D:114:PRO:HD3	2.26	0.65
1:A:127:PHE:CE2	1:A:150:VAL:HG11	2.31	0.65
1:E:202:ASP:OD1	1:E:204:ALA:HB3	1.97	0.65
1:A:93:GLN:N	1:A:93:GLN:OE1	2.30	0.65
1:C:201:VAL:HG23	1:C:207:GLU:HB3	1.77	0.65
1:E:202:ASP:CG	1:E:205:THR:HG22	2.21	0.65
1:E:200:VAL:HG22	1:E:208:LYS:HG2	1.79	0.65
1:G:198:GLU:OE2	4:G:401:HOH:O	2.14	0.65
1:B:113:TYR:OH	4:B:406:HOH:O	2.06	0.65
1:C:5:LYS:HD2	1:C:139:GLY:O	1.96	0.65
1:F:69:ASP:OD2	1:F:111:ARG:NH2	2.25	0.65
1:E:108:SER:OG	1:E:111:ARG:NE	2.23	0.65
1:G:130:ARG:O	1:G:134:THR:OG1	2.15	0.64
1:A:243:SER:O	1:A:246:ASP:HB2	1.98	0.64
1:D:64:ALA:O	1:D:70:GLN:NE2	2.29	0.64
2:E:301:FGD:C06	1:H:114:PRO:HD3	2.27	0.64
1:G:66:LEU:C	1:G:66:LEU:HD23	2.21	0.64
1:B:79:ALA:O	1:B:81:ARG:HD2	1.96	0.64
1:A:156:VAL:HG11	1:A:224:VAL:HG12	1.80	0.64
1:B:124:LYS:NZ	1:B:151:ILE:O	2.27	0.64
1:D:181:GLU:OE2	1:D:183:ARG:HG3	1.98	0.64
1:D:222:HIS:HE2	1:D:224:VAL:HG12	1.61	0.64
1:E:126:ASP:O	1:E:130:ARG:HG3	1.97	0.64
1:B:131:LEU:O	1:B:135:LEU:HD23	1.97	0.64
1:B:94:VAL:O	1:B:94:VAL:CG1	2.44	0.63
1:C:217:THR:HB	1:C:242:ILE:HD11	1.80	0.63
1:E:56:VAL:HG13	1:E:138:LEU:HD22	1.79	0.63
1:F:220:SER:OG	4:F:402:HOH:O	2.12	0.63
1:G:66:LEU:HD21	1:G:68:ARG:HG2	1.79	0.63
1:D:235:HIS:NE2	1:D:266:GLU:OE2	2.27	0.63
1:E:8:TYR:O	1:E:58:VAL:HA	1.98	0.63
1:D:6:LEU:HD12	1:D:142:VAL:O	1.99	0.63
1:D:164:ARG:O	1:D:223:TYR:HE1	1.80	0.63
1:D:106:VAL:CG1	1:D:131:LEU:HD23	2.27	0.63
1:E:266:GLU:O	1:E:270:LEU:CD1	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:TYR:CE2	1:G:99:LEU:HD23	2.34	0.63
1:G:188:THR:HG21	1:G:252:ARG:HE	1.63	0.63
1:H:222:HIS:CE1	1:H:229:ASP:HB3	2.34	0.63
1:H:81:ARG:O	1:H:84:GLN:CB	2.46	0.63
1:H:202:ASP:O	1:H:206:MSE:N	2.31	0.63
1:D:6:LEU:HD11	1:D:144:VAL:HG23	1.80	0.63
1:G:69:ASP:OD1	1:G:111:ARG:NH2	2.30	0.62
1:C:202:ASP:O	1:C:205:THR:O	2.16	0.62
1:C:128:GLU:CG	1:C:155:LEU:HB2	2.30	0.62
1:D:188:THR:HG21	1:D:252:ARG:NE	2.15	0.62
1:D:176:GLU:HG3	1:D:183:ARG:NH2	2.15	0.62
1:G:127:PHE:CZ	1:G:131:LEU:HD11	2.35	0.62
1:G:113:TYR:CB	1:G:120:HIS:HB2	2.28	0.62
1:G:14:ASN:HB2	1:G:149:LEU:HD11	1.82	0.61
1:F:256:PHE:HA	1:F:260:LEU:HB3	1.82	0.61
1:H:81:ARG:HB2	1:H:84:GLN:HG2	1.82	0.61
1:B:186:TYR:CZ	1:C:118:PRO:HD3	2.35	0.61
1:A:82:PRO:CB	1:E:65:GLU:OE1	2.48	0.61
1:F:128:GLU:OE2	1:F:152:LEU:HD22	2.01	0.61
1:E:14:ASN:HB2	1:E:149:LEU:HD21	1.81	0.61
1:H:181:GLU:HG2	1:H:183:ARG:HG3	1.83	0.61
1:F:157:ARG:HG2	1:F:158:PRO:HD2	1.81	0.61
1:B:154:GLU:O	1:B:157:ARG:CD	2.46	0.61
1:G:126:ASP:O	1:G:130:ARG:HG3	2.00	0.61
1:C:6:LEU:HD11	1:C:53:TYR:CE1	2.35	0.61
1:E:175:ARG:HG3	1:E:233:VAL:HG21	1.83	0.61
1:H:19:LYS:CD	1:H:22:GLN:OE1	2.34	0.61
1:D:128:GLU:OE2	1:D:153:ASP:N	2.26	0.61
1:G:66:LEU:HD21	1:G:68:ARG:CG	2.31	0.61
1:D:175:ARG:HD2	1:D:236:ASP:OD2	2.01	0.61
1:G:24:VAL:HG21	1:G:249:LEU:HB3	1.82	0.60
1:B:4:ARG:HG2	1:B:4:ARG:HH11	1.66	0.60
1:B:110:TYR:CD2	1:B:124:LYS:HA	2.36	0.60
1:E:164:ARG:O	1:E:164:ARG:HG2	2.00	0.60
1:B:156:VAL:HG11	1:B:224:VAL:HG23	1.84	0.60
1:C:188:THR:HG22	1:C:248:ILE:CD1	2.31	0.60
1:D:12:LEU:HB2	1:D:62:ASP:CG	2.27	0.60
1:A:135:LEU:O	1:A:138:LEU:N	2.33	0.60
1:B:261:PHE:O	1:B:265:HIS:ND1	2.35	0.60
1:E:249:LEU:HD23	1:E:249:LEU:O	2.02	0.60
1:G:6:LEU:HD11	1:G:144:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:TYR:HD2	1:G:120:HIS:CE1	2.19	0.60
1:F:26:TYR:CD2	1:F:31:ARG:CD	2.85	0.59
1:G:68:ARG:HH21	3:G:302:CIT:C5	2.06	0.59
1:A:107:PRO:HD2	1:A:130:ARG:HH12	1.67	0.59
1:A:175:ARG:HB2	1:A:178:SER:HB2	1.85	0.59
1:D:200:VAL:HG22	1:D:208:LYS:HD3	1.83	0.59
1:F:151:ILE:HG23	1:F:151:ILE:O	2.02	0.59
1:C:14:ASN:ND2	1:C:147:GLY:C	2.59	0.59
1:C:69:ASP:CG	1:C:111:ARG:HH22	2.10	0.59
1:E:262:PRO:O	1:E:266:GLU:HB2	2.02	0.59
1:H:19:LYS:HB3	1:H:22:GLN:HG3	1.83	0.59
1:F:217:THR:HB	1:F:242:ILE:HD11	1.84	0.59
1:C:236:ASP:OD1	4:C:402:HOH:O	2.16	0.59
1:E:5:LYS:HD2	1:E:139:GLY:O	2.03	0.59
1:E:8:TYR:OH	1:E:146:ASP:CG	2.45	0.59
1:G:48:ALA:O	1:G:51:ASP:HB2	2.02	0.59
1:A:94:VAL:HG13	1:A:94:VAL:O	2.03	0.59
1:C:6:LEU:CD1	1:C:53:TYR:HD1	2.10	0.59
1:B:61:ASP:HA	1:B:106:VAL:O	2.02	0.58
1:F:71:GLY:O	2:F:301:FGD:C16	2.51	0.58
1:H:156:VAL:HG11	1:H:224:VAL:HG23	1.85	0.58
1:D:235:HIS:HE2	1:D:266:GLU:CD	2.08	0.58
1:E:72:LYS:HZ1	2:E:301:FGD:C07	2.16	0.58
1:H:217:THR:O	1:H:238:LEU:HD12	2.03	0.58
1:A:80:TYR:HD2	1:F:74:LYS:CE	2.15	0.58
1:G:259:SER:C	1:G:262:PRO:HD2	2.27	0.58
1:B:92:LEU:HD23	1:B:99:LEU:HD23	1.84	0.58
1:D:128:GLU:OE1	1:D:154:GLU:HB3	2.04	0.58
1:A:143:VAL:CG1	1:A:166:ILE:CG1	2.79	0.58
1:D:197:GLY:O	1:D:211:VAL:N	2.31	0.58
1:A:20:ALA:O	1:A:76:TYR:OH	2.17	0.58
1:A:42:GLU:O	1:A:46:GLN:HG2	2.03	0.58
1:A:88:TYR:CZ	1:A:99:LEU:HD23	2.39	0.58
1:B:177:ASP:N	1:B:177:ASP:OD1	2.30	0.58
1:E:174:THR:HG23	1:E:220:SER:CB	2.34	0.58
1:A:106:VAL:HG11	1:A:131:LEU:HD23	1.85	0.58
1:H:88:TYR:CZ	1:H:99:LEU:HD23	2.39	0.58
1:B:27:LYS:HE3	1:B:250:GLU:OE1	2.04	0.57
1:F:3:LYS:HD2	1:F:3:LYS:O	2.04	0.57
1:A:217:THR:C	1:A:238:LEU:HD12	2.29	0.57
1:E:24:VAL:HG21	1:E:249:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ILE:HG23	1:E:169:ILE:O	2.04	0.57
1:H:126:ASP:OD1	1:H:129:ARG:NH2	2.35	0.57
1:A:134:THR:HA	1:A:137:GLU:HB2	1.85	0.57
1:E:222:HIS:HB3	1:E:233:VAL:HA	1.86	0.57
1:F:43:ALA:O	1:F:47:THR:OG1	2.22	0.57
1:G:174:THR:O	1:G:183:ARG:NE	2.35	0.57
1:C:8:TYR:CD2	1:C:144:VAL:HG13	2.40	0.57
1:F:235:HIS:CE1	1:F:266:GLU:OE1	2.58	0.57
1:H:57:GLY:HA2	1:H:102:LEU:HB3	1.87	0.57
1:E:24:VAL:CG2	1:E:249:LEU:HD21	2.35	0.56
1:C:41:VAL:HG21	1:C:99:LEU:CD2	2.35	0.56
1:C:70:GLN:HG2	1:C:78:PHE:HE1	1.69	0.56
1:C:107:PRO:HB2	1:C:109:THR:HG23	1.88	0.56
1:D:40:LEU:HD12	1:D:264:LEU:HD21	1.88	0.56
1:F:237:VAL:CG2	1:F:263:ALA:HB2	2.34	0.56
1:F:237:VAL:HB	1:F:263:ALA:HB2	1.88	0.56
1:A:4:ARG:HB2	1:A:53:TYR:CE1	2.41	0.56
1:F:144:VAL:O	1:F:144:VAL:HG13	2.05	0.56
1:A:213:PRO:O	1:A:214:LEU:HD12	2.05	0.56
1:E:26:TYR:O	1:E:250:GLU:OE2	2.23	0.56
1:E:201:VAL:HG12	1:E:201:VAL:O	2.04	0.56
1:G:110:TYR:HB3	1:G:123:GLY:HA3	1.88	0.56
1:C:183:ARG:HG2	1:C:183:ARG:HH21	1.71	0.56
1:D:191:ALA:O	4:D:402:HOH:O	2.18	0.56
1:A:106:VAL:HG12	1:A:106:VAL:O	2.06	0.56
1:D:194:GLY:O	1:D:213:PRO:HA	2.06	0.56
1:E:72:LYS:NZ	2:E:301:FGD:C07	2.69	0.56
1:E:80:TYR:CZ	1:E:90:ALA:HB2	2.41	0.56
1:F:26:TYR:CD2	1:F:31:ARG:HD3	2.41	0.56
1:H:84:GLN:OE1	1:H:84:GLN:HA	2.06	0.56
1:C:145:LEU:HD11	1:C:152:LEU:CD1	2.36	0.56
1:G:150:VAL:O	1:G:150:VAL:HG23	2.06	0.56
3:G:302:CIT:O3	3:G:302:CIT:O7	2.10	0.56
1:F:57:GLY:N	1:F:102:LEU:HD22	2.21	0.55
1:F:68:ARG:O	1:F:72:LYS:HG3	2.06	0.55
1:C:9:ILE:HD13	1:C:143:VAL:CG1	2.35	0.55
1:D:164:ARG:O	1:D:223:TYR:CE1	2.60	0.55
1:A:90:ALA:O	1:A:100:ASN:ND2	2.38	0.55
2:E:301:FGD:C06	1:H:114:PRO:CD	2.83	0.55
1:H:73:ILE:HD11	1:H:78:PHE:CE1	2.41	0.55
1:C:70:GLN:HG2	1:C:78:PHE:CE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LEU:HD11	1:C:162:PHE:CD2	2.42	0.55
1:C:188:THR:CG2	1:C:248:ILE:HD11	2.36	0.55
1:F:157:ARG:CG	1:F:158:PRO:HD2	2.37	0.55
1:H:67:PRO:HD2	2:H:301:FGD:O09	2.06	0.55
1:D:181:GLU:O	1:D:181:GLU:HG3	2.05	0.55
1:D:274:LYS:O	1:D:274:LYS:HG3	2.06	0.55
1:G:128:GLU:OE2	1:G:153:ASP:N	2.27	0.55
1:G:200:VAL:HG22	1:G:208:LYS:HG2	1.88	0.55
1:C:256:PHE:HA	1:C:260:LEU:HB3	1.89	0.54
1:D:68:ARG:O	1:D:72:LYS:HG3	2.06	0.54
1:E:145:LEU:HB2	1:E:168:ASN:OD1	2.07	0.54
1:F:114:PRO:HG2	1:F:117:THR:HG21	1.89	0.54
1:G:69:ASP:CG	1:G:111:ARG:HH22	2.15	0.54
1:B:195:ALA:HB3	4:B:404:HOH:O	2.08	0.54
1:C:5:LYS:HG2	1:C:56:VAL:HG11	1.89	0.54
1:G:256:PHE:HD2	1:G:261:PHE:CZ	2.25	0.54
1:F:166:ILE:HG23	1:F:224:VAL:HB	1.89	0.54
1:H:113:TYR:CB	1:H:120:HIS:HB2	2.38	0.54
1:B:44:LEU:O	1:B:50:GLY:HA3	2.07	0.54
1:C:6:LEU:HD12	1:C:53:TYR:CD1	2.35	0.54
1:F:217:THR:O	1:F:238:LEU:HD12	2.07	0.54
1:D:199:LYS:CD	1:D:211:VAL:HG11	2.37	0.54
1:F:243:SER:OG	1:F:244:PRO:HD2	2.07	0.54
1:G:7:ALA:O	1:G:143:VAL:HA	2.08	0.54
1:C:113:TYR:CD2	1:C:119:GLU:HB2	2.43	0.54
1:E:26:TYR:CG	1:E:31:ARG:HG3	2.43	0.54
1:B:23:TYR:CE1	1:B:32:TYR:HB2	2.43	0.53
1:A:82:PRO:O	1:A:82:PRO:HG2	2.08	0.53
1:B:86:TRP:HA	1:B:86:TRP:CE3	2.41	0.53
1:G:30:GLN:O	1:G:31:ARG:HG2	2.08	0.53
1:H:9:ILE:HG21	1:H:148:LEU:HD22	1.91	0.53
1:A:54:GLU:OE2	1:A:97:LYS:NZ	2.40	0.53
1:F:157:ARG:CB	1:F:158:PRO:HD2	2.37	0.53
1:C:222:HIS:HB2	1:C:232:GLU:O	2.07	0.53
1:D:110:TYR:HD1	1:D:120:HIS:CE1	2.27	0.53
1:E:174:THR:HG23	1:E:220:SER:HB3	1.89	0.53
1:A:73:ILE:O	1:A:77:GLY:N	2.34	0.53
1:A:9:ILE:HD12	1:A:145:LEU:HD21	1.91	0.53
1:B:111:ARG:CD	3:B:301:CIT:H42	2.39	0.53
1:F:259:SER:C	1:F:262:PRO:HD2	2.33	0.53
1:D:110:TYR:OH	1:D:150:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:THR:O	1:D:121:VAL:HG23	2.09	0.53
1:E:223:TYR:HB2	1:E:232:GLU:CD	2.29	0.53
1:D:141:ASP:O	1:D:165:ARG:HD2	2.09	0.52
1:E:80:TYR:CE2	1:E:90:ALA:HB1	2.45	0.52
1:A:164:ARG:NE	1:A:223:TYR:CE1	2.78	0.52
1:F:121:VAL:HG22	1:G:206:MSE:HE1	1.91	0.52
1:H:216:TRP:CZ3	1:H:241:GLU:HB2	2.44	0.52
1:C:72:LYS:HZ2	2:C:301:FGD:C06	2.23	0.52
1:D:5:LYS:HD3	1:D:54:GLU:CD	2.35	0.52
1:D:247:THR:HG23	1:D:250:GLU:OE1	2.09	0.52
1:E:112:ARG:O	2:F:301:FGD:O32	2.27	0.52
1:G:167:MSE:HE1	1:G:223:TYR:CD2	2.44	0.52
2:E:301:FGD:C06	1:H:114:PRO:CG	2.87	0.52
1:A:31:ARG:HG3	1:A:253:TRP:CZ2	2.44	0.52
1:F:4:ARG:CZ	1:F:272:ALA:HB1	2.40	0.52
1:G:201:VAL:HG23	1:G:207:GLU:HG3	1.90	0.52
1:H:110:TYR:CE2	1:H:124:LYS:HB2	2.45	0.52
1:D:126:ASP:O	1:D:130:ARG:HG3	2.10	0.52
1:D:195:ALA:HA	1:D:214:LEU:O	2.09	0.52
1:G:43:ALA:CB	1:G:265:HIS:CD2	2.90	0.52
1:C:65:GLU:HB2	1:C:112:ARG:NH2	2.25	0.52
1:F:57:GLY:HA2	1:F:102:LEU:HB3	1.92	0.52
1:A:143:VAL:HG13	1:A:166:ILE:HA	1.91	0.51
1:B:13:ARG:HG2	1:B:13:ARG:HH11	1.74	0.51
1:E:223:TYR:CG	1:E:232:GLU:OE2	2.62	0.51
1:F:128:GLU:CD	1:F:154:GLU:HG2	2.34	0.51
1:A:164:ARG:CD	1:A:223:TYR:CD1	2.93	0.51
1:B:202:ASP:O	1:B:206:MSE:N	2.43	0.51
1:G:167:MSE:HE1	1:G:223:TYR:CE2	2.46	0.51
1:H:156:VAL:HG11	1:H:224:VAL:CG2	2.41	0.51
1:D:99:LEU:O	1:D:99:LEU:HD12	2.10	0.51
1:A:64:ALA:HA	1:A:78:PHE:CE2	2.46	0.51
1:A:197:GLY:O	1:A:211:VAL:HG12	2.11	0.51
1:F:121:VAL:CG2	1:G:206:MSE:HE1	2.41	0.51
1:G:202:ASP:HB3	1:G:205:THR:HB	1.93	0.51
1:H:259:SER:C	1:H:262:PRO:HD2	2.36	0.51
1:F:251:LEU:HD12	1:F:251:LEU:O	2.10	0.51
1:G:205:THR:HG22	1:G:205:THR:O	2.09	0.51
1:B:154:GLU:HG3	1:B:157:ARG:NE	2.25	0.51
1:E:26:TYR:O	1:E:27:LYS:HG2	2.11	0.51
1:G:154:GLU:O	1:G:157:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HG2	1:A:253:TRP:CE2	2.45	0.51
1:C:115:ARG:NE	4:C:405:HOH:O	2.44	0.51
1:F:179:PRO:O	1:F:214:LEU:HD21	2.10	0.51
1:H:201:VAL:HG23	1:H:209:VAL:HG23	1.92	0.51
1:A:259:SER:C	1:A:262:PRO:HD2	2.36	0.51
1:D:126:ASP:OD1	1:D:129:ARG:NH1	2.44	0.50
1:D:173:VAL:HG23	4:D:420:HOH:O	2.10	0.50
1:H:201:VAL:HG12	1:H:201:VAL:O	2.10	0.50
1:F:156:VAL:HG23	1:F:156:VAL:O	2.11	0.50
1:H:58:VAL:HB	1:H:103:LEU:HD23	1.93	0.50
1:A:261:PHE:N	1:A:262:PRO:CD	2.74	0.50
1:E:113:TYR:O	1:E:114:PRO:C	2.51	0.50
1:F:151:ILE:O	1:F:151:ILE:CG2	2.60	0.50
1:H:37:LEU:HD21	1:H:99:LEU:HD11	1.94	0.50
1:H:113:TYR:HB2	1:H:120:HIS:HB2	1.94	0.50
1:A:4:ARG:HB2	1:A:53:TYR:CD1	2.47	0.50
1:G:223:TYR:O	1:G:231:GLY:CA	2.60	0.50
1:A:164:ARG:CD	1:A:223:TYR:CE1	2.95	0.50
1:A:256:PHE:HA	1:A:260:LEU:HB3	1.92	0.50
1:B:167:MSE:HE1	1:B:223:TYR:CZ	2.45	0.50
1:D:6:LEU:HA	1:D:142:VAL:O	2.11	0.50
1:H:8:TYR:OH	1:H:146:ASP:HB2	2.12	0.50
1:D:199:LYS:HD3	1:D:211:VAL:HG11	1.93	0.50
1:F:6:LEU:HD22	1:F:55:LEU:HD13	1.93	0.50
1:D:254:ASN:O	1:D:258:ASN:HB2	2.12	0.50
1:E:175:ARG:O	1:E:181:GLU:HG3	2.11	0.50
1:F:121:VAL:HG22	1:G:206:MSE:CE	2.41	0.50
1:B:111:ARG:HD2	3:B:301:CIT:H42	1.94	0.49
1:B:154:GLU:O	1:B:157:ARG:NE	2.45	0.49
1:A:6:LEU:HD13	1:A:53:TYR:CD1	2.47	0.49
1:A:98:THR:HB	1:A:101:ASP:OD2	2.10	0.49
1:H:91:ASP:O	1:H:93:GLN:NE2	2.38	0.49
1:C:167:MSE:HA	1:C:222:HIS:O	2.13	0.49
1:E:117:THR:O	1:E:121:VAL:HG23	2.12	0.49
1:F:179:PRO:O	1:F:214:LEU:CD2	2.61	0.49
1:H:181:GLU:CG	1:H:183:ARG:HG3	2.43	0.49
1:C:178:SER:HB3	1:C:181:GLU:HB3	1.94	0.49
1:E:128:GLU:CD	1:E:154:GLU:H	2.17	0.49
1:F:254:ASN:O	1:F:258:ASN:HB2	2.12	0.49
1:C:26:TYR:CD1	1:C:250:GLU:HG2	2.48	0.49
1:E:24:VAL:HB	1:E:249:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ASP:HB3	1:E:205:THR:HG22	1.95	0.49
1:H:80:TYR:CZ	1:H:90:ALA:HB2	2.47	0.49
1:C:8:TYR:CD2	1:C:144:VAL:CG1	2.96	0.49
1:A:223:TYR:HD2	1:A:232:GLU:HG3	1.78	0.49
1:C:72:LYS:NZ	2:C:301:FGD:C06	2.75	0.49
1:C:183:ARG:HD3	1:C:183:ARG:N	2.28	0.49
1:D:157:ARG:HB2	1:D:160:ALA:HB2	1.95	0.49
1:E:14:ASN:HB2	1:E:149:LEU:CD2	2.43	0.49
1:E:72:LYS:HE3	2:E:301:FGD:C11	2.43	0.49
1:E:94:VAL:O	1:E:94:VAL:CG1	2.61	0.49
1:E:223:TYR:CD2	1:E:232:GLU:OE2	2.66	0.49
1:B:128:GLU:HB3	1:B:155:LEU:CD1	2.43	0.48
1:E:259:SER:C	1:E:262:PRO:HD2	2.38	0.48
1:D:259:SER:O	1:D:262:PRO:HD2	2.14	0.48
1:A:25:PRO:HA	1:A:29:GLU:O	2.13	0.48
1:A:211:VAL:HG22	1:A:212:GLU:N	2.28	0.48
1:D:22:GLN:HG2	1:D:85:GLN:OE1	2.13	0.48
1:E:160:ALA:O	1:E:163:ALA:CB	2.61	0.48
1:B:243:SER:O	1:B:246:ASP:HB2	2.13	0.48
1:C:108:SER:HB3	1:C:127:PHE:CE1	2.48	0.48
1:F:5:LYS:HB2	1:F:141:ASP:OD2	2.14	0.48
1:D:216:TRP:CH2	1:D:241:GLU:HG3	2.48	0.48
1:A:31:ARG:NH2	4:A:404:HOH:O	2.46	0.48
1:E:261:PHE:N	1:E:262:PRO:CD	2.76	0.48
1:G:201:VAL:HG23	1:G:207:GLU:CG	2.43	0.48
1:C:4:ARG:HA	1:C:141:ASP:OD2	2.14	0.48
1:A:5:LYS:HG2	1:A:56:VAL:HG11	1.95	0.48
1:C:248:ILE:HG22	1:D:129:ARG:HH22	1.78	0.48
1:D:266:GLU:O	1:D:270:LEU:HD12	2.12	0.48
1:F:4:ARG:NH1	1:F:272:ALA:HB1	2.29	0.48
1:D:8:TYR:CZ	1:D:37:LEU:HB2	2.49	0.48
1:E:199:LYS:O	1:E:209:VAL:HG22	2.13	0.48
1:A:46:GLN:HG3	1:A:47:THR:HG23	1.96	0.47
1:B:27:LYS:HE3	1:B:246:ASP:OD1	2.12	0.47
1:C:75:ASP:O	1:C:84:GLN:NE2	2.47	0.47
1:F:13:ARG:HG2	1:F:13:ARG:HH11	1.78	0.47
1:F:94:VAL:O	1:F:94:VAL:HG13	2.14	0.47
1:E:74:LYS:NZ	4:E:403:HOH:O	2.41	0.47
1:G:247:THR:OG1	1:G:250:GLU:CG	2.55	0.47
1:B:128:GLU:OE1	1:B:155:LEU:HD13	2.15	0.47
1:D:80:TYR:CZ	1:D:90:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:THR:H	1:G:250:GLU:CD	2.20	0.47
1:B:128:GLU:HB3	1:B:155:LEU:HD13	1.96	0.47
1:D:33:MSE:O	1:D:33:MSE:HG3	2.13	0.47
1:E:110:TYR:CE2	1:E:124:LYS:HB2	2.49	0.47
1:E:252:ARG:HG2	1:E:252:ARG:HH11	1.80	0.47
1:A:9:ILE:HB	1:A:145:LEU:CD2	2.45	0.47
1:A:80:TYR:CD1	1:A:86:TRP:HB2	2.49	0.47
1:E:124:LYS:O	1:E:127:PHE:HB3	2.15	0.47
1:B:38:GLU:O	1:B:42:GLU:HG3	2.15	0.47
1:B:65:GLU:CG	1:B:112:ARG:NH2	2.77	0.47
1:E:202:ASP:HB3	1:E:205:THR:CG2	2.45	0.47
1:G:24:VAL:HG21	1:G:249:LEU:CB	2.44	0.47
1:G:58:VAL:O	1:G:104:LEU:N	2.45	0.47
1:H:261:PHE:N	1:H:262:PRO:CD	2.78	0.47
1:A:129:ARG:C	1:A:129:ARG:HD2	2.40	0.47
1:B:126:ASP:O	1:B:129:ARG:CB	2.57	0.47
1:D:99:LEU:HD12	1:D:99:LEU:C	2.40	0.47
1:E:222:HIS:CB	1:E:233:VAL:HA	2.45	0.47
1:A:200:VAL:HG21	1:A:203:TRP:CZ3	2.50	0.47
1:H:37:LEU:HD21	1:H:58:VAL:HG21	1.96	0.47
1:A:254:ASN:O	1:A:258:ASN:HB2	2.15	0.47
1:F:42:GLU:O	1:F:46:GLN:HG2	2.14	0.47
1:F:182:ARG:HH11	1:F:191:ALA:HA	1.80	0.47
1:A:143:VAL:HG11	1:A:166:ILE:CD1	2.45	0.46
1:B:251:LEU:O	1:B:251:LEU:HD12	2.15	0.46
1:E:23:TYR:CZ	1:E:32:TYR:HB2	2.49	0.46
1:G:19:LYS:HD2	1:G:19:LYS:N	2.30	0.46
1:H:143:VAL:HB	1:H:166:ILE:HG12	1.96	0.46
1:A:199:LYS:HG2	1:A:211:VAL:HG11	1.97	0.46
1:B:63:ASP:OD2	1:B:109:THR:HA	2.15	0.46
3:B:301:CIT:O4	3:B:301:CIT:H21	2.15	0.46
1:D:113:TYR:CD1	1:D:119:GLU:HB2	2.50	0.46
1:D:86:TRP:HA	1:D:86:TRP:CE3	2.51	0.46
1:D:219:ALA:CB	1:D:260:LEU:HA	2.45	0.46
1:E:80:TYR:CZ	1:E:90:ALA:CB	2.98	0.46
1:E:151:ILE:HD12	1:E:151:ILE:H	1.80	0.46
1:E:196:ARG:HD3	1:H:157:ARG:HH12	1.80	0.46
1:B:26:TYR:CB	1:B:31:ARG:HG3	2.45	0.46
1:B:261:PHE:N	1:B:262:PRO:CD	2.76	0.46
3:C:302:CIT:C6	3:C:302:CIT:O2	2.61	0.46
1:H:201:VAL:CG2	1:H:209:VAL:HG23	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:274:LYS:O	1:H:274:LYS:HG2	2.15	0.46
2:A:301:FGD:C19	1:B:113:TYR:CE2	2.99	0.46
1:B:155:LEU:N	1:B:155:LEU:HD12	2.31	0.46
1:B:211:VAL:HG22	1:B:212:GLU:N	2.30	0.46
1:C:188:THR:HG21	1:C:252[B]:ARG:HG3	1.96	0.46
1:D:58:VAL:O	1:D:103:LEU:HA	2.15	0.46
1:E:80:TYR:CE2	1:E:90:ALA:CB	2.98	0.46
1:E:112:ARG:HH11	2:F:301:FGD:C16	2.29	0.46
1:A:167:MSE:HE2	1:A:271:LEU:HD22	1.98	0.46
1:C:73:ILE:O	1:C:73:ILE:CD1	2.63	0.46
1:D:199:LYS:O	1:D:208:LYS:HA	2.15	0.46
1:D:235:HIS:NE2	1:D:266:GLU:CD	2.71	0.46
1:F:190:ASP:HB3	1:F:199:LYS:NZ	2.31	0.46
1:G:13:ARG:CD	3:G:302:CIT:O6	2.63	0.46
1:G:169:ILE:HB	1:G:264:LEU:HD13	1.97	0.46
1:G:256:PHE:CD2	1:G:261:PHE:CZ	3.03	0.46
1:H:216:TRP:CH2	1:H:241:GLU:HB2	2.50	0.46
1:A:31:ARG:CG	1:A:253:TRP:CE2	2.99	0.46
1:E:40:LEU:HD12	1:E:40:LEU:O	2.15	0.46
1:F:223:TYR:O	1:F:231:GLY:HA3	2.15	0.46
1:G:247:THR:N	1:G:250:GLU:OE1	2.43	0.46
1:D:199:LYS:HG2	1:D:211:VAL:CG1	2.46	0.46
1:F:217:THR:CG2	1:F:240:THR:HB	2.45	0.46
1:G:80:TYR:HB2	1:G:86:TRP:CE3	2.51	0.46
1:H:88:TYR:CE1	1:H:99:LEU:HD23	2.51	0.46
1:E:261:PHE:HB2	1:E:262:PRO:HD3	1.97	0.46
1:H:176:GLU:OE2	1:H:176:GLU:HA	2.15	0.46
1:A:234:PHE:HE2	1:A:267:GLY:O	1.99	0.45
1:B:106:VAL:HG11	1:B:131:LEU:HD23	1.97	0.45
1:B:174:THR:CG2	1:B:183:ARG:HD3	2.46	0.45
1:B:259:SER:C	1:B:262:PRO:HD2	2.40	0.45
1:E:64:ALA:HA	1:E:78:PHE:CZ	2.51	0.45
1:G:43:ALA:HB2	1:G:265:HIS:NE2	2.31	0.45
1:A:18:ASP:O	1:A:19:LYS:HB2	2.16	0.45
1:A:31:ARG:CG	1:A:253:TRP:CZ2	3.00	0.45
1:A:82:PRO:HB2	1:E:65:GLU:OE1	2.16	0.45
1:C:273:GLU:HG3	1:C:273:GLU:O	2.16	0.45
1:E:37:LEU:O	1:E:41:VAL:HG23	2.16	0.45
1:F:126:ASP:O	1:F:130:ARG:HG3	2.15	0.45
1:G:174:THR:O	1:G:183:ARG:CZ	2.63	0.45
1:A:166:ILE:HG23	1:A:224:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:TYR:CD1	1:E:37:LEU:HD13	2.52	0.45
1:G:261:PHE:N	1:G:262:PRO:CD	2.80	0.45
1:B:9:ILE:HB	1:B:145:LEU:HD23	1.98	0.45
1:H:6:LEU:CD2	1:H:55:LEU:HD12	2.47	0.45
1:D:19:LYS:O	1:D:22:GLN:HB2	2.16	0.45
1:E:194:GLY:O	1:E:213:PRO:HA	2.16	0.45
1:B:13:ARG:HG2	1:B:13:ARG:NH1	2.32	0.45
1:C:204:ALA:HB1	1:D:115:ARG:NH1	2.32	0.45
1:H:171:PRO:HG3	4:H:445:HOH:O	2.16	0.45
1:B:113:TYR:HA	1:B:114:PRO:HD3	1.79	0.45
1:C:169:ILE:HD13	1:C:264:LEU:HB2	1.99	0.45
1:E:173:VAL:CG2	1:E:238:LEU:HD13	2.38	0.45
1:G:43:ALA:HB2	1:G:265:HIS:HD2	1.75	0.45
1:A:5:LYS:CG	1:A:56:VAL:HG11	2.47	0.45
1:C:128:GLU:HG3	1:C:155:LEU:HB2	1.99	0.45
1:D:26:TYR:CG	1:D:31:ARG:HG3	2.52	0.45
1:D:261:PHE:O	1:D:265:HIS:ND1	2.50	0.45
1:G:110:TYR:CD2	1:G:120:HIS:CE1	3.04	0.45
1:G:201:VAL:CG2	1:G:207:GLU:HG3	2.46	0.44
1:A:14:ASN:HB2	1:A:149:LEU:HD21	1.99	0.44
1:A:197:GLY:C	1:A:211:VAL:CG1	2.88	0.44
1:B:143:VAL:HG13	1:B:166:ILE:HG23	1.99	0.44
1:D:180:TYR:HE1	1:D:216:TRP:N	2.08	0.44
1:E:121:VAL:HG13	1:F:206:MSE:SE	2.67	0.44
1:H:256:PHE:HB3	1:H:261:PHE:CZ	2.51	0.44
1:A:6:LEU:HA	1:A:142:VAL:O	2.18	0.44
1:B:209:VAL:HG23	1:B:209:VAL:O	2.16	0.44
1:C:110:TYR:HB3	4:C:403:HOH:O	2.16	0.44
1:D:157:ARG:O	1:D:163:ALA:HB2	2.17	0.44
1:D:182:ARG:HH11	1:D:191:ALA:HA	1.83	0.44
1:D:202:ASP:O	1:D:206:MSE:N	2.51	0.44
1:G:143:VAL:HB	1:G:166:ILE:HD13	2.00	0.44
1:E:6:LEU:HD13	1:E:142:VAL:CG1	2.45	0.44
1:F:154:GLU:O	1:F:157:ARG:HB2	2.16	0.44
1:F:261:PHE:N	1:F:262:PRO:CD	2.81	0.44
1:A:18:ASP:O	1:A:252:ARG:NH2	2.51	0.44
1:A:83:GLY:O	1:A:84:GLN:NE2	2.46	0.44
1:B:43:ALA:HB2	1:B:265:HIS:CD2	2.53	0.44
1:D:174:THR:O	1:D:183:ARG:NH2	2.46	0.44
1:G:147:GLY:HA3	4:G:402:HOH:O	2.17	0.44
1:E:76:TYR:O	4:E:402:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:ILE:HB	1:F:145:LEU:CD2	2.47	0.44
1:A:88:TYR:CZ	1:A:99:LEU:CD2	3.00	0.44
1:A:217:THR:O	1:A:238:LEU:HD12	2.18	0.44
1:B:174:THR:HG22	1:B:183:ARG:HD3	1.99	0.44
1:C:256:PHE:CD1	1:C:260:LEU:HD13	2.53	0.44
1:E:202:ASP:CB	1:E:205:THR:HG22	2.47	0.44
1:A:95:GLN:O	1:A:95:GLN:CD	2.60	0.44
1:F:180:TYR:CD1	1:F:214:LEU:HD23	2.53	0.44
1:G:127:PHE:CE2	1:G:131:LEU:HD11	2.52	0.44
1:F:132:HIS:HB2	1:F:155:LEU:CD1	2.48	0.44
1:D:222:HIS:HB2	1:D:232:GLU:O	2.18	0.43
1:F:237:VAL:CB	1:F:263:ALA:HB2	2.47	0.43
1:H:182:ARG:HB3	1:H:187:ALA:HB1	1.99	0.43
1:G:12:LEU:HB3	1:G:73:ILE:HD11	2.00	0.43
1:B:196:ARG:HG3	4:B:404:HOH:O	2.17	0.43
1:D:49:LEU:HD12	1:D:49:LEU:HA	1.85	0.43
1:H:60:TYR:HE2	1:H:103:LEU:HB3	1.83	0.43
1:A:186:TYR:CD1	1:A:203:TRP:CE2	3.06	0.43
1:D:188:THR:HG22	1:D:248:ILE:HD11	2.00	0.43
1:D:215:TYR:O	1:D:242:ILE:N	2.51	0.43
1:E:160:ALA:N	1:E:163:ALA:HB2	2.34	0.43
1:B:242:ILE:HG23	1:B:242:ILE:O	2.18	0.43
1:C:44:LEU:O	1:C:50:GLY:HA3	2.19	0.43
1:D:145:LEU:HB2	1:D:168:ASN:OD1	2.19	0.43
1:E:6:LEU:HD12	1:E:142:VAL:HG13	1.98	0.43
1:E:86:TRP:HA	1:E:86:TRP:CE3	2.52	0.43
1:G:106:VAL:CG1	1:G:131:LEU:HD23	2.45	0.43
1:G:129:ARG:HD2	1:G:129:ARG:C	2.43	0.43
1:G:237:VAL:HB	1:G:263:ALA:HB2	2.00	0.43
1:H:242:ILE:HD12	1:H:246:ASP:OD2	2.18	0.43
1:B:199:LYS:O	1:B:208:LYS:HA	2.18	0.43
1:E:26:TYR:C	1:E:27:LYS:HG2	2.43	0.43
1:G:66:LEU:HD21	1:G:68:ARG:HG3	2.01	0.43
1:G:175:ARG:CD	1:G:236:ASP:OD2	2.66	0.43
1:A:153:ASP:OD1	1:A:154:GLU:N	2.51	0.43
1:B:59:ILE:HA	1:B:104:LEU:O	2.19	0.43
1:D:182:ARG:HH22	1:D:214:LEU:CD1	2.28	0.43
1:F:182:ARG:NH2	1:F:199:LYS:HE2	2.33	0.43
1:G:68:ARG:HE	3:G:302:CIT:C4	2.31	0.43
1:A:114:PRO:O	1:A:120:HIS:HB2	2.18	0.43
1:D:65:GLU:OE1	1:D:65:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ASP:O	1:E:165:ARG:HD3	2.19	0.43
1:F:165:ARG:HD2	1:F:165:ARG:N	2.33	0.43
1:H:9:ILE:HG22	1:H:148:LEU:HB2	2.00	0.43
1:H:198:GLU:HG2	1:H:208:LYS:HD2	2.00	0.43
1:A:63:ASP:OD2	1:A:65:GLU:HB2	2.19	0.43
1:B:129:ARG:HD2	1:B:129:ARG:C	2.44	0.43
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.89	0.43
1:A:68:ARG:HB3	2:A:301:FGD:C05	2.49	0.42
1:B:49:LEU:O	1:B:52:ALA:HB3	2.19	0.42
1:D:8:TYR:CG	1:D:37:LEU:HD13	2.54	0.42
1:E:8:TYR:OH	1:E:146:ASP:CB	2.67	0.42
1:G:59:ILE:HA	1:G:104:LEU:O	2.20	0.42
1:B:5:LYS:HD3	1:B:56:VAL:HG11	2.02	0.42
1:D:222:HIS:CB	1:D:233:VAL:HA	2.49	0.42
1:D:266:GLU:HG2	1:D:270:LEU:CD1	2.49	0.42
1:G:59:ILE:HG12	1:G:104:LEU:HB2	2.01	0.42
1:H:81:ARG:HE	1:H:84:GLN:HG2	1.84	0.42
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.85	0.42
1:A:143:VAL:HG11	1:A:166:ILE:HD12	2.01	0.42
1:A:143:VAL:HG11	1:A:166:ILE:CG1	2.50	0.42
1:E:237:VAL:O	1:E:259:SER:HB3	2.20	0.42
1:H:129:ARG:C	1:H:129:ARG:HD2	2.45	0.42
1:H:237:VAL:HG11	1:H:259:SER:HA	2.02	0.42
1:G:73:ILE:O	1:G:73:ILE:CG2	2.67	0.42
1:B:73:ILE:O	1:B:76:TYR:O	2.37	0.42
1:C:169:ILE:HG12	1:C:260:LEU:CD2	2.49	0.42
1:G:34:LYS:HG3	1:G:38:GLU:OE1	2.19	0.42
1:E:148:LEU:HB3	4:E:414:HOH:O	2.18	0.42
1:F:260:LEU:C	1:F:260:LEU:HD23	2.43	0.42
1:A:157:ARG:NH1	1:D:244:PRO:O	2.52	0.42
1:C:113:TYR:CE2	1:C:119:GLU:CB	3.03	0.42
1:G:7:ALA:N	1:G:142:VAL:O	2.33	0.42
1:H:58:VAL:O	1:H:104:LEU:N	2.50	0.42
1:A:143:VAL:HG11	1:A:166:ILE:HG13	1.93	0.42
1:A:265:HIS:CD2	1:A:265:HIS:N	2.85	0.42
1:B:68:ARG:O	1:B:72:LYS:HG3	2.19	0.42
1:D:73:ILE:HG21	1:D:73:ILE:HD13	1.73	0.42
1:E:31:ARG:HH11	1:E:31:ARG:HG2	1.84	0.42
1:E:182:ARG:HD2	1:E:190:ASP:HB2	2.01	0.42
1:G:234:PHE:HE2	1:G:271:LEU:HB2	1.74	0.42
1:H:215:TYR:C	1:H:242:ILE:HG22	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:HE	3:C:302:CIT:H42	1.85	0.42
1:C:145:LEU:CD1	1:C:152:LEU:HD11	2.45	0.42
1:C:169:ILE:HG12	1:C:260:LEU:HD21	2.02	0.42
1:E:253:TRP:CH2	1:E:257:ASN:ND2	2.88	0.42
1:G:164:ARG:NH2	1:G:232:GLU:OE1	2.53	0.42
1:H:94:VAL:HG13	1:H:94:VAL:O	2.20	0.42
1:H:113:TYR:HB3	1:H:120:HIS:HB2	2.00	0.42
1:D:132:HIS:HB2	1:D:155:LEU:HD13	2.02	0.42
1:D:143:VAL:HB	1:D:166:ILE:HG12	2.02	0.42
1:H:200:VAL:HG22	1:H:208:LYS:HG2	2.02	0.42
1:E:41:VAL:O	1:E:45:ASN:ND2	2.53	0.41
1:E:113:TYR:O	1:E:120:HIS:ND1	2.53	0.41
1:F:248:ILE:HD12	1:F:248:ILE:HA	1.94	0.41
1:G:164:ARG:CZ	1:G:232:GLU:OE1	2.68	0.41
1:B:37:LEU:O	1:B:41:VAL:HG23	2.20	0.41
1:E:144:VAL:HA	1:E:167:MSE:O	2.21	0.41
1:G:143:VAL:CG2	1:G:166:ILE:HD13	2.50	0.41
1:G:170:HIS:ND1	1:G:171:PRO:HD2	2.35	0.41
1:B:4:ARG:HG2	1:B:4:ARG:NH1	2.33	0.41
1:E:169:ILE:HB	1:E:264:LEU:HD13	2.01	0.41
1:F:158:PRO:O	1:F:158:PRO:HG2	2.20	0.41
1:G:264:LEU:HD12	1:G:264:LEU:HA	1.79	0.41
1:H:132:HIS:O	1:H:136:VAL:HG23	2.19	0.41
1:A:53:TYR:CE2	1:A:268:LEU:HB3	2.55	0.41
1:A:98:THR:HB	1:A:101:ASP:CG	2.44	0.41
1:C:5:LYS:HB2	1:C:140:ALA:HA	2.03	0.41
1:F:73:ILE:HD13	1:F:73:ILE:HG21	1.84	0.41
1:G:132:HIS:HB2	1:G:155:LEU:HD13	2.03	0.41
1:G:168:ASN:HB2	1:G:224:VAL:CG1	2.50	0.41
1:A:132:HIS:NE2	1:A:161:PRO:HD2	2.35	0.41
1:D:189:LEU:HB3	1:D:203:TRP:CH2	2.56	0.41
1:G:143:VAL:HG21	1:G:166:ILE:HD13	2.02	0.41
1:E:145:LEU:HD21	1:E:166:ILE:HD11	2.03	0.41
1:F:216:TRP:CZ3	1:F:241:GLU:HB2	2.55	0.41
1:E:262:PRO:O	1:E:266:GLU:CB	2.67	0.41
1:G:126:ASP:OD2	1:G:130:ARG:HD3	2.20	0.41
1:D:221:PHE:CE1	1:D:264:LEU:HD12	2.56	0.41
1:D:261:PHE:N	1:D:262:PRO:CD	2.83	0.41
1:E:264:LEU:O	1:E:268:LEU:HD12	2.20	0.41
2:E:301:FGD:C06	2:E:301:FGD:O32	2.69	0.41
1:H:80:TYR:CE2	1:H:90:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:VAL:HB	1:H:203:TRP:CH2	2.55	0.41
1:A:132:HIS:O	1:A:136:VAL:HG23	2.21	0.41
1:B:13:ARG:NH1	1:B:62:ASP:OD2	2.51	0.41
1:C:9:ILE:HB	1:C:145:LEU:CD2	2.49	0.41
1:D:43:ALA:O	1:D:47:THR:OG1	2.29	0.41
1:E:8:TYR:CZ	1:E:146:ASP:HB3	2.55	0.41
1:E:38:GLU:O	1:E:41:VAL:HB	2.21	0.41
1:E:152:LEU:HD23	1:E:156:VAL:HG13	2.02	0.41
1:E:251:LEU:HA	1:E:254:ASN:HB2	2.03	0.41
1:F:4:ARG:HB3	1:F:53:TYR:HD1	1.83	0.41
1:G:80:TYR:HB2	1:G:86:TRP:CD2	2.56	0.41
1:G:114:PRO:HD2	1:G:117:THR:HG21	2.02	0.41
1:G:126:ASP:O	1:G:130:ARG:CG	2.69	0.41
1:A:73:ILE:HD11	1:A:78:PHE:CE2	2.56	0.41
1:F:191:ALA:HB3	1:F:251:LEU:HD21	2.03	0.41
1:G:115:ARG:HD3	1:H:204:ALA:HB1	2.03	0.41
1:C:141:ASP:O	1:C:165:ARG:NE	2.54	0.40
1:E:24:VAL:HB	1:E:249:LEU:HD21	2.02	0.40
1:E:73:ILE:O	1:E:73:ILE:CG2	2.69	0.40
1:E:75:ASP:OD2	2:E:301:FGD:O31	2.38	0.40
1:F:124:LYS:O	1:F:127:PHE:HB3	2.21	0.40
1:H:237:VAL:CG1	1:H:259:SER:HA	2.51	0.40
1:A:9:ILE:HG21	1:A:148:LEU:HD22	2.01	0.40
1:A:272:ALA:C	1:A:274:LYS:H	2.29	0.40
1:E:164:ARG:HG3	1:E:223:TYR:CD1	2.56	0.40
1:F:13:ARG:CZ	1:F:149:LEU:HD12	2.51	0.40
1:G:60:TYR:OH	1:G:105:SER:HB2	2.20	0.40
1:G:94:VAL:O	1:G:94:VAL:HG13	2.21	0.40
1:G:205:THR:O	1:G:205:THR:CG2	2.69	0.40
1:G:274:LYS:HD3	1:G:274:LYS:HA	1.82	0.40
1:A:9:ILE:HD12	1:A:145:LEU:CD2	2.51	0.40
1:A:143:VAL:CG1	1:A:166:ILE:HA	2.52	0.40
1:B:110:TYR:CZ	1:B:124:LYS:HG3	2.56	0.40
1:E:72:LYS:NZ	3:E:302:CIT:H42	2.36	0.40
1:F:129:ARG:HD2	1:F:129:ARG:C	2.47	0.40
1:G:7:ALA:O	1:G:144:VAL:N	2.44	0.40
1:A:182:ARG:NH2	1:A:191:ALA:HA	2.36	0.40
1:B:243:SER:HA	1:B:244:PRO:HD3	1.95	0.40
1:C:202:ASP:OD2	1:C:205:THR:OG1	2.30	0.40
1:D:195:ALA:HB2	1:D:214:LEU:O	2.22	0.40
1:E:34:LYS:HE3	1:E:34:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PRO:HB2	1:A:109:THR:HG23	2.02	0.40
1:B:149:LEU:HD23	1:B:149:LEU:HA	1.93	0.40
1:F:182:ARG:NH1	1:F:191:ALA:HA	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:406:HOH:O	4:G:424:HOH:O[2_545]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/275 (96%)	255 (97%)	8 (3%)	0	100	100
1	B	257/275 (94%)	248 (96%)	9 (4%)	0	100	100
1	C	264/275 (96%)	253 (96%)	11 (4%)	0	100	100
1	D	263/275 (96%)	254 (97%)	9 (3%)	0	100	100
1	E	260/275 (94%)	249 (96%)	11 (4%)	0	100	100
1	F	249/275 (90%)	243 (98%)	5 (2%)	1 (0%)	30	38
1	G	259/275 (94%)	249 (96%)	10 (4%)	0	100	100
1	H	261/275 (95%)	254 (97%)	7 (3%)	0	100	100
All	All	2076/2200 (94%)	2005 (97%)	70 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	5	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/225 (99%)	218 (98%)	4 (2%)	51	70
1	B	220/225 (98%)	219 (100%)	1 (0%)	81	90
1	C	223/225 (99%)	220 (99%)	3 (1%)	61	77
1	D	223/225 (99%)	221 (99%)	2 (1%)	70	84
1	E	219/225 (97%)	216 (99%)	3 (1%)	59	76
1	F	214/225 (95%)	212 (99%)	2 (1%)	70	84
1	G	221/225 (98%)	218 (99%)	3 (1%)	59	76
1	H	223/225 (99%)	223 (100%)	0	100	100
All	All	1765/1800 (98%)	1747 (99%)	18 (1%)	68	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	LEU
1	A	29	GLU
1	A	93	GLN
1	B	175	ARG
1	C	4	ARG
1	C	6	LEU
1	C	84	GLN
1	D	181	GLU
1	D	182	ARG
1	E	29	GLU
1	E	30	GLN
1	E	206	MSE
1	F	3	LYS
1	F	4	ARG
1	G	5	LYS
1	G	31	ARG
1	G	206	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	B	258	ASN
1	B	265	HIS
1	C	30	GLN
1	C	168	ASN
1	D	84	GLN
1	D	258	ASN
1	E	222	HIS
1	E	258	ASN
1	E	265	HIS
1	F	30	GLN
1	F	95	GLN
1	F	168	ASN
1	F	257	ASN
1	G	93	GLN
1	G	257	ASN
1	H	22	GLN
1	H	85	GLN
1	H	95	GLN
1	H	254	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CIT	E	302	-	12,12,12	1.16	1 (8%)	17,17,17	2.06	5 (29%)
3	CIT	A	302	-	12,12,12	0.99	0	17,17,17	2.11	6 (35%)
3	CIT	C	302	-	12,12,12	1.27	0	17,17,17	2.01	7 (41%)
3	CIT	D	302	-	12,12,12	1.05	0	17,17,17	1.81	4 (23%)
2	FGD	G	301	-	34,34,34	2.61	18 (52%)	46,47,47	1.95	14 (30%)
3	CIT	G	302	-	12,12,12	2.30	6 (50%)	17,17,17	2.63	9 (52%)
3	CIT	B	301	-	12,12,12	1.00	0	17,17,17	2.40	8 (47%)
3	CIT	F	302	-	12,12,12	1.65	2 (16%)	17,17,17	2.28	8 (47%)
2	FGD	E	301	-	34,34,34	2.34	13 (38%)	46,47,47	2.86	25 (54%)
2	FGD	H	301	-	34,34,34	2.12	15 (44%)	46,47,47	1.52	9 (19%)
3	CIT	H	302	-	12,12,12	1.09	0	17,17,17	1.67	3 (17%)
2	FGD	F	301	-	34,34,34	2.70	12 (35%)	46,47,47	2.52	16 (34%)
2	FGD	C	301	-	34,34,34	2.59	13 (38%)	46,47,47	3.14	28 (60%)
2	FGD	A	301	-	34,34,34	2.28	9 (26%)	46,47,47	0.91	1 (2%)
2	FGD	D	301	-	34,34,34	2.45	12 (35%)	46,47,47	1.64	12 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	E	302	-	-	8/16/16/16	-
3	CIT	A	302	-	-	7/16/16/16	-
3	CIT	C	302	-	-	5/16/16/16	-
3	CIT	D	302	-	-	10/16/16/16	-
2	FGD	G	301	-	-	10/22/22/22	0/3/3/3
3	CIT	G	302	-	-	2/16/16/16	-
3	CIT	B	301	-	-	8/16/16/16	-
3	CIT	F	302	-	-	11/16/16/16	-
2	FGD	E	301	-	-	8/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FGD	H	301	-	-	8/22/22/22	0/3/3/3
3	CIT	H	302	-	-	5/16/16/16	-
2	FGD	F	301	-	-	7/22/22/22	0/3/3/3
2	FGD	C	301	-	-	11/22/22/22	0/3/3/3
2	FGD	A	301	-	-	2/22/22/22	0/3/3/3
2	FGD	D	301	-	-	10/22/22/22	0/3/3/3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	FGD	C23-N26	8.43	1.54	1.39
2	C	301	FGD	O31-C30	-6.25	1.13	1.23
2	G	301	FGD	O31-C30	-6.06	1.13	1.23
2	D	301	FGD	O32-C11	-6.02	1.09	1.23
2	F	301	FGD	C27-N29	5.93	1.47	1.33
2	A	301	FGD	C23-N26	5.76	1.49	1.39
2	C	301	FGD	C22-C23	-5.71	1.32	1.41
2	E	301	FGD	C11-N10	5.62	1.47	1.34
2	D	301	FGD	C27-N28	5.44	1.46	1.34
2	E	301	FGD	O31-C30	-5.35	1.14	1.23
2	H	301	FGD	O31-C30	-5.33	1.14	1.23
2	G	301	FGD	O32-C11	-5.33	1.10	1.23
2	D	301	FGD	O31-C30	-5.24	1.14	1.23
2	C	301	FGD	C27-N28	5.13	1.46	1.34
2	A	301	FGD	C11-N10	5.11	1.46	1.34
2	C	301	FGD	C27-N29	4.94	1.45	1.33
2	A	301	FGD	C27-N29	4.91	1.45	1.33
2	A	301	FGD	C27-N28	4.81	1.45	1.34
2	G	301	FGD	C05-C04	-4.76	1.42	1.53
3	G	302	CIT	O2-C1	-4.61	1.15	1.30
2	D	301	FGD	C23-N26	4.37	1.47	1.39
2	E	301	FGD	C27-N29	4.34	1.43	1.33
2	F	301	FGD	C27-N26	4.24	1.47	1.37
2	D	301	FGD	C27-N29	4.23	1.43	1.33
2	E	301	FGD	C27-N28	4.04	1.43	1.34
2	A	301	FGD	C27-N26	3.97	1.47	1.37
2	C	301	FGD	O32-C11	-3.89	1.14	1.23
2	E	301	FGD	C23-N26	3.83	1.46	1.39
2	F	301	FGD	C30-N29	3.82	1.46	1.38
2	F	301	FGD	O31-C30	-3.82	1.17	1.23
2	G	301	FGD	O03-C02	-3.71	1.18	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	FGD	C27-N26	3.70	1.46	1.37
2	F	301	FGD	O03-C02	-3.67	1.19	1.30
2	G	301	FGD	C27-N29	3.55	1.41	1.33
2	C	301	FGD	C23-N26	3.55	1.45	1.39
2	F	301	FGD	C27-N28	3.54	1.42	1.34
2	D	301	FGD	C11-N10	3.47	1.42	1.34
2	D	301	FGD	C27-N26	3.41	1.45	1.37
2	G	301	FGD	O09-C07	-3.38	1.19	1.30
2	C	301	FGD	C27-N26	3.37	1.45	1.37
2	H	301	FGD	C23-N26	3.35	1.45	1.39
2	H	301	FGD	C22-C30	3.33	1.53	1.48
2	H	301	FGD	C27-N29	3.33	1.41	1.33
2	F	301	FGD	O32-C11	-3.30	1.15	1.23
2	H	301	FGD	C11-N10	3.25	1.41	1.34
2	D	301	FGD	C22-C23	-3.21	1.36	1.41
2	A	301	FGD	C22-C30	3.19	1.53	1.48
2	F	301	FGD	C04-C02	3.18	1.60	1.52
2	H	301	FGD	O32-C11	-3.15	1.16	1.23
2	G	301	FGD	C14-C17	-3.13	1.34	1.39
3	G	302	CIT	C3-C6	-3.13	1.50	1.53
2	C	301	FGD	C14-C17	-3.12	1.34	1.39
2	G	301	FGD	C04-N10	-3.07	1.39	1.45
2	G	301	FGD	C27-N28	3.06	1.41	1.34
2	G	301	FGD	C14-C13	-3.04	1.33	1.38
2	D	301	FGD	O03-C02	-3.02	1.21	1.30
3	G	302	CIT	C4-C3	-2.97	1.50	1.54
2	G	301	FGD	C16-C15	-2.96	1.34	1.38
2	H	301	FGD	C22-C23	-2.94	1.36	1.41
2	G	301	FGD	C15-C12	-2.89	1.35	1.39
3	F	302	CIT	O7-C3	2.84	1.48	1.43
2	G	301	FGD	C16-C17	-2.82	1.34	1.39
2	A	301	FGD	O31-C30	-2.79	1.19	1.23
3	G	302	CIT	O4-C5	-2.77	1.21	1.30
2	C	301	FGD	C22-C30	2.75	1.52	1.48
2	C	301	FGD	C17-N18	2.73	1.46	1.38
2	C	301	FGD	C12-C11	2.73	1.56	1.50
2	F	301	FGD	C22-C23	-2.72	1.36	1.41
2	E	301	FGD	C14-C13	-2.67	1.34	1.38
2	G	301	FGD	C21-C20	-2.60	1.34	1.39
2	E	301	FGD	O32-C11	-2.59	1.17	1.23
2	H	301	FGD	O03-C02	-2.58	1.22	1.30
2	A	301	FGD	C17-N18	2.52	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	FGD	O09-C07	-2.46	1.22	1.30
3	F	302	CIT	C4-C3	2.43	1.57	1.54
2	H	301	FGD	C15-C12	-2.40	1.35	1.39
2	E	301	FGD	C21-C20	-2.40	1.35	1.39
2	E	301	FGD	C22-C23	-2.40	1.37	1.41
2	E	301	FGD	C25-C20	2.39	1.43	1.38
2	H	301	FGD	O09-C07	-2.39	1.22	1.30
2	H	301	FGD	C14-C13	-2.38	1.35	1.38
3	G	302	CIT	O1-C1	-2.38	1.14	1.22
2	G	301	FGD	C22-C23	-2.37	1.37	1.41
2	C	301	FGD	C11-N10	2.32	1.39	1.34
2	F	301	FGD	C05-C06	-2.32	1.45	1.52
2	G	301	FGD	C11-N10	2.31	1.39	1.34
2	G	301	FGD	C04-C02	-2.30	1.46	1.52
3	G	302	CIT	O7-C3	-2.28	1.38	1.43
2	A	301	FGD	C30-N29	2.27	1.43	1.38
2	F	301	FGD	C11-N10	2.25	1.39	1.34
2	H	301	FGD	C27-N28	2.22	1.39	1.34
2	H	301	FGD	C13-C12	-2.17	1.36	1.39
2	C	301	FGD	C14-C13	2.16	1.42	1.38
2	D	301	FGD	C22-C30	2.16	1.51	1.48
2	E	301	FGD	O01-C02	2.09	1.28	1.22
2	G	301	FGD	C13-C12	-2.08	1.36	1.39
2	D	301	FGD	C21-C20	-2.07	1.35	1.39
2	E	301	FGD	C24-C23	2.07	1.43	1.39
3	E	302	CIT	O7-C3	2.04	1.47	1.43
2	H	301	FGD	C16-C15	-2.04	1.35	1.38
2	H	301	FGD	C16-C17	-2.02	1.35	1.39

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	FGD	C12-C11-N10	8.99	133.70	117.04
2	C	301	FGD	C05-C04-N10	-8.61	93.86	110.91
2	F	301	FGD	O03-C02-O01	-7.52	107.01	124.08
2	C	301	FGD	C02-C04-N10	6.80	126.34	110.57
3	E	302	CIT	O6-C6-C3	5.67	124.03	113.14
2	F	301	FGD	C12-C11-N10	5.51	127.25	117.04
2	F	301	FGD	C05-C04-C02	5.44	123.26	110.35
2	C	301	FGD	O31-C30-N29	-5.28	112.20	120.23
2	G	301	FGD	C05-C04-N10	-4.97	101.07	110.91
3	C	302	CIT	O6-C6-C3	4.89	122.52	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	CIT	O6-C6-C3	4.85	122.44	113.14
2	E	301	FGD	C22-C23-N26	-4.82	115.69	119.46
2	E	301	FGD	C23-C22-C30	4.72	125.21	120.11
3	F	302	CIT	O6-C6-C3	4.51	121.80	113.14
2	C	301	FGD	N26-C27-N29	-4.51	115.07	123.32
2	E	301	FGD	O32-C11-C12	-4.47	112.05	120.90
2	H	301	FGD	O03-C02-O01	-4.43	114.02	124.08
2	G	301	FGD	C02-C04-N10	4.43	120.85	110.57
2	F	301	FGD	C21-C22-C23	4.43	123.07	119.09
2	C	301	FGD	C22-C23-N26	4.37	122.87	119.46
2	E	301	FGD	O32-C11-N10	-4.37	114.17	122.47
2	C	301	FGD	O32-C11-C12	4.36	129.53	120.90
3	G	302	CIT	O2-C1-O1	-4.35	112.14	123.33
2	C	301	FGD	C15-C16-C17	4.35	125.30	120.30
3	G	302	CIT	O3-C5-C4	-4.33	110.69	122.95
2	C	301	FGD	C15-C12-C13	-4.27	113.14	118.57
2	F	301	FGD	O03-C02-C04	4.23	127.84	113.51
3	B	301	CIT	O6-C6-C3	4.22	121.24	113.14
3	B	301	CIT	O7-C3-C4	-4.14	99.94	109.38
2	E	301	FGD	O09-C07-C06	4.13	127.05	114.00
2	G	301	FGD	C20-C19-N18	-4.10	102.22	113.60
2	C	301	FGD	O32-C11-N10	-4.09	114.69	122.47
3	D	302	CIT	O6-C6-C3	4.05	120.91	113.14
2	C	301	FGD	C23-C22-C30	-4.03	115.76	120.11
2	D	301	FGD	O09-C07-C06	3.90	126.33	114.00
2	C	301	FGD	C19-N18-C17	3.90	134.38	121.87
2	E	301	FGD	O09-C07-O08	-3.82	113.50	123.33
2	E	301	FGD	C02-C04-N10	3.79	119.36	110.57
2	F	301	FGD	C05-C04-N10	3.77	118.38	110.91
2	F	301	FGD	O31-C30-C22	-3.77	115.26	121.33
3	B	301	CIT	O7-C3-C6	-3.76	103.62	108.96
2	E	301	FGD	C19-C20-C21	-3.76	112.61	120.63
2	C	301	FGD	O03-C02-O01	-3.73	115.63	124.08
2	F	301	FGD	O32-C11-C12	-3.72	113.52	120.90
3	F	302	CIT	O7-C3-C2	-3.68	100.99	109.38
2	C	301	FGD	C04-N10-C11	3.67	130.38	121.56
3	G	302	CIT	O6-C6-C3	3.67	120.17	113.14
3	F	302	CIT	C4-C3-C2	3.60	118.56	109.31
2	E	301	FGD	C14-C13-C12	3.57	124.61	120.80
2	E	301	FGD	C19-N18-C17	-3.56	110.47	121.87
2	C	301	FGD	O03-C02-C04	3.53	125.47	113.51
2	D	301	FGD	C12-C11-N10	3.53	123.58	117.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FGD	C16-C17-C14	-3.47	114.44	119.04
3	G	302	CIT	O2-C1-C2	3.45	125.27	114.35
2	C	301	FGD	C19-C20-C21	3.43	127.96	120.63
3	B	301	CIT	C4-C3-C6	3.43	117.61	110.03
3	G	302	CIT	O7-C3-C2	-3.41	101.59	109.38
3	G	302	CIT	C3-C2-C1	3.40	123.22	113.92
3	G	302	CIT	O4-C5-C4	3.38	125.06	114.35
2	H	301	FGD	O09-C07-C06	3.38	124.67	114.00
2	D	301	FGD	O32-C11-N10	-3.36	116.08	122.47
2	G	301	FGD	C19-C20-C21	-3.34	113.50	120.63
2	C	301	FGD	C14-C13-C12	3.32	124.35	120.80
3	A	302	CIT	O7-C3-C6	3.32	113.67	108.96
2	E	301	FGD	C25-C20-C21	3.32	123.12	118.55
2	G	301	FGD	C23-C22-C30	3.19	123.55	120.11
3	H	302	CIT	O6-C6-C3	3.18	119.23	113.14
2	G	301	FGD	O03-C02-O01	-3.17	116.89	124.08
2	D	301	FGD	N28-C27-N26	3.14	123.37	116.77
3	D	302	CIT	O4-C5-C4	3.08	124.10	114.35
2	E	301	FGD	O03-C02-C04	3.01	123.70	113.51
3	B	301	CIT	O4-C5-O3	-3.01	115.58	123.33
2	H	301	FGD	C05-C04-N10	-2.99	104.99	110.91
2	C	301	FGD	C05-C06-C07	-2.98	104.54	112.49
2	C	301	FGD	C14-C17-N18	2.93	127.58	120.96
2	E	301	FGD	C05-C06-C07	2.92	120.27	112.49
3	C	302	CIT	C4-C3-C6	-2.87	103.69	110.03
2	G	301	FGD	C16-C17-C14	2.87	122.85	119.04
2	C	301	FGD	C21-C22-C30	2.86	125.97	119.51
3	A	302	CIT	O4-C5-C4	2.85	123.38	114.35
2	G	301	FGD	C06-C05-C04	-2.85	107.91	113.16
2	E	301	FGD	C16-C17-N18	2.83	127.35	120.96
3	G	302	CIT	C2-C3-C6	2.83	116.28	110.03
3	F	302	CIT	O4-C5-O3	-2.82	116.08	123.33
2	D	301	FGD	C04-N10-C11	2.81	128.31	121.56
2	F	301	FGD	C20-C19-N18	2.79	121.33	113.60
3	E	302	CIT	O2-C1-C2	2.78	123.15	114.35
2	F	301	FGD	N26-C27-N29	-2.78	118.24	123.32
2	E	301	FGD	C15-C12-C11	2.77	129.57	120.60
2	G	301	FGD	O31-C30-N29	2.75	124.42	120.23
2	G	301	FGD	C14-C17-N18	-2.70	114.86	120.96
2	D	301	FGD	N26-C27-N29	-2.70	118.38	123.32
2	D	301	FGD	C02-C04-N10	2.68	116.78	110.57
2	F	301	FGD	C16-C15-C12	-2.64	117.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	302	CIT	C3-C2-C1	2.64	121.14	113.92
3	F	302	CIT	O2-C1-O1	-2.64	116.55	123.33
3	H	302	CIT	O4-C5-C4	2.63	122.67	114.35
2	H	301	FGD	O09-C07-O08	-2.62	116.59	123.33
3	C	302	CIT	O4-C5-O3	-2.59	116.67	123.33
3	C	302	CIT	O2-C1-O1	-2.58	116.70	123.33
3	E	302	CIT	O5-C6-C3	-2.53	117.19	122.09
2	C	301	FGD	C22-C30-N29	2.52	122.99	118.33
2	G	301	FGD	C19-C20-C25	2.51	126.06	120.94
3	F	302	CIT	O4-C5-C4	2.51	122.30	114.35
2	D	301	FGD	O08-C07-C06	-2.49	115.18	123.09
2	F	301	FGD	O31-C30-N29	2.49	124.02	120.23
2	D	301	FGD	O03-C02-O01	-2.49	118.44	124.08
2	H	301	FGD	C12-C11-N10	2.48	121.63	117.04
2	H	301	FGD	C06-C05-C04	2.47	117.71	113.16
2	F	301	FGD	C04-N10-C11	-2.46	115.66	121.56
2	E	301	FGD	C16-C17-C14	-2.46	115.78	119.04
2	E	301	FGD	C04-N10-C11	-2.46	115.67	121.56
3	A	302	CIT	C4-C3-C2	2.46	115.61	109.31
2	E	301	FGD	C21-C22-C30	-2.45	113.98	119.51
2	H	301	FGD	C05-C04-C02	2.42	116.10	110.35
2	C	301	FGD	C24-C23-N26	-2.41	115.86	119.91
3	B	301	CIT	O4-C5-C4	2.39	121.90	114.35
3	A	302	CIT	O4-C5-O3	-2.36	117.25	123.33
2	E	301	FGD	C24-C23-C22	2.32	122.40	119.37
3	H	302	CIT	C4-C3-C2	2.31	115.23	109.31
3	C	302	CIT	O7-C3-C4	2.30	114.63	109.38
2	C	301	FGD	C19-C20-C25	-2.30	116.25	120.94
2	H	301	FGD	O03-C02-C04	2.28	121.23	113.51
2	C	301	FGD	N28-C27-N26	2.28	121.57	116.77
3	B	301	CIT	O2-C1-C2	2.28	121.57	114.35
2	G	301	FGD	C15-C16-C17	-2.27	117.69	120.30
2	E	301	FGD	C22-C21-C20	-2.25	117.89	121.38
2	D	301	FGD	C21-C22-C23	2.20	121.07	119.09
3	E	302	CIT	C2-C3-C6	2.20	114.90	110.03
3	C	302	CIT	O2-C1-C2	2.20	121.31	114.35
3	G	302	CIT	C4-C3-C2	2.19	114.93	109.31
2	F	301	FGD	O09-C07-C06	2.17	120.87	114.00
2	C	301	FGD	C05-C04-C02	2.17	115.50	110.35
2	F	301	FGD	C13-C14-C17	-2.16	117.81	120.30
2	G	301	FGD	C04-N10-C11	2.16	126.74	121.56
2	H	301	FGD	O32-C11-N10	-2.15	118.38	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FGD	O31-C30-C22	2.15	124.79	121.33
3	A	302	CIT	O7-C3-C2	-2.14	104.49	109.38
3	E	302	CIT	O2-C1-O1	-2.14	117.84	123.33
2	F	301	FGD	C24-C23-C22	-2.13	116.59	119.37
2	E	301	FGD	C20-C19-N18	2.11	119.47	113.60
2	G	301	FGD	C05-C06-C07	-2.11	106.86	112.49
2	D	301	FGD	O31-C30-N29	-2.11	117.02	120.23
2	C	301	FGD	C06-C05-C04	2.10	117.03	113.16
3	F	302	CIT	O6-C6-O5	-2.10	117.14	123.86
2	E	301	FGD	O01-C02-C04	-2.09	115.51	122.26
3	D	302	CIT	C4-C3-C2	2.09	114.68	109.31
2	E	301	FGD	C13-C12-C11	-2.09	113.82	120.60
3	B	301	CIT	O1-C1-C2	-2.09	117.03	122.95
2	D	301	FGD	C05-C06-C07	2.08	118.04	112.49
3	C	302	CIT	O6-C6-O5	-2.05	117.28	123.86
3	D	302	CIT	O2-C1-O1	-2.04	118.09	123.33
2	A	301	FGD	N26-C27-N29	-2.01	119.63	123.32
2	C	301	FGD	C25-C20-C21	-2.01	115.77	118.55
2	E	301	FGD	C15-C16-C17	2.01	122.61	120.30

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	FGD	C02-C04-C05-C06
3	A	302	CIT	C2-C3-C6-O5
3	A	302	CIT	C2-C3-C6-O6
3	A	302	CIT	O7-C3-C6-O5
3	A	302	CIT	O7-C3-C6-O6
3	B	301	CIT	O7-C3-C4-C5
3	C	302	CIT	O7-C3-C4-C5
3	C	302	CIT	C6-C3-C4-C5
3	D	302	CIT	C2-C3-C4-C5
3	D	302	CIT	C6-C3-C4-C5
3	E	302	CIT	O7-C3-C6-O5
3	E	302	CIT	O7-C3-C6-O6
3	E	302	CIT	C4-C3-C6-O5
3	E	302	CIT	C4-C3-C6-O6
3	F	302	CIT	C1-C2-C3-O7
3	F	302	CIT	C1-C2-C3-C4
3	F	302	CIT	C1-C2-C3-C6
3	F	302	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	F	302	CIT	O7-C3-C4-C5
3	F	302	CIT	C2-C3-C6-O5
3	F	302	CIT	C2-C3-C6-O6
3	F	302	CIT	O7-C3-C6-O5
3	F	302	CIT	O7-C3-C6-O6
3	H	302	CIT	C1-C2-C3-O7
3	H	302	CIT	C1-C2-C3-C4
3	H	302	CIT	C1-C2-C3-C6
2	C	301	FGD	C02-C04-N10-C11
2	G	301	FGD	C02-C04-N10-C11
2	D	301	FGD	C02-C04-N10-C11
2	C	301	FGD	N10-C04-C05-C06
2	D	301	FGD	N10-C04-C05-C06
2	E	301	FGD	N10-C04-C05-C06
2	G	301	FGD	N10-C04-C05-C06
3	B	301	CIT	C1-C2-C3-C6
3	C	302	CIT	C2-C3-C4-C5
2	D	301	FGD	C02-C04-C05-C06
2	E	301	FGD	C02-C04-C05-C06
2	G	301	FGD	C02-C04-C05-C06
2	C	301	FGD	C14-C17-N18-C19
3	B	301	CIT	C1-C2-C3-O7
3	F	302	CIT	C6-C3-C4-C5
2	C	301	FGD	C16-C17-N18-C19
3	D	302	CIT	C4-C3-C6-O6
2	G	301	FGD	O01-C02-C04-N10
2	F	301	FGD	C02-C04-C05-C06
3	B	301	CIT	C6-C3-C4-C5
2	G	301	FGD	O03-C02-C04-N10
3	D	302	CIT	O7-C3-C4-C5
2	H	301	FGD	O03-C02-C04-C05
2	D	301	FGD	O03-C02-C04-N10
2	C	301	FGD	C20-C19-N18-C17
2	H	301	FGD	O01-C02-C04-C05
3	D	302	CIT	O7-C3-C6-O6
2	D	301	FGD	O01-C02-C04-N10
3	C	302	CIT	O1-C1-C2-C3
2	C	301	FGD	C04-C05-C06-C07
2	F	301	FGD	C20-C19-N18-C17
3	C	302	CIT	O2-C1-C2-C3
3	B	301	CIT	C2-C3-C4-C5
3	G	302	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	C	301	FGD	O03-C02-C04-C05
3	D	302	CIT	C2-C3-C6-O5
2	E	301	FGD	C05-C04-N10-C11
2	D	301	FGD	O03-C02-C04-C05
2	F	301	FGD	O03-C02-C04-C05
2	H	301	FGD	C04-C05-C06-C07
2	C	301	FGD	O01-C02-C04-C05
2	D	301	FGD	O01-C02-C04-C05
2	G	301	FGD	O03-C02-C04-C05
3	B	301	CIT	C1-C2-C3-C4
2	E	301	FGD	O01-C02-C04-C05
2	F	301	FGD	O01-C02-C04-C05
3	D	302	CIT	C2-C3-C6-O6
3	D	302	CIT	C4-C3-C6-O5
2	E	301	FGD	O03-C02-C04-C05
2	G	301	FGD	O01-C02-C04-C05
2	E	301	FGD	C16-C17-N18-C19
3	A	302	CIT	C1-C2-C3-C4
2	G	301	FGD	C05-C06-C07-O08
2	H	301	FGD	C05-C06-C07-O09
2	H	301	FGD	C05-C06-C07-O08
2	F	301	FGD	C04-C05-C06-C07
3	H	302	CIT	C4-C3-C6-O5
2	A	301	FGD	C05-C06-C07-O09
2	G	301	FGD	C05-C06-C07-O09
2	E	301	FGD	C05-C06-C07-O09
2	G	301	FGD	C04-C05-C06-C07
3	E	302	CIT	C3-C4-C5-O4
3	D	302	CIT	C1-C2-C3-O7
3	G	302	CIT	C1-C2-C3-O7
2	C	301	FGD	C05-C06-C07-O08
2	D	301	FGD	C14-C17-N18-C19
2	C	301	FGD	C05-C06-C07-O09
2	E	301	FGD	C05-C06-C07-O08
2	A	301	FGD	C05-C06-C07-O08
2	H	301	FGD	N10-C04-C05-C06
2	F	301	FGD	C05-C06-C07-O08
3	E	302	CIT	O2-C1-C2-C3
3	E	302	CIT	C3-C4-C5-O3
2	F	301	FGD	C05-C06-C07-O09
3	D	302	CIT	O7-C3-C6-O5
3	H	302	CIT	C4-C3-C6-O6

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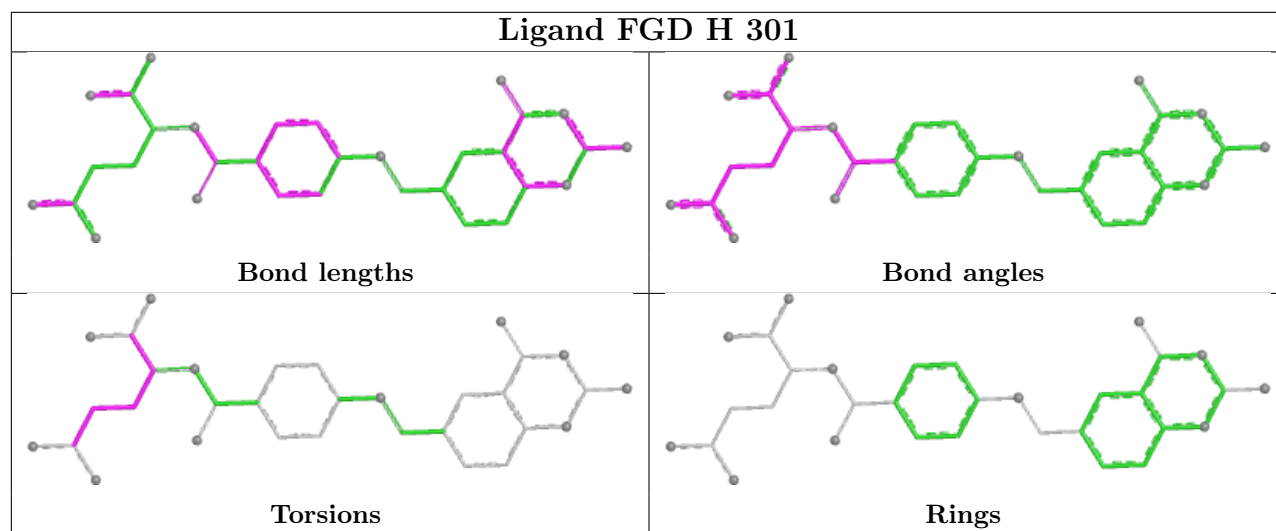
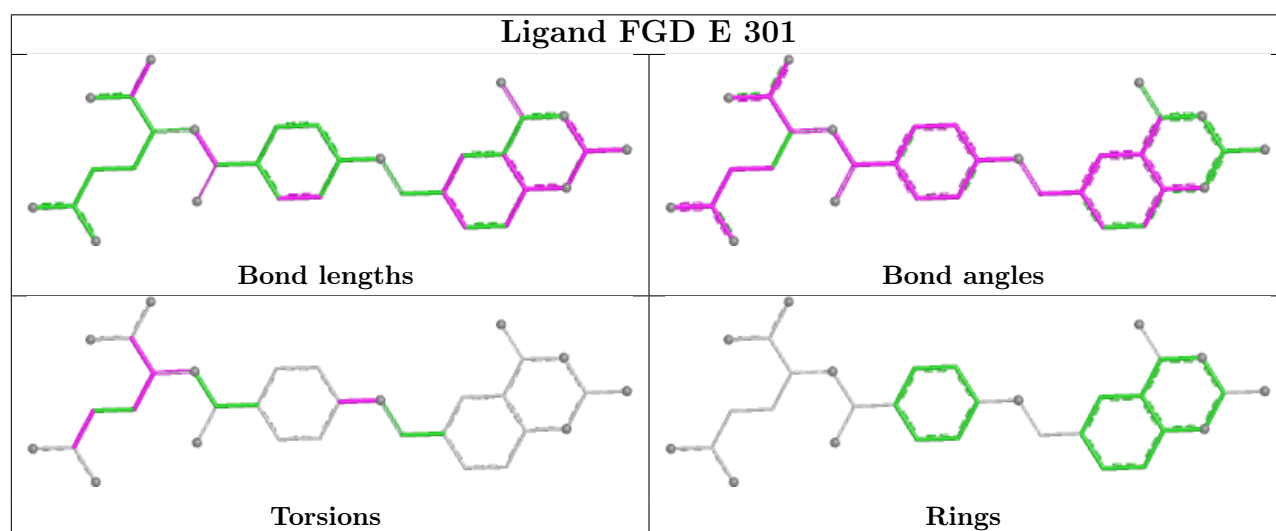
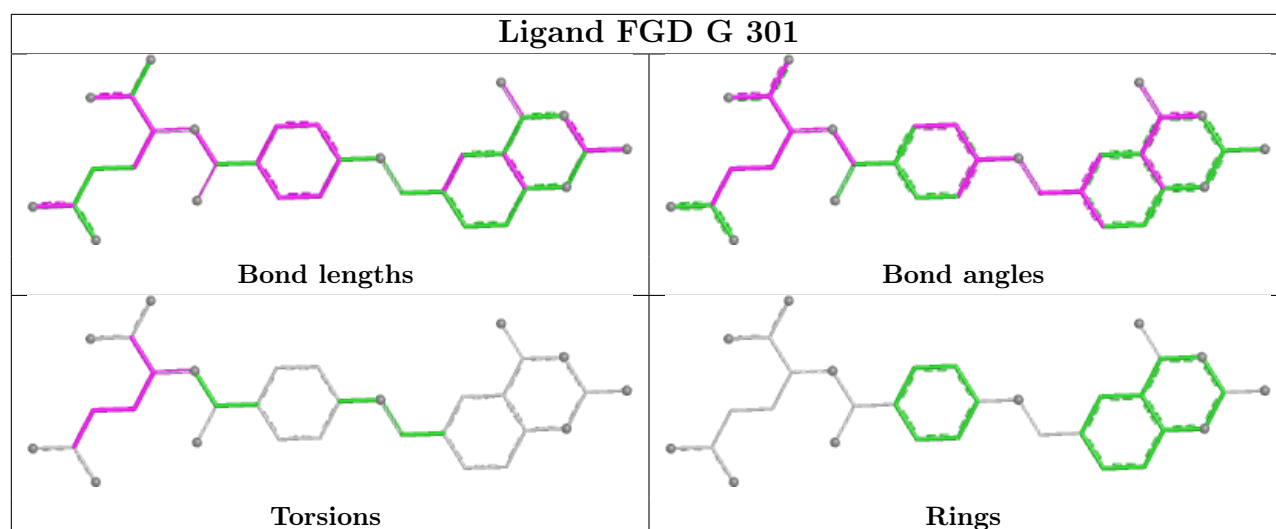
Mol	Chain	Res	Type	Atoms
3	E	302	CIT	O1-C1-C2-C3
2	D	301	FGD	C16-C17-N18-C19
3	A	302	CIT	C3-C4-C5-O3
3	B	301	CIT	O1-C1-C2-C3
2	H	301	FGD	O03-C02-C04-N10
3	F	302	CIT	C3-C4-C5-O3
2	H	301	FGD	O01-C02-C04-N10
3	A	302	CIT	C3-C4-C5-O4
3	B	301	CIT	O2-C1-C2-C3
2	D	301	FGD	C05-C06-C07-O09

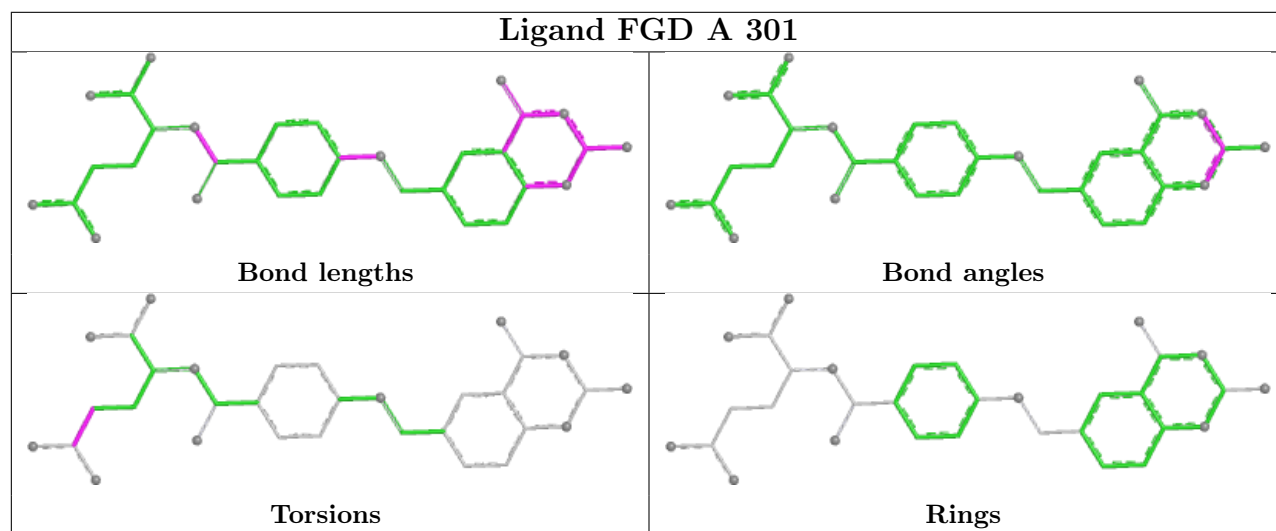
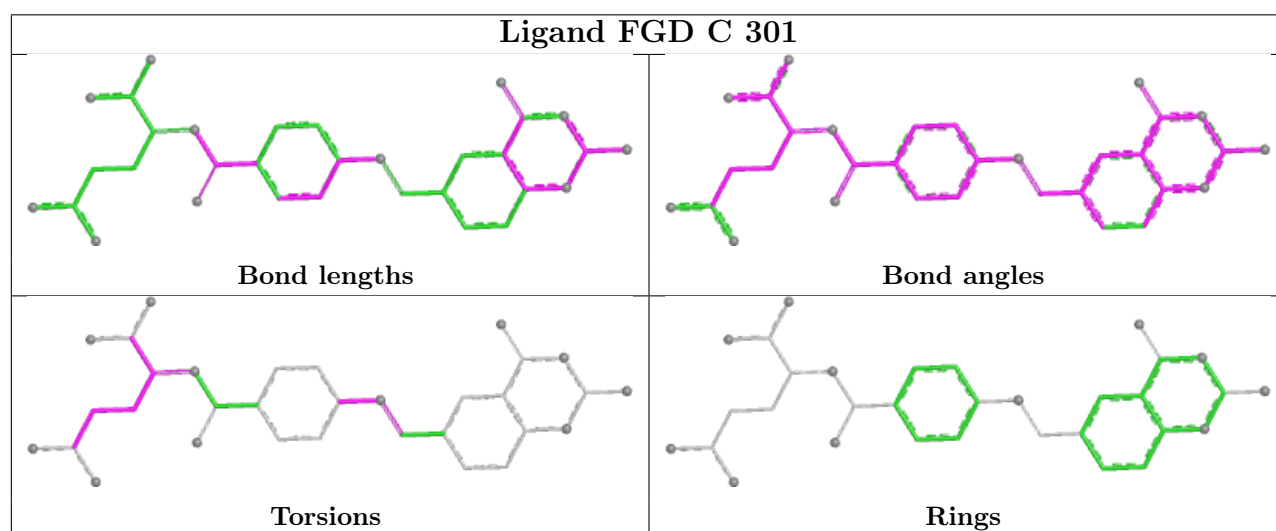
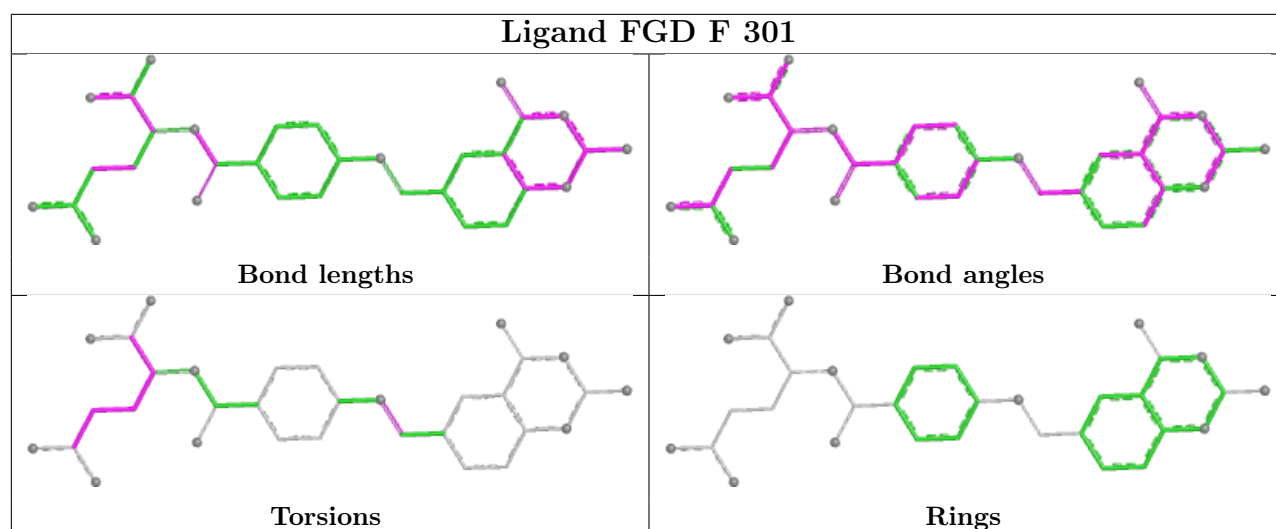
There are no ring outliers.

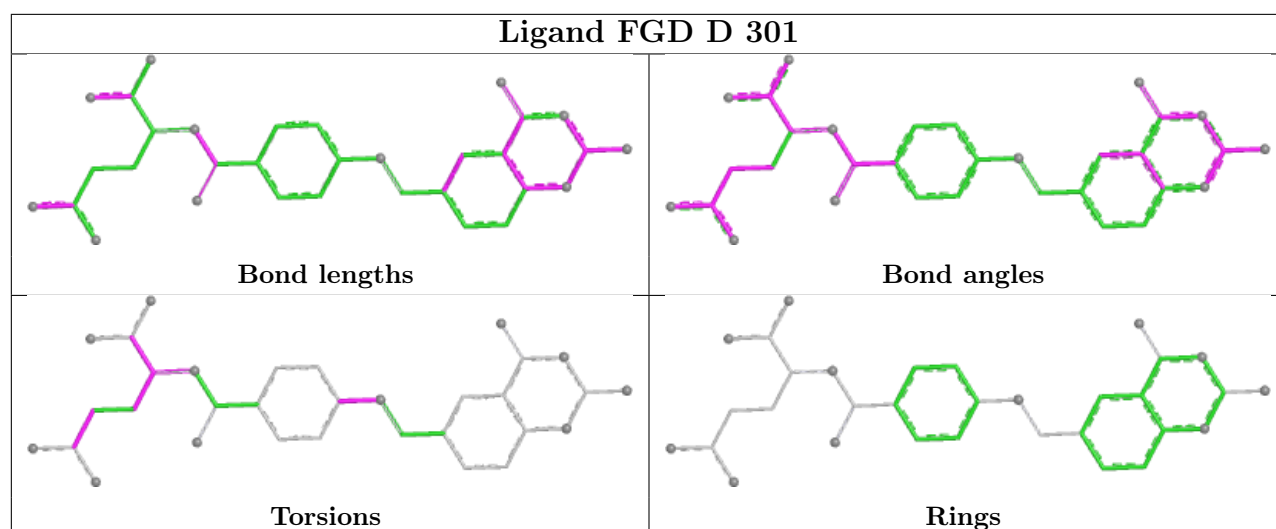
10 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	CIT	1	0
3	A	302	CIT	1	0
3	C	302	CIT	2	0
3	G	302	CIT	9	0
3	B	301	CIT	3	0
2	E	301	FGD	9	0
2	H	301	FGD	1	0
2	F	301	FGD	3	0
2	C	301	FGD	3	0
2	A	301	FGD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/275 (96%)	-0.93	0 100 100	25, 42, 70, 89	0
1	B	260/275 (94%)	-0.99	0 100 100	24, 40, 64, 82	0
1	C	264/275 (96%)	-0.97	0 100 100	20, 43, 64, 90	1 (0%)
1	D	264/275 (96%)	-1.03	0 100 100	20, 40, 61, 76	0
1	E	261/275 (94%)	-0.95	0 100 100	29, 43, 66, 87	0
1	F	254/275 (92%)	-0.89	0 100 100	32, 48, 70, 90	0
1	G	262/275 (95%)	-1.04	0 100 100	19, 38, 57, 73	0
1	H	264/275 (96%)	-1.01	0 100 100	19, 37, 56, 74	0
All	All	2093/2200 (95%)	-0.98	0 100 100	19, 41, 65, 90	1 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

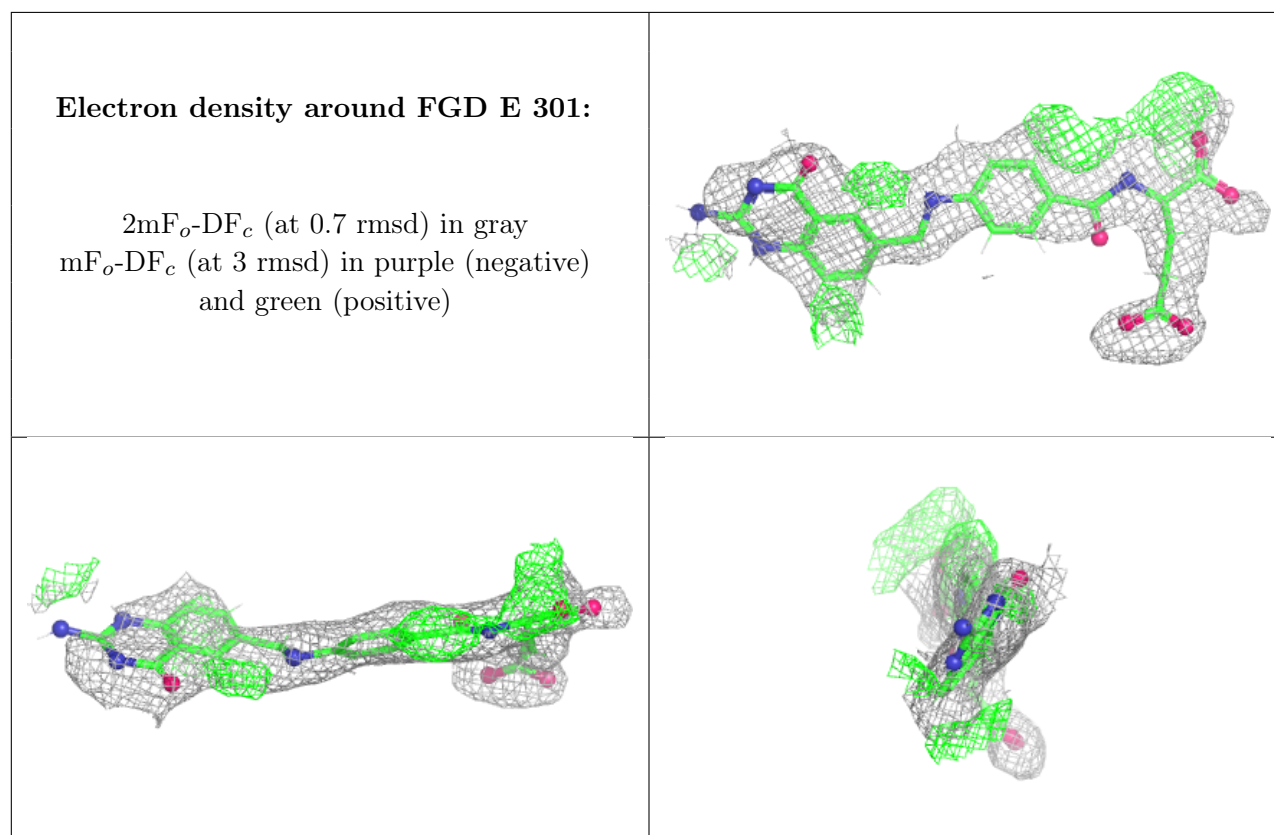
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

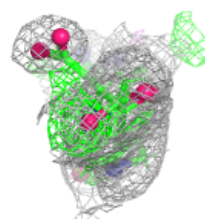
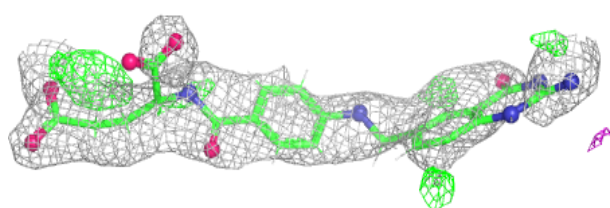
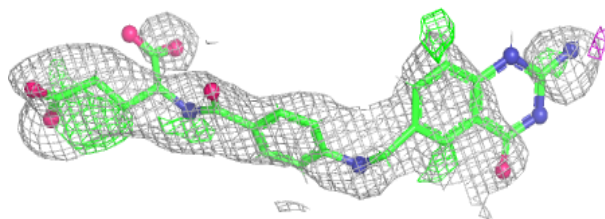
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FGD	E	301	32/32	0.97	0.08	20,25,30,31	51
2	FGD	F	301	32/32	0.97	0.09	18,25,29,30	51
3	CIT	D	302	13/13	0.97	0.05	17,34,49,49	0
2	FGD	A	301	32/32	0.98	0.04	15,26,44,59	0
2	FGD	C	301	32/32	0.98	0.06	20,25,30,32	51
2	FGD	G	301	32/32	0.98	0.04	19,20,24,24	0
2	FGD	H	301	32/32	0.98	0.05	13,25,45,54	0
3	CIT	A	302	13/13	0.98	0.04	18,29,39,39	0
3	CIT	B	301	13/13	0.98	0.06	25,33,49,49	0
2	FGD	D	301	32/32	0.98	0.05	21,29,43,51	0
3	CIT	E	302	13/13	0.98	0.05	24,34,53,53	0
3	CIT	F	302	13/13	0.98	0.06	27,44,53,54	0
3	CIT	G	302	13/13	0.98	0.05	27,33,41,41	0
3	CIT	H	302	13/13	0.98	0.05	18,32,47,50	0
3	CIT	C	302	13/13	0.99	0.05	22,37,45,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

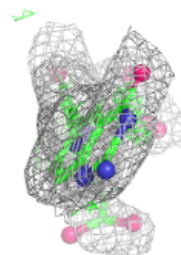
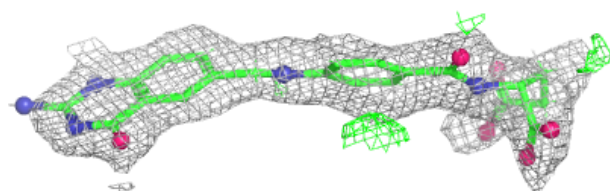
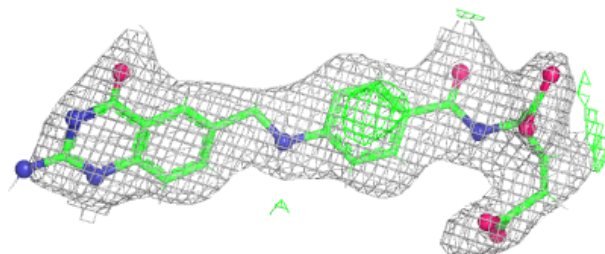


Electron density around FGD F 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

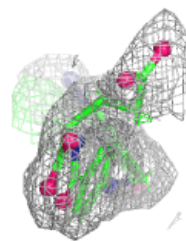
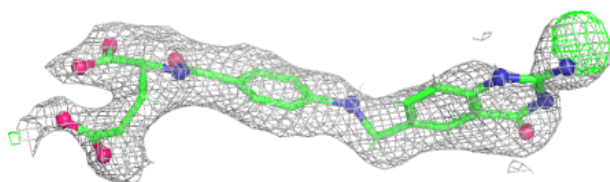
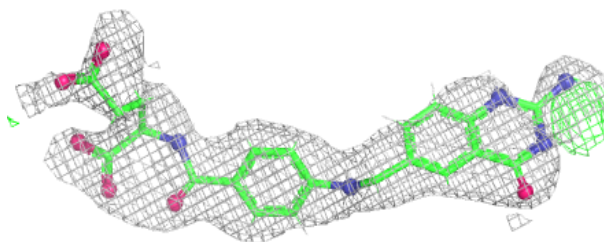
**Electron density around FGD A 301:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

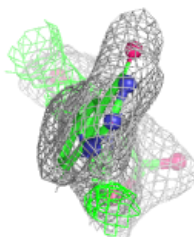
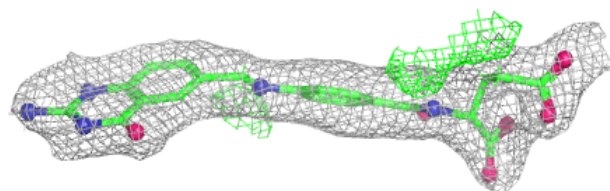
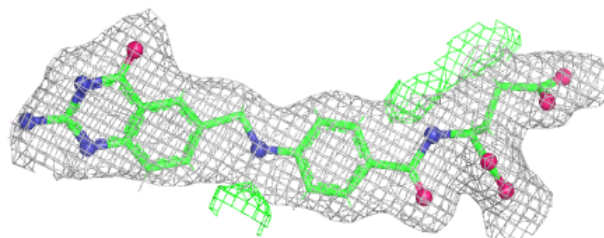


Electron density around FGD C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

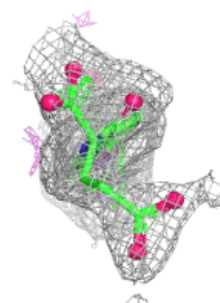
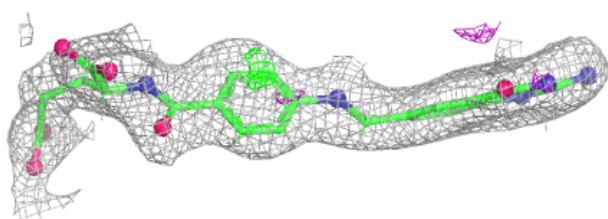
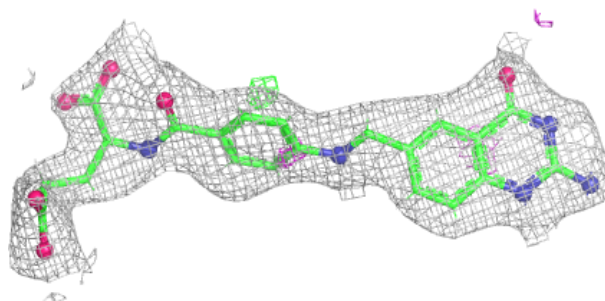
**Electron density around FGD G 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

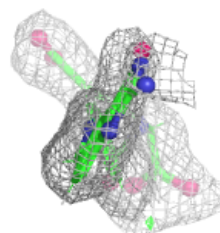
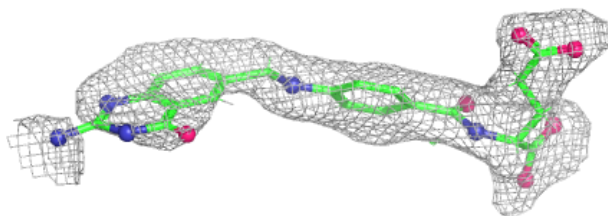
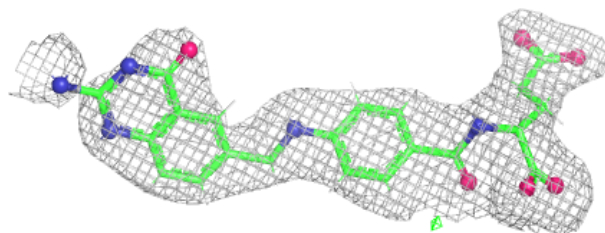


Electron density around FGD H 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FGD D 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.