Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 05:56 AM EDT

PDB ID	:	1DIO / pdb_00001dio
Title	:	DIOL DEHYDRATASE-CYANOCOBALAMIN COMPLEX FROM KLEBSIELLA OXYTOCA
Authors	:	Shibata, N.; Masuda, J.; Tobimatsu, T.; Toraya, T.; Suto, K.; Morimoto, Y.; Yasuoka, N.
Deposited on	:	1999-01-27
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

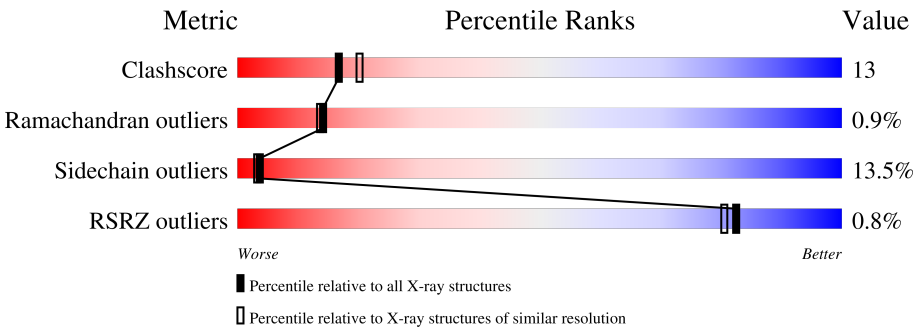
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 <=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	554	% 60% 30% 8% ••
1	L	554	61% 30% 7% ••
2	B	224	% 50% 21% 8% • 20%
2	E	224	% 38% 30% 9% • 20%
3	G	173	% 39% 28% 12% • 21%
3	M	173	2% 47% 22% 8% • 21%

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
5	PGO	L	602	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13912 atoms, of which 0 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 PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	551	4201	2620	727	825	29	0	0	0
1	L	551	4201	2620	727	825	29	0	0	0

- Molecule 2 is a protein called PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	179	1367	865	245	255	2	0	0	0
2	E	179	1367	865	245	255	2	0	0	0

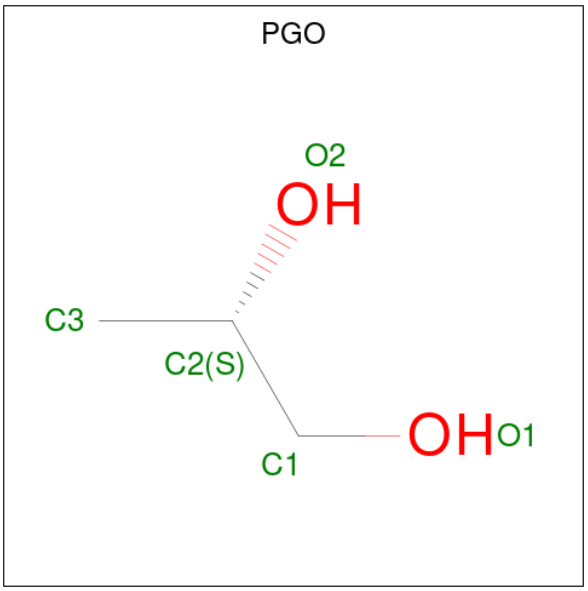
- Molecule 3 is a protein called PROTEIN (DIOL DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	137	1093	681	195	214	3	0	0	0
3	M	137	1093	681	195	214	3	0	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

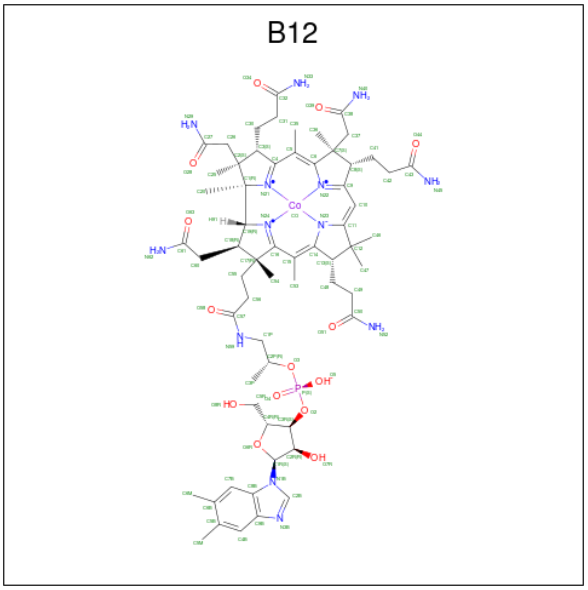
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0
4	L	1	1	1	0	0

- Molecule 5 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	5	3	2	0	0
			Total	C	O		
5	L	1	5	3	2	0	0

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
6	B	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
6	E	1	91	62	1	13	14	1	0	0

- Molecule 7 is water.

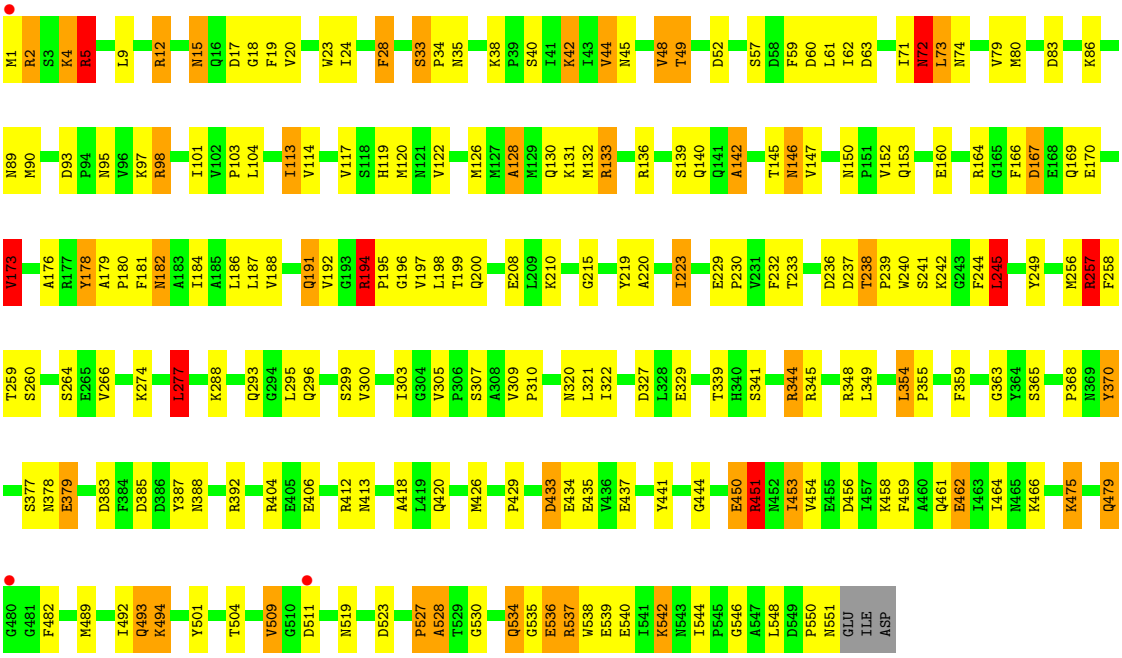
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	144	Total O 144 144	0	0
7	B	41	Total O 41 41	0	0
7	G	24	Total O 24 24	0	0
7	L	150	Total O 150 150	0	0
7	E	22	Total O 22 22	0	0
7	M	15	Total O 15 15	0	0

3 Residue-property plots (i)

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.

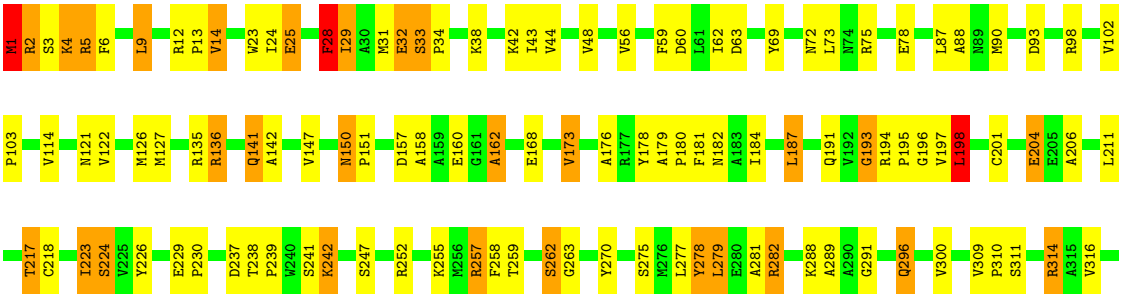
• Molecule 1: PROTEIN (DIOL DEHYDRATASE)

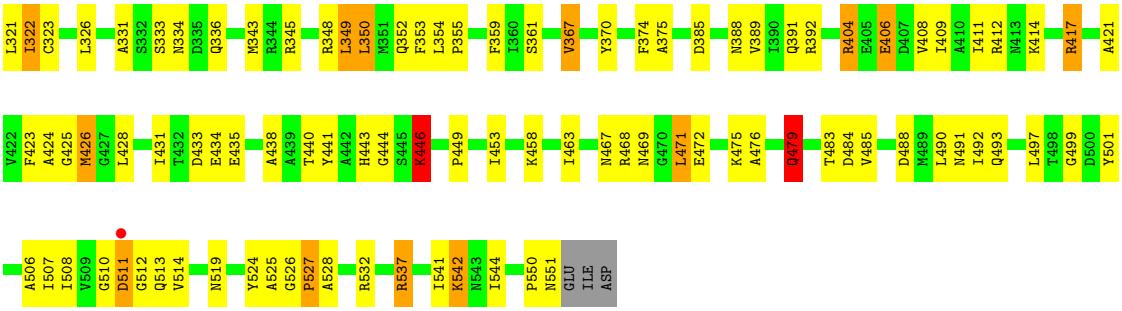
Chain A:



• Molecule 1: PROTEIN (DIOL DEHYDRATASE)

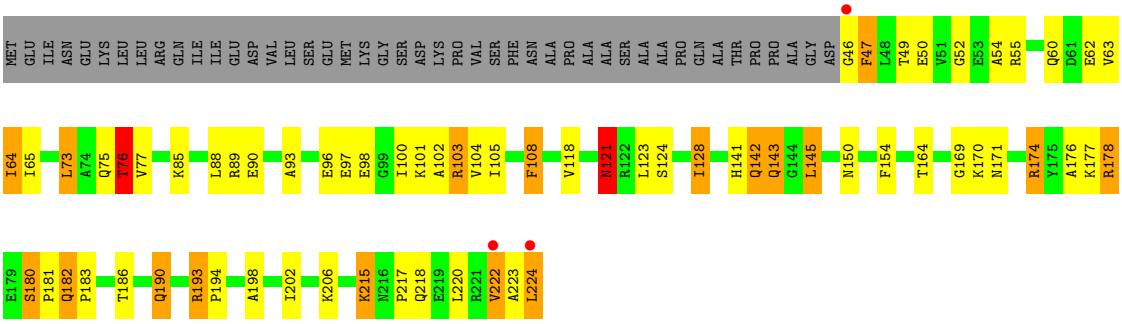
Chain L:





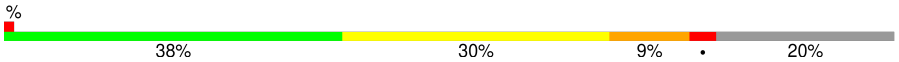
- Molecule 2: PROTEIN (DIOL DEHYDRATASE)

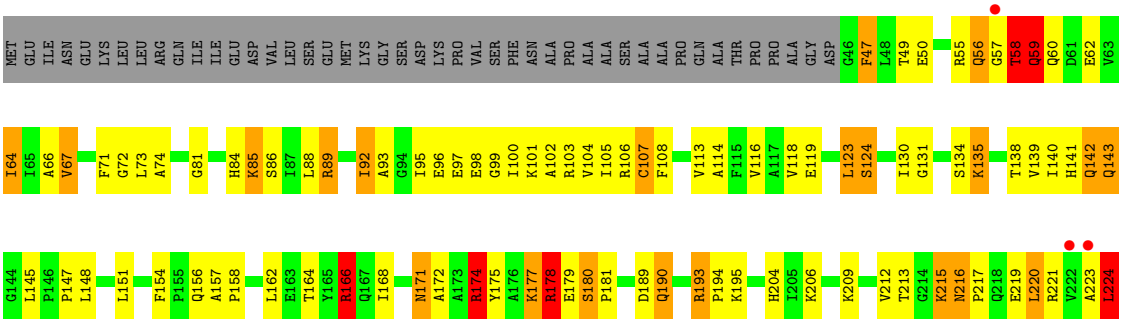
Chain B:



- Molecule 2: PROTEIN (DIOL DEHYDRATASE)

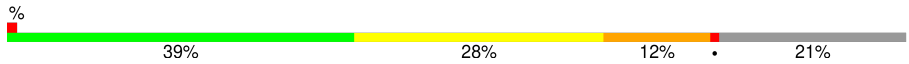
Chain E:

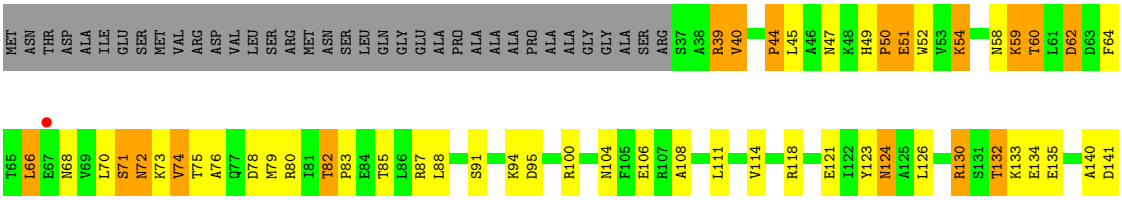




- Molecule 3: PROTEIN (DIOL DEHYDRATASE)

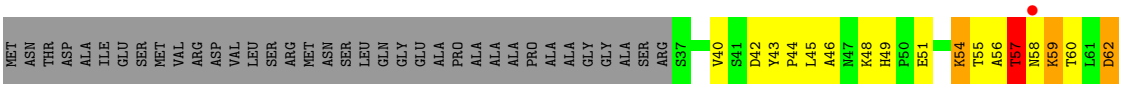
Chain G:

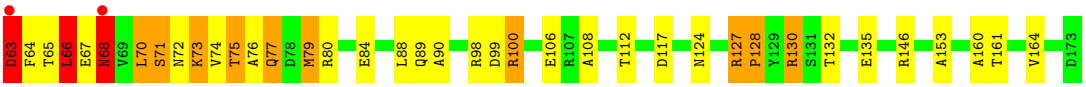




• Molecule 3: PROTEIN (DIOL DEHYDRATASE)

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.20Å 122.30Å 209.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.5 (10.00-2.20) 84.1 (10.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.236 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13912	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, B12, PGO

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	0.99	1/4273 (0.0%)	2.11	140/5787 (2.4%)
1	L	0.90	1/4273 (0.0%)	2.03	124/5787 (2.1%)
2	B	0.77	0/1389	1.92	28/1879 (1.5%)
2	E	0.68	0/1389	1.88	28/1879 (1.5%)
3	G	0.80	0/1108	2.09	36/1497 (2.4%)
3	M	0.74	0/1108	1.95	33/1497 (2.2%)
All	All	0.88	2/13540 (0.0%)	2.03	389/18326 (2.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	L	0	1
All	All	1	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	LEU	N-CA	5.52	1.51	1.46
1	L	14	VAL	N-CA	-5.17	1.40	1.46

All (389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	47	PHE	N-CA-C	15.57	133.05	111.56
1	A	237	ASP	CA-CB-CG	14.97	127.57	112.60
1	A	12	ARG	NE-CZ-NH1	12.99	134.49	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	47	PHE	N-CA-CB	-12.33	93.67	111.54
1	A	511	ASP	CA-CB-CG	10.85	123.45	112.60
1	A	379	GLU	CA-CB-CG	10.47	135.04	114.10
1	A	136	ARG	CD-NE-CZ	10.29	138.80	124.40
1	A	1	MET	N-CA-CB	9.92	127.36	110.50
3	G	173	ASP	CA-CB-CG	9.83	122.43	112.60
1	A	12	ARG	NE-CZ-NH2	-9.65	110.51	119.20
3	G	114	VAL	CA-C-O	9.64	127.38	119.47
2	E	193	ARG	CD-NE-CZ	9.62	137.87	124.40
1	A	93	ASP	O-C-N	-9.61	112.95	121.31
1	A	413	ASN	OD1-CG-ND2	9.55	132.15	122.60
1	A	320	ASN	CA-CB-CG	9.51	122.11	112.60
1	A	44	VAL	CA-C-O	9.32	130.54	120.57
3	M	99	ASP	CA-CB-CG	-9.31	103.29	112.60
1	A	93	ASP	CA-C-O	9.20	128.53	119.51
3	G	123	TYR	CA-C-O	-9.18	111.19	120.82
1	A	344	ARG	NH1-CZ-NH2	9.12	131.16	119.30
2	E	156	GLN	OE1-CD-NE2	-9.03	113.57	122.60
1	L	12	ARG	CD-NE-CZ	8.93	136.90	124.40
1	A	537	ARG	NE-CZ-NH2	-8.87	111.22	119.20
1	A	48	VAL	O-C-N	-8.79	113.70	122.67
1	A	345	ARG	NE-CZ-NH2	8.79	127.11	119.20
1	L	336	GLN	OE1-CD-NE2	8.73	131.33	122.60
3	M	130	ARG	NE-CZ-NH2	-8.69	111.38	119.20
3	G	44	PRO	N-CA-CB	8.67	112.13	102.60
1	A	72	ASN	OD1-CG-ND2	8.59	131.19	122.60
1	L	519	ASN	CB-CG-ND2	8.55	129.22	116.40
1	L	257	ARG	CA-CB-CG	8.40	130.90	114.10
1	A	1	MET	O-C-N	-8.39	109.57	123.00
1	L	532	ARG	NE-CZ-NH2	8.34	126.70	119.20
1	A	288	LYS	CA-C-N	8.30	131.41	120.28
1	A	288	LYS	C-N-CA	8.30	131.41	120.28
3	G	133	LYS	CA-C-N	8.28	131.38	120.28
3	G	133	LYS	C-N-CA	8.28	131.38	120.28
2	E	130	ILE	CA-C-N	-8.17	114.88	122.80
2	E	130	ILE	C-N-CA	-8.17	114.88	122.80
1	L	141	GLN	OE1-CD-NE2	-8.16	114.44	122.60
1	L	224	SER	N-CA-C	8.13	122.20	110.24
1	A	348	ARG	CA-C-O	-8.13	112.33	120.70
1	A	72	ASN	CB-CG-ND2	-8.10	104.25	116.40
1	A	133	ARG	CG-CD-NE	8.10	129.82	112.00
1	A	167	ASP	CA-CB-CG	-8.09	104.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	178	ARG	CD-NE-CZ	8.08	135.71	124.40
1	A	257	ARG	NE-CZ-NH2	8.02	126.42	119.20
2	E	47	PHE	CA-CB-CG	8.02	121.82	113.80
1	L	443	HIS	N-CA-C	-8.02	103.45	113.55
1	L	391	GLN	CA-C-N	7.91	130.88	120.28
1	L	391	GLN	C-N-CA	7.91	130.88	120.28
1	A	412	ARG	CD-NE-CZ	7.85	135.39	124.40
2	E	154	PHE	CA-CB-CG	-7.83	105.97	113.80
1	A	551	ASN	OD1-CG-ND2	7.82	130.41	122.60
1	L	257	ARG	CD-NE-CZ	7.75	135.25	124.40
1	A	378	ASN	OD1-CG-ND2	7.73	130.33	122.60
1	A	296	GLN	CA-C-O	-7.68	112.55	120.54
1	L	181	PHE	CA-CB-CG	7.68	121.48	113.80
1	L	532	ARG	CD-NE-CZ	7.63	135.08	124.40
3	M	153	ALA	N-CA-C	-7.60	102.93	111.14
1	L	262	SER	O-C-N	-7.57	113.13	122.82
3	M	62	ASP	CA-C-O	-7.55	112.46	120.92
1	L	288	LYS	N-CA-C	-7.52	103.02	111.07
1	A	293	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	A	537	ARG	NH1-CZ-NH2	7.50	129.05	119.30
1	L	9	LEU	CA-C-N	7.45	131.26	120.38
1	L	9	LEU	C-N-CA	7.45	131.26	120.38
1	A	130	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	A	509	VAL	N-CA-C	-7.38	98.81	109.29
2	B	154	PHE	CA-CB-CG	-7.38	106.42	113.80
1	A	238	THR	CA-C-O	-7.36	113.50	120.94
1	A	191	GLN	OE1-CD-NE2	-7.30	115.30	122.60
3	G	39	ARG	CD-NE-CZ	7.24	134.53	124.40
1	L	519	ASN	CA-CB-CG	7.18	119.78	112.60
1	L	5	ARG	CB-CG-CD	7.18	127.81	111.30
1	L	226	TYR	CA-C-O	-7.10	113.38	121.40
1	A	164	ARG	CD-NE-CZ	7.07	134.30	124.40
3	G	45	LEU	CA-C-O	-7.07	112.28	120.20
1	A	344	ARG	NE-CZ-NH1	-7.03	114.47	121.50
2	B	180	SER	O-C-N	7.02	126.92	121.23
1	A	451	ARG	CD-NE-CZ	-7.01	114.59	124.40
2	B	102	ALA	CA-C-N	-7.00	113.12	122.99
2	B	102	ALA	C-N-CA	-7.00	113.12	122.99
1	A	451	ARG	CB-CG-CD	6.99	127.37	111.30
1	L	127	MET	N-CA-C	-6.98	103.75	111.36
3	M	63	ASP	CA-CB-CG	6.98	119.58	112.60
1	L	114	VAL	CA-C-N	6.96	129.94	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	114	VAL	C-N-CA	6.96	129.94	120.54
1	L	195	PRO	CA-C-N	-6.96	115.28	123.08
1	L	195	PRO	C-N-CA	-6.96	115.28	123.08
1	A	146	ASN	OD1-CG-ND2	6.93	129.53	122.60
1	A	15	ASN	CA-CB-CG	-6.92	105.68	112.60
1	A	150	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	33	SER	CA-C-N	6.91	126.88	119.28
1	A	33	SER	C-N-CA	6.91	126.88	119.28
1	L	291	GLY	CA-C-O	6.90	127.00	119.06
2	B	52	GLY	CA-C-O	6.89	127.87	122.29
1	A	169	GLN	CG-CD-NE2	6.88	126.72	116.40
1	A	74	ASN	CA-C-O	-6.88	113.25	120.55
2	B	186	THR	CA-C-N	6.88	131.59	122.30
2	B	186	THR	C-N-CA	6.88	131.59	122.30
1	A	169	GLN	CB-CG-CD	6.85	124.25	112.60
3	M	117	ASP	CA-C-O	6.84	127.79	119.38
1	A	341	SER	O-C-N	-6.83	115.56	123.27
1	A	277	LEU	CA-C-O	-6.81	113.68	120.70
3	G	151	ILE	CA-C-O	-6.81	113.64	120.85
3	G	151	ILE	N-CA-CB	6.80	120.77	110.58
1	L	193	GLY	N-CA-C	6.79	120.86	112.64
1	A	35	ASN	OD1-CG-ND2	6.78	129.38	122.60
1	L	361	SER	CB-CA-C	-6.77	98.05	109.50
2	B	75	GLN	OE1-CD-NE2	-6.75	115.84	122.60
2	B	76	THR	CA-C-O	6.74	126.25	118.77
2	E	216	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	259	THR	CA-C-O	-6.72	112.86	120.32
3	M	128	PRO	CA-C-N	6.71	132.14	122.40
3	M	128	PRO	C-N-CA	6.71	132.14	122.40
1	A	307	SER	CA-CB-OG	6.71	124.52	111.10
1	A	296	GLN	O-C-N	6.68	131.00	123.05
1	L	5	ARG	CG-CD-NE	-6.66	97.34	112.00
3	M	49	HIS	CB-CA-C	-6.63	102.25	111.41
1	A	223	ILE	N-CA-CB	-6.61	104.76	111.90
1	L	6	PHE	CA-CB-CG	-6.59	107.21	113.80
3	G	141	ASP	CA-C-O	-6.59	113.57	120.55
3	G	44	PRO	CA-N-CD	-6.58	102.29	111.50
1	L	467	ASN	CA-CB-CG	-6.56	106.04	112.60
1	L	511	ASP	CA-C-O	6.55	131.79	120.85
1	L	275	SER	CA-C-O	-6.54	114.28	121.87
3	M	43	TYR	CA-C-O	-6.54	114.11	120.19
1	A	385	ASP	N-CA-C	-6.52	103.67	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	84	GLU	CB-CG-CD	6.48	123.62	112.60
1	A	266	VAL	N-CA-C	-6.48	104.44	110.53
1	A	237	ASP	N-CA-CB	6.44	121.35	111.56
1	A	329	GLU	CA-C-O	-6.43	113.59	120.92
1	L	537	ARG	NE-CZ-NH1	-6.43	115.07	121.50
3	G	124	ASN	CA-CB-CG	-6.42	106.18	112.60
1	A	451	ARG	CG-CD-NE	6.40	126.09	112.00
1	A	456	ASP	CA-CB-CG	6.40	119.00	112.60
2	B	182	GLN	OE1-CD-NE2	6.40	129.00	122.60
1	L	257	ARG	NE-CZ-NH2	-6.36	113.47	119.20
1	L	367	VAL	N-CA-CB	-6.36	102.30	111.21
1	L	511	ASP	CA-C-N	6.31	132.17	120.87
1	L	511	ASP	C-N-CA	6.31	132.17	120.87
3	G	132	THR	CA-C-O	-6.31	114.51	121.89
2	B	193	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	A	140	GLN	CG-CD-NE2	6.30	125.86	116.40
1	A	5	ARG	CD-NE-CZ	-6.28	115.60	124.40
1	A	178	TYR	N-CA-CB	-6.28	99.97	110.39
1	A	83	ASP	CB-CG-OD1	6.26	132.81	118.40
3	M	68	ASN	OD1-CG-ND2	6.26	128.86	122.60
1	A	128	ALA	O-C-N	-6.25	115.63	122.07
1	L	121	ASN	CA-CB-CG	6.25	118.85	112.60
1	L	3	SER	CA-C-O	6.25	128.04	120.92
1	L	201	CYS	CA-C-O	-6.23	113.64	120.24
2	E	148	LEU	N-CA-C	-6.23	104.16	112.94
1	A	2	ARG	N-CA-C	6.23	118.88	108.73
1	A	420	GLN	OE1-CD-NE2	6.22	128.82	122.60
2	E	58	THR	CA-C-O	6.22	125.62	118.97
3	G	149	ALA	CA-C-O	6.21	129.28	121.58
1	A	378	ASN	CA-CB-CG	6.21	118.81	112.60
3	M	130	ARG	NH1-CZ-NH2	6.20	127.36	119.30
2	B	62	GLU	CA-C-O	6.18	128.09	121.11
3	G	62	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	383	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	98	ARG	NH1-CZ-NH2	6.16	127.30	119.30
1	L	510	GLY	CA-C-N	-6.15	113.24	123.33
1	L	510	GLY	C-N-CA	-6.15	113.24	123.33
1	A	368	PRO	CA-C-O	-6.15	114.43	121.56
2	B	65	ILE	CA-C-N	-6.14	114.52	123.00
2	B	65	ILE	C-N-CA	-6.14	114.52	123.00
1	A	244	PHE	CA-CB-CG	-6.14	107.66	113.80
1	L	48	VAL	O-C-N	-6.12	116.11	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	99	GLY	N-CA-C	-6.12	106.80	115.43
1	A	173	VAL	N-CA-CB	6.12	121.48	111.45
3	G	124	ASN	N-CA-C	6.11	117.94	111.28
1	L	33	SER	CA-C-N	6.09	125.98	119.28
1	L	33	SER	C-N-CA	6.09	125.98	119.28
3	G	152	CYS	CA-C-O	-6.08	111.90	119.38
1	L	388	ASN	CA-C-O	-6.08	113.23	120.10
1	A	244	PHE	CA-C-O	6.07	127.20	120.82
1	L	333	SER	CA-C-O	-6.07	111.83	120.51
1	L	361	SER	CA-C-O	-6.07	114.12	121.28
1	L	479	GLN	CB-CG-CD	6.06	122.90	112.60
2	E	193	ARG	CA-C-O	6.05	124.66	118.73
2	B	65	ILE	CA-C-O	-6.05	114.00	120.59
1	L	551	ASN	CA-CB-CG	6.04	118.64	112.60
1	L	316	VAL	CA-CB-CG1	6.01	120.62	110.40
1	L	12	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	153	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	15	ASN	CB-CG-ND2	5.95	125.33	116.40
1	L	259	THR	CA-C-O	-5.95	112.97	120.28
1	A	71	ILE	O-C-N	-5.93	116.16	123.10
2	E	162	LEU	O-C-N	-5.92	115.84	122.12
1	A	544	ILE	CA-C-O	5.92	127.89	119.95
1	A	232	PHE	O-C-N	-5.91	115.86	122.12
1	A	305	VAL	CA-C-N	5.91	125.45	119.19
1	A	305	VAL	C-N-CA	5.91	125.45	119.19
1	A	83	ASP	CA-C-O	5.90	127.48	120.70
1	A	153	GLN	CG-CD-NE2	5.88	125.22	116.40
1	L	255	LYS	O-C-N	-5.88	116.00	123.06
1	A	120	MET	CG-SD-CE	5.86	113.80	100.90
1	A	528	ALA	N-CA-CB	-5.86	103.60	113.15
1	A	413	ASN	CA-CB-CG	-5.86	106.74	112.60
1	L	217	THR	CA-C-O	-5.85	113.53	120.43
1	L	12	ARG	CA-C-N	5.85	127.15	119.84
1	L	12	ARG	C-N-CA	5.85	127.15	119.84
2	E	224	LEU	CA-CB-CG	5.85	136.77	116.30
1	A	387	TYR	N-CA-C	-5.84	104.99	111.36
1	A	519	ASN	CB-CG-ND2	5.82	125.14	116.40
3	M	80	ARG	NE-CZ-NH2	5.80	124.42	119.20
3	M	99	ASP	CA-C-O	-5.80	114.72	120.82
1	L	88	ALA	O-C-N	-5.80	115.97	122.12
3	M	106	GLU	CA-CB-CG	-5.80	102.50	114.10
3	M	160	ALA	CA-C-O	-5.79	114.41	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	93	ASP	O-C-N	-5.79	116.15	121.30
2	E	166	ARG	CD-NE-CZ	-5.79	116.30	124.40
3	G	50	PRO	CA-C-N	5.78	129.94	120.63
3	G	50	PRO	C-N-CA	5.78	129.94	120.63
1	L	88	ALA	CA-C-O	5.78	126.67	120.55
3	G	133	LYS	N-CA-C	5.78	117.25	111.07
3	M	58	ASN	CA-CB-CG	-5.77	106.83	112.60
1	A	208	GLU	CG-CD-OE2	-5.77	105.14	118.40
1	L	278	TYR	CA-C-N	5.76	127.93	120.44
1	L	278	TYR	C-N-CA	5.76	127.93	120.44
1	L	282	ARG	CD-NE-CZ	5.76	132.46	124.40
1	L	252	ARG	CD-NE-CZ	-5.75	116.35	124.40
1	A	142	ALA	N-CA-C	5.75	119.09	109.95
2	B	150	ASN	CB-CG-ND2	5.74	125.00	116.40
1	A	392	ARG	CB-CA-C	-5.74	101.10	110.85
1	L	257	ARG	N-CA-CB	-5.74	101.71	111.69
3	G	133	LYS	O-C-N	-5.73	116.17	122.07
1	L	345	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	L	44	VAL	O-C-N	-5.70	117.19	123.18
2	B	174	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	L	136	ARG	CD-NE-CZ	-5.68	116.45	124.40
1	A	236	ASP	O-C-N	-5.67	116.27	122.67
1	L	417	ARG	CD-NE-CZ	5.66	132.33	124.40
1	L	391	GLN	OE1-CD-NE2	-5.66	116.94	122.60
3	M	98	ARG	NE-CZ-NH2	-5.65	114.12	119.20
2	B	169	GLY	CA-C-O	5.64	126.86	121.05
2	E	195	LYS	CA-C-N	-5.64	113.37	122.23
2	E	195	LYS	C-N-CA	-5.64	113.37	122.23
1	L	343	MET	N-CA-C	-5.62	105.07	111.14
3	M	46	ALA	CA-C-N	5.62	132.34	122.79
3	M	46	ALA	C-N-CA	5.62	132.34	122.79
1	L	311	SER	CA-C-N	5.62	126.18	120.00
1	L	311	SER	C-N-CA	5.62	126.18	120.00
1	A	437	GLU	CB-CG-CD	5.59	122.10	112.60
1	L	196	GLY	O-C-N	5.58	128.47	122.22
1	A	264	SER	CA-CB-OG	-5.56	99.97	111.10
1	L	321	LEU	CA-C-O	-5.56	114.06	120.24
3	M	43	TYR	CB-CA-C	-5.56	100.95	108.68
2	B	103	ARG	CD-NE-CZ	-5.56	116.62	124.40
1	A	181	PHE	CA-C-N	5.56	128.51	120.79
1	A	181	PHE	C-N-CA	5.56	128.51	120.79
1	A	249	TYR	CA-C-O	5.56	126.85	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	74	ALA	N-CA-C	-5.54	106.36	113.23
3	G	111	LEU	N-CA-C	-5.54	106.53	113.28
3	M	89	GLN	CG-CD-NE2	5.54	124.70	116.40
1	A	370	TYR	CA-C-O	-5.53	114.68	120.55
1	L	3	SER	O-C-N	-5.53	116.09	122.95
1	L	13	PRO	CA-C-N	5.52	128.31	120.53
1	L	13	PRO	C-N-CA	5.52	128.31	120.53
2	E	47	PHE	N-CA-C	-5.52	107.79	114.75
1	L	198	LEU	CA-C-O	-5.51	114.87	120.71
1	L	194	ARG	NH1-CZ-NH2	-5.50	112.15	119.30
1	L	150	ASN	OD1-CG-ND2	5.50	128.10	122.60
3	M	42	ASP	CA-CB-CG	-5.50	107.10	112.60
3	M	90	ALA	CA-C-O	-5.49	114.73	120.55
1	A	133	ARG	CD-NE-CZ	5.49	132.08	124.40
1	A	264	SER	CB-CA-C	-5.48	101.65	110.74
1	L	194	ARG	CG-CD-NE	5.48	124.05	112.00
2	E	130	ILE	O-C-N	5.47	128.87	123.18
2	E	135	LYS	CA-C-O	-5.46	112.67	119.38
1	A	194	ARG	CB-CG-CD	5.46	123.85	111.30
1	L	43	ILE	N-CA-C	5.46	115.44	107.37
1	A	327	ASP	CA-CB-CG	-5.45	107.15	112.60
1	A	344	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	L	237	ASP	CA-CB-CG	5.44	118.04	112.60
2	E	143	GLN	N-CA-CB	5.44	117.97	109.97
3	M	106	GLU	CB-CG-CD	5.44	121.84	112.60
1	A	293	GLN	CG-CD-NE2	5.43	124.55	116.40
1	L	224	SER	N-CA-CB	-5.43	101.06	109.48
3	M	57	THR	CA-C-O	5.43	126.11	119.05
1	A	320	ASN	O-C-N	-5.43	116.37	122.12
1	L	1	MET	CA-C-N	5.42	131.89	121.54
1	L	1	MET	C-N-CA	5.42	131.89	121.54
1	L	314	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	L	98	ARG	CA-C-O	5.41	126.47	120.63
2	E	107	CYS	CA-C-O	-5.41	114.90	121.28
1	L	333	SER	O-C-N	-5.40	115.41	122.59
1	L	173	VAL	O-C-N	5.40	129.04	123.05
1	L	162	ALA	N-CA-C	-5.38	105.49	111.36
1	L	488	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	458	LYS	N-CA-CB	5.38	117.87	110.07
3	G	153	ALA	CA-C-O	5.38	126.12	120.42
1	A	236	ASP	CA-C-O	5.38	127.80	121.40
1	A	245	LEU	N-CA-C	5.35	117.53	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	HIS	N-CA-C	-5.35	106.75	113.28
3	G	108	ALA	O-C-N	5.35	128.24	122.15
3	G	82	THR	N-CA-CB	5.34	116.49	110.03
1	L	160	GLU	N-CA-C	-5.33	105.55	111.36
3	G	39	ARG	CG-CD-NE	5.32	123.71	112.00
1	A	388	ASN	N-CA-C	5.32	117.83	111.71
1	L	525	ALA	N-CA-CB	-5.32	103.83	111.54
1	A	18	GLY	O-C-N	-5.31	120.00	123.35
3	G	104	ASN	OD1-CG-ND2	-5.31	117.29	122.60
2	B	121	ASN	CA-CB-CG	5.31	117.91	112.60
1	L	258	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	113	ILE	CA-C-N	5.30	127.24	120.56
1	A	113	ILE	C-N-CA	5.30	127.24	120.56
1	L	142	ALA	N-CA-C	5.30	118.37	109.95
3	G	161	THR	O-C-N	5.29	127.52	122.07
1	L	352	GLN	CG-CD-NE2	5.29	124.33	116.40
1	A	392	ARG	CD-NE-CZ	-5.29	117.00	124.40
2	E	178	ARG	NH1-CZ-NH2	5.28	126.16	119.30
1	A	348	ARG	O-C-N	5.26	127.78	122.09
1	A	245	LEU	CA-C-O	5.25	126.52	120.90
1	L	259	THR	O-C-N	5.25	129.76	123.36
1	A	95	ASN	OD1-CG-ND2	-5.24	117.36	122.60
2	B	193	ARG	NH1-CZ-NH2	5.24	126.11	119.30
1	L	135	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	L	506	ALA	CA-C-O	5.23	126.94	121.19
1	A	238	THR	O-C-N	5.21	125.75	121.32
2	B	108	PHE	CA-C-O	5.21	124.49	118.55
1	A	89	ASN	CA-C-O	5.21	126.29	120.82
1	A	74	ASN	N-CA-C	5.20	116.95	111.28
3	G	72	ASN	CA-CB-CG	-5.20	107.40	112.60
1	L	72	ASN	CB-CG-ND2	5.20	124.19	116.40
1	L	296	GLN	N-CA-CB	5.20	118.09	110.35
3	M	127	ARG	CD-NE-CZ	5.19	131.67	124.40
2	B	46	GLY	N-CA-C	5.19	128.34	113.30
2	E	174	ARG	NE-CZ-NH2	5.18	123.87	119.20
1	A	345	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	240	TRP	CA-C-N	-5.18	113.34	120.28
1	A	240	TRP	C-N-CA	-5.18	113.34	120.28
2	B	171	ASN	CA-CB-CG	-5.18	107.42	112.60
1	L	158	ALA	N-CA-C	-5.17	105.64	111.28
1	L	507	ILE	O-C-N	5.17	128.46	122.82
1	L	519	ASN	OD1-CG-ND2	-5.17	117.43	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	316	VAL	O-C-N	5.17	127.15	121.83
1	A	136	ARG	CG-CD-NE	-5.16	100.65	112.00
1	L	270	TYR	CA-CB-CG	5.15	123.18	113.90
3	M	66	LEU	CA-CB-CG	5.15	134.31	116.30
1	L	28	PHE	CB-CG-CD2	-5.14	111.96	120.70
1	A	434	GLU	CB-CG-CD	5.14	121.34	112.60
3	G	157	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	L	242	LYS	CA-CB-CG	-5.14	103.82	114.10
3	G	39	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	A	57	SER	CA-C-O	-5.12	115.10	120.63
1	A	359	PHE	CA-CB-CG	-5.12	108.68	113.80
2	E	98	GLU	CA-C-O	5.12	125.82	119.12
1	A	433	ASP	CA-C-N	5.11	127.55	120.29
1	A	433	ASP	C-N-CA	5.11	127.55	120.29
1	A	196	GLY	CA-C-O	-5.11	114.26	119.37
1	L	72	ASN	CA-C-O	5.11	126.70	120.62
3	M	72	ASN	CA-CB-CG	-5.09	107.50	112.60
1	A	44	VAL	O-C-N	-5.09	117.38	123.03
2	E	81	GLY	N-CA-C	5.09	121.84	114.67
3	G	85	THR	CA-CB-OG1	-5.08	101.97	109.60
1	L	352	GLN	CA-C-O	5.08	124.98	119.24
2	E	189	ASP	CA-CB-CG	5.08	117.68	112.60
1	L	241	SER	CA-CB-OG	5.08	121.25	111.10
1	A	345	ARG	CA-CB-CG	5.07	124.25	114.10
3	M	75	THR	CB-CA-C	-5.07	100.26	110.30
1	L	491	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	392	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	321	LEU	N-CA-C	-5.06	105.67	111.14
1	A	19	PHE	O-C-N	5.06	129.23	123.31
1	L	263	GLY	N-CA-C	5.06	121.85	115.42
1	L	499	GLY	O-C-N	-5.06	115.91	122.34
1	A	160	GLU	CA-C-N	5.05	125.59	119.98
1	A	160	GLU	C-N-CA	5.05	125.59	119.98
1	A	232	PHE	CA-C-O	5.05	125.90	120.55
1	L	444	GLY	CA-C-O	5.05	126.12	121.38
1	A	456	ASP	N-CA-C	-5.05	105.69	111.14
3	M	71	SER	CA-C-N	5.05	129.28	122.07
3	M	71	SER	C-N-CA	5.05	129.28	122.07
3	G	44	PRO	N-CD-CG	5.04	109.85	103.80
1	L	2	ARG	CA-C-O	5.04	127.71	120.51
1	L	512	GLY	CA-C-N	-5.04	115.50	122.30
1	L	512	GLY	C-N-CA	-5.04	115.50	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	98	ARG	O-C-N	-5.03	116.79	122.12
2	B	142	GLN	N-CA-C	5.03	116.70	108.55
1	L	223	ILE	CA-C-N	5.02	128.23	121.05
1	L	223	ILE	C-N-CA	5.02	128.23	121.05
3	G	108	ALA	N-CA-C	-5.02	105.89	111.36
2	E	178	ARG	CG-CD-NE	-5.01	100.97	112.00
1	A	509	VAL	CA-C-O	-5.01	116.91	121.72
3	G	158	GLU	CB-CA-C	-5.01	103.02	110.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ALA	Mainchain
1	L	322	ILE	Mainchain

5.2 Too-close contacts (i)

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	4201	0	4140	96	0
1	L	4201	0	4140	86	0
2	B	1367	0	1419	40	0
2	E	1367	0	1419	52	0
3	G	1093	0	1101	39	0
3	M	1093	0	1101	34	0
4	A	1	0	0	0	0
4	L	1	0	0	0	0
5	A	5	0	6	1	0
5	L	5	0	5	1	0
6	B	91	0	88	5	0
6	E	91	0	88	9	0
7	A	144	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	41	0	0	1	0
7	E	22	0	0	3	0
7	G	24	0	0	1	0
7	L	150	0	0	2	0
7	M	15	0	0	0	0
All	All	13912	0	13507	347	0

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 13.

All (347) 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)
3:M:59:LYS:HE3	3:M:60:THR:H	1.20	1.01
2:B:76:THR:HG22	2:B:77:VAL:HG13	1.39	1.00
2:E:64:ILE:HG13	2:E:124:SER:HB2	1.41	1.00
3:M:59:LYS:HE2	3:M:63:ASP:HB2	1.46	0.93
2:E:179:GLU:O	2:E:180:SER:HB2	1.67	0.91
2:B:190:GLN:H	2:B:190:GLN:HE21	1.23	0.83
6:B:601:B12:H1R	7:B:630:HOH:O	1.78	0.81
2:B:128:ILE:HD13	2:B:176:ALA:HA	1.61	0.81
1:A:98:ARG:HA	1:A:132:MET:HE1	1.64	0.78
1:A:132:MET:HA	1:A:132:MET:HE2	1.68	0.76
2:E:72:GLY:H	2:E:84:HIS:HD2	1.34	0.75
1:L:475:LYS:HG2	3:M:70:LEU:HD12	1.70	0.73
1:A:462:GLU:HG3	1:A:466:LYS:HD3	1.70	0.72
1:A:441:TYR:HE1	1:L:1:MET:HG3	1.53	0.72
3:G:54:LYS:HD2	3:G:58:ASN:HD21	1.55	0.72
2:B:121:ASN:C	2:B:121:ASN:HD22	1.98	0.71
3:G:134:GLU:CD	3:G:134:GLU:H	1.99	0.70
1:A:180:PRO:HG3	1:A:464:ILE:HD11	1.73	0.69
1:A:475:LYS:HD3	3:G:70:LEU:HD23	1.74	0.69
1:A:182:ASN:HD22	1:A:182:ASN:N	1.91	0.69
3:G:132:THR:OG1	3:G:135:GLU:HG3	1.93	0.69
1:L:484:ASP:OD1	1:L:485:VAL:HG23	1.93	0.69
2:E:72:GLY:H	2:E:84:HIS:CD2	2.10	0.69
2:B:47:PHE:HB2	2:B:223:ALA:HB3	1.76	0.68
1:A:23:TRP:HB2	1:L:550:PRO:HG3	1.75	0.68
1:A:131:LYS:HG2	1:A:132:MET:HE3	1.75	0.68
1:A:475:LYS:O	1:A:479:GLN:HG2	1.94	0.67
2:E:190:GLN:H	2:E:190:GLN:HE21	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:55:THR:HG22	3:M:57:THR:H	1.60	0.67
1:L:426:MET:HB2	1:L:428:LEU:HG	1.77	0.66
1:A:182:ASN:HD22	1:A:182:ASN:H	1.44	0.66
2:E:95:ILE:HG21	2:E:102:ALA:HB2	1.77	0.66
1:L:309:VAL:HB	1:L:310:PRO:HD2	1.78	0.66
1:A:534:GLN:HG2	1:A:535:GLY:N	2.11	0.66
1:L:198:LEU:HD11	1:L:508:ILE:HD12	1.77	0.66
3:G:60:THR:HG22	3:G:62:ASP:H	1.60	0.65
2:E:142:GLN:HG3	2:E:145:LEU:HD22	1.78	0.65
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.77	0.65
2:E:58:THR:O	2:E:59:GLN:HB3	1.96	0.65
1:L:404:ARG:HG3	7:L:688:HOH:O	1.95	0.64
1:L:173:VAL:HG12	1:L:182:ASN:ND2	2.11	0.64
2:E:47:PHE:HA	2:E:223:ALA:HB2	1.79	0.64
1:A:441:TYR:CE1	1:L:1:MET:HG3	2.33	0.64
2:E:100:ILE:HD11	2:E:177:LYS:CD	2.28	0.64
2:B:104:VAL:HG12	2:B:220:LEU:HD12	1.79	0.64
3:G:153:ALA:O	3:G:157:ARG:HB2	1.98	0.64
2:E:223:ALA:O	2:E:224:LEU:HD13	1.98	0.63
1:A:114:VAL:HG13	1:A:277:LEU:HD13	1.79	0.63
1:L:23:TRP:HB3	1:L:28:PHE:HB2	1.80	0.63
1:A:494:LYS:HD3	3:G:64:PHE:HB2	1.80	0.63
2:B:141:HIS:HE1	2:B:145:LEU:HB3	1.64	0.62
1:A:23:TRP:HB3	1:A:28:PHE:HB2	1.80	0.62
2:E:103:ARG:HD2	2:E:219:GLU:OE2	1.99	0.62
2:E:47:PHE:HB2	2:E:223:ALA:HB3	1.82	0.62
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.80	0.62
3:G:54:LYS:HD2	3:G:58:ASN:ND2	2.14	0.62
2:E:177:LYS:O	2:E:178:ARG:HB2	1.96	0.62
2:E:174:ARG:HG2	2:E:181:PRO:HB3	1.81	0.62
3:M:59:LYS:HE2	3:M:63:ASP:CB	2.25	0.62
6:B:601:B12:H362	6:B:601:B12:H351	1.82	0.61
1:L:180:PRO:O	1:L:184:ILE:HD12	1.99	0.61
1:L:87:LEU:HA	1:L:90:MET:HE3	1.82	0.61
3:M:59:LYS:CE	3:M:63:ASP:HB2	2.25	0.61
6:E:601:B12:C2B	6:E:601:B12:H492	2.30	0.61
2:E:113:VAL:HG12	7:E:613:HOH:O	1.99	0.60
2:B:121:ASN:O	2:B:143:GLN:HG3	2.01	0.60
2:B:174:ARG:HB2	2:B:181:PRO:HG3	1.83	0.60
1:A:48:VAL:CG2	1:A:73:LEU:HD11	2.32	0.60
3:M:100:ARG:H	3:M:100:ARG:HE	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:409:ILE:HG23	1:L:440:THR:HG22	1.82	0.60
2:E:179:GLU:O	2:E:180:SER:CB	2.47	0.59
1:A:238:THR:HB	1:A:239:PRO:HD2	1.83	0.59
1:L:204:GLU:OE2	1:L:206:ALA:N	2.35	0.59
3:M:75:THR:HG22	3:M:76:ALA:N	2.18	0.59
2:B:50:GLU:HG2	2:B:218:GLN:HB3	1.83	0.59
1:A:132:MET:O	1:A:133:ARG:C	2.46	0.59
1:A:223:ILE:HG13	1:A:256:MET:HE2	1.84	0.59
2:B:142:GLN:O	2:B:145:LEU:HB2	2.02	0.59
1:A:538:TRP:CE2	1:A:542:LYS:HD2	2.37	0.59
3:M:60:THR:OG1	3:M:62:ASP:HB2	2.03	0.59
6:E:601:B12:H1R	7:E:618:HOH:O	2.03	0.59
1:A:80:MET:HE2	7:A:729:HOH:O	2.01	0.58
3:G:118:ARG:NH1	3:G:121:GLU:OE1	2.35	0.58
1:L:475:LYS:HG2	3:M:70:LEU:CD1	2.33	0.58
3:G:60:THR:HG22	3:G:62:ASP:N	2.18	0.58
2:E:67:VAL:HG13	2:E:71:PHE:HB3	1.85	0.58
3:G:71:SER:OG	3:G:73:LYS:HE2	2.04	0.58
1:L:513:GLN:NE2	1:L:514:VAL:O	2.37	0.57
2:E:100:ILE:HD11	2:E:177:LYS:HD2	1.85	0.57
3:M:68:ASN:HB3	3:M:73:LYS:HD2	1.85	0.57
3:G:144:GLU:O	3:G:148:GLN:HA	2.04	0.57
1:A:435:GLU:OE2	1:A:451:ARG:HD2	2.05	0.57
1:A:131:LYS:HG2	1:A:132:MET:CE	2.34	0.56
1:A:220:ALA:HB1	1:A:223:ILE:HD11	1.88	0.56
3:G:87:ARG:NH1	7:G:185:HOH:O	2.39	0.55
2:E:66:ALA:O	2:E:131:GLY:HA2	2.07	0.55
3:G:64:PHE:CD1	3:G:79:MET:HE3	2.41	0.55
1:A:86:LYS:O	1:A:90:MET:HG3	2.06	0.55
1:A:527:PRO:O	1:A:528:ALA:HB3	2.05	0.55
2:B:93:ALA:O	2:B:97:GLU:HG3	2.06	0.55
6:E:601:B12:H362	6:E:601:B12:H351	1.87	0.55
1:A:229:GLU:N	1:A:230:PRO:HD2	2.22	0.55
1:L:31:MET:HG3	1:L:32:GLU:HG2	1.88	0.54
1:L:322:ILE:O	1:L:323:CYS:C	2.50	0.54
2:E:177:LYS:O	2:E:178:ARG:CB	2.53	0.54
2:B:64:ILE:HG13	2:B:124:SER:HB2	1.88	0.54
3:G:74:VAL:HA	3:G:78:ASP:OD2	2.08	0.54
2:B:190:GLN:H	2:B:190:GLN:NE2	2.01	0.54
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.89	0.54
1:A:9:LEU:O	1:A:12:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:GLU:OE2	2:E:166:ARG:NH2	2.41	0.54
2:E:157:ALA:N	2:E:158:PRO:HD2	2.23	0.54
2:E:85:LYS:O	2:E:89:ARG:HB2	2.07	0.54
1:A:122:VAL:O	1:A:126:MET:HG3	2.07	0.54
2:B:63:VAL:HG23	2:B:100:ILE:HG21	1.89	0.53
2:B:198:ALA:O	2:B:202:ILE:HD12	2.08	0.53
1:L:370:TYR:CE1	1:L:446:LYS:HD3	2.43	0.53
3:G:68:ASN:HA	3:G:73:LYS:HE3	1.90	0.53
1:L:421:ALA:O	1:L:424:ALA:HB3	2.09	0.53
2:E:100:ILE:HD11	2:E:177:LYS:HD3	1.90	0.53
1:L:334:ASN:ND2	1:L:348:ARG:HD3	2.22	0.53
6:B:601:B12:C2B	6:B:601:B12:H492	2.39	0.53
3:M:68:ASN:HB3	3:M:73:LYS:CD	2.39	0.53
3:G:145:SER:HA	3:G:148:GLN:NE2	2.23	0.52
3:G:64:PHE:CE1	3:G:79:MET:HG2	2.45	0.52
2:B:47:PHE:H	2:B:47:PHE:HD1	1.58	0.52
3:G:49:HIS:N	3:G:50:PRO:HD3	2.25	0.52
3:M:75:THR:HG22	3:M:77:GLN:H	1.75	0.52
3:G:140:ALA:HB1	3:G:157:ARG:HD3	1.91	0.52
2:E:140:ILE:O	2:E:151:LEU:HB2	2.09	0.52
1:A:365:SER:HB2	1:A:377:SER:HB3	1.93	0.51
1:L:468:ARG:NH2	1:L:472:GLU:OE1	2.35	0.51
2:E:84:HIS:HE1	2:E:134:SER:O	1.94	0.51
1:L:238:THR:HB	1:L:239:PRO:HD2	1.92	0.51
1:L:331:ALA:HA	1:L:359:PHE:HB2	1.93	0.51
1:L:404:ARG:NH1	1:L:406:GLU:OE1	2.43	0.51
3:M:124:ASN:O	3:M:130:ARG:HG3	2.11	0.51
1:L:223:ILE:CG2	1:L:242:LYS:HE2	2.41	0.51
2:E:96:GLU:HA	2:E:100:ILE:O	2.11	0.50
3:G:75:THR:HG22	3:G:76:ALA:N	2.26	0.50
1:A:61:LEU:HG	3:G:166:ARG:HG3	1.94	0.50
1:A:450:GLU:HA	1:A:450:GLU:OE1	2.11	0.50
1:L:354:LEU:HB2	1:L:355:PRO:HD3	1.94	0.50
2:E:212:VAL:HG11	2:E:215:LYS:HG3	1.93	0.50
3:M:59:LYS:HE3	3:M:60:THR:N	2.05	0.50
2:B:193:ARG:HB3	2:B:194:PRO:HD3	1.94	0.50
2:B:89:ARG:HH11	2:B:90:GLU:HG2	1.77	0.49
2:B:222:VAL:HG12	2:B:223:ALA:H	1.78	0.49
1:A:233:THR:OG1	3:G:168:LYS:HE3	2.11	0.49
1:A:260:SER:OG	1:A:295:LEU:HD11	2.12	0.49
3:G:124:ASN:O	3:G:130:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:309:VAL:HB	1:L:310:PRO:CD	2.42	0.49
1:L:204:GLU:OE2	1:L:206:ALA:HB3	2.13	0.49
1:A:188:VAL:O	1:A:192:VAL:HG23	2.13	0.49
1:A:453:ILE:HD11	2:B:183:PRO:HD2	1.95	0.49
1:L:469:ASN:OD1	1:L:471:LEU:HB2	2.13	0.49
2:E:93:ALA:O	2:E:97:GLU:HG3	2.13	0.49
2:E:104:VAL:HG12	2:E:220:LEU:HD12	1.94	0.49
1:A:12:ARG:HA	1:A:12:ARG:HD3	1.68	0.48
1:A:418:ALA:HA	1:A:482:PHE:CE2	2.48	0.48
1:A:170:GLU:OE2	5:A:602:PGO:O1	2.30	0.48
1:A:98:ARG:CA	1:A:132:MET:HE1	2.39	0.48
3:M:66:LEU:O	3:M:70:LEU:HB2	2.14	0.48
1:A:113:ILE:HD13	1:A:322:ILE:HG23	1.96	0.48
2:B:105:ILE:HD12	2:B:217:PRO:HB3	1.95	0.48
3:M:127:ARG:HB3	3:M:128:PRO:HD2	1.95	0.48
1:A:5:ARG:HH11	1:A:5:ARG:HD2	1.53	0.48
2:B:108:PHE:HB2	2:B:215:LYS:HB3	1.96	0.48
2:E:71:PHE:CE1	2:E:84:HIS:HB3	2.48	0.48
1:A:4:LYS:HG3	1:L:441:TYR:O	2.14	0.48
2:B:141:HIS:CE1	2:B:145:LEU:HB3	2.47	0.48
1:L:229:GLU:N	1:L:230:PRO:CD	2.77	0.48
1:L:484:ASP:OD1	1:L:485:VAL:N	2.47	0.48
3:M:55:THR:HG22	3:M:56:ALA:N	2.28	0.47
2:E:123:LEU:HD11	2:E:217:PRO:HG2	1.95	0.47
1:L:354:LEU:N	1:L:355:PRO:HD2	2.29	0.47
1:L:423:PHE:HA	1:L:428:LEU:HD12	1.97	0.47
2:B:108:PHE:CG	2:B:215:LYS:HD2	2.50	0.47
3:G:44:PRO:HG2	3:G:47:ASN:OD1	2.14	0.47
3:G:51:GLU:H	3:G:51:GLU:HG3	1.33	0.47
1:L:24:ILE:HG22	1:L:25:GLU:OE1	2.15	0.47
1:L:392:ARG:HG3	1:L:542:LYS:HA	1.95	0.47
1:L:122:VAL:O	1:L:126:MET:HG3	2.15	0.47
2:E:62:GLU:CD	2:E:103:ARG:HE	2.22	0.47
1:A:536:GLU:CD	1:A:536:GLU:H	2.21	0.47
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.97	0.47
1:A:489:MET:HE3	1:A:489:MET:HB3	1.68	0.47
2:B:89:ARG:NH1	2:B:90:GLU:OE2	2.46	0.47
1:A:180:PRO:O	1:A:184:ILE:HD12	2.15	0.46
1:A:242:LYS:HE3	1:A:245:LEU:HD12	1.97	0.46
3:M:132:THR:OG1	3:M:135:GLU:HG3	2.15	0.46
3:G:54:LYS:O	3:G:82:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:NH1	1:A:540:GLU:OE1	2.49	0.46
1:L:296:GLN:HE22	5:L:602:PGO:H12	1.79	0.46
1:A:229:GLU:N	1:A:230:PRO:CD	2.79	0.46
1:A:537:ARG:HA	1:A:537:ARG:HD2	1.64	0.46
1:L:75:ARG:HH21	1:L:78:GLU:CD	2.24	0.46
1:A:170:GLU:HA	1:A:200:GLN:HG3	1.98	0.46
2:E:47:PHE:HB2	2:E:223:ALA:CB	2.45	0.46
2:E:172:ALA:O	2:E:175:TYR:HB2	2.15	0.46
6:E:601:B12:H491	6:E:601:B12:C11	2.46	0.46
2:E:177:LYS:HE3	2:E:177:LYS:HA	1.98	0.46
6:E:601:B12:H261	6:E:601:B12:H601	1.97	0.46
1:L:136:ARG:HH11	1:L:136:ARG:HD3	1.50	0.46
1:L:408:VAL:O	1:L:411:ILE:HG22	2.16	0.46
3:M:44:PRO:O	3:M:48:LYS:HG2	2.16	0.46
2:E:138:THR:HG21	2:E:168:ILE:HD13	1.98	0.45
2:E:171:ASN:ND2	2:E:181:PRO:HB2	2.30	0.45
3:G:71:SER:O	3:G:72:ASN:HB2	2.14	0.45
1:A:200:GLN:HG2	1:A:219:TYR:CZ	2.51	0.45
1:A:546:GLY:O	1:A:548:LEU:HG	2.16	0.45
1:A:131:LYS:HE3	1:A:132:MET:HE3	1.97	0.45
1:L:23:TRP:HB3	1:L:28:PHE:CB	2.46	0.45
1:A:40:SER:H	1:A:52:ASP:HA	1.80	0.45
2:E:64:ILE:HD11	2:E:103:ARG:NH2	2.31	0.45
1:L:60:ASP:OD1	1:L:62:ILE:N	2.50	0.45
1:L:162:ALA:HB3	1:L:193:GLY:HA3	1.99	0.45
3:M:55:THR:HB	3:M:59:LYS:H	1.81	0.45
2:B:182:GLN:HG3	2:B:183:PRO:HD2	1.99	0.45
3:G:140:ALA:CB	3:G:157:ARG:HD3	2.47	0.45
3:M:68:ASN:HB3	3:M:73:LYS:HG2	1.98	0.45
1:L:56:VAL:HA	1:L:59:PHE:CD1	2.52	0.45
1:L:314:ARG:HH11	1:L:314:ARG:HD3	1.60	0.45
3:M:124:ASN:HA	3:M:127:ARG:HG3	1.98	0.45
1:A:17:ASP:OD2	1:A:339:THR:OG1	2.18	0.45
1:L:141:GLN:HB2	1:L:168:GLU:HB2	1.99	0.45
1:A:23:TRP:CE3	1:L:550:PRO:HB2	2.52	0.44
1:A:42:LYS:HB3	1:A:49:THR:HG22	1.99	0.44
1:A:309:VAL:HB	1:A:310:PRO:HD2	1.98	0.44
2:B:73:LEU:HD12	2:B:73:LEU:HA	1.86	0.44
1:A:194:ARG:HB3	1:A:197:VAL:HG23	1.99	0.44
1:L:476:ALA:O	1:L:479:GLN:HG3	2.18	0.44
1:L:4:LYS:HE3	1:L:4:LYS:HB2	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:135:LYS:HG2	7:E:615:HOH:O	2.18	0.44
3:M:108:ALA:O	3:M:112:THR:HG23	2.18	0.44
1:A:191:GLN:OE1	1:A:195:PRO:HA	2.18	0.44
6:E:601:B12:C2B	6:E:601:B12:O7R	2.66	0.44
3:M:55:THR:HG21	3:M:57:THR:HB	1.99	0.44
2:B:47:PHE:CD1	2:B:47:PHE:N	2.85	0.44
2:B:222:VAL:HG12	2:B:223:ALA:N	2.32	0.44
3:M:100:ARG:H	3:M:100:ARG:NE	2.15	0.44
1:A:131:LYS:CG	1:A:132:MET:HE3	2.46	0.44
1:A:339:THR:HG21	1:A:344:ARG:HB3	1.99	0.44
1:L:431:ILE:HA	1:L:435:GLU:OE1	2.17	0.44
1:A:182:ASN:N	1:A:182:ASN:ND2	2.63	0.44
3:M:54:LYS:HB2	3:M:59:LYS:O	2.17	0.44
1:L:157:ASP:OD1	1:L:412:ARG:NH1	2.39	0.43
1:A:145:THR:O	1:A:146:ASN:HB3	2.18	0.43
1:L:223:ILE:HG23	1:L:242:LYS:HE2	1.99	0.43
2:E:135:LYS:HE2	2:E:204:HIS:HB2	1.99	0.43
1:L:374:PHE:O	1:L:375:ALA:HB3	2.18	0.43
3:M:75:THR:CG2	3:M:76:ALA:N	2.80	0.43
1:L:198:LEU:CD1	1:L:508:ILE:HD12	2.47	0.43
3:M:55:THR:CG2	3:M:57:THR:HB	2.49	0.43
3:M:127:ARG:HB3	3:M:128:PRO:CD	2.48	0.43
1:A:257:ARG:HG3	1:A:258:PHE:O	2.18	0.43
1:A:435:GLU:HG2	7:A:619:HOH:O	2.17	0.43
2:B:128:ILE:HD13	2:B:176:ALA:CA	2.40	0.43
2:B:224:LEU:N	2:B:224:LEU:HD12	2.33	0.43
1:L:238:THR:HB	1:L:239:PRO:CD	2.49	0.43
1:L:426:MET:HE3	1:L:426:MET:HB3	1.93	0.43
2:E:118:VAL:HG21	2:E:147:PRO:HB3	1.99	0.43
1:L:424:ALA:O	1:L:425:GLY:C	2.62	0.43
2:E:114:ALA:HB2	6:E:601:B12:HM62	2.00	0.43
1:A:142:ALA:HB2	1:A:166:PHE:CD1	2.54	0.43
6:B:601:B12:H481	6:B:601:B12:H533	2.01	0.43
1:A:139:SER:OG	1:A:167:ASP:OD2	2.30	0.43
1:L:102:VAL:HB	1:L:103:PRO:HD3	2.00	0.43
1:L:187:LEU:O	1:L:191:GLN:HG2	2.19	0.43
1:A:299:SER:OG	1:A:303:ILE:HA	2.18	0.42
1:L:279:LEU:HD12	1:L:279:LEU:HA	1.83	0.42
3:M:64:PHE:CD1	3:M:79:MET:HE3	2.54	0.42
1:A:59:PHE:HB3	1:A:63:ASP:HB2	2.01	0.42
3:G:169:LEU:O	3:G:172:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:537:ARG:O	1:L:541:ILE:HG13	2.18	0.42
2:E:106:ARG:O	2:E:217:PRO:HA	2.19	0.42
1:A:60:ASP:OD1	1:A:62:ILE:HB	2.19	0.42
1:A:97:LYS:O	1:A:101:ILE:HD12	2.19	0.42
2:B:88:LEU:HD12	2:B:88:LEU:HA	1.86	0.42
1:L:278:TYR:O	1:L:281:ALA:HB3	2.19	0.42
2:B:89:ARG:HH11	2:B:90:GLU:CG	2.31	0.42
1:A:215:GLY:O	1:A:493:GLN:NE2	2.52	0.42
1:L:385:ASP:O	1:L:389:VAL:HG13	2.19	0.42
3:M:161:THR:O	3:M:164:VAL:HB	2.20	0.42
3:G:66:LEU:HD12	3:G:66:LEU:HA	1.84	0.42
1:L:282:ARG:HD2	7:L:620:HOH:O	2.19	0.42
2:E:88:LEU:O	2:E:92:ILE:HD12	2.19	0.42
1:A:98:ARG:HG3	1:A:132:MET:CE	2.50	0.42
2:B:224:LEU:HD12	2:B:224:LEU:H	1.83	0.42
1:L:463:ILE:H	1:L:463:ILE:HG12	1.70	0.42
2:E:107:CYS:HB3	2:E:119:GLU:OE1	2.20	0.42
1:A:418:ALA:HA	1:A:482:PHE:CD2	2.55	0.42
1:L:179:ALA:HB3	1:L:180:PRO:HD3	2.02	0.42
2:E:105:ILE:HD12	2:E:217:PRO:HB3	2.01	0.42
1:A:238:THR:HG1	1:A:241:SER:H	1.68	0.42
2:B:103:ARG:HH11	2:B:103:ARG:HD2	1.63	0.42
1:L:438:ALA:CB	1:L:449:PRO:HD3	2.50	0.42
1:A:539:GLU:OE2	1:A:542:LYS:NZ	2.52	0.41
3:G:83:PRO:O	3:G:87:ARG:HG3	2.20	0.41
1:L:162:ALA:HB1	1:L:197:VAL:HG21	2.01	0.41
1:A:33:SER:HA	1:A:34:PRO:HD2	1.78	0.41
1:A:370:TYR:OH	1:A:444:GLY:HA3	2.20	0.41
1:L:349:LEU:HD22	1:L:353:PHE:HB2	2.03	0.41
1:L:526:GLY:O	1:L:527:PRO:C	2.62	0.41
1:A:523:ASP:OD1	1:A:530:GLY:HA2	2.20	0.41
2:B:54:ALA:HB3	2:B:123:LEU:HD13	2.00	0.41
1:L:414:LYS:HA	1:L:417:ARG:NH2	2.35	0.41
6:E:601:B12:N3B	6:E:601:B12:H202	2.36	0.41
1:L:350:LEU:HA	1:L:353:PHE:HB3	2.03	0.41
2:E:106:ARG:HD2	2:E:108:PHE:CE2	2.54	0.41
1:A:44:VAL:O	1:A:45:ASN:C	2.64	0.41
1:A:241:SER:O	1:A:245:LEU:HB2	2.21	0.41
1:A:550:PRO:HG2	1:L:23:TRP:HB2	2.02	0.41
2:B:100:ILE:HD11	2:B:177:LYS:CG	2.50	0.41
1:A:142:ALA:HB2	1:A:166:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:CD2	1:A:199:THR:HB	2.50	0.41
6:B:601:B12:H362	6:B:601:B12:C35	2.48	0.41
3:G:49:HIS:HB3	3:G:52:TRP:CG	2.55	0.41
1:L:524:TYR:CZ	1:L:526:GLY:HA2	2.55	0.41
2:B:98:GLU:HG3	2:B:177:LYS:NZ	2.36	0.41
2:B:105:ILE:O	2:B:105:ILE:HG13	2.19	0.41
3:G:54:LYS:HE2	3:G:54:LYS:HB2	1.63	0.41
3:G:150:LYS:NZ	3:G:150:LYS:HB2	2.35	0.41
3:G:40:VAL:HG13	3:G:95:ASP:OD2	2.20	0.41
3:G:59:LYS:HB3	3:G:59:LYS:NZ	2.36	0.41
1:L:229:GLU:HB3	1:L:230:PRO:HD3	2.03	0.41
1:A:12:ARG:HB2	1:A:15:ASN:HD22	1.86	0.41
1:A:23:TRP:HB3	1:A:28:PHE:CB	2.47	0.41
1:A:429:PRO:HD3	1:A:459:PHE:CG	2.56	0.41
1:L:354:LEU:N	1:L:355:PRO:CD	2.83	0.41
2:E:108:PHE:CD1	2:E:215:LYS:HD2	2.56	0.41
6:E:601:B12:H362	6:E:601:B12:C35	2.50	0.41
3:G:75:THR:O	3:G:78:ASP:HB2	2.21	0.41
1:L:392:ARG:HD2	1:L:544:ILE:HG12	2.03	0.41
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.88	0.40
2:E:113:VAL:HG22	2:E:139:VAL:HG12	2.02	0.40
1:L:33:SER:HA	1:L:34:PRO:HD2	1.73	0.40
1:L:150:ASN:HA	1:L:151:PRO:HD3	1.96	0.40
3:M:51:GLU:O	3:M:54:LYS:HE3	2.22	0.40
1:A:79:VAL:HG22	1:A:104:LEU:HD22	2.04	0.40
1:L:63:ASP:OD1	1:L:282:ARG:NH1	2.54	0.40
1:A:354:LEU:N	1:A:355:PRO:HD2	2.36	0.40
1:A:534:GLN:CG	1:A:535:GLY:N	2.83	0.40
3:G:70:LEU:HD23	3:G:70:LEU:HA	1.86	0.40
1:L:527:PRO:O	1:L:528:ALA:HB3	2.21	0.40
2:E:193:ARG:O	2:E:194:PRO:C	2.63	0.40
3:M:65:THR:HB	3:M:68:ASN:ND2	2.37	0.40

There are no symmetry-related clashes.

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	549/554 (99%)	512 (93%)	33 (6%)	4 (1%)	18	19
1	L	549/554 (99%)	508 (92%)	37 (7%)	4 (1%)	18	19
2	B	177/224 (79%)	171 (97%)	6 (3%)	0	100	100
2	E	177/224 (79%)	155 (88%)	16 (9%)	6 (3%)	3	1
3	G	135/173 (78%)	130 (96%)	5 (4%)	0	100	100
3	M	135/173 (78%)	128 (95%)	6 (4%)	1 (1%)	18	19
All	All	1722/1902 (90%)	1604 (93%)	103 (6%)	15 (1%)	14	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	180	SER
1	L	2	ARG
1	L	446	LYS
2	E	59	GLN
2	E	178	ARG
1	A	72	ASN
2	E	56	GLN
1	A	300	VAL
1	A	504	THR
1	L	300	VAL
2	E	123	LEU
3	M	67	GLU
2	E	57	GLY
1	A	363	GLY
1	L	29	ILE

5.3.2 Protein sidechains (i)

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	450/453 (99%)	401 (89%)	49 (11%)	6 6
1	L	450/453 (99%)	401 (89%)	49 (11%)	6 6
2	B	147/183 (80%)	124 (84%)	23 (16%)	2 2
2	E	147/183 (80%)	113 (77%)	34 (23%)	1 0
3	G	116/141 (82%)	95 (82%)	21 (18%)	2 1
3	M	116/141 (82%)	99 (85%)	17 (15%)	3 2
All	All	1426/1554 (92%)	1233 (86%)	193 (14%)	4 3

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	LYS
1	A	5	ARG
1	A	20	VAL
1	A	24	ILE
1	A	28	PHE
1	A	38	LYS
1	A	42	LYS
1	A	49	THR
1	A	72	ASN
1	A	73	LEU
1	A	103	PRO
1	A	117	VAL
1	A	147	VAL
1	A	152	VAL
1	A	173	VAL
1	A	178	TYR
1	A	182	ASN
1	A	187	LEU
1	A	194	ARG
1	A	198	LEU
1	A	210	LYS
1	A	245	LEU
1	A	257	ARG
1	A	274	LYS
1	A	277	LEU
1	A	349	LEU
1	A	379	GLU
1	A	404	ARG
1	A	406	GLU

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Mol	Chain	Res	Type
1	A	426	MET
1	A	433	ASP
1	A	450	GLU
1	A	451	ARG
1	A	453	ILE
1	A	454	VAL
1	A	461	GLN
1	A	462	GLU
1	A	475	LYS
1	A	479	GLN
1	A	492	ILE
1	A	493	GLN
1	A	494	LYS
1	A	501	TYR
1	A	509	VAL
1	A	527	PRO
1	A	534	GLN
1	A	536	GLU
1	A	542	LYS
2	B	49	THR
2	B	55	ARG
2	B	60	GLN
2	B	64	ILE
2	B	73	LEU
2	B	76	THR
2	B	85	LYS
2	B	96	GLU
2	B	101	LYS
2	B	118	VAL
2	B	121	ASN
2	B	128	ILE
2	B	143	GLN
2	B	145	LEU
2	B	164	THR
2	B	170	LYS
2	B	178	ARG
2	B	180	SER
2	B	190	GLN
2	B	206	LYS
2	B	215	LYS
2	B	222	VAL
2	B	224	LEU

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Mol	Chain	Res	Type
3	G	39	ARG
3	G	40	VAL
3	G	51	GLU
3	G	54	LYS
3	G	59	LYS
3	G	60	THR
3	G	66	LEU
3	G	71	SER
3	G	74	VAL
3	G	80	ARG
3	G	88	LEU
3	G	91	SER
3	G	94	LYS
3	G	100	ARG
3	G	106	GLU
3	G	126	LEU
3	G	130	ARG
3	G	150	LYS
3	G	157	ARG
3	G	167	LYS
3	G	173	ASP
1	L	1	MET
1	L	4	LYS
1	L	5	ARG
1	L	9	LEU
1	L	14	VAL
1	L	25	GLU
1	L	28	PHE
1	L	29	ILE
1	L	32	GLU
1	L	38	LYS
1	L	42	LYS
1	L	73	LEU
1	L	147	VAL
1	L	178	TYR
1	L	187	LEU
1	L	198	LEU
1	L	204	GLU
1	L	211	LEU
1	L	217	THR
1	L	218	CYS
1	L	224	SER

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Mol	Chain	Res	Type
1	L	247	SER
1	L	257	ARG
1	L	262	SER
1	L	277	LEU
1	L	279	LEU
1	L	326	LEU
1	L	349	LEU
1	L	350	LEU
1	L	367	VAL
1	L	404	ARG
1	L	406	GLU
1	L	426	MET
1	L	433	ASP
1	L	434	GLU
1	L	446	LYS
1	L	453	ILE
1	L	458	LYS
1	L	471	LEU
1	L	479	GLN
1	L	483	THR
1	L	490	LEU
1	L	492	ILE
1	L	493	GLN
1	L	497	LEU
1	L	501	TYR
1	L	511	ASP
1	L	527	PRO
1	L	542	LYS
2	E	49	THR
2	E	50	GLU
2	E	55	ARG
2	E	56	GLN
2	E	58	THR
2	E	59	GLN
2	E	60	GLN
2	E	64	ILE
2	E	67	VAL
2	E	73	LEU
2	E	85	LYS
2	E	86	SER
2	E	89	ARG
2	E	92	ILE

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Mol	Chain	Res	Type
2	E	101	LYS
2	E	116	VAL
2	E	124	SER
2	E	141	HIS
2	E	142	GLN
2	E	143	GLN
2	E	164	THR
2	E	166	ARG
2	E	171	ASN
2	E	174	ARG
2	E	177	LYS
2	E	190	GLN
2	E	206	LYS
2	E	209	LYS
2	E	213	THR
2	E	215	LYS
2	E	216	ASN
2	E	220	LEU
2	E	221	ARG
2	E	224	LEU
3	M	40	VAL
3	M	45	LEU
3	M	54	LYS
3	M	57	THR
3	M	59	LYS
3	M	63	ASP
3	M	66	LEU
3	M	68	ASN
3	M	70	LEU
3	M	71	SER
3	M	73	LYS
3	M	74	VAL
3	M	77	GLN
3	M	79	MET
3	M	88	LEU
3	M	100	ARG
3	M	146	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN

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Mol	Chain	Res	Type
1	A	16	GLN
1	A	89	ASN
1	A	182	ASN
1	A	452	ASN
1	A	465	ASN
1	A	467	ASN
1	A	493	GLN
2	B	75	GLN
2	B	121	ASN
2	B	167	GLN
2	B	190	GLN
3	G	58	ASN
3	G	148	GLN
1	L	15	ASN
1	L	95	ASN
1	L	153	GLN
1	L	334	ASN
1	L	452	ASN
1	L	465	ASN
1	L	487	GLN
1	L	513	GLN
2	E	56	GLN
2	E	84	HIS
2	E	142	GLN
2	E	143	GLN
2	E	190	GLN
2	E	216	ASN
3	M	49	HIS
3	M	68	ASN
3	M	77	GLN

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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
5	PGO	A	602	4	4,4,4	0.67	0	4,4,4	1.23	0
6	B12	B	601	-	94,101,101	1.29	12 (12%)	149,166,166	1.99	37 (24%)
6	B12	E	601	-	94,101,101	1.15	9 (9%)	149,166,166	1.91	39 (26%)
5	PGO	L	602	4	4,4,4	0.73	0	4,4,4	1.89	2 (50%)

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
5	PGO	A	602	4	-	2/2/2/2	-
6	B12	B	601	-	-	11/56/223/223	0/3/11/11
6	B12	E	601	-	-	9/56/223/223	0/3/11/11
5	PGO	L	602	4	-	2/2/2/2	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	B12	O58-C57	3.61	1.30	1.23
6	B	601	B12	C14-N23	3.48	1.39	1.35
6	E	601	B12	O58-C57	3.41	1.30	1.23
6	E	601	B12	C14-N23	3.39	1.39	1.35
6	E	601	B12	C19-N24	3.16	1.53	1.49
6	E	601	B12	P-O5	-2.72	1.42	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	B12	C19-N24	2.64	1.52	1.49
6	B	601	B12	C2B-N1B	-2.59	1.33	1.37
6	E	601	B12	C9-N22	2.42	1.36	1.30
6	B	601	B12	C17-C18	2.38	1.59	1.54
6	E	601	B12	C48-C49	2.35	1.59	1.52
6	E	601	B12	C1-C19	2.27	1.60	1.55
6	B	601	B12	C20-C1	-2.23	1.49	1.53
6	E	601	B12	C17-C18	2.17	1.58	1.54
6	B	601	B12	P-O5	-2.09	1.45	1.55
6	B	601	B12	C60-C18	-2.08	1.49	1.54
6	B	601	B12	C46-C12	2.07	1.58	1.54
6	B	601	B12	C9-N22	2.05	1.35	1.30
6	B	601	B12	C11-N23	2.05	1.40	1.36
6	E	601	B12	C54-C17	2.04	1.57	1.54
6	B	601	B12	C30-C3	2.03	1.59	1.54

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	601	B12	O58-C57-C56	-6.49	110.25	122.02
6	E	601	B12	C8B-N1B-C2B	5.88	111.60	106.26
6	B	601	B12	C1R-N1B-C2B	-5.82	114.18	127.09
6	B	601	B12	C8B-N1B-C2B	5.70	111.43	106.26
6	B	601	B12	C7B-C8B-C9B	-5.42	115.98	122.47
6	B	601	B12	C8B-N1B-C1R	5.31	134.39	125.41
6	E	601	B12	C1R-N1B-C2B	-5.09	115.79	127.09
6	E	601	B12	O58-C57-C56	-5.07	112.84	122.02
6	B	601	B12	C1-C19-N24	-4.81	100.89	106.25
6	B	601	B12	C4B-C9B-C8B	4.71	124.49	120.16
6	E	601	B12	C1-C19-N24	-4.69	101.03	106.25
6	E	601	B12	C7B-C8B-C9B	-4.53	117.05	122.47
6	B	601	B12	C26-C2-C1	4.42	116.84	110.00
6	E	601	B12	O6R-C1R-N1B	-4.38	99.67	108.09
6	B	601	B12	C25-C2-C1	-4.34	107.26	113.75
6	E	601	B12	O3-C2P-C1P	-4.26	98.50	106.94
6	E	601	B12	C8B-N1B-C1R	4.22	132.55	125.41
6	E	601	B12	N1B-C2B-N3B	-4.13	108.08	113.94
6	B	601	B12	O5-P-O2	4.03	123.11	106.70
6	E	601	B12	C20-C1-C19	3.99	113.19	109.35
6	E	601	B12	C55-C17-C16	3.95	124.31	116.59
6	B	601	B12	C7B-C8B-N1B	3.71	138.72	131.39
6	B	601	B12	N1B-C2B-N3B	-3.68	108.71	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	601	B12	C26-C2-C1	3.66	115.66	110.00
6	E	601	B12	C7B-C8B-N1B	3.62	138.55	131.39
6	B	601	B12	C13-C12-C11	-3.52	97.04	100.97
6	B	601	B12	C9-N22-C6	3.44	109.42	105.28
6	E	601	B12	C2-C3-C4	3.41	105.48	101.64
6	B	601	B12	C3P-C2P-C1P	3.36	117.92	111.42
6	B	601	B12	O2-P-O3	-3.35	93.51	102.87
6	E	601	B12	O2-P-O3	-3.33	93.57	102.87
6	E	601	B12	C47-C12-C46	-3.20	104.11	109.41
6	E	601	B12	C9B-N3B-C2B	3.19	108.32	104.40
6	B	601	B12	C56-C57-N59	3.18	122.13	116.34
6	B	601	B12	C36-C7-C37	3.13	116.06	110.74
6	B	601	B12	C1-C19-C18	-3.13	116.84	121.90
6	B	601	B12	O6R-C1R-N1B	-3.05	102.24	108.09
6	E	601	B12	O5-P-O2	3.03	119.02	106.70
6	B	601	B12	C2-C26-C27	2.97	123.45	115.19
6	E	601	B12	C36-C7-C37	2.85	115.58	110.74
6	E	601	B12	C56-C57-N59	2.83	121.51	116.34
6	E	601	B12	O5-P-O3	2.82	118.18	106.70
6	B	601	B12	C54-C17-C18	-2.79	108.98	112.99
6	B	601	B12	C8B-C9B-N3B	-2.69	107.09	110.00
6	E	601	B12	C13-C12-C11	-2.68	97.98	100.97
6	B	601	B12	C15-C16-N24	-2.62	118.69	122.42
6	E	601	B12	O44-C43-C42	-2.62	113.13	121.04
6	E	601	B12	C53-C15-C16	2.60	124.77	120.36
6	B	601	B12	O44-C43-C42	-2.59	113.22	121.04
5	L	602	PGO	O2-C2-C3	2.55	120.45	109.45
6	E	601	B12	C35-C5-C6	-2.55	118.30	122.41
6	E	601	B12	C1-C19-C18	-2.52	117.82	121.90
6	B	601	B12	C9B-N3B-C2B	2.48	107.45	104.40
6	E	601	B12	C9-C10-C11	-2.48	122.42	125.97
5	L	602	PGO	C3-C2-C1	2.47	120.94	110.80
6	B	601	B12	C49-C48-C13	2.45	121.59	114.65
6	E	601	B12	O51-C50-N52	2.45	129.06	122.53
6	E	601	B12	C53-C15-C14	-2.44	113.57	118.42
6	B	601	B12	C17-C18-C19	-2.44	98.67	102.36
6	B	601	B12	C53-C15-C14	-2.43	113.60	118.42
6	E	601	B12	C54-C17-C18	-2.42	109.52	112.99
6	E	601	B12	C26-C2-C3	2.40	111.61	107.42
6	B	601	B12	C47-C12-C46	-2.38	105.46	109.41
6	E	601	B12	C42-C43-N45	2.34	123.99	116.49
6	B	601	B12	O58-C57-N59	2.33	127.61	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	601	B12	C55-C17-C18	-2.27	106.78	111.12
6	E	601	B12	C8B-C9B-N3B	-2.23	107.58	110.00
6	B	601	B12	C55-C17-C16	2.19	120.88	116.59
6	B	601	B12	C3R-C2R-C1R	-2.19	95.07	99.89
6	E	601	B12	C47-C12-C11	2.19	117.90	110.08
6	E	601	B12	O2-P-O4	-2.18	102.83	109.81
6	B	601	B12	C7-C6-C5	-2.15	124.71	128.07
6	E	601	B12	C7-C6-N22	2.13	111.82	107.94
6	B	601	B12	C53-C15-C16	2.06	123.87	120.36
6	B	601	B12	O6R-C4R-C5R	-2.06	104.87	109.22
6	E	601	B12	C20-C1-C2	-2.05	109.90	113.28
6	E	601	B12	C9B-C8B-N1B	-2.03	104.40	105.30
6	E	601	B12	C5-C6-N22	-2.02	120.82	123.88

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	PGO	O1-C1-C2-O2
5	L	602	PGO	O1-C1-C2-O2
6	B	601	B12	C12-C13-C48-C49
6	E	601	B12	C12-C13-C48-C49
6	E	601	B12	C30-C31-C32-O34
6	B	601	B12	C30-C31-C32-O34
5	A	602	PGO	O1-C1-C2-C3
5	L	602	PGO	O1-C1-C2-C3
6	E	601	B12	C30-C31-C32-N33
6	B	601	B12	C1-C2-C26-C27
6	B	601	B12	C25-C2-C26-C27
6	E	601	B12	C1-C2-C26-C27
6	E	601	B12	C25-C2-C26-C27
6	B	601	B12	C8-C41-C42-C43
6	B	601	B12	C30-C31-C32-N33
6	E	601	B12	C42-C41-C8-C9
6	B	601	B12	C17-C18-C60-C61
6	E	601	B12	C17-C18-C60-C61
6	B	601	B12	C42-C41-C8-C9
6	B	601	B12	C19-C18-C60-C61
6	E	601	B12	C19-C18-C60-C61
6	E	601	B12	C1P-C2P-O3-P
6	B	601	B12	C3R-O2-P-O4
6	B	601	B12	C7-C37-C38-N40

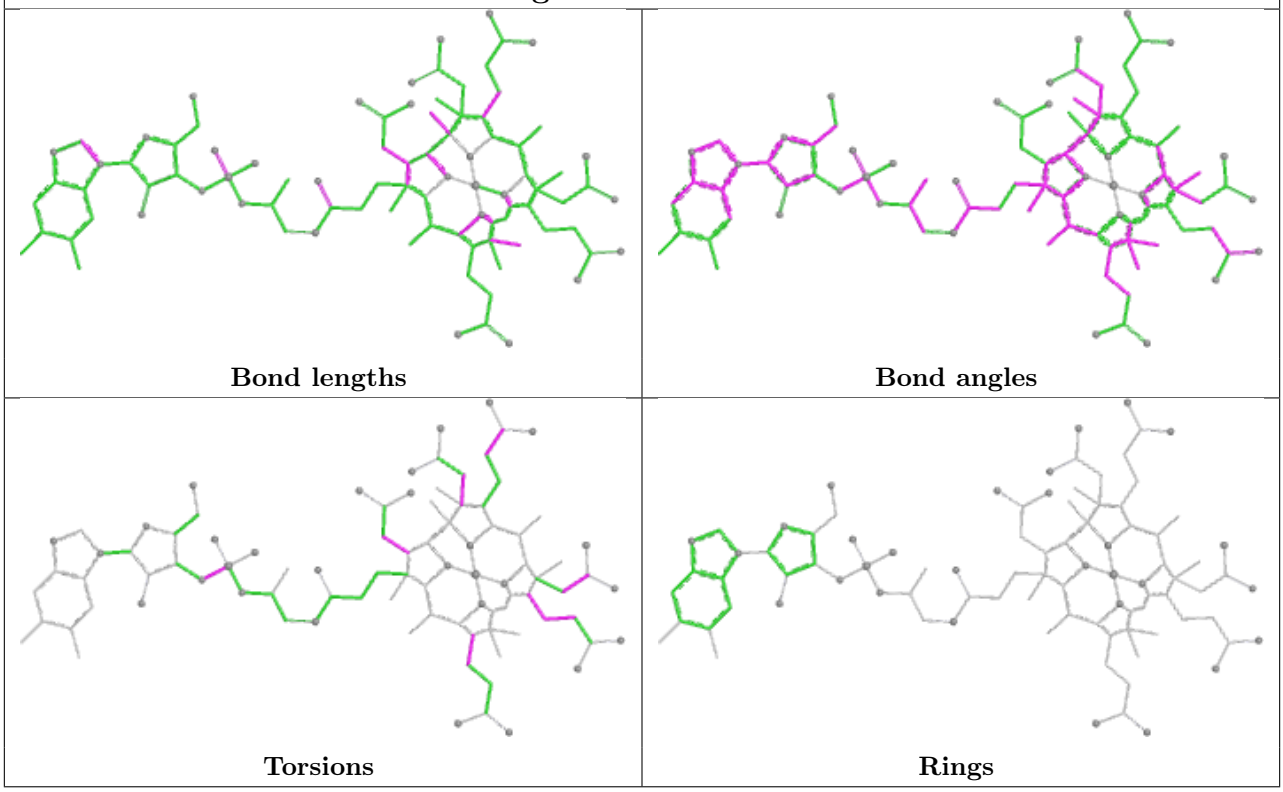
There are no ring outliers.

4 monomers are involved in 16 short contacts:

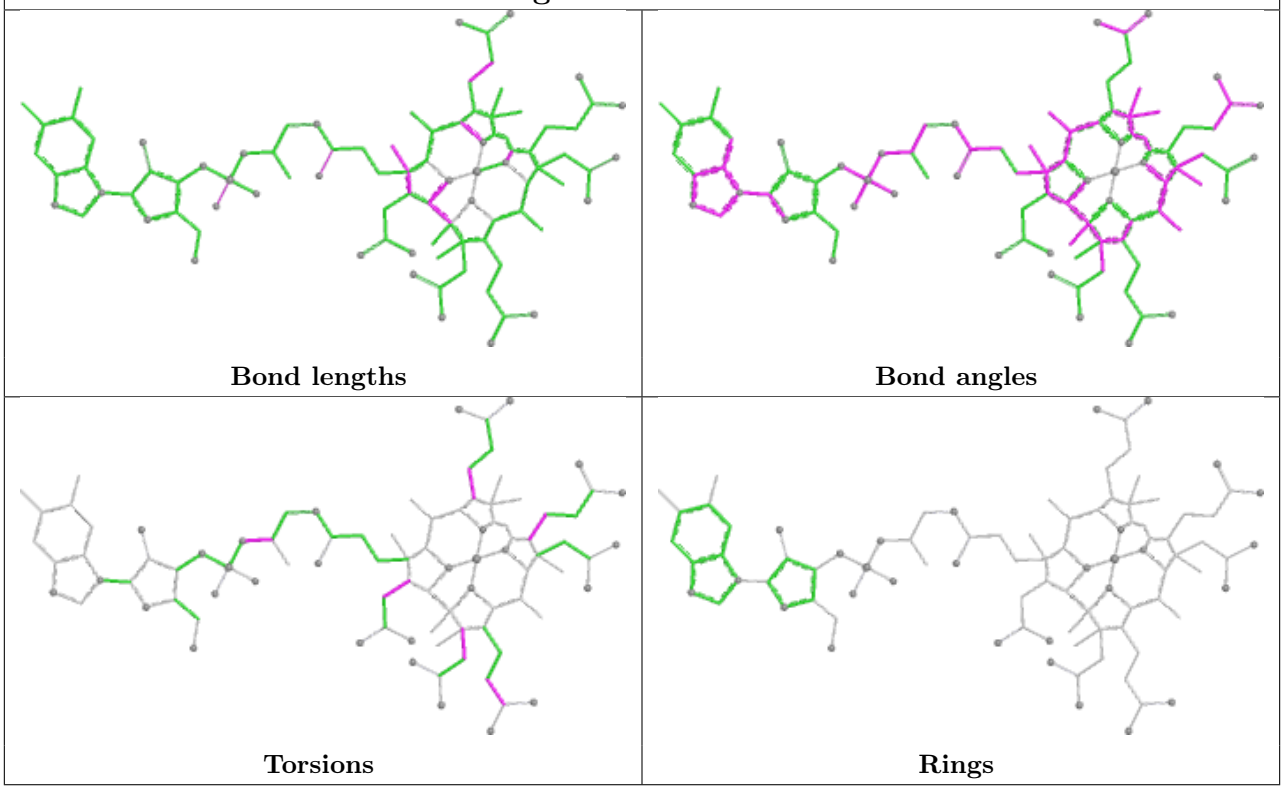
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	PGO	1	0
6	B	601	B12	5	0
6	E	601	B12	9	0
5	L	602	PGO	1	0

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 then 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.

Ligand B12 B 601



Ligand B12 E 601



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	551/554 (99%)	-0.77	3 (0%)	87	85	12, 24, 52, 90	0
1	L	551/554 (99%)	-0.69	1 (0%)	91	90	11, 27, 54, 76	0
2	B	179/224 (79%)	-0.32	3 (1%)	69	66	18, 37, 64, 99	0
2	E	179/224 (79%)	-0.03	3 (1%)	69	66	21, 45, 82, 117	0
3	G	137/173 (79%)	-0.24	1 (0%)	84	82	24, 35, 65, 78	0
3	M	137/173 (79%)	-0.15	3 (2%)	62	59	25, 37, 73, 86	0
All	All	1734/1902 (91%)	-0.53	14 (0%)	82	80	11, 31, 62, 117	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	223	ALA	3.6
3	M	58	ASN	3.2
3	M	68	ASN	2.7
3	M	63	ASP	2.5
2	B	46	GLY	2.4
1	A	480	GLY	2.3
2	E	57	GLY	2.3
1	A	1	MET	2.3
2	B	222	VAL	2.3
2	B	224	LEU	2.2
2	E	222	VAL	2.1
3	G	67	GLU	2.1
1	A	511	ASP	2.0
1	L	511	ASP	2.0

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)

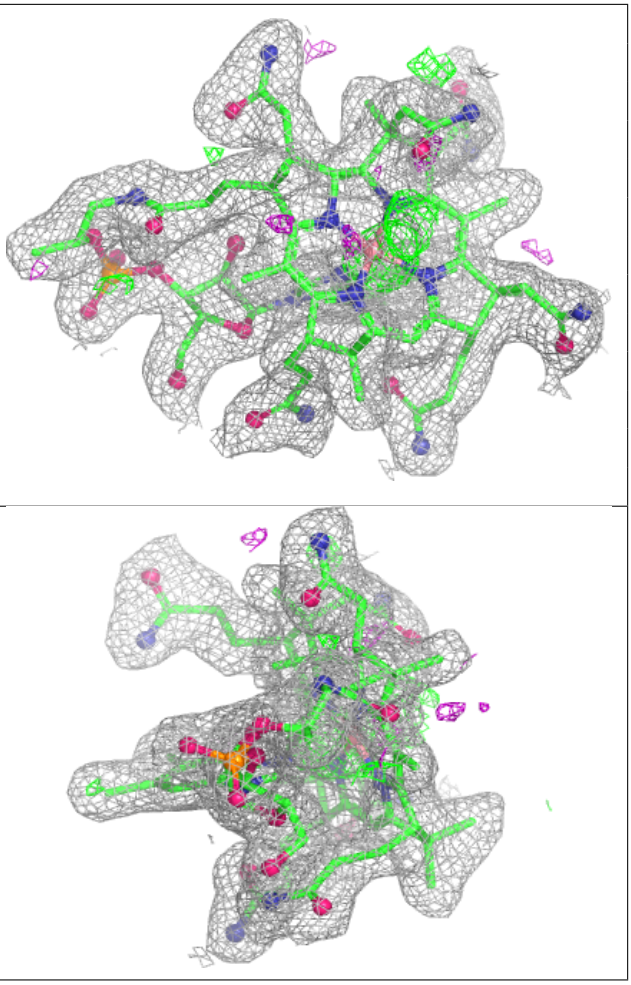
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGO	A	602	5/5	0.96	0.07	23,23,24,25	0
5	PGO	L	602	5/5	0.96	0.05	21,23,25,25	0
4	K	A	603	1/1	0.97	0.02	18,18,18,18	0
4	K	L	603	1/1	0.97	0.03	19,19,19,19	0
6	B12	B	601	91/91	0.97	0.06	17,23,27,40	0
6	B12	E	601	91/91	0.97	0.06	22,28,31,38	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.

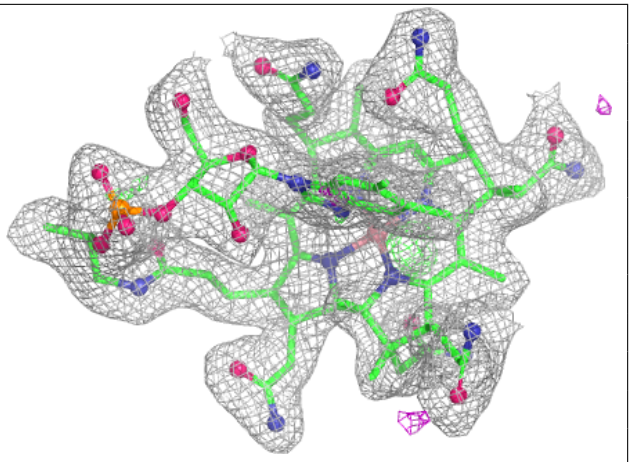
Electron density around B12 B 601:

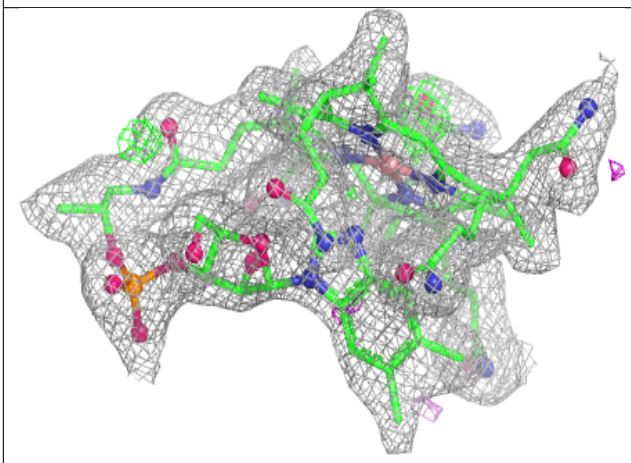
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

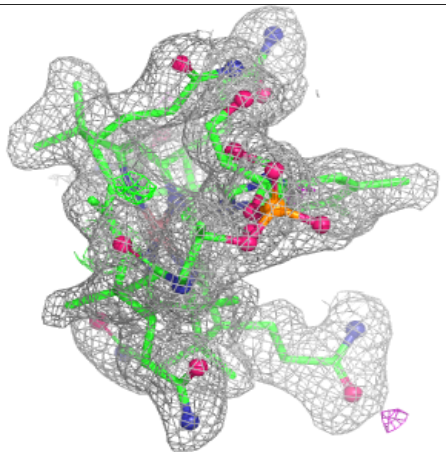


Electron density around B12 E 601:

$2mF_o$-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.