



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:25 AM EDT

PDB ID : 2INN / pdb_00002inn
Title : Structure of the Phenol Hydroxylase-Regulatory Protein Complex
Authors : Sazinsky, M.H.; Dunten, P.W.; McCormick, M.S.; Lippard, S.J.
Deposited on : 2006-10-08
Resolution : 2.70 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:

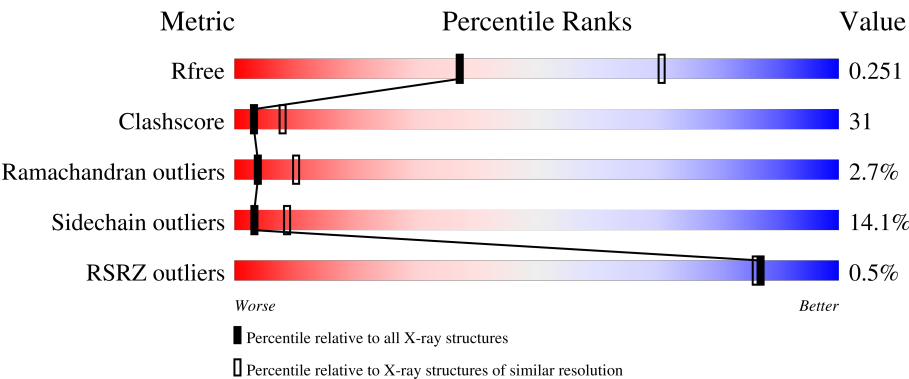
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	511	43%41%11%..
1	B	511	% 40%41%13%..
2	C	333	34%40%19%..
2	D	333	49%36%11%..
3	E	119	45%41%13%..

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Mol	Chain	Length	Quality of chain
3	F	119	
4	L	89	

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
7	MOO	B	515	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16389 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 Phenol hydroxylase component pHN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	Se	0	0	0
			4129	2655	694	756	8	16			
1	B	493	Total	C	N	O	S	Se	0	3	0
			4140	2665	694	757	8	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q84AQ2
A	21	MSE	MET	modified residue	UNP Q84AQ2
A	58	MSE	MET	modified residue	UNP Q84AQ2
A	133	MSE	MET	modified residue	UNP Q84AQ2
A	149	MSE	MET	modified residue	UNP Q84AQ2
A	165	MSE	MET	modified residue	UNP Q84AQ2
A	211	MSE	MET	modified residue	UNP Q84AQ2
A	220	MSE	MET	modified residue	UNP Q84AQ2
A	237	MSE	MET	modified residue	UNP Q84AQ2
A	278	MSE	MET	modified residue	UNP Q84AQ2
A	279	MSE	MET	modified residue	UNP Q84AQ2
A	280	MSE	MET	modified residue	UNP Q84AQ2
A	283	MSE	MET	modified residue	UNP Q84AQ2
A	289	MSE	MET	modified residue	UNP Q84AQ2
A	358	MSE	MET	modified residue	UNP Q84AQ2
A	361	MSE	MET	modified residue	UNP Q84AQ2
A	416	MSE	MET	modified residue	UNP Q84AQ2
A	510	ASP	ALA	conflict	UNP Q84AQ2
B	1	MSE	MET	modified residue	UNP Q84AQ2
B	21	MSE	MET	modified residue	UNP Q84AQ2
B	58	MSE	MET	modified residue	UNP Q84AQ2
B	133	MSE	MET	modified residue	UNP Q84AQ2
B	149	MSE	MET	modified residue	UNP Q84AQ2
B	165	MSE	MET	modified residue	UNP Q84AQ2
B	211	MSE	MET	modified residue	UNP Q84AQ2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	220	MSE	MET	modified residue	UNP Q84AQ2
B	237	MSE	MET	modified residue	UNP Q84AQ2
B	278	MSE	MET	modified residue	UNP Q84AQ2
B	279	MSE	MET	modified residue	UNP Q84AQ2
B	280	MSE	MET	modified residue	UNP Q84AQ2
B	283	MSE	MET	modified residue	UNP Q84AQ2
B	289	MSE	MET	modified residue	UNP Q84AQ2
B	358	MSE	MET	modified residue	UNP Q84AQ2
B	361	MSE	MET	modified residue	UNP Q84AQ2
B	416	MSE	MET	modified residue	UNP Q84AQ2
B	510	ASP	ALA	conflict	UNP Q84AQ2

- Molecule 2 is a protein called Phenol hydroxylase component pH_L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	319	Total	C	N	O	S	Se	0	0	0
			2593	1632	450	493	2	16			
2	D	325	Total	C	N	O	S	Se	0	0	0
			2643	1663	458	504	2	16			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	MET	modified residue	UNP Q84AQ4
C	67	MSE	MET	modified residue	UNP Q84AQ4
C	91	MSE	MET	modified residue	UNP Q84AQ4
C	135	MSE	MET	modified residue	UNP Q84AQ4
C	152	MSE	MET	modified residue	UNP Q84AQ4
C	158	MSE	MET	modified residue	UNP Q84AQ4
C	173	MSE	MET	modified residue	UNP Q84AQ4
C	190	MSE	MET	modified residue	UNP Q84AQ4
C	194	MSE	MET	modified residue	UNP Q84AQ4
C	198	MSE	MET	modified residue	UNP Q84AQ4
C	225	MSE	MET	modified residue	UNP Q84AQ4
C	226	MSE	MET	modified residue	UNP Q84AQ4
C	234	MSE	MET	modified residue	UNP Q84AQ4
C	248	MSE	MET	modified residue	UNP Q84AQ4
C	253	MSE	MET	modified residue	UNP Q84AQ4
C	267	MSE	MET	modified residue	UNP Q84AQ4
C	268	MSE	MET	modified residue	UNP Q84AQ4
D	1	MSE	MET	modified residue	UNP Q84AQ4
D	67	MSE	MET	modified residue	UNP Q84AQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	91	MSE	MET	modified residue	UNP Q84AQ4
D	135	MSE	MET	modified residue	UNP Q84AQ4
D	152	MSE	MET	modified residue	UNP Q84AQ4
D	158	MSE	MET	modified residue	UNP Q84AQ4
D	173	MSE	MET	modified residue	UNP Q84AQ4
D	190	MSE	MET	modified residue	UNP Q84AQ4
D	194	MSE	MET	modified residue	UNP Q84AQ4
D	198	MSE	MET	modified residue	UNP Q84AQ4
D	225	MSE	MET	modified residue	UNP Q84AQ4
D	226	MSE	MET	modified residue	UNP Q84AQ4
D	234	MSE	MET	modified residue	UNP Q84AQ4
D	248	MSE	MET	modified residue	UNP Q84AQ4
D	253	MSE	MET	modified residue	UNP Q84AQ4
D	267	MSE	MET	modified residue	UNP Q84AQ4
D	268	MSE	MET	modified residue	UNP Q84AQ4

- Molecule 3 is a protein called Phenol hydroxylase component phO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	118	Total	C	N	O	S	Se	0	0	0
			925	602	145	173	1	4			
3	F	118	Total	C	N	O	S	Se	0	0	0
			925	602	145	173	1	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	MET	modified residue	UNP Q84AQ1
E	23	MSE	MET	modified residue	UNP Q84AQ1
E	48	MSE	MET	modified residue	UNP Q84AQ1
E	103	MSE	MET	modified residue	UNP Q84AQ1
E	114	MSE	MET	modified residue	UNP Q84AQ1
F	1	MSE	MET	modified residue	UNP Q84AQ1
F	23	MSE	MET	modified residue	UNP Q84AQ1
F	48	MSE	MET	modified residue	UNP Q84AQ1
F	103	MSE	MET	modified residue	UNP Q84AQ1
F	114	MSE	MET	modified residue	UNP Q84AQ1

- Molecule 4 is a protein called Phenol hydroxylase component phM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	87	Total	C	N	O	Se	0	0	0
			719	446	122	146	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	MSE	MET	modified residue	UNP Q84AQ3
L	23	MSE	MET	modified residue	UNP Q84AQ3
L	31	MSE	MET	modified residue	UNP Q84AQ3
L	37	MSE	MET	modified residue	UNP Q84AQ3
L	53	MSE	MET	modified residue	UNP Q84AQ3
L	66	MSE	MET	modified residue	UNP Q84AQ3

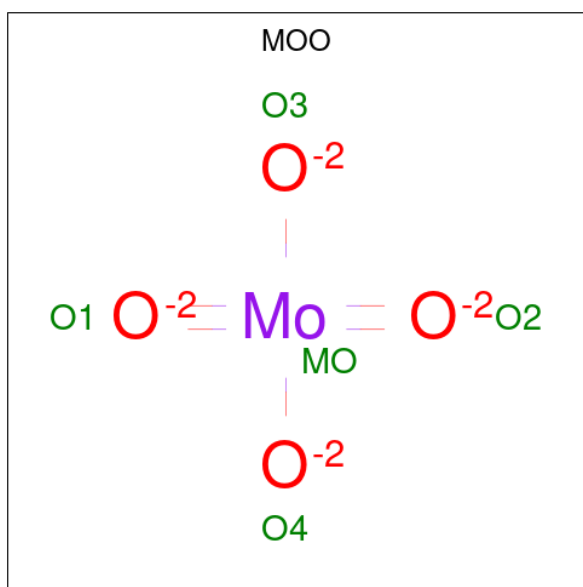
- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		
5	B	2	Total	Fe	0	0
			2	2		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is MOLYBDATE ION (CCD ID: MOO) (formula: MoO₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Mo	O	0	0
			5	1	4		

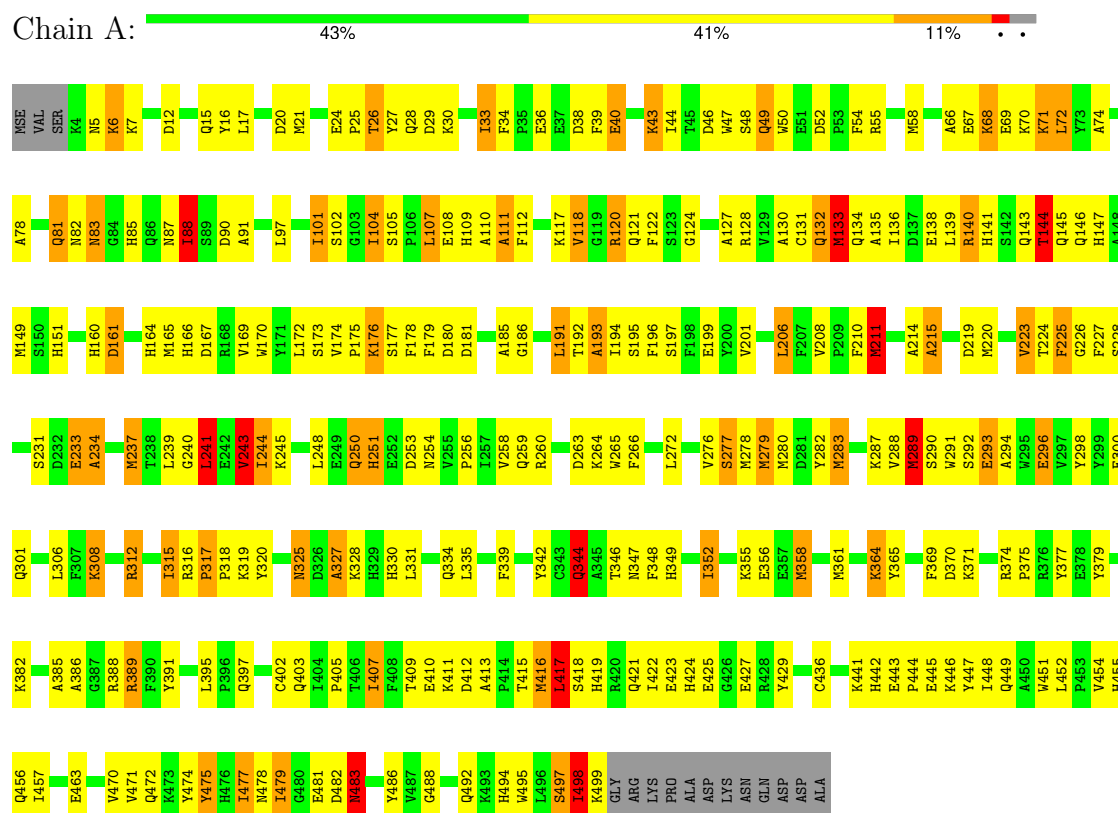
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	80	Total	O	0	0
			80	80		
8	B	71	Total	O	0	0
			71	71		
8	C	53	Total	O	0	0
			53	53		
8	D	60	Total	O	0	0
			60	60		
8	E	23	Total	O	0	0
			23	23		
8	F	13	Total	O	0	0
			13	13		
8	L	4	Total	O	0	0
			4	4		

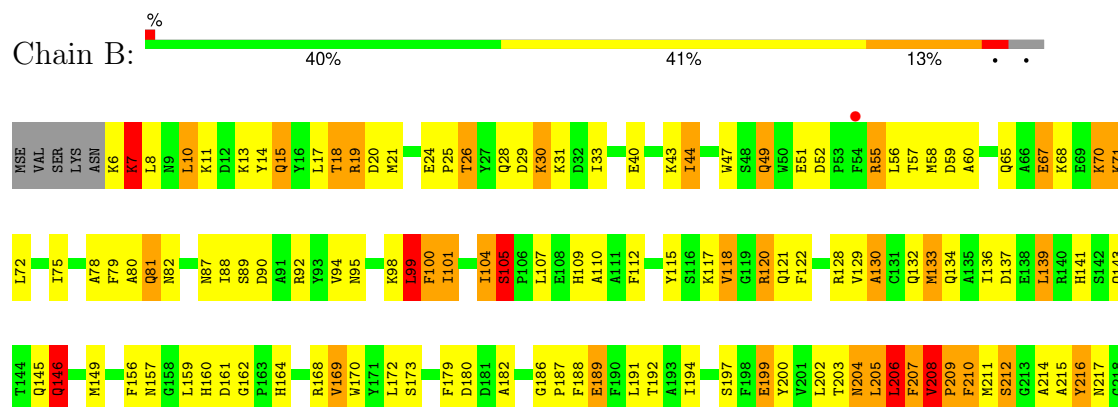
3 Residue-property plots

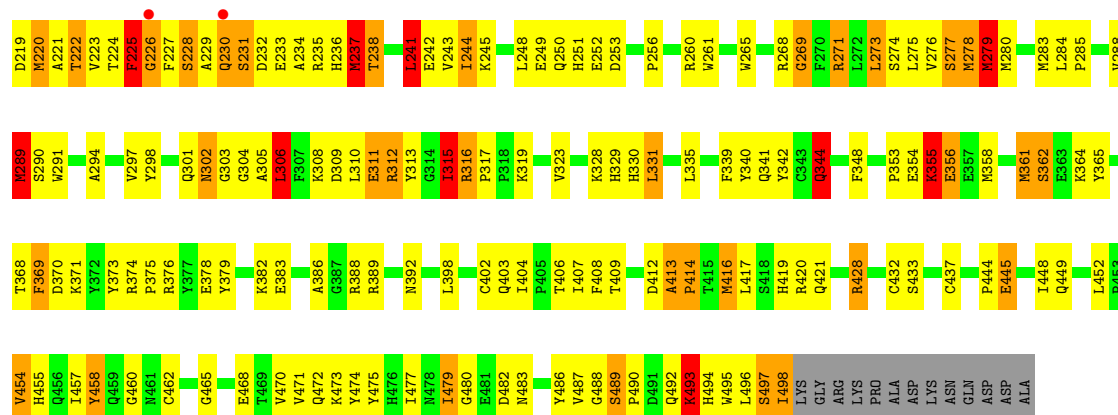
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phenol hydroxylase component pHN



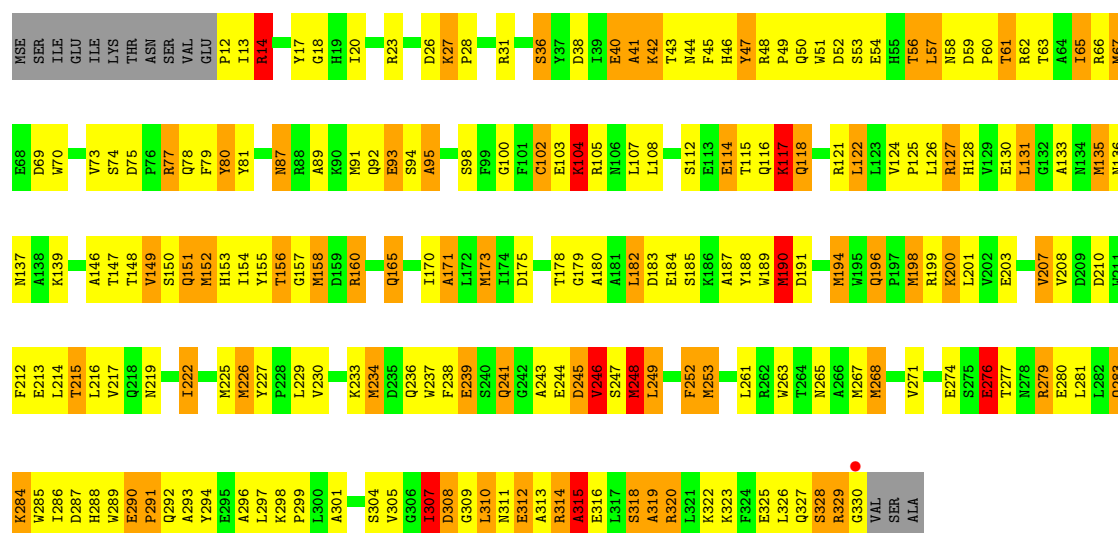
• Molecule 1: Phenol hydroxylase component pHN





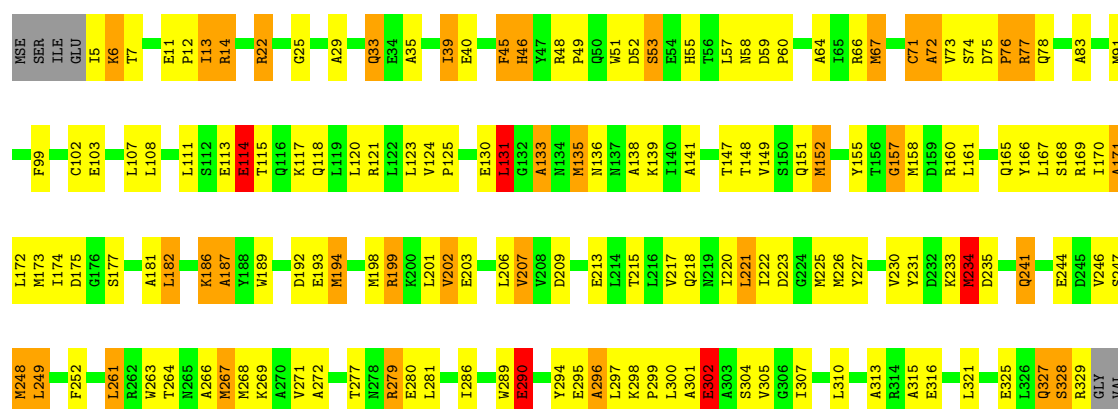
• Molecule 2: Phenol hydroxylase component pH_L

Chain C: 34% 40% 19%



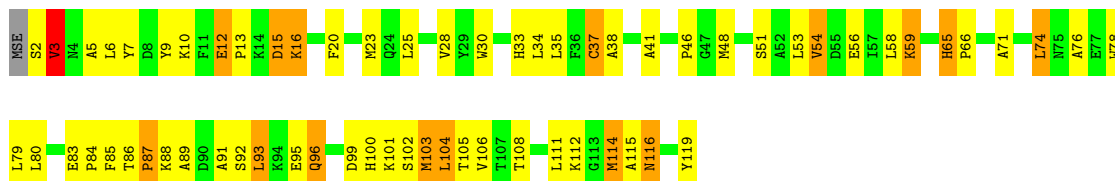
• Molecule 2: Phenol hydroxylase component pH_L

Chain D: 49% 36% 11%

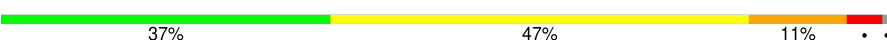
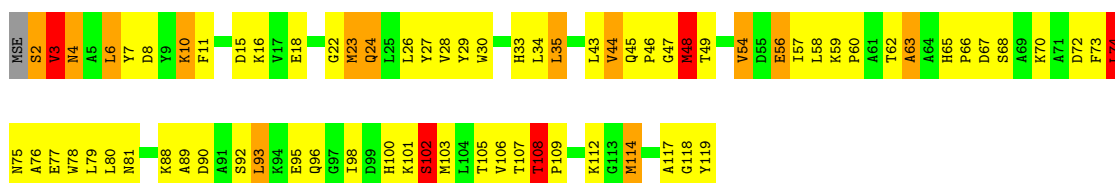


SER
ALA

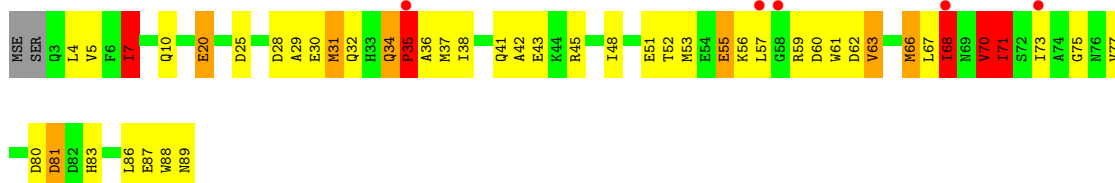
- Molecule 3: Phenol hydroxylase component phO

Chain E:  45% 41% 13% ..

- Molecule 3: Phenol hydroxylase component phO

Chain F:  37% 47% 11% . .

- Molecule 4: Phenol hydroxylase component phM

Chain L:  6% 45% 39% 8% 6% .

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.45Å 146.93Å 189.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.3 (30.00-2.70) 86.2 (30.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.37 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.252 0.164 , 0.251	Depositor DCC
R_{free} test set	2973 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16389	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MOO, FE, ZN

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	1.81	64/4247 (1.5%)	1.63	62/5728 (1.1%)
1	B	1.76	51/4260 (1.2%)	1.61	69/5746 (1.2%)
2	C	1.88	45/2636 (1.7%)	1.67	35/3537 (1.0%)
2	D	1.74	23/2686 (0.9%)	1.64	35/3606 (1.0%)
3	E	1.95	20/949 (2.1%)	1.74	20/1285 (1.6%)
3	F	1.86	17/949 (1.8%)	1.59	12/1285 (0.9%)
4	L	1.39	8/725 (1.1%)	1.48	10/971 (1.0%)
All	All	1.79	228/16452 (1.4%)	1.63	243/22158 (1.1%)

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	B	0	1

All (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	23	MSE	SE-CE	15.41	2.41	1.95
1	A	416	MSE	SE-CE	15.28	2.41	1.95
1	A	237	MSE	SE-CE	15.18	2.40	1.95
3	E	114	MSE	SE-CE	15.13	2.40	1.95
3	F	114	MSE	SE-CE	14.71	2.39	1.95
2	D	39	ILE	CA-CB	12.73	1.68	1.55
1	B	237	MSE	SE-CE	11.44	2.29	1.95
2	D	234	MSE	SE-CE	11.28	2.29	1.95
2	C	149	VAL	CA-CB	11.11	1.66	1.54
2	D	248	MSE	SE-CE	10.89	2.28	1.95
1	B	220	MSE	SE-CE	10.33	2.26	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	SER	CA-C	9.36	1.64	1.53
2	C	226	MSE	SE-CE	9.31	2.23	1.95
1	A	194	ILE	CA-CB	-9.04	1.42	1.54
3	F	48	MSE	SE-CE	8.99	2.22	1.95
2	C	253	MSE	SE-CE	8.96	2.22	1.95
1	B	208	VAL	N-CA	8.91	1.57	1.46
2	C	248	MSE	SE-CE	8.71	2.21	1.95
3	F	4	ASN	CA-C	-8.61	1.42	1.52
1	B	210	PHE	CA-C	8.46	1.64	1.52
2	C	222	ILE	CA-CB	-8.40	1.45	1.54
2	C	198	MSE	SE-CE	8.37	2.20	1.95
1	B	99	LEU	CG-CD2	8.31	1.79	1.52
2	C	207	VAL	CA-C	8.22	1.62	1.52
2	C	103	GLU	N-CA	-8.01	1.36	1.46
1	A	279	MSE	SE-CE	7.91	2.19	1.95
2	C	61	THR	CA-CB	7.87	1.64	1.53
2	D	152	MSE	SE-CE	-7.83	1.72	1.95
2	D	187	ALA	CA-CB	7.71	1.65	1.53
3	E	41	ALA	CA-CB	-7.71	1.42	1.53
3	F	24	GLN	CA-C	7.71	1.62	1.52
1	B	210	PHE	CD1-CE1	7.50	1.61	1.38
3	E	38	ALA	CA-CB	-7.48	1.43	1.53
2	D	67	MSE	SE-CE	7.45	2.17	1.95
3	E	103	MSE	SE-CE	7.40	2.17	1.95
3	F	4	ASN	C-O	-7.40	1.15	1.24
1	B	416	MSE	SE-CE	7.34	2.17	1.95
2	C	67	MSE	SE-CE	7.31	2.17	1.95
2	C	149	VAL	CA-C	7.29	1.61	1.52
1	B	221	ALA	CA-CB	-7.24	1.41	1.53
1	A	327	ALA	CA-C	7.21	1.62	1.52
2	D	83	ALA	CA-CB	-7.21	1.42	1.53
1	A	110	ALA	CA-CB	-7.11	1.41	1.53
2	C	31	ARG	N-CA	7.11	1.54	1.46
4	L	31	MSE	SE-CE	7.11	2.16	1.95
2	C	65	ILE	CA-CB	-7.11	1.47	1.54
1	A	166	HIS	CA-C	7.08	1.62	1.52
1	B	214	ALA	N-CA	-6.99	1.37	1.46
4	L	70	VAL	CA-C	6.97	1.60	1.52
1	A	289	MSE	SE-CE	6.91	2.16	1.95
1	A	234	ALA	CA-CB	-6.88	1.42	1.53
2	C	274	GLU	C-O	-6.86	1.16	1.23
1	A	5	ASN	CA-CB	6.81	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	GLU	CA-C	6.79	1.61	1.52
1	A	225	PHE	C-O	6.74	1.32	1.24
1	B	130	ALA	CA-CB	-6.74	1.42	1.53
1	A	447	TYR	C-O	6.69	1.32	1.24
1	A	147	HIS	C-O	-6.69	1.16	1.24
4	L	66	MSE	SE-CE	6.66	2.15	1.95
2	D	64	ALA	CA-CB	-6.66	1.41	1.53
3	F	23	MSE	CA-C	-6.65	1.44	1.53
2	D	135	MSE	SE-CE	6.64	2.15	1.95
2	C	268	MSE	SE-CE	6.60	2.15	1.95
2	C	234	MSE	SE-CE	6.58	2.15	1.95
1	A	454	VAL	CA-CB	6.57	1.61	1.54
3	E	12	GLU	CA-C	6.57	1.59	1.53
1	A	146	GLN	N-CA	-6.56	1.38	1.46
1	A	498	ILE	CA-C	6.55	1.61	1.52
2	C	318	SER	N-CA	6.54	1.54	1.46
1	A	447	TYR	CA-C	6.53	1.61	1.52
2	C	61	THR	N-CA	6.51	1.53	1.46
1	B	364	LYS	CA-C	6.50	1.62	1.52
2	D	72	ALA	CA-CB	6.45	1.64	1.53
1	A	131	CYS	C-O	-6.42	1.16	1.24
3	F	44	VAL	CA-C	6.42	1.60	1.52
1	A	215	ALA	CA-CB	-6.41	1.43	1.53
2	D	313	ALA	CA-CB	-6.39	1.43	1.53
1	A	499	LYS	CA-CB	6.38	1.66	1.53
3	E	89	ALA	CA-CB	-6.38	1.43	1.53
4	L	71	ILE	CA-CB	-6.37	1.45	1.54
1	A	294	ALA	CA-CB	-6.35	1.43	1.53
2	C	190	MSE	SE-CE	6.34	2.14	1.95
2	C	102	CYS	CB-SG	-6.32	1.60	1.81
1	A	55	ARG	CA-CB	6.31	1.59	1.53
2	C	208	VAL	CA-CB	-6.31	1.48	1.54
1	B	21	MSE	SE-CE	6.24	2.14	1.95
1	B	133	MSE	SE-CE	6.22	2.14	1.95
3	F	10	LYS	N-CA	6.20	1.53	1.46
1	A	201	VAL	C-O	-6.19	1.17	1.24
3	E	86	THR	CA-CB	6.18	1.60	1.53
2	C	285	TRP	CA-C	6.17	1.61	1.52
2	C	180	ALA	CA-CB	-6.08	1.43	1.53
1	A	15	GLN	CA-CB	-6.07	1.43	1.53
2	C	263	TRP	N-CA	-6.07	1.38	1.46
1	B	33	ILE	CA-CB	-6.04	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	TYR	CA-C	6.04	1.61	1.52
2	C	56	THR	CA-CB	6.02	1.62	1.53
1	A	282	TYR	CA-C	-6.01	1.44	1.52
1	B	487	VAL	CA-CB	6.01	1.61	1.54
1	B	60	ALA	CA-C	5.97	1.60	1.52
1	A	192	THR	CA-CB	5.96	1.63	1.53
1	A	289	MSE	CA-C	-5.96	1.45	1.52
1	A	352	ILE	C-O	-5.96	1.17	1.24
1	A	132	GLN	N-CA	-5.95	1.39	1.46
2	D	267	MSE	SE-CE	5.95	2.13	1.95
2	C	171	ALA	CA-CB	-5.93	1.44	1.53
1	B	71	LYS	N-CA	-5.93	1.39	1.46
1	A	211	MSE	CG-SE	5.92	2.13	1.95
1	A	120	ARG	CZ-NH2	5.92	1.41	1.33
1	B	160	HIS	C-O	5.90	1.31	1.24
2	D	202	VAL	CA-CB	-5.90	1.47	1.54
1	B	407	ILE	CA-CB	-5.89	1.46	1.54
1	B	271	ARG	CZ-NH2	-5.89	1.25	1.33
1	B	19	ARG	CD-NE	5.89	1.54	1.46
1	B	204	ASN	N-CA	-5.89	1.38	1.46
2	C	14	ARG	CA-C	-5.88	1.45	1.52
2	C	216	LEU	C-O	5.88	1.30	1.24
1	B	465	GLY	C-O	-5.86	1.16	1.23
1	A	483	ASN	CB-CG	-5.86	1.37	1.52
2	D	266	ALA	CA-CB	-5.86	1.44	1.53
1	B	216	TYR	CA-CB	-5.86	1.43	1.53
1	A	111	ALA	CA-C	5.86	1.60	1.52
4	L	35	PRO	N-CA	-5.84	1.39	1.47
1	B	118	VAL	CB-CG2	-5.82	1.33	1.52
1	A	12	ASP	CB-CG	5.79	1.66	1.52
3	E	6	LEU	CA-C	5.78	1.60	1.52
3	E	13	PRO	CA-C	5.77	1.59	1.52
1	B	378	GLU	C-O	5.76	1.30	1.24
2	C	173	MSE	SE-CE	5.75	2.12	1.95
1	B	206	LEU	CA-C	5.74	1.58	1.52
1	B	306	LEU	CA-C	5.74	1.60	1.52
3	E	71	ALA	CA-C	-5.73	1.45	1.52
1	A	71	LYS	CA-C	-5.72	1.44	1.52
1	B	404	ILE	CA-CB	5.70	1.61	1.54
2	C	20	ILE	CA-CB	5.70	1.61	1.54
2	D	133	ALA	CA-CB	-5.70	1.43	1.53
4	L	7	ILE	CA-CB	5.68	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	VAL	CA-CB	5.68	1.61	1.54
2	C	152	MSE	SE-CE	5.68	2.12	1.95
2	D	296	ALA	CA-CB	5.68	1.62	1.53
2	D	186	LYS	C-O	-5.66	1.16	1.24
1	A	306	LEU	CA-C	5.66	1.60	1.52
2	C	150	SER	N-CA	-5.65	1.39	1.46
3	F	28	VAL	C-O	5.65	1.29	1.24
1	A	83	ASN	N-CA	-5.65	1.38	1.46
2	D	192	ASP	CA-C	5.64	1.60	1.52
1	A	258	VAL	CA-CB	-5.64	1.47	1.54
2	C	133	ALA	N-CA	-5.62	1.39	1.46
1	B	118	VAL	N-CA	-5.62	1.39	1.46
2	D	209	ASP	CA-C	-5.60	1.45	1.52
1	B	279	MSE	CG-SE	5.60	2.12	1.95
2	D	45	PHE	C-O	-5.59	1.17	1.23
2	D	117	LYS	CG-CD	5.58	1.69	1.52
1	A	193	ALA	CA-CB	-5.57	1.44	1.53
1	A	250	GLN	N-CA	-5.57	1.39	1.46
1	A	233	GLU	CG-CD	5.54	1.65	1.52
1	B	19	ARG	CG-CD	5.52	1.69	1.52
1	B	182	ALA	C-O	-5.51	1.17	1.24
3	E	105	THR	N-CA	5.51	1.52	1.46
1	A	127	ALA	CA-CB	-5.51	1.44	1.53
1	B	379	TYR	C-O	5.51	1.30	1.24
2	C	222	ILE	N-CA	-5.50	1.40	1.46
1	B	197	SER	C-O	-5.50	1.17	1.24
2	C	118	GLN	C-O	5.50	1.30	1.24
1	A	151	HIS	C-O	-5.50	1.17	1.24
2	D	235	ASP	CA-C	5.48	1.60	1.52
1	A	470	VAL	CA-CB	-5.48	1.48	1.54
1	A	243	VAL	N-CA	-5.46	1.40	1.46
3	E	54	VAL	N-CA	-5.45	1.40	1.46
3	F	49	THR	CA-CB	5.45	1.62	1.53
1	A	481	GLU	CA-C	5.44	1.57	1.52
2	C	26	ASP	CG-OD1	5.44	1.35	1.25
2	C	252	PHE	N-CA	-5.43	1.39	1.46
2	D	328	SER	C-O	-5.42	1.17	1.24
3	E	104	LEU	N-CA	-5.42	1.39	1.46
1	A	133	MSE	SE-CE	5.41	2.11	1.95
1	B	454	VAL	N-CA	5.41	1.52	1.46
4	L	37	MSE	SE-CE	5.39	2.11	1.95
2	C	80	TYR	C-O	5.39	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	95	GLU	CG-CD	5.39	1.65	1.52
1	B	449	GLN	C-O	-5.39	1.17	1.24
1	A	301	GLN	CA-C	-5.38	1.46	1.53
1	B	493	LYS	CG-CD	5.38	1.68	1.52
2	C	236	GLN	CG-CD	5.37	1.65	1.52
1	B	222	THR	CA-CB	-5.36	1.45	1.53
2	C	315	ALA	CA-CB	5.35	1.62	1.53
1	B	355	LYS	CG-CD	5.35	1.68	1.52
1	A	260	ARG	N-CA	-5.33	1.40	1.46
1	B	26	THR	CA-CB	5.33	1.62	1.53
1	B	244	ILE	CA-C	5.32	1.59	1.52
2	C	135	MSE	SE-CE	5.30	2.11	1.95
3	E	56	GLU	CG-CD	5.30	1.65	1.52
1	A	358	MSE	CA-C	-5.30	1.45	1.52
3	F	46	PRO	C-O	5.30	1.31	1.24
1	A	308	LYS	CD-CE	5.28	1.68	1.52
2	C	154	ILE	CA-CB	-5.28	1.47	1.54
3	F	63	ALA	N-CA	5.27	1.52	1.46
3	F	29	TYR	C-O	-5.23	1.17	1.24
1	A	231	SER	N-CA	-5.22	1.39	1.46
1	B	445	GLU	CB-CG	5.22	1.68	1.52
3	E	5	ALA	CA-C	-5.22	1.46	1.52
1	A	5	ASN	CA-C	5.21	1.60	1.53
2	C	171	ALA	N-CA	-5.19	1.40	1.46
1	A	102	SER	CA-C	-5.19	1.45	1.52
2	C	94	SER	C-O	-5.18	1.17	1.24
1	A	365	TYR	N-CA	-5.17	1.41	1.46
1	A	88	ILE	C-O	-5.14	1.18	1.24
3	E	96	GLN	CA-C	-5.14	1.46	1.53
1	A	228	SER	CA-C	5.13	1.60	1.52
3	E	46	PRO	CA-C	5.12	1.59	1.52
3	F	63	ALA	CA-CB	5.12	1.62	1.53
1	A	293	GLU	C-O	-5.11	1.17	1.24
1	A	105	SER	N-CA	-5.09	1.41	1.46
1	B	313	TYR	N-CA	5.08	1.52	1.46
3	F	3	VAL	CB-CG2	-5.07	1.35	1.52
3	E	15	ASP	CA-C	5.07	1.59	1.52
1	B	180	ASP	CA-C	5.06	1.59	1.52
3	F	23	MSE	CA-CB	-5.05	1.45	1.53
1	A	407	ILE	CA-CB	-5.05	1.48	1.54
1	A	417	LEU	N-CA	-5.04	1.39	1.46
1	A	424	HIS	N-CA	-5.04	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	LEU	C-O	-5.04	1.17	1.24
1	B	137	ASP	C-O	5.03	1.30	1.24
1	A	370	ASP	CB-CG	5.03	1.64	1.52
2	C	107	LEU	C-O	5.03	1.30	1.24
1	B	319	LYS	N-CA	-5.01	1.39	1.45
4	L	5	VAL	N-CA	5.01	1.52	1.46
3	E	87	PRO	N-CA	-5.00	1.41	1.47

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	SER	N-CA-C	-11.73	98.95	113.38
3	F	108	THR	CA-C-N	-10.34	110.17	120.31
3	F	108	THR	C-N-CA	-10.34	110.17	120.31
1	A	352	ILE	CA-C-N	-9.68	110.83	120.31
1	A	352	ILE	C-N-CA	-9.68	110.83	120.31
2	C	62	ARG	N-CA-C	-9.58	101.58	113.18
1	A	48	SER	N-CA-C	-9.50	101.24	112.92
1	A	225	PHE	N-CA-C	-9.40	101.04	111.28
4	L	83	HIS	N-CA-C	8.92	122.25	108.96
1	B	273	LEU	CA-CB-CG	-8.66	85.98	116.30
2	D	114	GLU	N-CA-C	-8.55	100.56	112.45
1	A	127	ALA	N-CA-C	-8.48	101.99	111.82
4	L	80	ASP	N-CA-C	8.39	119.65	108.07
1	A	28	GLN	CA-C-N	-8.38	109.43	121.42
1	A	28	GLN	C-N-CA	-8.38	109.43	121.42
1	B	67	GLU	CB-CA-C	8.29	124.55	110.79
3	E	5	ALA	N-CA-C	-8.28	96.63	108.96
4	L	87	GLU	N-CA-C	8.21	120.61	108.14
1	A	186	GLY	CA-C-N	-8.07	111.49	119.64
1	A	186	GLY	C-N-CA	-8.07	111.49	119.64
3	E	20	PHE	N-CA-C	8.04	122.40	112.59
1	A	38	ASP	N-CA-C	8.04	123.17	113.12
2	C	158	MSE	N-CA-C	-7.93	101.43	112.45
1	B	457	ILE	N-CA-C	-7.91	102.73	110.72
2	C	213	GLU	N-CA-C	-7.90	102.61	111.14
1	B	214	ALA	N-CA-C	-7.87	102.01	111.69
2	D	213	GLU	N-CA-C	-7.57	103.00	111.71
3	F	93	LEU	N-CA-C	-7.46	103.09	111.14
2	C	165	GLN	N-CA-C	-7.45	102.53	111.69
1	B	104	ILE	N-CA-C	7.42	118.35	111.45
2	D	39	ILE	N-CA-C	-7.37	104.67	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	81	ASP	N-CA-C	-7.37	104.44	113.50
2	D	33	GLN	N-CA-C	7.32	119.94	111.02
2	D	313	ALA	N-CA-C	-7.25	103.45	111.36
1	B	480	GLY	N-CA-C	-7.19	106.13	114.69
2	D	76	PRO	N-CA-C	-7.18	103.96	113.65
2	D	289	TRP	N-CA-C	7.13	122.31	112.04
1	B	216	TYR	N-CA-C	7.11	125.94	110.80
3	E	71	ALA	N-CA-C	-7.10	99.41	110.42
1	B	249	GLU	N-CA-C	-7.09	104.64	112.72
1	B	121	GLN	N-CA-C	7.06	118.97	111.28
1	A	178	PHE	CB-CA-C	-7.06	99.52	110.81
2	D	235	ASP	N-CA-C	7.04	119.85	111.33
1	B	110	ALA	N-CA-C	-6.93	103.78	111.82
1	A	243	VAL	N-CA-C	6.93	117.69	110.62
1	A	208	VAL	CA-C-N	-6.91	111.68	119.28
1	A	208	VAL	C-N-CA	-6.91	111.68	119.28
1	B	311	GLU	N-CA-C	-6.89	103.55	112.23
2	D	77	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	A	317	PRO	CA-C-N	6.87	126.91	119.90
1	A	317	PRO	C-N-CA	6.87	126.91	119.90
2	C	107	LEU	N-CA-C	6.83	118.72	111.28
1	B	216	TYR	CB-CA-C	-6.80	96.88	110.42
1	B	437	CYS	N-CA-C	6.80	119.27	111.11
1	B	189	GLU	N-CA-C	-6.80	103.87	111.28
1	A	102	SER	N-CA-C	-6.76	105.16	113.41
1	B	483	ASN	N-CA-CB	-6.73	100.67	110.70
1	B	94	VAL	N-CA-C	-6.70	103.95	113.07
2	C	79	PHE	N-CA-C	6.62	119.22	108.63
1	B	306	LEU	N-CA-C	6.59	120.18	111.75
1	A	33	ILE	N-CA-C	6.55	118.08	110.62
3	E	30	TRP	CA-C-N	-6.54	112.78	120.11
3	E	30	TRP	C-N-CA	-6.54	112.78	120.11
2	C	246	VAL	CB-CA-C	-6.50	101.72	112.26
1	B	284	LEU	CA-C-N	-6.49	112.49	119.24
1	B	284	LEU	C-N-CA	-6.49	112.49	119.24
2	D	78	GLN	N-CA-C	6.48	120.77	112.86
2	D	171	ALA	CA-C-N	-6.48	110.95	120.28
2	D	171	ALA	C-N-CA	-6.48	110.95	120.28
1	A	413	ALA	CA-C-N	6.41	126.53	119.87
1	A	413	ALA	C-N-CA	6.41	126.53	119.87
2	C	36	SER	N-CA-C	6.39	122.15	113.97
2	C	77	ARG	N-CA-C	-6.34	105.51	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ASN	N-CA-C	-6.34	104.86	112.59
4	L	75	GLY	N-CA-C	6.31	118.45	112.08
2	D	131	LEU	CA-CB-CG	-6.29	94.29	116.30
2	C	314	ARG	N-CA-C	-6.29	104.12	110.97
2	C	284	LYS	CA-C-N	6.25	128.94	120.38
2	C	284	LYS	C-N-CA	6.25	128.94	120.38
2	D	141	ALA	N-CA-C	-6.25	104.53	111.71
1	B	265	TRP	N-CA-C	6.23	119.05	111.82
2	D	25	GLY	CA-C-O	-6.23	117.82	122.37
1	B	279	MSE	N-CA-C	-6.23	104.03	111.69
1	A	325	ASN	N-CA-C	-6.22	104.58	111.36
1	B	316	ARG	CA-C-N	-6.22	113.97	120.38
1	B	316	ARG	C-N-CA	-6.22	113.97	120.38
4	L	28	ASP	N-CA-C	6.21	120.98	113.41
2	D	221	LEU	N-CA-C	6.21	118.59	111.02
2	D	107	LEU	N-CA-C	6.16	120.41	113.01
3	F	101	LYS	N-CA-C	6.16	120.58	113.38
1	A	409	THR	N-CA-C	6.14	119.66	110.14
1	B	362	SER	N-CA-C	-6.14	104.65	111.71
1	B	493	LYS	N-CA-C	-6.12	104.61	111.28
2	C	44	ASN	N-CA-C	6.11	120.04	112.47
1	B	112	PHE	N-CA-C	-6.09	104.55	111.07
2	D	174	ILE	N-CA-C	6.07	116.81	110.62
1	A	118	VAL	N-CA-C	-6.06	103.16	111.89
1	A	237	MSE	CG-SE-CE	6.05	112.24	98.92
1	A	447	TYR	N-CA-C	6.03	118.81	111.82
1	B	169	VAL	N-CA-C	6.03	117.50	109.37
3	F	75	ASN	N-CA-C	-6.02	104.59	112.41
2	D	199	ARG	N-CA-C	-6.01	104.80	111.71
3	F	24	GLN	N-CA-CB	-6.01	101.47	111.20
1	B	243	VAL	CA-C-N	-5.99	113.01	120.56
1	B	243	VAL	C-N-CA	-5.99	113.01	120.56
1	B	489	SER	N-CA-C	5.99	118.35	110.08
2	C	95	ALA	N-CA-C	-5.96	104.72	112.23
1	B	261	TRP	O-C-N	5.95	128.20	122.07
2	C	236	GLN	N-CA-C	-5.93	104.90	111.36
2	C	100	GLY	N-CA-C	-5.92	105.32	112.49
1	A	102	SER	CB-CA-C	-5.92	98.88	109.24
3	E	6	LEU	CA-CB-CG	5.88	136.90	116.30
2	C	43	THR	CA-C-O	-5.88	115.12	121.36
3	F	89	ALA	N-CA-C	5.86	121.05	111.37
1	B	99	LEU	CB-CG-CD1	-5.86	93.12	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	GLN	N-CA-C	-5.84	106.01	113.01
1	A	40	GLU	N-CA-C	-5.83	106.12	113.18
2	C	117	LYS	N-CA-C	-5.83	104.83	111.07
1	A	475	TYR	N-CA-C	5.83	119.49	112.38
4	L	71	ILE	N-CA-C	-5.81	97.25	109.34
1	A	272	LEU	N-CA-C	-5.78	104.67	110.97
3	F	102	SER	N-CA-CB	5.76	118.28	110.38
4	L	68	ILE	N-CA-C	5.76	121.33	109.34
2	C	230	VAL	N-CA-C	5.76	116.41	110.82
1	A	91	ALA	N-CA-C	5.76	119.82	112.34
3	E	65	HIS	CA-C-N	-5.76	113.88	119.87
3	E	65	HIS	C-N-CA	-5.76	113.88	119.87
3	E	37	CYS	N-CA-C	5.75	119.82	112.34
3	F	54	VAL	N-CA-C	5.75	121.30	109.34
1	A	180	ASP	N-CA-C	-5.75	105.16	111.82
1	A	298	TYR	CA-C-N	-5.74	113.52	122.42
1	A	298	TYR	C-N-CA	-5.74	113.52	122.42
2	C	13	ILE	CB-CA-C	-5.74	104.30	112.22
2	C	263	TRP	N-CA-C	5.74	117.61	111.36
1	A	283	MSE	CG-SE-CE	-5.68	86.43	98.92
1	A	334	GLN	N-CA-C	-5.68	105.08	112.23
1	B	428	ARG	N-CA-C	5.68	119.17	110.20
3	E	65	HIS	N-CA-C	5.67	116.80	109.65
1	B	369	PHE	N-CA-C	5.66	117.14	110.97
1	A	395	LEU	N-CA-C	5.64	117.69	109.84
1	A	263	ASP	N-CA-C	-5.64	104.75	111.69
2	C	74	SER	CA-C-O	-5.64	114.95	121.49
1	B	118	VAL	N-CA-C	-5.64	104.04	111.09
1	A	457	ILE	N-CA-C	-5.63	105.04	110.72
4	L	70	VAL	N-CA-C	5.62	116.52	108.93
2	D	201	LEU	N-CA-C	-5.62	105.07	111.14
2	D	46	HIS	N-CA-C	5.59	119.82	112.89
1	B	207	PHE	N-CA-CB	5.58	119.92	110.49
3	E	3	VAL	CA-C-N	-5.57	113.84	122.09
3	E	3	VAL	C-N-CA	-5.57	113.84	122.09
1	B	173	SER	N-CA-C	-5.57	106.46	113.20
2	C	215	THR	N-CA-C	-5.56	105.22	112.23
2	C	41	ALA	N-CA-C	-5.56	102.66	110.50
1	B	146	GLN	N-CA-C	-5.55	104.61	111.33
1	A	298	TYR	N-CA-C	-5.53	106.69	113.50
2	D	271	VAL	N-CA-C	-5.53	105.46	110.82
2	D	138	ALA	N-CA-C	-5.52	105.17	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	GLY	N-CA-C	-5.51	101.09	112.34
2	D	13	ILE	N-CA-C	5.50	116.13	110.36
1	A	176	LYS	N-CA-C	-5.49	105.19	111.07
2	C	152	MSE	N-CA-C	-5.49	105.84	112.54
4	L	4	LEU	N-CA-C	5.49	117.17	108.67
3	F	23	MSE	CG-SE-CE	5.49	110.99	98.92
2	D	71	CYS	N-CA-C	5.48	122.47	110.80
1	A	483	ASN	N-CA-CB	-5.47	101.98	110.46
2	D	77	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	B	315	ILE	N-CA-C	5.45	115.80	108.17
1	A	55	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	A	144	THR	CB-CA-C	5.44	120.65	110.70
1	A	427	GLU	N-CA-C	-5.44	100.16	109.24
1	A	477	ILE	CB-CA-C	-5.43	104.39	110.96
1	B	105	SER	CA-C-N	-5.41	113.33	119.28
1	B	105	SER	C-N-CA	-5.41	113.33	119.28
3	E	23	MSE	N-CA-C	-5.41	101.54	109.81
2	C	191	ASP	CA-C-N	-5.40	115.58	122.77
2	C	191	ASP	C-N-CA	-5.40	115.58	122.77
1	B	445	GLU	N-CA-C	-5.39	105.96	112.54
2	D	290	GLU	N-CA-C	5.39	120.81	113.16
1	B	468	GLU	CB-CA-C	5.38	119.33	110.88
1	A	68	LYS	CD-CE-NZ	-5.38	94.68	111.90
1	B	344	GLN	N-CA-C	-5.38	105.97	112.54
1	B	139	LEU	N-CA-C	-5.38	105.50	111.36
2	C	237	TRP	N-CA-C	5.36	117.87	111.71
1	B	237	MSE	CG-SE-CE	5.32	110.62	98.92
2	D	22	ARG	NE-CZ-NH1	-5.32	116.18	121.50
2	D	136	ASN	CA-C-N	-5.30	111.77	121.52
2	D	136	ASN	C-N-CA	-5.30	111.77	121.52
3	E	87	PRO	CA-C-N	-5.30	115.72	122.77
3	E	87	PRO	C-N-CA	-5.30	115.72	122.77
1	B	317	PRO	CA-C-N	5.29	125.21	119.76
1	B	317	PRO	C-N-CA	5.29	125.21	119.76
2	C	102	CYS	CB-CA-C	-5.29	101.90	110.79
2	D	302	GLU	N-CA-CB	5.29	117.99	110.06
1	B	316	ARG	N-CA-CB	5.28	115.86	109.74
1	B	207	PHE	CA-C-O	-5.28	112.97	120.51
2	D	157	GLY	N-CA-C	-5.27	100.68	113.18
3	F	98	ILE	N-CA-C	5.27	111.85	106.21
1	B	21	MSE	N-CA-C	5.26	117.93	111.82
1	B	56	LEU	CB-CG-CD1	-5.22	95.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	VAL	CA-C-N	-5.21	113.33	119.84
1	A	174	VAL	C-N-CA	-5.21	113.33	119.84
2	C	307	ILE	N-CA-C	5.21	120.17	109.34
2	C	104	LYS	CB-CA-C	5.19	120.97	110.38
3	E	105	THR	CA-C-N	-5.18	115.96	123.11
3	E	105	THR	C-N-CA	-5.18	115.96	123.11
1	B	8	LEU	N-CA-C	5.18	117.81	110.50
1	B	421	GLN	N-CA-C	5.16	117.23	109.23
1	B	99	LEU	CB-CG-CD2	5.15	126.16	110.70
1	B	118	VAL	N-CA-CB	-5.15	101.44	110.77
1	A	385	ALA	N-CA-C	-5.15	105.56	111.07
2	C	54	GLU	CA-C-N	-5.14	114.25	122.53
2	C	54	GLU	C-N-CA	-5.14	114.25	122.53
1	A	52	ASP	N-CA-C	5.14	115.90	109.57
1	A	266	PHE	N-CA-C	-5.14	105.86	111.82
1	B	205	LEU	CA-CB-CG	-5.14	98.32	116.30
2	D	99	PHE	N-CA-C	5.12	116.86	111.28
1	B	386	ALA	N-CA-C	-5.12	107.04	113.28
2	C	276	GLU	CB-CA-C	5.11	121.10	110.32
1	B	413	ALA	CA-C-N	5.10	126.22	119.84
1	B	413	ALA	C-N-CA	5.10	126.22	119.84
1	A	54	PHE	N-CA-C	-5.10	101.15	108.60
3	E	108	THR	N-CA-CB	5.09	117.85	110.32
1	B	473	LYS	N-CA-C	5.08	117.72	111.82
1	B	120	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	436	CYS	N-CA-C	-5.08	105.44	111.69
1	B	208	VAL	N-CA-C	5.08	119.84	108.88
3	E	95	GLU	CA-CB-CG	5.07	124.23	114.10
1	B	365	TYR	CA-C-N	5.06	124.67	119.56
1	B	365	TYR	C-N-CA	5.06	124.67	119.56
1	B	260	ARG	N-CA-C	-5.06	105.21	111.33
1	B	100	PHE	CB-CA-C	-5.06	102.25	110.85
2	C	245	ASP	N-CA-CB	5.05	119.24	110.39
2	D	48	ARG	CG-CD-NE	-5.05	100.89	112.00
2	D	194	MSE	N-CA-C	5.04	117.50	111.71
1	A	346	THR	CA-C-N	-5.03	114.67	122.67
1	A	346	THR	C-N-CA	-5.03	114.67	122.67
1	A	109	HIS	CA-C-N	-5.03	113.04	120.28
1	A	109	HIS	C-N-CA	-5.03	113.04	120.28
1	A	441	LYS	N-CA-C	-5.02	105.81	111.28
1	B	289	MSE	CB-CA-C	5.02	117.36	110.34
3	E	116	ASN	N-CA-C	-5.01	104.42	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	LEU	N-CA-C	-5.01	106.86	113.12
3	F	23	MSE	CA-CB-CG	-5.01	104.09	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	482	ASP	Peptide

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	4129	0	3860	235	0
1	B	4140	0	3863	352	0
2	C	2593	0	2504	219	0
2	D	2643	0	2557	130	0
3	E	925	0	898	34	0
3	F	925	0	898	66	0
4	L	719	0	677	26	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	B	5	0	0	9	0
8	A	80	0	0	14	0
8	B	71	0	0	6	0
8	C	53	0	0	8	0
8	D	60	0	0	1	0
8	E	23	0	0	0	0
8	F	13	0	0	3	0
8	L	4	0	0	0	0
All	All	16389	0	15257	966	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 31.

All (966) 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:B:99:LEU:CD2	1:B:99:LEU:CG	1.80	1.57
2:C:190:MSE:SE	2:C:190:MSE:CE	2.14	1.46
1:A:289:MSE:CE	1:A:289:MSE:SE	2.16	1.44
2:D:135:MSE:SE	2:D:135:MSE:CE	2.15	1.44
2:C:234:MSE:SE	2:C:234:MSE:CE	2.15	1.44
1:A:58:MSE:HE1	1:A:133:MSE:CE	1.47	1.44
2:C:268:MSE:SE	2:C:268:MSE:CE	2.15	1.44
2:C:67:MSE:SE	2:C:67:MSE:CE	2.17	1.43
2:D:67:MSE:SE	2:D:67:MSE:CE	2.17	1.42
1:B:416:MSE:CE	1:B:416:MSE:SE	2.17	1.42
3:E:103:MSE:CE	3:E:103:MSE:SE	2.17	1.42
1:A:279:MSE:SE	1:A:279:MSE:CE	2.19	1.39
2:C:253:MSE:SE	2:C:253:MSE:CE	2.22	1.38
2:C:248:MSE:SE	2:C:248:MSE:CE	2.21	1.37
2:C:198:MSE:SE	2:C:198:MSE:CE	2.20	1.37
3:F:48:MSE:SE	3:F:48:MSE:CE	2.22	1.37
1:B:361:MSE:HE3	1:B:369:PHE:CE1	1.58	1.36
2:C:226:MSE:SE	2:C:226:MSE:CE	2.23	1.36
2:C:290:GLU:HG3	2:C:291:PRO:CD	1.54	1.36
1:B:220:MSE:SE	1:B:220:MSE:CE	2.26	1.33
2:D:248:MSE:SE	2:D:248:MSE:CE	2.28	1.32
2:D:234:MSE:SE	2:D:234:MSE:CE	2.29	1.31
1:B:237:MSE:SE	1:B:237:MSE:CE	2.29	1.30
1:A:58:MSE:CE	1:A:133:MSE:HE1	1.69	1.21
1:B:361:MSE:CE	1:B:369:PHE:CZ	2.25	1.20
3:E:114:MSE:SE	3:E:114:MSE:CE	2.40	1.20
3:F:114:MSE:SE	3:F:114:MSE:CE	2.39	1.19
1:A:416:MSE:SE	1:A:416:MSE:CE	2.41	1.18
1:A:237:MSE:SE	1:A:237:MSE:CE	2.41	1.17
3:F:23:MSE:CE	3:F:23:MSE:SE	2.41	1.17
2:D:225:MSE:HE1	2:D:294:TYR:HA	1.25	1.16
1:B:212:SER:HB3	4:L:35:PRO:HG3	1.28	1.15
2:C:225:MSE:HE1	2:C:294:TYR:HA	1.29	1.14
1:B:227:PHE:HB3	4:L:10:GLN:HE22	1.12	1.12
1:B:210:PHE:CD1	1:B:279:MSE:HE2	1.83	1.12
3:F:30:TRP:HE1	3:F:108:THR:CG2	1.66	1.08
2:C:190:MSE:HE1	2:C:199:ARG:HD2	1.29	1.08
2:C:190:MSE:HE1	2:C:199:ARG:CD	1.83	1.07
1:A:26:THR:HB	2:C:199:ARG:NH2	1.70	1.07
1:A:278:MSE:HE3	1:A:283:MSE:CE	1.85	1.06
2:C:290:GLU:HG3	2:C:291:PRO:HD2	1.30	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:190:MSE:HE2	2:C:190:MSE:HA	1.32	1.06
1:B:361:MSE:HE3	1:B:369:PHE:CZ	1.87	1.05
2:C:190:MSE:CE	2:C:199:ARG:HD2	1.86	1.05
1:A:278:MSE:HE3	1:A:283:MSE:HE1	1.05	1.04
1:B:353:PRO:HB2	1:B:358:MSE:HE2	1.38	1.04
1:B:361:MSE:HE2	1:B:369:PHE:CZ	1.92	1.04
1:B:55:ARG:HH21	1:B:55:ARG:CG	1.67	1.04
1:A:206:LEU:O	1:A:206:LEU:HD12	1.58	1.03
1:B:216:TYR:CE1	1:B:288:VAL:HG22	1.93	1.03
1:A:410:GLU:HG3	1:A:416:MSE:HE2	1.37	1.03
1:B:274:SER:HB2	1:B:335:LEU:HD11	1.40	1.02
1:B:216:TYR:CD1	1:B:288:VAL:HG22	1.96	1.01
1:A:312:ARG:HH11	1:A:312:ARG:HG3	1.26	1.01
2:C:276:GLU:HA	2:C:279:ARG:NH1	1.76	1.01
1:B:200:TYR:CE2	1:B:241:LEU:HD23	1.96	1.00
1:B:361:MSE:CE	1:B:369:PHE:CE1	2.43	1.00
1:A:27:TYR:OH	2:C:196:GLN:HG3	1.60	1.00
1:A:344:GLN:H	1:A:344:GLN:HE21	1.04	0.99
1:B:6:LYS:O	1:B:7:LYS:HB2	1.63	0.99
1:A:278:MSE:CE	1:A:283:MSE:HE1	1.91	0.99
1:A:97:LEU:HB3	1:A:149:MSE:HE1	1.45	0.99
3:F:30:TRP:HE1	3:F:108:THR:HG21	1.22	0.98
1:A:402:CYS:HG	6:A:514:ZN:ZN	0.72	0.98
1:A:488:GLY:H	1:A:492:GLN:HE22	1.11	0.97
1:B:203:THR:HG23	1:B:204:ASN:H	1.30	0.97
2:C:225:MSE:HE1	2:C:294:TYR:CA	1.95	0.95
2:C:225:MSE:CE	2:C:294:TYR:HA	1.96	0.95
1:A:220:MSE:HE2	1:B:78:ALA:HB1	1.48	0.95
2:D:75:ASP:CB	2:D:152:MSE:HE3	1.97	0.95
2:D:172:LEU:HD21	2:D:182:LEU:HD22	1.49	0.94
2:D:130:GLU:OE1	2:D:160:ARG:HD2	1.66	0.94
1:B:225[A]:PHE:CD1	1:B:226:GLY:N	2.36	0.94
2:C:290:GLU:HG3	2:C:291:PRO:HD3	1.47	0.93
2:D:225:MSE:HE1	2:D:294:TYR:CA	1.98	0.93
2:C:308:ASP:O	2:C:312:GLU:HG3	1.68	0.93
1:A:241:LEU:HD11	1:A:245:LYS:HE3	1.49	0.93
1:B:344:GLN:H	1:B:344:GLN:HE21	0.97	0.93
1:A:358:MSE:HE2	1:A:374:ARG:HG3	1.53	0.91
1:A:494:HIS:HB2	8:A:586:HOH:O	1.70	0.91
2:C:53:SER:HB3	3:F:7:TYR:CD2	2.05	0.91
3:F:16:LYS:HB3	3:F:18:GLU:OE1	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:73:PHE:O	3:F:74:LEU:HB2	1.69	0.90
1:B:227:PHE:HB3	4:L:10:GLN:NE2	1.84	0.90
1:B:55:ARG:HH21	1:B:55:ARG:HG2	1.38	0.89
3:F:92:SER:OG	3:F:95:GLU:HG2	1.72	0.89
1:B:302[A]:ASN:H	1:B:302[A]:ASN:ND2	1.70	0.88
1:A:241:LEU:CD1	1:A:245:LYS:HE3	2.03	0.88
2:C:329:ARG:HD3	2:C:330:GLY:N	1.88	0.88
2:C:276:GLU:CB	2:C:279:ARG:NH1	2.37	0.88
7:B:515:MOO:MO	7:B:515:MOO:O3	1.43	0.88
7:B:515:MOO:MO	7:B:515:MOO:O2	1.43	0.88
1:B:312:ARG:CB	1:B:312:ARG:HH11	1.86	0.88
2:C:190:MSE:HE1	2:C:199:ARG:NE	1.88	0.88
1:B:206:LEU:C	1:B:206:LEU:HD22	1.99	0.87
1:B:244:ILE:HD12	1:B:245:LYS:N	1.90	0.87
7:B:515:MOO:MO	7:B:515:MOO:O1	1.45	0.87
1:A:397:GLN:OE1	3:F:103:MSE:HE1	1.73	0.87
1:B:99:LEU:CD2	1:B:99:LEU:HG	2.04	0.87
1:B:341:GLN:HE22	3:E:37:CYS:H	1.20	0.87
1:B:361:MSE:HE3	1:B:369:PHE:HE1	1.29	0.87
1:B:161:ASP:OD1	2:D:22:ARG:NH2	2.06	0.87
1:B:18:THR:HG22	1:B:19:ARG:H	1.40	0.86
2:C:276:GLU:CA	2:C:279:ARG:NH1	2.38	0.86
2:D:225:MSE:CE	2:D:294:TYR:HA	2.05	0.86
1:A:250:GLN:O	1:A:251:HIS:HB2	1.73	0.86
1:B:308:LYS:HA	1:B:311:GLU:OE2	1.76	0.86
7:B:515:MOO:MO	7:B:515:MOO:O4	1.45	0.85
1:B:206:LEU:HD22	1:B:206:LEU:O	1.75	0.85
2:C:190:MSE:CE	2:C:199:ARG:CD	2.51	0.85
2:C:276:GLU:HB2	2:C:279:ARG:NH1	1.91	0.85
3:F:35:LEU:HA	3:F:119:TYR:CE2	2.11	0.84
1:B:361:MSE:CE	1:B:369:PHE:HZ	1.90	0.84
1:B:302[A]:ASN:N	1:B:302[A]:ASN:HD22	1.71	0.84
1:B:18:THR:HG22	1:B:19:ARG:N	1.90	0.84
1:B:133:MSE:HA	1:B:136:ILE:HG22	1.60	0.84
1:B:132:GLN:OE1	2:D:158:MSE:HE1	1.78	0.83
1:B:120:ARG:HG2	2:D:139:LYS:HB2	1.58	0.83
1:B:312:ARG:HH11	1:B:312:ARG:HB3	1.41	0.83
1:A:206:LEU:HD12	1:A:206:LEU:C	2.04	0.83
1:B:225[B]:PHE:CD1	1:B:226:GLY:N	2.46	0.83
2:C:56:THR:HG23	2:C:57:LEU:O	1.78	0.83
1:A:361:MSE:HE3	1:A:369:PHE:CZ	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225[B]:PHE:O	1:B:227:PHE:N	2.13	0.82
2:C:104:LYS:HZ3	2:C:105:ARG:HE	1.28	0.82
1:B:212:SER:O	1:B:215:ALA:HB3	1.80	0.81
2:C:45:PHE:CZ	2:C:58:ASN:HB2	2.16	0.81
1:B:225[B]:PHE:HD1	1:B:226:GLY:HA2	1.45	0.81
1:B:212:SER:HB3	4:L:35:PRO:CG	2.10	0.81
2:C:290:GLU:CG	2:C:291:PRO:HD2	2.10	0.81
1:B:14:TYR:O	1:B:18:THR:HB	1.80	0.81
1:A:488:GLY:H	1:A:492:GLN:NE2	1.78	0.81
1:A:58:MSE:H	2:C:165:GLN:HE22	1.26	0.81
1:B:225[B]:PHE:CD1	1:B:226:GLY:HA2	2.16	0.81
2:C:190:MSE:CE	2:C:190:MSE:HA	2.10	0.80
2:D:75:ASP:HB2	2:D:152:MSE:HE3	1.61	0.80
1:B:204:ASN:HB2	8:B:531:HOH:O	1.82	0.80
1:B:212:SER:HA	4:L:35:PRO:HB3	1.63	0.80
1:B:403:GLN:HE22	2:D:46:HIS:CD2	2.00	0.80
1:A:26:THR:CB	2:C:199:ARG:NH2	2.45	0.80
1:B:302[A]:ASN:ND2	1:B:302[A]:ASN:N	2.27	0.80
3:F:27:TYR:HB3	3:F:103:MSE:HE2	1.64	0.80
1:B:225[B]:PHE:CZ	1:B:229:ALA:CB	2.64	0.79
2:D:75:ASP:HA	2:D:152:MSE:HE1	1.64	0.79
2:D:91:MSE:HE2	2:D:252:PHE:CD1	2.18	0.79
2:C:118:GLN:HE22	2:C:241:GLN:HE21	1.28	0.79
2:C:276:GLU:HA	2:C:279:ARG:HH11	1.44	0.79
3:F:45:GLN:HB2	3:F:48:MSE:HG2	1.64	0.79
1:A:58:MSE:HE1	1:A:133:MSE:HE1	0.82	0.79
2:C:276:GLU:CA	2:C:279:ARG:HH12	1.95	0.78
1:B:225[B]:PHE:HD1	1:B:226:GLY:CA	1.95	0.78
2:C:171:ALA:CB	2:C:182:LEU:HD13	2.13	0.78
2:D:75:ASP:HA	2:D:152:MSE:CE	2.14	0.78
2:D:300:LEU:O	2:D:304:SER:HB2	1.83	0.78
1:A:344:GLN:H	1:A:344:GLN:NE2	1.80	0.78
1:A:141:HIS:O	1:A:145:GLN:HG3	1.84	0.77
1:B:225[B]:PHE:CZ	1:B:229:ALA:HB1	2.19	0.77
1:B:312:ARG:CB	1:B:312:ARG:NH1	2.47	0.77
2:C:276:GLU:CB	2:C:279:ARG:HH12	1.97	0.77
1:A:241:LEU:HD11	1:A:245:LYS:CE	2.14	0.77
3:F:72:ASP:HB3	8:F:123:HOH:O	1.85	0.77
1:A:196:PHE:CD1	1:A:244:ILE:HG12	2.20	0.76
1:B:55:ARG:NH2	1:B:55:ARG:HG3	1.99	0.76
1:B:49:GLN:HE21	1:B:49:GLN:HA	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ARG:HH21	1:B:55:ARG:HG3	1.51	0.76
2:C:198:MSE:HA	2:C:296:ALA:HB1	1.68	0.75
3:F:30:TRP:HE1	3:F:108:THR:HG22	1.49	0.75
1:B:216:TYR:CD1	1:B:288:VAL:CG2	2.68	0.75
1:B:344:GLN:H	1:B:344:GLN:NE2	1.81	0.75
2:D:172:LEU:CD2	2:D:182:LEU:HD22	2.17	0.74
1:A:455:HIS:HD2	3:F:15:ASP:OD1	1.70	0.74
1:B:355:LYS:HD3	1:B:356:GLU:OE2	1.86	0.74
1:B:18:THR:CG2	1:B:19:ARG:N	2.51	0.74
1:B:490:PRO:HA	1:B:493:LYS:CD	2.18	0.73
1:B:203:THR:HG23	1:B:204:ASN:N	1.99	0.73
1:B:413:ALA:N	1:B:414:PRO:HD3	2.02	0.73
2:D:172:LEU:HD21	2:D:182:LEU:CD2	2.18	0.73
1:B:273:LEU:CD2	1:B:276:VAL:HG21	2.18	0.73
1:A:140:ARG:O	1:A:144:THR:HB	1.89	0.73
2:C:104:LYS:NZ	2:C:105:ARG:HE	1.86	0.73
1:B:248:LEU:CD2	1:B:315:ILE:HD13	2.18	0.73
1:A:214:ALA:HB1	1:A:219:ASP:HB3	1.71	0.73
1:B:225[B]:PHE:CD1	1:B:226:GLY:CA	2.71	0.73
1:B:72:LEU:HD12	1:B:224:THR:HG22	1.71	0.72
1:B:211:MSE:SE	1:B:226:GLY:HA3	2.37	0.72
1:B:156:PHE:O	2:D:14:ARG:NH2	2.22	0.72
1:A:220:MSE:HE2	1:B:78:ALA:CB	2.20	0.72
1:A:344:GLN:HE21	1:A:344:GLN:N	1.84	0.72
1:B:6:LYS:O	1:B:7:LYS:CB	2.38	0.71
2:C:27:LYS:HB2	2:C:28:PRO:HD2	1.70	0.71
1:B:230:GLN:NE2	1:B:233:GLU:HG3	2.05	0.71
1:B:225[B]:PHE:HD1	1:B:226:GLY:N	1.85	0.71
1:B:455:HIS:HD2	3:E:15:ASP:OD2	1.73	0.71
2:C:189:TRP:CD1	2:C:190:MSE:HE3	2.25	0.71
2:D:118:GLN:HE22	2:D:241:GLN:HG2	1.56	0.71
1:A:58:MSE:CE	1:A:133:MSE:CE	2.44	0.71
1:A:382:LYS:HG2	8:A:588:HOH:O	1.90	0.70
1:B:20:ASP:O	2:D:186:LYS:NZ	2.23	0.70
2:D:121:ARG:NH2	2:D:194:MSE:HE3	2.06	0.70
1:B:312:ARG:NH1	1:B:312:ARG:HB2	2.05	0.70
1:B:210:PHE:CG	1:B:279:MSE:HE2	2.26	0.70
1:B:472:GLN:HB2	1:B:479:ILE:HD12	1.73	0.70
1:B:55:ARG:CG	1:B:55:ARG:NH2	2.37	0.70
1:A:165:MSE:HB3	1:A:169:VAL:HG21	1.72	0.70
1:A:122:PHE:CZ	1:A:191:LEU:HD22	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLN:CD	3:F:103:MSE:HE1	2.17	0.69
2:C:117:LYS:HE2	2:C:184:GLU:OE1	1.92	0.69
1:B:208:VAL:O	1:B:212:SER:OG	2.10	0.69
2:C:212:PHE:CE1	2:C:271:VAL:HG21	2.27	0.69
1:B:200:TYR:C	1:B:200:TYR:CD1	2.68	0.69
1:B:353:PRO:HB2	1:B:358:MSE:CE	2.19	0.69
1:B:490:PRO:HA	1:B:493:LYS:HD2	1.75	0.69
1:A:132:GLN:OE1	2:C:158:MSE:HE1	1.92	0.69
1:A:397:GLN:HE22	3:F:103:MSE:CE	2.06	0.69
2:C:311:ASN:O	2:C:313:ALA:N	2.25	0.69
1:A:27:TYR:CG	2:C:200:LYS:HB2	2.28	0.69
2:C:290:GLU:CG	2:C:291:PRO:CD	2.50	0.69
1:B:231:SER:CA	4:L:70:VAL:O	2.41	0.68
1:B:248:LEU:HD22	1:B:315:ILE:HD13	1.73	0.68
1:B:494:HIS:CD2	8:B:585:HOH:O	2.46	0.68
2:D:151:GLN:HG3	2:D:155:TYR:CE1	2.27	0.68
1:B:149:MSE:HE3	1:B:225[A]:PHE:HE2	1.58	0.68
1:A:211:MSE:HE2	1:A:211:MSE:N	2.07	0.68
1:B:228:SER:N	4:L:10:GLN:HE22	1.92	0.68
1:A:410:GLU:OE2	1:A:418:SER:HA	1.94	0.68
1:B:279:MSE:C	1:B:279:MSE:SE	2.86	0.68
1:A:144:THR:CG2	1:A:225:PHE:CD1	2.77	0.68
1:B:231:SER:HA	4:L:70:VAL:O	1.93	0.68
1:B:233:GLU:HA	1:B:236:HIS:HB2	1.76	0.67
2:C:312:GLU:O	2:C:315:ALA:HB3	1.94	0.67
1:B:100:PHE:HA	1:B:104:ILE:HD12	1.76	0.67
1:B:199:GLU:O	1:B:203:THR:HB	1.94	0.67
2:D:118:GLN:NE2	2:D:241:GLN:HG2	2.09	0.67
1:A:165:MSE:HB3	1:A:169:VAL:CG2	2.24	0.67
1:B:341:GLN:HE21	1:B:392:ASN:HD22	1.42	0.67
1:B:488:GLY:H	1:B:492:GLN:NE2	1.92	0.67
1:A:58:MSE:H	2:C:165:GLN:NE2	1.93	0.67
2:D:121:ARG:CZ	2:D:194:MSE:CE	2.72	0.67
2:D:11:GLU:OE2	2:D:12:PRO:HD2	1.95	0.67
2:C:148:THR:O	2:C:152:MSE:HG3	1.95	0.67
1:A:259:GLN:NE2	1:A:316:ARG:HG3	2.10	0.66
1:B:203:THR:CG2	1:B:204:ASN:H	2.05	0.66
2:C:265:ASN:HB2	8:C:340:HOH:O	1.95	0.66
1:B:230:GLN:C	1:B:232:ASP:N	2.52	0.66
1:B:49:GLN:HA	1:B:49:GLN:NE2	2.11	0.66
1:A:122:PHE:CE2	1:A:191:LEU:HD22	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:HIS:CE1	3:F:27:TYR:OH	2.48	0.66
1:B:132:GLN:HB3	2:D:158:MSE:HE1	1.78	0.66
2:C:56:THR:HG22	2:C:59:ASP:HB2	1.78	0.66
1:A:167:ASP:HA	1:A:176:LYS:HE3	1.77	0.66
2:C:12:PRO:HD2	8:C:382:HOH:O	1.95	0.66
3:F:30:TRP:NE1	3:F:108:THR:HG21	2.04	0.66
1:B:330:HIS:HD2	1:B:373:TYR:OH	1.79	0.66
1:B:356:GLU:CD	1:B:356:GLU:H	2.04	0.66
3:F:27:TYR:CB	3:F:103:MSE:HE2	2.27	0.65
1:B:225[B]:PHE:CE1	1:B:229:ALA:HB3	2.31	0.65
1:A:319:LYS:O	1:A:320:TYR:HB2	1.96	0.65
2:D:74:SER:O	2:D:76:PRO:HD3	1.97	0.65
1:A:472:GLN:HB2	1:A:479:ILE:HD12	1.77	0.65
1:A:58:MSE:HE1	1:A:133:MSE:HE3	1.69	0.65
1:B:228:SER:N	4:L:10:GLN:NE2	2.45	0.65
1:B:273:LEU:HD23	1:B:276:VAL:CG2	2.27	0.65
2:C:87:ASN:HD22	2:C:87:ASN:C	2.05	0.65
1:B:403:GLN:HE22	2:D:46:HIS:HD2	1.44	0.64
3:F:73:PHE:O	3:F:74:LEU:CB	2.45	0.64
1:A:397:GLN:NE2	3:F:103:MSE:CE	2.61	0.64
1:B:210:PHE:CE1	1:B:279:MSE:HG2	2.32	0.64
2:D:161:LEU:O	2:D:165:GLN:HG3	1.97	0.64
2:C:328:SER:O	2:C:329:ARG:CB	2.45	0.64
2:D:198:MSE:HA	2:D:296:ALA:HB1	1.80	0.64
1:B:65:GLN:HE22	1:B:68:LYS:NZ	1.96	0.64
1:B:353:PRO:CB	1:B:358:MSE:HE2	2.23	0.64
2:C:27:LYS:CB	2:C:28:PRO:HD2	2.27	0.64
2:C:23:ARG:HD3	8:C:342:HOH:O	1.95	0.63
1:B:225[B]:PHE:CE2	1:B:229:ALA:CB	2.82	0.63
1:B:458:TYR:C	1:B:460:GLY:H	2.05	0.63
2:D:194:MSE:O	2:D:194:MSE:HG2	1.94	0.63
1:A:143:GLN:HE22	2:C:151:GLN:HE22	1.45	0.63
1:A:403:GLN:HE22	2:C:46:HIS:CD2	2.17	0.63
2:D:121:ARG:NH2	2:D:194:MSE:CE	2.61	0.63
1:A:455:HIS:CD2	3:F:15:ASP:OD1	2.52	0.63
1:A:210:PHE:CB	1:A:211:MSE:HE2	2.28	0.63
1:B:212:SER:CA	4:L:35:PRO:HB3	2.29	0.62
1:B:308:LYS:C	1:B:310:LEU:H	2.07	0.62
1:A:97:LEU:HB3	1:A:149:MSE:CE	2.24	0.62
2:C:171:ALA:HB1	2:C:182:LEU:HD13	1.80	0.62
2:C:229:LEU:HD23	2:C:297:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:HB2	1:B:71:LYS:HG2	1.80	0.62
1:B:206:LEU:HD11	1:B:207:PHE:CD2	2.34	0.62
1:B:273:LEU:CD2	1:B:276:VAL:CG2	2.77	0.62
2:D:160:ARG:HH22	2:D:223:ASP:CG	2.07	0.62
1:A:27:TYR:HH	2:C:196:GLN:HG3	1.65	0.62
1:B:44:ILE:HG21	1:B:47:TRP:CD1	2.35	0.62
3:F:30:TRP:NE1	3:F:108:THR:CG2	2.51	0.62
1:A:40:GLU:HG2	8:A:523:HOH:O	1.99	0.62
1:B:203:THR:HG23	1:B:204:ASN:HD22	1.63	0.62
2:C:283:GLN:HA	2:C:283:GLN:NE2	2.14	0.62
2:D:203:GLU:HA	2:D:206:LEU:HD12	1.81	0.62
2:D:207:VAL:O	2:D:207:VAL:HG13	1.99	0.62
1:B:67:GLU:HG3	4:L:68:ILE:HD13	1.82	0.62
2:C:93:GLU:HA	2:C:93:GLU:OE1	1.99	0.62
3:F:88:LYS:H	3:F:96:GLN:HE22	1.48	0.61
1:A:211:MSE:O	1:A:223:VAL:HG23	1.99	0.61
2:C:194:MSE:HG2	2:C:299:PRO:HB2	1.82	0.61
3:F:67:ASP:O	3:F:68:SER:C	2.41	0.61
1:B:271:ARG:CZ	1:B:408:PHE:CD1	2.83	0.61
1:A:374:ARG:N	1:A:375:PRO:HD2	2.15	0.61
1:B:200:TYR:C	1:B:200:TYR:HD1	2.09	0.61
1:B:344:GLN:HE21	1:B:344:GLN:N	1.83	0.61
2:C:201:LEU:CD2	2:C:293:ALA:HA	2.30	0.61
1:B:99:LEU:HD23	1:B:210:PHE:CZ	2.36	0.61
1:B:342:TYR:C	1:B:344:GLN:NE2	2.59	0.61
2:D:75:ASP:CA	2:D:152:MSE:CE	2.78	0.61
1:A:210:PHE:HB3	1:A:211:MSE:HE2	1.82	0.61
1:B:90:ASP:HB3	1:B:285:PRO:HG2	1.82	0.61
2:D:160:ARG:NH2	2:D:223:ASP:OD2	2.31	0.61
1:B:98:LYS:HE2	1:B:157:ASN:O	2.01	0.61
1:B:164:HIS:HE1	1:B:474:TYR:O	1.83	0.61
1:B:206:LEU:HD11	1:B:207:PHE:CE2	2.35	0.60
2:D:299:PRO:HA	2:D:302:GLU:HG2	1.83	0.60
1:A:67:GLU:OE2	1:A:71:LYS:HE3	2.01	0.60
1:B:128:ARG:O	1:B:132:GLN:HG3	2.00	0.60
1:B:206:LEU:CD1	1:B:207:PHE:CD2	2.83	0.60
1:A:26:THR:HB	2:C:199:ARG:HH21	1.65	0.60
2:D:75:ASP:CA	2:D:152:MSE:HE3	2.30	0.60
2:D:152:MSE:HE2	2:D:263:TRP:HB2	1.82	0.60
1:A:21:MSE:HB3	2:C:131:LEU:HD13	1.83	0.60
1:A:193:ALA:O	1:A:197:SER:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:LEU:HB2	3:F:105:THR:HB	1.84	0.60
1:A:69:GLU:OE1	1:A:140:ARG:NH1	2.34	0.60
1:B:92:ARG:HG3	1:B:486:TYR:CE2	2.36	0.60
2:C:311:ASN:O	2:C:312:GLU:C	2.44	0.60
1:A:78:ALA:HB2	1:B:75:ILE:HD13	1.83	0.60
2:C:77:ARG:O	2:C:78:GLN:HB2	2.01	0.60
1:A:279:MSE:HA	1:A:283:MSE:HE3	1.84	0.59
1:B:11:LYS:O	1:B:15:GLN:HG3	2.02	0.59
1:B:413:ALA:N	1:B:414:PRO:CD	2.66	0.59
2:C:234:MSE:CE	2:C:234:MSE:HB2	2.32	0.59
1:A:6:LYS:HA	1:A:6:LYS:HE2	1.82	0.59
1:A:81:GLN:HG3	4:L:36:ALA:HB1	1.84	0.59
1:A:164:HIS:HE1	1:A:474:TYR:O	1.84	0.59
1:A:215:ALA:HB2	1:A:223:VAL:HG21	1.85	0.59
1:B:24:GLU:OE2	1:B:30:LYS:HE2	2.02	0.59
1:B:95:ASN:CB	1:B:283:MSE:CE	2.80	0.59
1:B:289:MSE:HE2	4:L:34:GLN:HE22	1.68	0.59
1:B:72:LEU:CD1	1:B:224:THR:HG22	2.33	0.59
1:A:442:HIS:O	3:F:2:SER:N	2.36	0.59
1:B:10:LEU:HD21	4:L:81:ASP:CG	2.27	0.59
1:A:293:GLU:OE2	1:A:364:LYS:HE3	2.03	0.59
2:C:95:ALA:O	2:C:98:SER:HB2	2.03	0.59
2:C:318:SER:O	2:C:322:LYS:HG3	2.03	0.59
2:D:272:ALA:O	2:D:279:ARG:HD3	2.03	0.59
3:E:99:ASP:OD1	3:E:102:SER:OG	2.20	0.59
1:A:33:ILE:HG22	1:A:34:PHE:CD1	2.37	0.59
1:B:88:ILE:HA	1:B:217:ASN:O	2.03	0.58
1:B:206:LEU:HD13	1:B:207:PHE:N	2.18	0.58
2:C:102:CYS:SG	2:C:249:LEU:HD21	2.42	0.58
2:C:52:ASP:OD1	2:C:52:ASP:C	2.42	0.58
2:D:49:PRO:HG2	2:D:55:HIS:O	2.03	0.58
1:A:327:ALA:O	1:A:328:LYS:C	2.45	0.58
1:A:472:GLN:HB2	1:A:479:ILE:CD1	2.33	0.58
1:A:58:MSE:N	2:C:165:GLN:HE22	1.99	0.58
1:B:273:LEU:HD23	1:B:276:VAL:HG23	1.85	0.58
1:B:132:GLN:HB3	2:D:158:MSE:CE	2.34	0.58
1:B:248:LEU:CD2	1:B:315:ILE:CD1	2.81	0.58
2:C:190:MSE:CE	2:C:199:ARG:NE	2.63	0.58
2:D:75:ASP:CG	2:D:152:MSE:HE3	2.27	0.58
1:A:477:ILE:O	1:A:477:ILE:HG22	2.03	0.58
1:B:428:ARG:O	3:E:101:LYS:NZ	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:VAL:O	2:D:207:VAL:CG1	2.52	0.58
1:A:241:LEU:CD1	1:A:245:LYS:CE	2.76	0.58
2:C:175:ASP:O	2:C:178:THR:HG23	2.04	0.58
1:B:139:LEU:O	1:B:143:GLN:HG3	2.04	0.58
1:B:329:HIS:HB3	1:B:368:THR:HG21	1.86	0.58
1:A:161:ASP:O	1:A:165:MSE:HG3	2.04	0.58
1:A:488:GLY:N	1:A:492:GLN:HE22	1.92	0.58
2:C:171:ALA:CB	2:C:182:LEU:CD1	2.82	0.58
1:B:210:PHE:HA	1:B:279:MSE:HE1	1.86	0.57
3:F:30:TRP:NE1	3:F:108:THR:HG22	2.17	0.57
1:B:68:LYS:HG2	4:L:68:ILE:HD12	1.86	0.57
1:B:194:ILE:O	1:B:199:GLU:HB2	2.04	0.57
1:B:225[A]:PHE:CD1	1:B:225[A]:PHE:C	2.82	0.57
1:B:253:ASP:O	1:B:256:PRO:HD2	2.04	0.57
1:B:273:LEU:O	1:B:274:SER:C	2.46	0.57
1:A:26:THR:CB	2:C:199:ARG:HH22	2.15	0.57
1:B:490:PRO:HA	1:B:493:LYS:HD3	1.85	0.57
1:B:305:ALA:O	1:B:308:LYS:HB2	2.05	0.57
2:D:225:MSE:HE2	2:D:297:LEU:HD12	1.86	0.57
1:B:26:THR:HB	2:D:199:ARG:NH2	2.19	0.57
1:B:302[A]:ASN:O	1:B:305:ALA:HB3	2.03	0.57
1:B:330:HIS:CD2	1:B:373:TYR:OH	2.57	0.57
3:E:65:HIS:ND1	3:E:66:PRO:HD2	2.20	0.57
1:A:39:PHE:CD2	3:F:6:LEU:HD13	2.40	0.57
1:A:397:GLN:HE22	3:F:103:MSE:HE3	1.70	0.57
1:B:494:HIS:HD2	8:B:585:HOH:O	1.87	0.57
2:D:171:ALA:HB3	2:D:182:LEU:HD13	1.85	0.57
1:A:241:LEU:HD13	1:A:245:LYS:HE3	1.86	0.57
1:B:376:ARG:HG2	3:E:119:TYR:CE1	2.39	0.57
3:F:2:SER:HB3	8:F:130:HOH:O	2.04	0.57
1:B:232:ASP:O	1:B:235:ARG:N	2.38	0.57
2:C:126:LEU:C	2:C:128:HIS:N	2.63	0.57
1:B:99:LEU:CD2	1:B:210:PHE:HZ	2.18	0.56
1:B:40:GLU:OE2	1:B:188:PHE:HD1	1.89	0.56
2:C:188:TYR:O	2:C:189:TRP:C	2.48	0.56
2:C:329:ARG:HD3	2:C:329:ARG:C	2.29	0.56
1:B:206:LEU:CD1	1:B:207:PHE:HD2	2.18	0.56
1:B:228:SER:H	4:L:10:GLN:HE22	1.54	0.56
2:D:123:LEU:O	2:D:124:VAL:C	2.49	0.56
1:B:122:PHE:CE1	1:B:187:PRO:HB2	2.41	0.56
1:B:206:LEU:C	1:B:206:LEU:CD2	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HB2	1:B:273:LEU:HD21	1.87	0.56
2:C:309:GLY:O	2:C:310:LEU:C	2.48	0.56
3:E:28:VAL:HA	3:E:104:LEU:O	2.05	0.56
2:D:120:LEU:HD21	2:D:181:ALA:HB1	1.88	0.55
1:B:234:ALA:O	1:B:238:THR:HG23	2.07	0.55
2:D:220:ILE:CD1	2:D:264:THR:HB	2.36	0.55
2:D:226:MSE:O	2:D:230:VAL:HG23	2.07	0.55
2:D:91:MSE:HE2	2:D:252:PHE:CE1	2.42	0.55
2:C:157:GLY:C	2:C:158:MSE:HE2	2.31	0.55
1:A:259:GLN:NE2	1:A:316:ARG:CG	2.70	0.55
3:F:76:ALA:HB1	3:F:107:THR:O	2.06	0.55
2:C:212:PHE:CZ	2:C:271:VAL:HG21	2.40	0.55
1:B:497:SER:O	1:B:498:ILE:HG12	2.07	0.55
2:C:38:ASP:OD1	2:C:42:LYS:NZ	2.39	0.55
1:A:259:GLN:NE2	1:A:316:ARG:H	2.05	0.55
1:A:278:MSE:HG2	1:A:283:MSE:HE3	1.87	0.55
1:B:230:GLN:C	1:B:232:ASP:H	2.13	0.55
1:B:251:HIS:ND1	1:B:253:ASP:HB2	2.21	0.55
1:B:210:PHE:HA	1:B:279:MSE:CE	2.37	0.55
1:B:388:ARG:HB3	8:B:547:HOH:O	2.06	0.55
1:B:206:LEU:HD13	1:B:207:PHE:HD2	1.70	0.55
2:D:220:ILE:HD11	2:D:264:THR:HB	1.89	0.55
1:A:167:ASP:OD1	1:A:176:LYS:HE3	2.07	0.54
1:B:219:ASP:OD2	1:B:222:THR:HB	2.07	0.54
2:C:87:ASN:C	2:C:87:ASN:ND2	2.64	0.54
2:C:75:ASP:HB2	2:C:152:MSE:SE	2.57	0.54
2:C:121:ARG:CZ	2:C:194:MSE:CE	2.85	0.54
2:C:185:SER:HA	2:C:188:TYR:HD1	1.70	0.54
2:D:198:MSE:O	2:D:202:VAL:HG23	2.07	0.54
2:D:75:ASP:CG	2:D:77:ARG:HE	2.16	0.54
1:A:16:TYR:CD2	2:C:182:LEU:HD23	2.43	0.54
1:A:471:VAL:O	1:A:475:TYR:HB2	2.07	0.54
1:B:26:THR:CB	2:D:199:ARG:HH22	2.21	0.54
1:B:95:ASN:CB	1:B:283:MSE:HE2	2.38	0.54
2:C:289:TRP:O	2:C:290:GLU:C	2.51	0.54
1:A:101:ILE:HG12	1:A:101:ILE:O	2.08	0.54
1:B:225[A]:PHE:HD1	1:B:226:GLY:N	1.93	0.54
1:B:95:ASN:HB2	1:B:283:MSE:HE2	1.89	0.53
1:B:99:LEU:CD2	1:B:99:LEU:CD1	2.76	0.53
1:B:225[B]:PHE:CE1	1:B:229:ALA:CB	2.89	0.53
2:C:126:LEU:C	2:C:128:HIS:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:ALA:HA	2:D:218:GLN:OE1	2.07	0.53
1:A:259:GLN:HE22	1:A:316:ARG:HG3	1.72	0.53
1:B:227:PHE:CB	4:L:10:GLN:HE22	2.01	0.53
1:B:489:SER:O	1:B:493:LYS:HD2	2.09	0.53
2:D:218:GLN:HA	2:D:222:ILE:HD12	1.91	0.53
1:A:410:GLU:CG	1:A:416:MSE:HE2	2.25	0.53
1:B:95:ASN:HB3	1:B:283:MSE:CE	2.38	0.53
1:B:248:LEU:HD22	1:B:315:ILE:CD1	2.39	0.53
2:C:320:ARG:HD3	8:C:352:HOH:O	2.09	0.53
3:E:3:VAL:HG11	3:E:9:TYR:CD2	2.42	0.53
3:F:47:GLY:O	3:F:48:MSE:O	2.27	0.53
1:A:122:PHE:O	1:A:128:ARG:NH2	2.35	0.53
1:B:40:GLU:OE2	1:B:187:PRO:HD2	2.09	0.53
1:A:288:VAL:HG12	1:A:289:MSE:HG2	1.90	0.53
1:A:358:MSE:HG2	1:A:361:MSE:CE	2.39	0.53
1:A:397:GLN:NE2	3:F:103:MSE:HE1	2.23	0.53
2:D:147:THR:O	2:D:148:THR:C	2.50	0.53
1:B:65:GLN:HE22	1:B:68:LYS:HZ1	1.56	0.52
1:B:115:TYR:CD2	1:B:134:GLN:HG2	2.43	0.52
1:B:305:ALA:O	1:B:308:LYS:CB	2.57	0.52
1:B:419:HIS:O	1:B:420:ARG:HD3	2.08	0.52
2:C:199:ARG:O	2:C:203:GLU:HG3	2.09	0.52
2:D:227:TYR:CD2	2:D:231:TYR:CD1	2.97	0.52
1:B:136:ILE:HD12	2:D:158:MSE:HG3	1.90	0.52
2:C:156:THR:O	2:C:160:ARG:HG2	2.10	0.52
2:C:225:MSE:HE2	2:C:297:LEU:HD12	1.91	0.52
3:F:78:TRP:O	3:F:79:LEU:HD12	2.10	0.52
1:A:87:ASN:HB3	1:B:87:ASN:ND2	2.24	0.52
1:A:278:MSE:HG2	1:A:283:MSE:CE	2.39	0.52
1:A:358:MSE:HE1	1:A:377:TYR:HB2	1.91	0.52
3:E:106:VAL:O	3:E:106:VAL:HG13	2.09	0.52
1:A:259:GLN:HE22	1:A:316:ARG:H	1.55	0.52
1:B:290:SER:O	1:B:291:TRP:C	2.53	0.52
1:B:294:ALA:O	1:B:298:TYR:HB2	2.09	0.52
2:C:329:ARG:C	2:C:329:ARG:CD	2.83	0.52
1:A:27:TYR:CD2	2:C:200:LYS:HB2	2.45	0.52
1:A:312:ARG:HG3	1:A:312:ARG:NH1	2.03	0.52
1:A:349:HIS:CE1	8:A:535:HOH:O	2.63	0.52
2:C:171:ALA:HB3	2:C:182:LEU:HD13	1.91	0.52
1:B:248:LEU:HD21	1:B:315:ILE:HD13	1.90	0.52
2:C:130:GLU:OE2	2:C:160:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:OE1	1:A:199:GLU:OE1	2.26	0.52
1:A:167:ASP:OD1	1:A:176:LYS:CE	2.58	0.52
1:B:225[B]:PHE:CE2	1:B:229:ALA:HB2	2.45	0.52
3:F:3:VAL:HG13	3:F:4:ASN:N	2.25	0.52
1:B:342:TYR:HA	1:B:344:GLN:NE2	2.25	0.51
2:C:56:THR:CG2	2:C:59:ASP:HB2	2.40	0.51
1:A:374:ARG:H	1:A:375:PRO:HD2	1.75	0.51
1:B:458:TYR:C	1:B:460:GLY:N	2.67	0.51
2:D:121:ARG:CZ	2:D:194:MSE:HE3	2.37	0.51
3:F:59:LYS:HB3	3:F:60:PRO:HD3	1.92	0.51
1:A:241:LEU:HD11	1:A:245:LYS:NZ	2.25	0.51
2:D:249:LEU:HD23	2:D:249:LEU:N	2.24	0.51
2:C:322:LYS:HA	2:C:326:LEU:O	2.10	0.51
2:D:29:ALA:HB1	2:D:33:GLN:OE1	2.10	0.51
2:D:118:GLN:HE22	2:D:241:GLN:CG	2.23	0.51
2:C:184:GLU:O	2:C:187:ALA:HB3	2.10	0.51
3:F:24:GLN:HG3	3:F:100:HIS:HA	1.93	0.51
1:A:43:LYS:NZ	1:A:253:ASP:OD1	2.38	0.51
2:C:12:PRO:CD	8:C:379:HOH:O	2.59	0.51
2:C:92:GLN:OE1	2:C:92:GLN:C	2.54	0.51
1:A:330:HIS:O	1:A:331:LEU:C	2.53	0.51
1:A:446:LYS:O	1:A:449:GLN:HB2	2.11	0.51
1:B:277:SER:HB2	1:B:291:TRP:CD2	2.45	0.51
1:B:104:ILE:O	1:B:105:SER:C	2.48	0.51
2:C:294:TYR:CD1	2:C:314:ARG:HD2	2.46	0.51
2:C:316:GLU:O	2:C:319:ALA:HB3	2.11	0.51
1:B:164:HIS:CE1	1:B:474:TYR:O	2.64	0.51
1:B:342:TYR:HA	1:B:344:GLN:HE22	1.76	0.51
1:A:143:GLN:HE22	2:C:151:GLN:NE2	2.09	0.50
1:B:362:SER:OG	1:B:370:ASP:OD1	2.26	0.50
2:C:229:LEU:HD22	2:C:310:LEU:HD13	1.91	0.50
1:A:68:LYS:NZ	8:A:516:HOH:O	2.43	0.50
1:A:210:PHE:HB3	1:A:211:MSE:CE	2.40	0.50
2:C:201:LEU:HD22	2:C:293:ALA:HA	1.92	0.50
1:A:379:TYR:CD1	3:F:114:MSE:HE1	2.46	0.50
1:A:411:LYS:NZ	1:A:412:ASP:OD2	2.44	0.50
1:A:419:HIS:CE1	1:A:421:GLN:HB2	2.46	0.50
1:A:443:GLU:HB3	3:F:3:VAL:HG23	1.93	0.50
2:C:57:LEU:O	2:C:58:ASN:C	2.54	0.50
2:C:198:MSE:CA	2:C:296:ALA:HB1	2.40	0.50
1:A:244:ILE:HD12	1:A:245:LYS:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:HIS:O	1:B:495:TRP:C	2.55	0.50
2:C:53:SER:HB3	3:F:7:TYR:CE2	2.45	0.50
2:C:69:ASP:O	2:C:70:TRP:C	2.52	0.50
2:C:121:ARG:NH2	2:C:194:MSE:HE3	2.26	0.50
2:C:126:LEU:O	2:C:128:HIS:N	2.44	0.50
1:A:145:GLN:O	1:A:149:MSE:HG2	2.11	0.50
1:B:348:PHE:CD1	1:B:348:PHE:C	2.89	0.50
1:A:27:TYR:OH	2:C:196:GLN:CG	2.49	0.50
1:B:225[A]:PHE:CD1	1:B:226:GLY:CA	2.95	0.50
2:C:215:THR:OG1	2:C:267:MSE:HE1	2.11	0.50
3:F:34:LEU:O	3:F:35:LEU:C	2.55	0.50
1:B:354:GLU:HB3	1:B:356:GLU:OE1	2.12	0.50
2:C:233:LYS:HE3	2:C:312:GLU:HB2	1.94	0.50
2:D:246:VAL:O	2:D:247:SER:C	2.55	0.50
1:A:195:SER:HB3	1:A:240:GLY:HA2	1.94	0.49
1:B:200:TYR:CE1	1:B:306:LEU:HD13	2.47	0.49
1:B:308:LYS:C	1:B:310:LEU:N	2.70	0.49
1:B:26:THR:CB	2:D:199:ARG:NH2	2.76	0.49
1:B:244:ILE:HD12	1:B:244:ILE:C	2.37	0.49
2:C:121:ARG:CZ	2:C:194:MSE:HE3	2.42	0.49
1:A:172:LEU:C	1:A:175:PRO:HD2	2.37	0.49
1:B:462:CYS:O	1:B:470:VAL:HG22	2.12	0.49
2:C:115:THR:O	2:C:116:GLN:C	2.54	0.49
2:C:283:GLN:NE2	2:C:283:GLN:CA	2.75	0.49
2:C:102:CYS:HB3	2:C:173:MSE:SE	2.63	0.49
1:B:115:TYR:CE2	1:B:134:GLN:HG2	2.47	0.49
2:C:112:SER:O	2:C:116:GLN:HG3	2.11	0.49
1:B:134:GLN:NE2	1:B:236:HIS:ND1	2.61	0.49
1:B:209:PRO:HB3	1:B:280:MSE:SE	2.63	0.49
1:B:382:LYS:O	1:B:383:GLU:C	2.55	0.49
2:C:287:ASP:O	2:C:291:PRO:HG2	2.13	0.49
1:A:244:ILE:O	1:A:248:LEU:HD12	2.13	0.49
1:B:303:GLY:O	1:B:305:ALA:N	2.45	0.49
2:C:311:ASN:C	2:C:313:ALA:N	2.70	0.49
2:C:311:ASN:C	2:C:313:ALA:H	2.21	0.49
2:D:217:VAL:HA	2:D:221:LEU:HD12	1.93	0.49
2:D:301:ALA:O	2:D:302:GLU:C	2.54	0.49
3:F:47:GLY:O	3:F:48:MSE:C	2.54	0.49
3:F:117:ALA:O	3:F:118:GLY:C	2.55	0.49
1:B:129:VAL:HG23	1:B:130:ALA:N	2.27	0.49
7:B:515:MOO:O2	7:B:515:MOO:O4	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:246:VAL:O	2:C:247:SER:C	2.53	0.49
2:D:171:ALA:CB	2:D:182:LEU:HD13	2.43	0.49
1:B:230:GLN:CD	1:B:233:GLU:HG3	2.37	0.49
2:C:171:ALA:HB3	2:C:182:LEU:CD1	2.41	0.49
1:A:276:VAL:O	1:A:277:SER:C	2.54	0.49
1:A:134:GLN:O	1:A:135:ALA:C	2.56	0.48
1:A:279:MSE:O	1:A:283:MSE:HB2	2.13	0.48
1:A:342:TYR:HA	1:A:344:GLN:HE22	1.78	0.48
7:B:515:MOO:O3	7:B:515:MOO:O1	2.31	0.48
3:F:57:ILE:HG22	3:F:58:LEU:N	2.28	0.48
3:F:77:GLU:OE2	3:F:109:PRO:HG3	2.13	0.48
1:A:374:ARG:N	1:A:375:PRO:CD	2.76	0.48
2:C:286:ILE:HD11	2:C:326:LEU:HD13	1.94	0.48
2:D:225:MSE:HE3	2:D:310:LEU:HD11	1.95	0.48
1:A:130:ALA:HB1	1:A:239:LEU:HD13	1.95	0.48
1:A:287:LYS:HD3	1:A:287:LYS:N	2.27	0.48
2:C:243:ALA:O	2:C:244:GLU:C	2.56	0.48
2:D:102:CYS:SG	2:D:249:LEU:HD21	2.53	0.48
1:A:389:ARG:HG3	1:A:391:TYR:CE1	2.48	0.48
2:C:226:MSE:HE3	2:C:227:TYR:CE1	2.49	0.48
1:A:233:GLU:O	1:A:234:ALA:C	2.56	0.48
1:B:388:ARG:O	1:B:389:ARG:C	2.53	0.48
1:A:253:ASP:O	1:A:256:PRO:HD2	2.13	0.48
1:B:99:LEU:HD23	1:B:210:PHE:CE1	2.49	0.48
1:B:495:TRP:O	1:B:498:ILE:HG13	2.14	0.48
2:C:146:ALA:HB3	2:C:149:VAL:HG23	1.96	0.48
2:D:133:ALA:CB	2:D:160:ARG:HG3	2.44	0.48
2:D:221:LEU:HD22	2:D:290:GLU:HB3	1.96	0.48
2:D:295:GLU:CD	2:D:298:LYS:HZ3	2.21	0.48
7:B:515:MOO:O3	7:B:515:MOO:O2	2.32	0.48
2:D:286:ILE:HD13	2:D:321:LEU:HD13	1.95	0.48
1:A:224:THR:O	1:A:225:PHE:C	2.53	0.48
1:A:446:LYS:NZ	2:C:50:GLN:HE22	2.12	0.48
1:B:26:THR:HB	2:D:199:ARG:HH22	1.78	0.48
1:B:122:PHE:CZ	1:B:191:LEU:HD22	2.49	0.48
1:B:277:SER:HB2	1:B:291:TRP:CG	2.49	0.48
1:B:303:GLY:C	1:B:305:ALA:N	2.69	0.48
1:A:220:MSE:HG3	1:B:82:ASN:ND2	2.29	0.48
2:C:91:MSE:HE2	2:C:252:PHE:CE1	2.49	0.48
3:F:35:LEU:HA	3:F:119:TYR:CZ	2.48	0.48
1:A:220:MSE:HE1	1:B:79:PHE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ARG:HG2	1:B:486:TYR:CD2	2.49	0.48
1:B:225[A]:PHE:O	1:B:227:PHE:N	2.47	0.48
2:C:63:THR:O	2:C:66:ARG:NH2	2.46	0.48
1:A:483:ASN:HD22	1:A:483:ASN:HA	1.18	0.47
1:B:59:ASP:OD1	1:B:59:ASP:N	2.47	0.47
1:B:122:PHE:CZ	1:B:187:PRO:HB2	2.48	0.47
1:A:342:TYR:HA	1:A:344:GLN:NE2	2.28	0.47
1:B:68:LYS:CG	4:L:68:ILE:HD12	2.44	0.47
1:B:204:ASN:N	1:B:204:ASN:HD22	2.13	0.47
2:C:310:LEU:HD12	2:C:310:LEU:HA	1.49	0.47
2:C:81:TYR:CD2	2:C:81:TYR:C	2.92	0.47
3:E:100:HIS:O	3:E:101:LYS:HB2	2.14	0.47
1:B:99:LEU:CD2	1:B:210:PHE:CZ	2.96	0.47
1:B:225[B]:PHE:C	1:B:227:PHE:N	2.71	0.47
1:B:471:VAL:HG13	1:B:477:ILE:HB	1.96	0.47
2:C:308:ASP:O	2:C:312:GLU:CG	2.53	0.47
2:D:71:CYS:C	2:D:73:VAL:N	2.70	0.47
1:A:356:GLU:OE2	1:A:356:GLU:N	2.38	0.47
1:B:329:HIS:CB	1:B:368:THR:HG21	2.44	0.47
1:B:219:ASP:OD2	1:B:222:THR:CB	2.62	0.47
1:B:231:SER:HB2	4:L:70:VAL:O	2.15	0.47
2:C:56:THR:HG22	2:C:59:ASP:CB	2.43	0.47
1:B:72:LEU:HD12	1:B:224:THR:CG2	2.42	0.47
1:B:188:PHE:O	1:B:189:GLU:C	2.56	0.47
1:B:225[B]:PHE:CD1	1:B:225[B]:PHE:C	2.92	0.47
2:C:310:LEU:O	2:C:313:ALA:HB3	2.14	0.47
1:B:57:THR:O	1:B:58:MSE:C	2.56	0.47
2:C:170:ILE:HG12	2:C:249:LEU:HD12	1.96	0.47
2:C:179:GLY:O	2:C:182:LEU:N	2.47	0.47
1:B:71:LYS:O	1:B:75:ILE:HG13	2.15	0.47
1:B:89:SER:N	1:B:217:ASN:O	2.44	0.47
1:B:92:ARG:CG	1:B:486:TYR:CD2	2.97	0.47
2:C:219:ASN:ND2	8:C:343:HOH:O	2.48	0.47
3:E:91:ALA:HB3	3:E:96:GLN:NE2	2.29	0.47
1:A:160:HIS:HE1	1:A:482:ASP:OD1	1.98	0.47
1:A:497:SER:O	1:A:498:ILE:C	2.58	0.47
1:B:212:SER:HA	4:L:35:PRO:CB	2.38	0.47
1:B:95:ASN:HB2	1:B:283:MSE:CE	2.45	0.46
1:B:192:THR:HG22	1:B:192:THR:O	2.15	0.46
1:B:203:THR:O	1:B:204:ASN:C	2.57	0.46
1:B:283:MSE:O	1:B:285:PRO:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:ALA:O	2:D:316:GLU:C	2.56	0.46
1:B:268:ARG:O	1:B:269:GLY:C	2.58	0.46
2:C:328:SER:O	2:C:329:ARG:HB3	2.15	0.46
3:F:47:GLY:O	3:F:92:SER:HB2	2.15	0.46
1:A:358:MSE:HE3	1:A:377:TYR:HD2	1.79	0.46
2:C:233:LYS:O	2:C:234:MSE:C	2.56	0.46
2:C:328:SER:O	2:C:329:ARG:HB2	2.14	0.46
1:B:212:SER:CB	4:L:35:PRO:HB3	2.45	0.46
1:A:117:LYS:HE2	2:C:51:TRP:CZ3	2.50	0.46
1:B:13:LYS:O	1:B:13:LYS:HG2	2.16	0.46
1:B:40:GLU:OE2	1:B:188:PHE:CD1	2.69	0.46
2:C:196:GLN:OE1	2:C:199:ARG:NH1	2.48	0.46
2:C:298:LYS:HD3	2:C:307:ILE:HD11	1.97	0.46
2:D:115:THR:O	2:D:118:GLN:HB2	2.15	0.46
2:D:166:TYR:O	2:D:167:LEU:C	2.56	0.46
2:D:189:TRP:CZ2	2:D:199:ARG:HG3	2.50	0.46
2:D:233:LYS:HB3	2:D:305:VAL:HG11	1.98	0.46
1:B:65:GLN:HE22	1:B:68:LYS:CE	2.28	0.46
1:B:143:GLN:NE2	2:D:35:ALA:O	2.44	0.46
1:B:203:THR:CG2	1:B:204:ASN:N	2.68	0.46
2:D:171:ALA:O	2:D:172:LEU:C	2.54	0.46
1:A:33:ILE:HG22	1:A:34:PHE:CG	2.51	0.46
1:B:78:ALA:O	1:B:79:PHE:C	2.59	0.46
1:B:168:ARG:HB3	1:B:474:TYR:CE1	2.51	0.46
1:B:311:GLU:O	1:B:312:ARG:C	2.56	0.46
1:B:341:GLN:NE2	1:B:392:ASN:HD22	2.11	0.46
1:A:97:LEU:CB	1:A:149:MSE:HE1	2.33	0.46
1:A:388:ARG:HH21	1:A:388:ARG:HG3	1.82	0.46
1:B:301:GLN:O	1:B:302[A]:ASN:C	2.59	0.46
1:A:241:LEU:HD13	1:A:241:LEU:O	2.16	0.45
1:A:475:TYR:N	1:A:475:TYR:CD1	2.83	0.45
1:B:200:TYR:O	1:B:203:THR:HG22	2.16	0.45
1:B:339:PHE:O	1:B:340:TYR:C	2.59	0.45
1:B:341:GLN:HE22	3:E:37:CYS:N	2.01	0.45
1:B:355:LYS:H	1:B:355:LYS:HG3	1.57	0.45
1:A:210:PHE:CB	1:A:211:MSE:CE	2.94	0.45
1:A:300:GLU:OE1	1:A:328:LYS:HE3	2.17	0.45
1:B:99:LEU:HD21	1:B:210:PHE:HZ	1.81	0.45
1:B:206:LEU:HD13	1:B:207:PHE:CD2	2.48	0.45
1:B:223:VAL:HG13	1:B:224:THR:N	2.31	0.45
1:B:271:ARG:HH21	1:B:433:SER:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:ALA:O	2:C:147:THR:C	2.57	0.45
2:D:299:PRO:HA	2:D:302:GLU:CG	2.44	0.45
1:A:160:HIS:CD2	8:A:520:HOH:O	2.68	0.45
1:B:241:LEU:CD1	1:B:245:LYS:HD2	2.46	0.45
1:A:478:ASN:O	1:A:479:ILE:C	2.57	0.45
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.67	0.45
1:B:358:MSE:O	1:B:362:SER:N	2.48	0.45
1:A:107:LEU:O	1:A:108:GLU:C	2.59	0.45
1:B:225[B]:PHE:CD2	1:B:229:ALA:HB2	2.52	0.45
1:B:428:ARG:N	8:B:543:HOH:O	2.35	0.45
2:C:294:TYR:CD1	2:C:314:ARG:NH1	2.85	0.45
2:D:167:LEU:HA	2:D:170:ILE:HD12	1.99	0.45
3:E:12:GLU:OE2	3:E:16:LYS:NZ	2.47	0.45
1:B:244:ILE:O	1:B:245:LYS:C	2.59	0.45
3:E:15:ASP:O	3:E:16:LYS:C	2.60	0.45
1:A:169:VAL:O	1:A:170:TRP:C	2.58	0.45
1:A:443:GLU:HG3	8:A:561:HOH:O	2.17	0.45
1:A:451:TRP:CE2	1:A:456:GLN:HG3	2.52	0.45
1:B:455:HIS:CD2	3:E:15:ASP:OD2	2.61	0.45
2:C:17:TYR:O	2:C:18:GLY:C	2.59	0.45
2:C:36:SER:O	2:C:147:THR:HB	2.15	0.45
2:D:187:ALA:HB1	8:D:391:HOH:O	2.16	0.45
1:A:50:TRP:HZ3	1:A:243:VAL:HG23	1.81	0.45
1:A:160:HIS:CE1	1:A:482:ASP:OD1	2.70	0.45
1:B:169:VAL:HG22	1:B:475:TYR:CG	2.52	0.45
1:B:312:ARG:NE	4:L:89:ASN:HD22	2.15	0.45
2:C:194:MSE:CG	2:C:299:PRO:HB2	2.47	0.45
2:C:234:MSE:HB2	2:C:234:MSE:HE3	1.96	0.45
1:A:85:HIS:O	1:A:88:ILE:HG12	2.16	0.45
1:A:111:ALA:O	1:A:112:PHE:C	2.60	0.45
1:B:101:ILE:HA	1:B:105:SER:OG	2.16	0.45
1:B:277:SER:O	1:B:278:MSE:C	2.58	0.45
2:C:59:ASP:HA	2:C:60:PRO:HD3	1.79	0.45
2:C:108:LEU:HD21	2:C:246:VAL:HG13	1.99	0.45
2:C:190:MSE:CE	2:C:190:MSE:CA	2.89	0.45
1:A:277:SER:OG	1:A:278:MSE:N	2.48	0.45
1:A:277:SER:HB2	1:A:291:TRP:CD2	2.52	0.45
1:A:160:HIS:HD2	8:A:520:HOH:O	2.00	0.44
1:B:409:THR:HG21	1:B:414:PRO:O	2.17	0.44
2:C:48:ARG:HH21	3:F:11:PHE:HE1	1.64	0.44
2:C:151:GLN:HG3	2:C:155:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:322:LYS:O	2:C:325:GLU:N	2.50	0.44
1:B:252:GLU:CB	8:B:584:HOH:O	2.65	0.44
2:D:227:TYR:CD2	2:D:231:TYR:HD1	2.34	0.44
1:B:497:SER:C	1:B:498:ILE:CG1	2.90	0.44
2:D:234:MSE:CE	2:D:234:MSE:CB	2.95	0.44
3:E:33:HIS:HD2	3:E:65:HIS:CD2	2.35	0.44
1:A:455:HIS:HE1	3:F:27:TYR:OH	1.96	0.44
1:B:65:GLN:NE2	1:B:68:LYS:HE2	2.31	0.44
2:C:53:SER:HA	3:F:7:TYR:CE2	2.53	0.44
2:C:73:VAL:CG1	2:C:267:MSE:HB2	2.48	0.44
2:C:114:GLU:O	2:C:118:GLN:HG3	2.18	0.44
1:A:407:ILE:HG21	1:A:407:ILE:HD13	1.72	0.44
2:C:126:LEU:O	2:C:127:ARG:C	2.60	0.44
2:D:75:ASP:CB	2:D:152:MSE:CE	2.83	0.44
1:B:129:VAL:CG2	1:B:130:ALA:N	2.81	0.44
1:B:230:GLN:CD	1:B:233:GLU:CG	2.91	0.44
1:B:273:LEU:HD21	1:B:276:VAL:HG21	1.97	0.44
2:C:121:ARG:NH1	2:C:194:MSE:CE	2.81	0.44
2:D:131:LEU:O	2:D:131:LEU:HG	2.13	0.44
2:D:175:ASP:OD1	2:D:175:ASP:C	2.61	0.44
1:A:289:MSE:HE2	2:D:6:LYS:HD3	1.99	0.44
2:C:225:MSE:HB3	2:C:297:LEU:CD1	2.47	0.44
2:D:45:PHE:CZ	2:D:58:ASN:HB2	2.52	0.44
2:D:267:MSE:O	2:D:268:MSE:C	2.60	0.44
1:A:374:ARG:HB3	1:A:375:PRO:HD3	1.99	0.43
1:B:356:GLU:CD	1:B:356:GLU:N	2.73	0.43
2:C:131:LEU:O	2:C:131:LEU:HG	2.17	0.43
3:F:81:ASN:HD21	3:F:102:SER:HB3	1.82	0.43
1:A:36:GLU:HB2	8:A:544:HOH:O	2.18	0.43
1:A:144:THR:CG2	1:A:225:PHE:CE1	3.02	0.43
1:B:169:VAL:O	1:B:170:TRP:C	2.59	0.43
2:C:40:GLU:H	2:C:40:GLU:HG3	1.45	0.43
3:E:74:LEU:O	3:E:74:LEU:HD22	2.18	0.43
1:A:27:TYR:CD1	1:A:27:TYR:N	2.86	0.43
1:A:319:LYS:O	1:A:320:TYR:CB	2.62	0.43
1:B:204:ASN:H	1:B:204:ASN:HD22	1.65	0.43
1:B:402:CYS:O	1:B:403:GLN:HB2	2.18	0.43
2:D:52:ASP:OD2	2:D:55:HIS:HD2	2.01	0.43
1:B:194:ILE:O	1:B:199:GLU:N	2.43	0.43
2:C:308:ASP:OD2	2:C:308:ASP:N	2.38	0.43
1:A:40:GLU:HB2	8:A:547:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ALA:CB	2:C:89:ALA:HB2	2.48	0.43
1:A:82:ASN:O	1:A:83:ASN:C	2.59	0.43
1:A:104:ILE:O	1:A:107:LEU:HB2	2.18	0.43
1:A:358:MSE:CE	1:A:377:TYR:HB2	2.48	0.43
1:B:224:THR:O	1:B:225[B]:PHE:O	2.36	0.43
7:B:515:MOO:O3	7:B:515:MOO:O4	2.37	0.43
2:C:136:ASN:CG	2:C:214:LEU:HD11	2.43	0.43
2:C:309:GLY:O	2:C:312:GLU:N	2.51	0.43
1:B:210:PHE:CZ	1:B:279:MSE:HG2	2.53	0.43
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.50	0.43
1:A:122:PHE:CE2	1:A:191:LEU:CD2	3.00	0.43
1:B:141:HIS:O	1:B:145:GLN:HG3	2.18	0.43
1:B:203:THR:HG23	1:B:204:ASN:ND2	2.31	0.43
1:B:308:LYS:O	1:B:310:LEU:N	2.52	0.43
2:C:46:HIS:C	2:C:47:TYR:CG	2.96	0.43
2:D:182:LEU:HD12	2:D:182:LEU:HA	1.80	0.43
1:A:25:PRO:HA	2:C:203:GLU:OE1	2.19	0.43
1:A:214:ALA:CB	1:A:219:ASP:HB3	2.47	0.43
1:B:225[A]:PHE:C	1:B:225[A]:PHE:HD1	2.24	0.43
2:C:238:PHE:O	2:C:239:GLU:C	2.61	0.43
1:A:44:ILE:HD12	1:A:44:ILE:HG23	1.73	0.43
1:A:47:TRP:CE3	1:A:124:GLY:HA3	2.54	0.43
1:A:144:THR:HG22	1:A:225:PHE:CE1	2.54	0.43
1:B:161:ASP:CG	2:D:22:ARG:NH2	2.75	0.43
2:D:298:LYS:HA	2:D:310:LEU:CD2	2.49	0.43
3:E:25:LEU:H	3:E:100:HIS:CE1	2.35	0.43
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.44	0.43
1:B:342:TYR:CA	1:B:344:GLN:NE2	2.82	0.43
2:D:120:LEU:O	2:D:125:PRO:HD3	2.18	0.43
2:D:261:LEU:HD12	2:D:261:LEU:HA	1.91	0.43
3:E:65:HIS:ND1	3:E:66:PRO:CD	2.82	0.43
3:F:88:LYS:H	3:F:96:GLN:NE2	2.14	0.43
1:A:405:PRO:HB2	1:A:407:ILE:HG23	2.01	0.42
1:B:11:LYS:O	1:B:15:GLN:CG	2.66	0.42
7:B:515:MOO:O2	7:B:515:MOO:O1	2.37	0.42
2:C:329:ARG:HD3	2:C:330:GLY:H	1.76	0.42
1:B:11:LYS:HE3	1:B:51:GLU:OE2	2.20	0.42
1:B:271:ARG:NH1	1:B:408:PHE:CD1	2.87	0.42
2:C:225:MSE:HE1	2:C:294:TYR:CB	2.46	0.42
1:A:165:MSE:HB3	1:A:169:VAL:HG23	2.00	0.42
1:A:325:ASN:O	1:A:328:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ILE:HG23	1:A:482:ASP:HB2	2.02	0.42
1:B:70:LYS:HB2	1:B:70:LYS:HE2	1.55	0.42
1:B:88:ILE:O	1:B:89:SER:C	2.58	0.42
1:B:280:MSE:HE3	1:B:280:MSE:HB2	1.95	0.42
3:E:34:LEU:O	3:E:35:LEU:C	2.63	0.42
1:B:231:SER:CB	4:L:70:VAL:O	2.68	0.42
2:C:53:SER:CA	3:F:7:TYR:CE2	3.02	0.42
2:C:61:THR:HA	2:C:66:ARG:NH2	2.35	0.42
2:C:91:MSE:HE2	2:C:252:PHE:CD1	2.54	0.42
2:C:190:MSE:CE	2:C:199:ARG:CZ	2.98	0.42
1:B:49:GLN:NE2	1:B:49:GLN:CA	2.80	0.42
1:B:274:SER:HB2	1:B:335:LEU:CD1	2.30	0.42
1:B:303:GLY:C	1:B:305:ALA:H	2.27	0.42
2:C:288:HIS:CD2	2:C:292:GLN:HE22	2.38	0.42
2:D:166:TYR:O	2:D:169:ARG:N	2.52	0.42
1:B:145:GLN:O	1:B:146:GLN:C	2.62	0.42
1:B:289:MSE:CE	4:L:34:GLN:HE22	2.32	0.42
1:B:398:LEU:HD11	1:B:454:VAL:HG23	2.02	0.42
2:C:65:ILE:HG22	2:C:66:ARG:N	2.35	0.42
1:A:144:THR:CG2	1:A:225:PHE:HD1	2.29	0.42
1:B:288:VAL:HG12	1:B:289:MSE:HB3	2.00	0.42
2:C:137:ASN:HD22	2:C:153:HIS:HD2	1.68	0.42
3:E:58:LEU:O	3:E:59:LYS:C	2.60	0.42
3:E:92:SER:O	3:E:93:LEU:C	2.62	0.42
1:A:44:ILE:HG21	1:A:47:TRP:NE1	2.35	0.42
8:A:533:HOH:O	2:C:41:ALA:HA	2.20	0.42
1:B:227:PHE:C	1:B:229:ALA:N	2.77	0.42
1:B:444:PRO:O	1:B:448:ILE:HG23	2.20	0.42
2:C:276:GLU:HB2	2:C:279:ARG:HH11	1.81	0.42
2:D:39:ILE:HD13	2:D:39:ILE:HA	1.80	0.42
3:F:22:GLY:N	8:F:120:HOH:O	2.52	0.42
1:A:181:ASP:OD1	1:A:264:LYS:NZ	2.53	0.42
1:B:143:GLN:O	1:B:146:GLN:HB2	2.20	0.42
1:B:306:LEU:HB2	4:L:88:TRP:CH2	2.55	0.42
2:C:14:ARG:NH1	8:C:357:HOH:O	2.53	0.42
2:D:59:ASP:HA	2:D:60:PRO:HD2	1.88	0.42
2:C:49:PRO:HB3	2:C:51:TRP:CE2	2.55	0.42
2:C:201:LEU:HD12	2:C:201:LEU:O	2.20	0.42
2:D:114:GLU:CD	2:D:114:GLU:N	2.78	0.42
1:A:316:ARG:HB2	1:A:317:PRO:CD	2.50	0.41
1:B:374:ARG:N	1:B:375:PRO:CD	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:114:MSE:C	3:E:115:ALA:O	2.60	0.41
1:A:72:LEU:HD12	1:A:224:THR:HG22	2.01	0.41
1:A:161:ASP:CB	1:A:165:MSE:HE3	2.50	0.41
1:A:264:LYS:HD3	1:A:265:TRP:NE1	2.35	0.41
1:B:413:ALA:H	1:B:414:PRO:HD3	1.77	0.41
2:C:93:GLU:OE1	2:C:93:GLU:CA	2.66	0.41
2:C:124:VAL:N	2:C:125:PRO:CD	2.83	0.41
2:C:217:VAL:O	2:C:222:ILE:HG13	2.20	0.41
2:C:182:LEU:O	2:C:183:ASP:C	2.63	0.41
2:C:318:SER:CB	2:C:328:SER:OG	2.68	0.41
2:D:121:ARG:CZ	2:D:194:MSE:HE1	2.49	0.41
3:F:43:LEU:HA	3:F:43:LEU:HD12	1.76	0.41
1:A:46:ASP:HB3	1:A:49:GLN:NE2	2.36	0.41
1:B:199:GLU:O	1:B:203:THR:CB	2.65	0.41
2:D:71:CYS:C	2:D:73:VAL:H	2.29	0.41
2:D:75:ASP:CG	2:D:152:MSE:CE	2.92	0.41
3:E:48:MSE:O	3:E:93:LEU:HD13	2.20	0.41
3:F:106:VAL:HG13	3:F:106:VAL:O	2.21	0.41
1:A:88:ILE:HG13	1:A:495:TRP:CH2	2.56	0.41
1:A:121:GLN:HB3	8:A:544:HOH:O	2.21	0.41
1:B:80:ALA:O	1:B:81:GLN:C	2.63	0.41
1:B:117:LYS:HE2	2:D:51:TRP:CZ3	2.55	0.41
1:B:199:GLU:HG2	1:B:236:HIS:HB3	2.02	0.41
1:B:289:MSE:O	1:B:290:SER:C	2.64	0.41
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.88	0.41
3:E:53:LEU:O	3:E:54:VAL:C	2.61	0.41
3:F:8:ASP:OD2	3:F:10:LYS:CD	2.68	0.41
1:A:251:HIS:O	1:A:254:ASN:HB2	2.21	0.41
1:A:429:TYR:CZ	1:A:448:ILE:HG22	2.55	0.41
2:D:234:MSE:CE	2:D:234:MSE:HB2	2.51	0.41
3:E:85:PHE:CE2	3:E:87:PRO:HA	2.55	0.41
1:B:472:GLN:HB2	1:B:479:ILE:CD1	2.48	0.41
1:A:66:ALA:HB2	2:C:89:ALA:HB2	2.03	0.41
1:A:226:GLY:O	1:A:227:PHE:C	2.63	0.41
1:A:241:LEU:HD13	1:A:241:LEU:C	2.45	0.41
2:C:298:LYS:O	2:C:301:ALA:HB3	2.20	0.41
3:E:83:GLU:HA	3:E:84:PRO:HD3	1.90	0.41
1:A:379:TYR:HD1	3:F:114:MSE:HE1	1.86	0.41
1:B:204:ASN:C	1:B:206:LEU:N	2.79	0.41
1:B:238:THR:HG21	4:L:77:VAL:HG21	2.02	0.41
2:C:27:LYS:HB2	2:C:28:PRO:CD	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:GLU:CG	2:C:147:THR:OG1	2.69	0.41
2:C:122:LEU:H	2:C:122:LEU:HG	1.69	0.41
2:C:190:MSE:HE2	2:C:199:ARG:CD	2.48	0.41
2:D:52:ASP:OD2	2:D:55:HIS:CD2	2.73	0.41
1:A:210:PHE:C	1:A:211:MSE:HE2	2.45	0.41
1:A:211:MSE:HB3	2:D:5:ILE:HG12	2.02	0.41
1:A:328:LYS:HB3	8:A:567:HOH:O	2.20	0.41
1:A:356:GLU:H	1:A:356:GLU:CD	2.25	0.41
1:A:452:LEU:N	1:A:452:LEU:CD1	2.84	0.41
2:C:158:MSE:HE2	2:C:158:MSE:N	2.35	0.41
2:C:210:ASP:OD1	2:C:210:ASP:C	2.64	0.41
2:D:73:VAL:HG11	2:D:149:VAL:HG22	2.02	0.41
2:D:160:ARG:HA	2:D:160:ARG:HD3	1.64	0.41
2:D:295:GLU:O	2:D:299:PRO:HD3	2.21	0.41
3:F:59:LYS:HB3	3:F:60:PRO:CD	2.51	0.41
1:A:315:ILE:HD13	1:A:315:ILE:HA	1.89	0.40
1:A:317:PRO:HA	1:A:318:PRO:HD3	1.88	0.40
1:A:339:PHE:CD2	1:A:348:PHE:HZ	2.38	0.40
1:A:443:GLU:O	1:A:444:PRO:C	2.63	0.40
1:A:446:LYS:HE3	2:C:50:GLN:NE2	2.36	0.40
2:C:298:LYS:O	2:C:299:PRO:C	2.64	0.40
2:D:281:LEU:HD23	2:D:281:LEU:HA	1.78	0.40
1:A:112:PHE:CD1	1:A:139:LEU:HB2	2.56	0.40
1:B:28:GLN:HA	1:B:28:GLN:NE2	2.36	0.40
2:C:40:GLU:HG2	2:C:147:THR:OG1	2.20	0.40
2:C:304:SER:HB3	2:C:305:VAL:H	1.27	0.40
2:C:307:ILE:C	2:C:309:GLY:N	2.79	0.40
2:D:108:LEU:HD11	2:D:170:ILE:HG23	2.01	0.40
2:D:157:GLY:O	2:D:160:ARG:HB2	2.21	0.40
3:F:56:GLU:O	3:F:57:ILE:HD13	2.22	0.40
1:A:280:MSE:HE2	1:A:289:MSE:O	2.21	0.40
1:B:29:ASP:O	1:B:30:LYS:C	2.64	0.40
1:B:376:ARG:HG2	3:E:119:TYR:CZ	2.56	0.40
1:B:496:LEU:HD23	1:B:496:LEU:HA	1.93	0.40
1:B:497:SER:O	1:B:498:ILE:CG1	2.68	0.40
2:C:118:GLN:O	2:C:122:LEU:HG	2.21	0.40
2:D:53:SER:HB3	3:E:7:TYR:CD2	2.56	0.40
2:D:103:GLU:HG3	2:D:173:MSE:SE	2.72	0.40
2:D:147:THR:O	2:D:151:GLN:HB3	2.20	0.40
2:D:304:SER:HB3	2:D:305:VAL:H	1.44	0.40
3:F:8:ASP:OD2	3:F:10:LYS:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:33:HIS:HD2	3:F:65:HIS:CE1	2.40	0.40
1:A:292:SER:O	1:A:296:GLU:HB2	2.21	0.40
1:A:349:HIS:HB3	1:A:486:TYR:N	2.36	0.40
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.41	0.40
1:B:24:GLU:HA	1:B:25:PRO:HD2	1.85	0.40
1:B:132:GLN:OE1	2:D:158:MSE:CE	2.61	0.40
1:B:169:VAL:HB	1:B:172:LEU:HD12	2.03	0.40
2:C:12:PRO:HD2	8:C:379:HOH:O	2.19	0.40
2:C:80:TYR:O	2:C:81:TYR:C	2.64	0.40
2:D:327:GLN:HE21	2:D:327:GLN:HB2	1.60	0.40
3:E:48:MSE:HG2	3:E:93:LEU:HD22	2.02	0.40
3:E:76:ALA:O	3:E:78:TRP:CD1	2.75	0.40
1:A:16:TYR:HA	1:A:20:ASP:HB2	2.03	0.40
1:A:349:HIS:NE2	8:A:535:HOH:O	2.37	0.40
1:B:44:ILE:HD12	1:B:250:GLN:HG2	2.04	0.40
1:B:199:GLU:C	1:B:203:THR:HB	2.47	0.40
1:B:225[A]:PHE:CD1	1:B:226:GLY:HA2	2.56	0.40
1:B:251:HIS:O	1:B:252:GLU:C	2.64	0.40
1:B:271:ARG:O	1:B:274:SER:OG	2.28	0.40
1:B:408:PHE:HD1	1:B:432:CYS:HB2	1.86	0.40
2:C:92:GLN:C	2:C:92:GLN:CD	2.90	0.40
3:E:111:LEU:HD23	3:E:111:LEU:HA	1.80	0.40
3:F:54:VAL:O	3:F:54:VAL:HG12	2.21	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	494/511 (97%)	444 (90%)	45 (9%)	5 (1%)	12	32
1	B	494/511 (97%)	416 (84%)	60 (12%)	18 (4%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	317/333 (95%)	271 (86%)	38 (12%)	8 (2%)	4	11
2	D	323/333 (97%)	298 (92%)	21 (6%)	4 (1%)	10	27
3	E	116/119 (98%)	107 (92%)	8 (7%)	1 (1%)	14	35
3	F	116/119 (98%)	95 (82%)	18 (16%)	3 (3%)	4	11
4	L	85/89 (96%)	55 (65%)	15 (18%)	15 (18%)	0	0
All	All	1945/2015 (96%)	1686 (87%)	205 (10%)	54 (3%)	4	9

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	A	498	ILE
1	B	7	LYS
1	B	228	SER
2	C	329	ARG
3	F	48	MSE
3	F	63	ALA
4	L	20	GLU
4	L	34	GLN
4	L	52	THR
4	L	63	VAL
1	A	185	ALA
1	A	386	ALA
1	A	497	SER
1	B	81	GLN
1	B	162	GLY
1	B	205	LEU
1	B	226	GLY
1	B	231	SER
1	B	269	GLY
1	B	297	VAL
1	B	304	GLY
1	B	309	ASP
1	B	331	LEU
2	C	291	PRO
2	C	312	GLU
2	C	315	ALA
2	D	72	ALA
2	D	325	GLU
3	E	16	LYS

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Mol	Chain	Res	Type
3	F	74	LEU
4	L	29	ALA
4	L	35	PRO
1	B	209	PRO
1	B	225[A]	PHE
1	B	225[B]	PHE
2	C	127	ARG
2	C	310	LEU
2	C	323	LYS
2	D	328	SER
4	L	42	ALA
4	L	53	MSE
4	L	57	LEU
1	B	241	LEU
1	B	328	LYS
2	C	319	ALA
2	D	244	GLU
4	L	59	ARG
4	L	45	ARG
4	L	55	GLU
1	B	414	PRO
4	L	7	ILE
4	L	71	ILE
4	L	68	ILE

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	433/431 (100%)	378 (87%)	55 (13%)	4	11
1	B	435/431 (101%)	378 (87%)	57 (13%)	4	10
2	C	272/268 (102%)	228 (84%)	44 (16%)	2	6
2	D	279/268 (104%)	248 (89%)	31 (11%)	6	15
3	E	98/94 (104%)	86 (88%)	12 (12%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	98/94 (104%)	80 (82%)	18 (18%)	1	4
4	L	79/75 (105%)	55 (70%)	24 (30%)	0	1
All	All	1694/1661 (102%)	1453 (86%)	241 (14%)	3	8

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	LYS
1	A	24	GLU
1	A	26	THR
1	A	29	ASP
1	A	30	LYS
1	A	43	LYS
1	A	49	GLN
1	A	70	LYS
1	A	72	LEU
1	A	81	GLN
1	A	88	ILE
1	A	90	ASP
1	A	101	ILE
1	A	104	ILE
1	A	107	LEU
1	A	118	VAL
1	A	120	ARG
1	A	133	MSE
1	A	136	ILE
1	A	140	ARG
1	A	144	THR
1	A	161	ASP
1	A	177	SER
1	A	179	PHE
1	A	191	LEU
1	A	206	LEU
1	A	211	MSE
1	A	223	VAL
1	A	241	LEU
1	A	243	VAL
1	A	244	ILE
1	A	277	SER
1	A	289	MSE

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Mol	Chain	Res	Type
1	A	290	SER
1	A	296	GLU
1	A	308	LYS
1	A	312	ARG
1	A	315	ILE
1	A	335	LEU
1	A	344	GLN
1	A	352	ILE
1	A	355	LYS
1	A	364	LYS
1	A	371	LYS
1	A	389	ARG
1	A	415	THR
1	A	417	LEU
1	A	422	ILE
1	A	423	GLU
1	A	425	GLU
1	A	445	GLU
1	A	463	GLU
1	A	479	ILE
1	A	483	ASN
1	B	7	LYS
1	B	10	LEU
1	B	15	GLN
1	B	17	LEU
1	B	18	THR
1	B	30	LYS
1	B	31	LYS
1	B	43	LYS
1	B	44	ILE
1	B	49	GLN
1	B	52	ASP
1	B	55	ARG
1	B	70	LYS
1	B	99	LEU
1	B	101	ILE
1	B	105	SER
1	B	107	LEU
1	B	109	HIS
1	B	118	VAL
1	B	146	GLN
1	B	159	LEU

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Mol	Chain	Res	Type
1	B	179	PHE
1	B	199	GLU
1	B	202	LEU
1	B	206	LEU
1	B	208	VAL
1	B	212	SER
1	B	225[A]	PHE
1	B	225[B]	PHE
1	B	230	GLN
1	B	237	MSE
1	B	238	THR
1	B	241	LEU
1	B	242	GLU
1	B	277	SER
1	B	278	MSE
1	B	279	MSE
1	B	289	MSE
1	B	302[A]	ASN
1	B	302[B]	ASN
1	B	306	LEU
1	B	312	ARG
1	B	315	ILE
1	B	316	ARG
1	B	331	LEU
1	B	344	GLN
1	B	355	LYS
1	B	356	GLU
1	B	361	MSE
1	B	371	LYS
1	B	406	THR
1	B	412	ASP
1	B	417	LEU
1	B	445	GLU
1	B	479	ILE
1	B	493	LYS
1	B	498	ILE
2	C	14	ARG
2	C	27	LYS
2	C	40	GLU
2	C	42	LYS
2	C	47	TYR
2	C	57	LEU

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Mol	Chain	Res	Type
2	C	87	ASN
2	C	93	GLU
2	C	104	LYS
2	C	114	GLU
2	C	117	LYS
2	C	122	LEU
2	C	131	LEU
2	C	135	MSE
2	C	139	LYS
2	C	151	GLN
2	C	156	THR
2	C	160	ARG
2	C	182	LEU
2	C	190	MSE
2	C	194	MSE
2	C	196	GLN
2	C	200	LYS
2	C	207	VAL
2	C	239	GLU
2	C	241	GLN
2	C	245	ASP
2	C	246	VAL
2	C	248	MSE
2	C	249	LEU
2	C	261	LEU
2	C	276	GLU
2	C	277	THR
2	C	279	ARG
2	C	280	GLU
2	C	281	LEU
2	C	283	GLN
2	C	284	LYS
2	C	290	GLU
2	C	307	ILE
2	C	308	ASP
2	C	320	ARG
2	C	327	GLN
2	C	328	SER
2	D	6	LYS
2	D	7	THR
2	D	13	ILE
2	D	14	ARG

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Mol	Chain	Res	Type
2	D	40	GLU
2	D	53	SER
2	D	57	LEU
2	D	66	ARG
2	D	111	LEU
2	D	113	GLU
2	D	114	GLU
2	D	131	LEU
2	D	168	SER
2	D	177	SER
2	D	182	LEU
2	D	193	GLU
2	D	207	VAL
2	D	215	THR
2	D	234	MSE
2	D	241	GLN
2	D	249	LEU
2	D	261	LEU
2	D	269	LYS
2	D	277	THR
2	D	279	ARG
2	D	280	GLU
2	D	290	GLU
2	D	302	GLU
2	D	307	ILE
2	D	327	GLN
2	D	329	ARG
3	E	2	SER
3	E	3	VAL
3	E	10	LYS
3	E	51	SER
3	E	59	LYS
3	E	74	LEU
3	E	79	LEU
3	E	80	LEU
3	E	88	LYS
3	E	93	LEU
3	E	112	LYS
3	E	116	ASN
3	F	2	SER
3	F	3	VAL
3	F	6	LEU

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Mol	Chain	Res	Type
3	F	26	LEU
3	F	35	LEU
3	F	44	VAL
3	F	48	MSE
3	F	56	GLU
3	F	62	THR
3	F	66	PRO
3	F	70	LYS
3	F	74	LEU
3	F	80	LEU
3	F	90	ASP
3	F	93	LEU
3	F	102	SER
3	F	108	THR
3	F	112	LYS
4	L	7	ILE
4	L	20	GLU
4	L	25	ASP
4	L	30	GLU
4	L	31	MSE
4	L	32	GLN
4	L	38	ILE
4	L	41	GLN
4	L	43	GLU
4	L	48	ILE
4	L	51	GLU
4	L	55	GLU
4	L	56	LYS
4	L	60	ASP
4	L	61	TRP
4	L	62	ASP
4	L	63	VAL
4	L	66	MSE
4	L	67	LEU
4	L	68	ILE
4	L	70	VAL
4	L	71	ILE
4	L	73	ILE
4	L	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	49	GLN
1	A	65	GLN
1	A	81	GLN
1	A	153	ASN
1	A	155	HIS
1	A	160	HIS
1	A	164	HIS
1	A	259	GLN
1	A	330	HIS
1	A	341	GLN
1	A	344	GLN
1	A	400	GLN
1	A	455	HIS
1	A	478	ASN
1	A	483	ASN
1	A	492	GLN
1	B	28	GLN
1	B	49	GLN
1	B	65	GLN
1	B	83	ASN
1	B	87	ASN
1	B	155	HIS
1	B	160	HIS
1	B	204	ASN
1	B	330	HIS
1	B	341	GLN
1	B	344	GLN
1	B	349	HIS
1	B	400	GLN
1	B	421	GLN
1	B	424	HIS
1	B	455	HIS
1	B	476	HIS
1	B	483	ASN
1	B	492	GLN
1	B	494	HIS
2	C	46	HIS
2	C	50	GLN
2	C	87	ASN
2	C	137	ASN
2	C	151	GLN
2	C	165	GLN

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Mol	Chain	Res	Type
2	C	219	ASN
2	C	241	GLN
2	C	292	GLN
2	D	46	HIS
2	D	50	GLN
2	D	55	HIS
2	D	78	GLN
2	D	136	ASN
2	D	137	ASN
2	D	151	GLN
2	D	165	GLN
2	D	219	ASN
2	D	288	HIS
2	D	327	GLN
3	F	24	GLN
3	F	96	GLN
4	L	10	GLN
4	L	32	GLN
4	L	34	GLN
4	L	83	HIS
4	L	89	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](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
7	MOO	B	515	-	2,4,4	14.04	2 (100%)	-		

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	515	MOO	O2-MO	-14.50	1.43	1.75
7	B	515	MOO	O1-MO	-13.56	1.45	1.75

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	515	MOO	9	0

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	480/511 (93%)	-0.85	0 100 100	17, 32, 47, 61	0
1	B	477/511 (93%)	-0.76	3 (0%) 85 85	18, 32, 57, 69	3 (0%)
2	C	303/333 (90%)	-0.73	1 (0%) 90 89	17, 34, 55, 74	0
2	D	309/333 (92%)	-0.85	0 100 100	18, 34, 52, 73	0
3	E	114/119 (95%)	-0.82	0 100 100	20, 34, 45, 50	0
3	F	114/119 (95%)	-0.49	0 100 100	30, 48, 62, 64	0
4	L	82/89 (92%)	0.69	5 (6%) 27 24	12, 20, 24, 25	82 (100%)
All	All	1879/2015 (93%)	-0.72	9 (0%) 87 86	12, 33, 55, 74	85 (4%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	330	GLY	4.1
4	L	58	GLY	3.8
4	L	73	ILE	3.2
4	L	57	LEU	3.0
1	B	226	GLY	2.5
4	L	68	ILE	2.2
1	B	54[A]	PHE	2.1
1	B	230	GLN	2.1
4	L	35	PRO	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($\text{\AA}^2$)	Q<0.9
7	MOO	B	515	5/5	0.75	0.40	84,86,87,88	0
5	FE	B	512	1/1	0.99	0.04	28,28,28,28	0
5	FE	B	513	1/1	0.99	0.04	47,47,47,47	0
5	FE	A	512	1/1	0.99	0.04	35,35,35,35	0
6	ZN	A	514	1/1	1.00	0.01	32,32,32,32	0
6	ZN	B	514	1/1	1.00	0.01	36,36,36,36	0
5	FE	A	513	1/1	1.00	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.