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PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 05:56 pm BST

PDB ID	:	2INN
Title	:	Structure of the Phenol Hydroxyalse-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 (i) symbol.

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

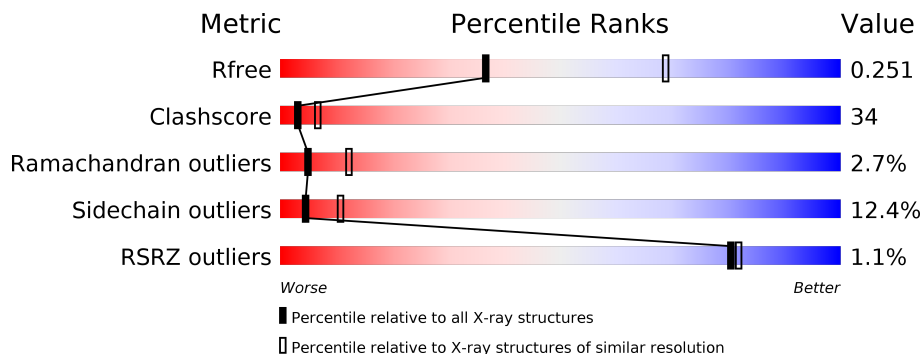|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	Percentile Ranks	Value
Rfree		0.251
Clashscore		34
Ramachandran outliers		2.7%
Sidechain outliers		12.4%
RSRZ outliers		1.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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	511	52% 34% 10% • •
1	B	511	% 46% 37% 11% • •
2	C	333	% 40% 40% 14% • •
2	D	333	53% 36% 8% • •
3	E	119	59% 35% 5% •
3	F	119	42% 48% 7% • •

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Mol	Chain	Length	Quality of chain
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 (i)

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 4129	C 2655	N 694	O 756	S 8	Se 16	0	0	0
1	B	493	Total 4140	C 2665	N 694	O 757	S 8	Se 16	0	3	0

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 phL.

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

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 925	C 602	N 145	O 173	S 1	Se 4	0	0	0
3	F	118	Total 925	C 602	N 145	O 173	S 1	Se 4	0	0	0

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
			Total	C	N	O	Se			
4	L	87	719	446	122	146	5	0	0	0

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 (three-letter code: FE) (formula: Fe).

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is MOLYBDATE ION (three-letter code: MOO) (formula: MoO_4).
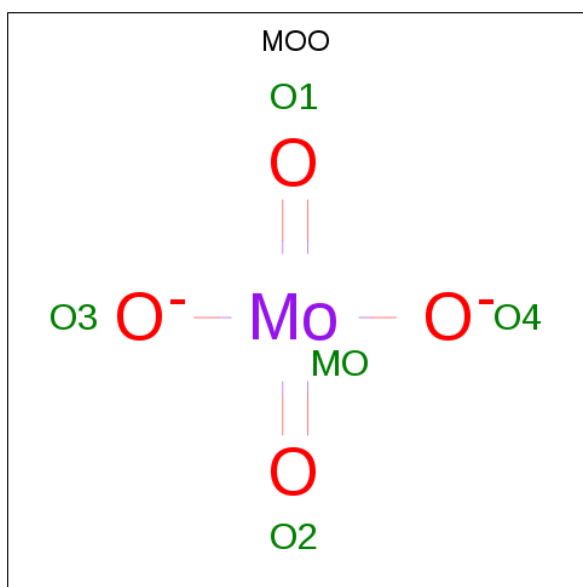
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 5	Mo 1	O 4	0	0

- Molecule 8 is water.

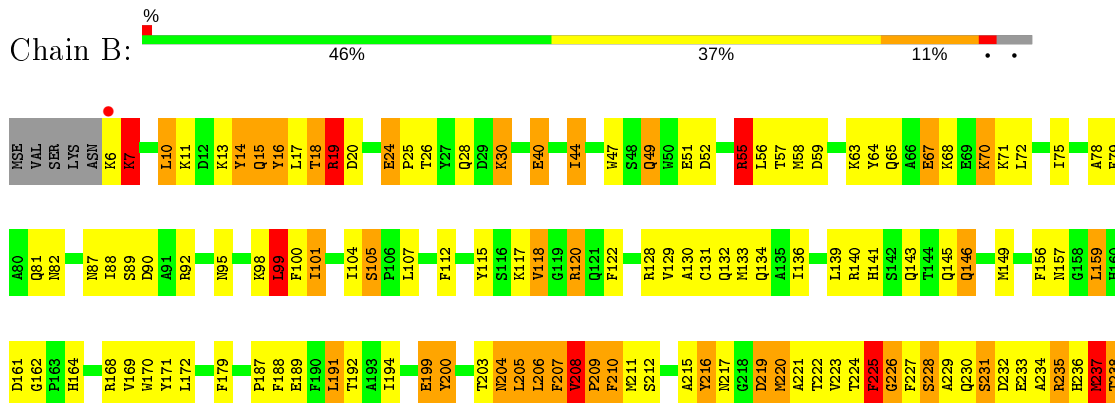| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	80	Total 80	O 80	0	0
8	B	71	Total 71	O 71	0	0
8	C	53	Total 53	O 53	0	0
8	D	60	Total 60	O 60	0	0
8	E	23	Total 23	O 23	0	0
8	F	13	Total 13	O 13	0	0
8	L	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
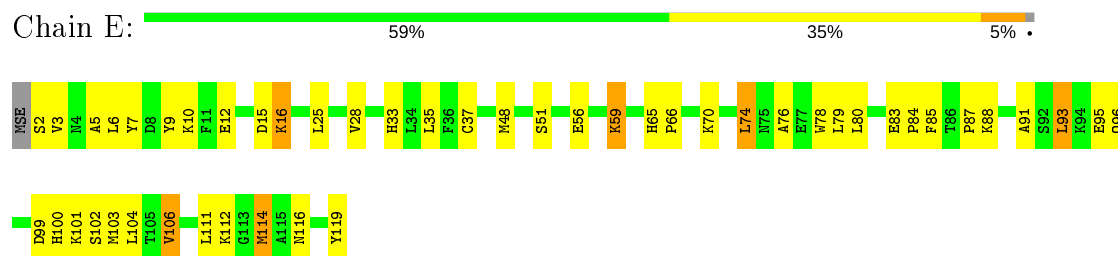
- Molecule 1: Phenol hydroxylase component phN
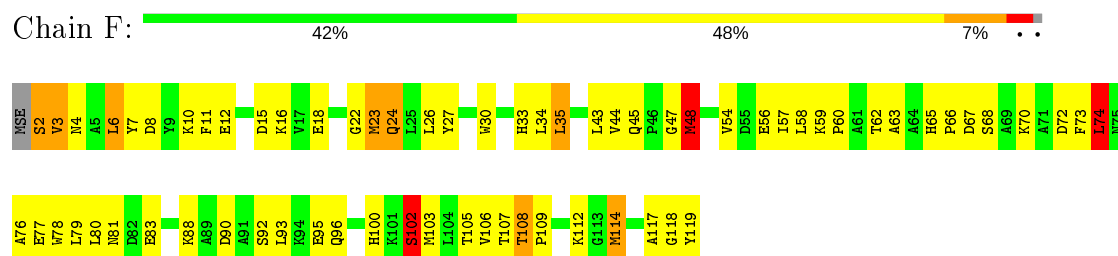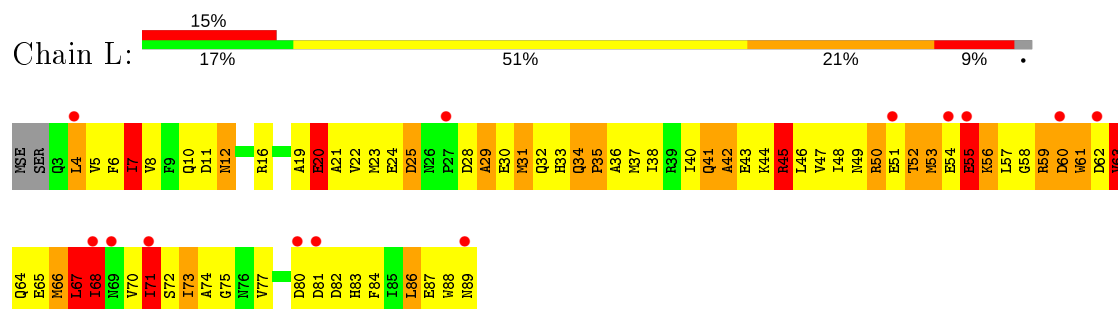
Chain A:

- Molecule 1: Phenol hydroxylase component phN

Chain B:

L241 E242 V243 I244 K245 L248 E249 Q250 H251 E252 D253 P256 D263 R268 G269 F270 R271 L272 S274 L275 V276 S277 M278 M279 M280 M283 L284 P285 V288 M289 S290 W291 A294 W295 E296 V297 Y298 Q301 N302 G303 G304 A305 L306 F307 K308 D309 L310 E311 R312 Y313

G314 I315 R316 K319 D326 A327 K328 H329 H330 L331 L335 F339 Y340 Q341 Y342 C343 Q344 F348 P353 E354 K355 E356 E357 M358 M361 S362 E363 T368 F369 Y373 R374 P375 Y377 E378 K382 E383 R388 R389 N392 L398 C402 Q403 I404 F408

T409 D412 A413 P414 T415 M416 L417 S418 H419 R420 R428 C432 S433 P444 E445 K446 Y447 I448 L452 P453 V454 H455 Y458 Q459 G460 N461 C462 E468 T469 V470 V471 Q472 K473 Y474 Y475 H476 I477 N478 I479 D482 N483 Y486 V487 G488 S489 P490 D491 Q492 K493 H494 W495

L496 S497 I498 LYS GLY ARG LYS PRO ALA ASP LYS ASN GLN ASP ASP ALA

• Molecule 2: Phenol hydroxylase component phL

Chain C:
% 40% 40% 14% • •

MSE SER ILE GLU ILE LYS ASN SER VAL GLU P12 I13 R14 Y17 G18 R23 D26 K27 P28 S36 Y37 D38 I39 E40 A41 K42 F45 H46 Y47 R48 P49 Q50 W51 D52 S53 E54 H55 T56 L57 N58 D59 P60 T61 R62 T63 A64 I65 R66 M67 E68 D69 W70 C71 A72

V73 S74 D75 P76 R77 Q78 F79 Y80 Y81 N87 R88 A89 K90 M91 Q92 E93 S94 A95 E96 T97 S98 C102 E103 K104 R105 L108 S112 E113 E114 T115 Q116 K117 Q118 R121 L122 V123 P125 L126 R127 H128 V129 E130 L131 G132 A133 N137 A138 K139 A146 T147 T148 V149

S150 Q151 M152 H153 I154 Y155 T156 G157 M158 D159 R160 Q165 Y166 R169 I170 A171 L172 M173 I174 D175 T178 G179 L182 D183 E184 S185 K186 A187 Y188 W189 M190 M194 W195 Q196 P197 M198 R199 K200 L201 V202 E203 V207 V208 D209 F212 E213 I214 T215 L216 V217 Q218 N219

I222 D223 G224 M225 M226 Y227 P228 L229 K233 M234 I235 Q236 Q241 G242 A243 E244 D245 Y246 S247 M248 L249 F252 M253 Y257 K258 E259 S260 L261 N265 A266 M267 N268 V271 E276 T277 N278 R279 E280 Q283 K284 W285 I286 D287 D288 W289 P290 P291 Q292 Q293 Y294 E295 A296

L297 K298 P299 L300 A301 S304 V305 G306 I307 D308 G309 L310 N311 E312 A313 R314 A315 E316 L317 S318 A319 R320 L321 K322 K323 F324 E325 L326 Q327 S328 R329 G330 VAL SER ALA

• Molecule 2: Phenol hydroxylase component phL

Chain D:
53% 36% 8% • •

MSE SER ILE GLU I5 K6 T7 V10 E11 P12 I13 R14 R22 D26 K27 P28 A29 Q33 E34 A35 S36 Y37 D38 I39 E40 F45 H46 Y47 R48 P49 Q50 W51 D52 S53 E54 H55 T56 L57 N58 D59 P60 A64 I65 R66 M67 E68 C71 A72 V73 S74 D75 P76 R77

R88 M91 C102 E103 L107 L108 L111 S112 E113 E114 T115 Q118 L119 L120 R121 L122 L123 V124 P125 E130 L131 G132 A133 N134 M135 K139 T147 T148 V149 S150 Q151 M152 Y155 T156 G157 M158 D159 R160 L161 Q165 Y166 L167 S168 R169 I170 A171 L172 M173

S177 A181 L182 K186 A187 Y188 W189 E193 M194 M198 R199 V202 E203 L206 V207 T215 L216 V217 Q218 M219 I220 L221 I222 D223 G224 M225 M226 Y227 V230 V231 D232 K233 M234 F238 Q241 E244 D245 V246 S247 M248 L249 F252 M253 R254 L261 R262 W263

T264 K269 A270 V271 A272 T277 N278 R279 E280 L281 W285 I286 E290 Y294 E295 A296 L297 K298 P299 L300 A301 E302 A303 S304 V305 G306 I307 L310 A315 E316 L321 E325 L326 Q327 S328 R329 GLY VAL SER ALA

• Molecule 3: Phenol hydroxylase component phO

Chain E:

• Molecule 3: Phenol hydroxylase component phO

Chain F:

• Molecule 4: Phenol hydroxylase component phM

Chain L:

4 Data and refinement statistics (i)

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 29.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.3 (30.00-2.70) 86.3 (29.86-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [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 (5.08%)	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)	0.32 , 45.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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[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: ZN, MOO, FE

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	1.53	38/4247 (0.9%)	1.29	33/5728 (0.6%)
1	B	1.54	45/4260 (1.1%)	1.33	37/5746 (0.6%)
2	C	1.58	24/2636 (0.9%)	1.38	24/3537 (0.7%)
2	D	1.43	17/2686 (0.6%)	1.33	24/3606 (0.7%)
3	E	1.54	5/949 (0.5%)	1.32	5/1285 (0.4%)
3	F	1.42	5/949 (0.5%)	1.23	4/1285 (0.3%)
4	L	1.03	0/725	1.15	4/971 (0.4%)
All	All	1.50	134/16452 (0.8%)	1.31	131/22158 (0.6%)

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 (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	102	CYS	CB-SG	-12.86	1.60	1.82
1	B	210	PHE	CD1-CE1	10.94	1.61	1.39
2	C	71	CYS	CB-SG	-9.38	1.66	1.82
1	A	233	GLU	CG-CD	9.30	1.65	1.51
1	B	118	VAL	CB-CG2	-9.28	1.33	1.52
3	E	95	GLU	CG-CD	9.05	1.65	1.51
3	E	56	GLU	CG-CD	8.90	1.65	1.51
1	B	210	PHE	CE2-CZ	8.53	1.53	1.37
1	A	402	CYS	CB-SG	-8.53	1.67	1.82
1	A	432	CYS	CB-SG	-8.47	1.67	1.82
1	B	445	GLU	CB-CG	8.39	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	TYR	CE2-CZ	8.14	1.49	1.38
1	B	445	GLU	CG-CD	8.11	1.64	1.51
3	F	3	VAL	CB-CG2	-8.11	1.35	1.52
1	B	402	CYS	CB-SG	-8.09	1.68	1.82
2	D	193	GLU	CG-CD	8.02	1.64	1.51
3	F	23	MSE	SE-CE	7.83	2.41	1.95
1	A	416	MSE	SE-CE	7.77	2.41	1.95
1	A	237	MSE	SE-CE	7.72	2.40	1.95
3	E	114	MSE	SE-CE	7.69	2.40	1.95
1	B	171	TYR	CG-CD2	7.61	1.49	1.39
1	B	99	LEU	CG-CD2	7.60	1.79	1.51
3	F	114	MSE	SE-CE	7.48	2.39	1.95
1	A	225	PHE	CE1-CZ	7.39	1.51	1.37
2	C	96	GLU	CD-OE1	7.18	1.33	1.25
1	B	210	PHE	CD2-CE2	7.13	1.53	1.39
1	A	12	ASP	CB-CG	7.04	1.66	1.51
2	C	184	GLU	CD-OE1	6.96	1.33	1.25
1	A	391	TYR	CD2-CE2	6.89	1.49	1.39
1	B	19	ARG	CG-CD	6.83	1.69	1.51
1	A	308	LYS	CD-CE	6.82	1.68	1.51
1	B	354	GLU	CD-OE2	6.79	1.33	1.25
1	B	216	TYR	CB-CG	-6.73	1.41	1.51
1	B	171	TYR	CE2-CZ	6.62	1.47	1.38
1	A	207	PHE	CE2-CZ	6.60	1.49	1.37
2	C	114	GLU	CG-CD	6.53	1.61	1.51
1	A	227	PHE	CD2-CE2	6.53	1.52	1.39
1	B	64	TYR	CG-CD1	6.39	1.47	1.39
1	A	117	LYS	CD-CE	6.35	1.67	1.51
1	B	131	CYS	CB-SG	-6.30	1.71	1.82
1	B	378	GLU	CD-OE2	6.28	1.32	1.25
2	C	236	GLN	CG-CD	6.27	1.65	1.51
2	D	187	ALA	CA-CB	6.23	1.65	1.52
1	A	120	ARG	CZ-NH2	6.23	1.41	1.33
2	C	54	GLU	CG-CD	6.21	1.61	1.51
1	A	198	PHE	CE1-CZ	6.21	1.49	1.37
2	D	114	GLU	CB-CG	6.19	1.64	1.52
2	D	37	TYR	CD1-CE1	-6.16	1.30	1.39
1	A	370	ASP	CB-CG	6.13	1.64	1.51
1	B	210	PHE	CG-CD1	6.11	1.48	1.38
1	B	112	PHE	CE1-CZ	6.07	1.48	1.37
1	A	225	PHE	CD2-CE2	6.06	1.51	1.39
1	B	14	TYR	CD1-CE1	-6.05	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GLU	CG-CD	6.05	1.61	1.51
1	A	225	PHE	CG-CD1	5.98	1.47	1.38
1	A	440	PHE	CE2-CZ	5.95	1.48	1.37
1	A	483	ASN	CB-CG	-5.94	1.37	1.51
1	A	390	PHE	CE1-CZ	5.91	1.48	1.37
2	D	39	ILE	CA-CB	5.87	1.68	1.54
1	A	170	TRP	CB-CG	-5.85	1.39	1.50
1	B	378	GLU	CG-CD	5.85	1.60	1.51
1	B	112	PHE	CD2-CE2	5.85	1.50	1.39
2	C	259	GLU	CD-OE1	5.83	1.32	1.25
2	D	68	GLU	CG-CD	5.82	1.60	1.51
1	B	210	PHE	CB-CG	5.82	1.61	1.51
1	B	237	MSE	SE-CE	5.82	2.29	1.95
2	C	213	GLU	CD-OE2	5.80	1.32	1.25
1	B	446	LYS	CD-CE	5.78	1.65	1.51
2	C	149	VAL	CA-CB	5.78	1.66	1.54
3	F	12	GLU	CG-CD	5.77	1.60	1.51
1	B	468	GLU	CD-OE2	5.75	1.31	1.25
1	A	227	PHE	CE1-CZ	5.74	1.48	1.37
2	D	246	VAL	CB-CG2	-5.73	1.40	1.52
2	D	234	MSE	SE-CE	5.73	2.29	1.95
1	A	348	PHE	CD1-CE1	5.73	1.50	1.39
1	B	252	GLU	CG-CD	5.73	1.60	1.51
2	C	295	GLU	CB-CG	5.70	1.62	1.52
2	C	70	TRP	CB-CG	-5.70	1.40	1.50
2	D	72	ALA	CA-CB	5.67	1.64	1.52
2	C	318	SER	CB-OG	5.59	1.49	1.42
1	B	208	VAL	N-CA	5.59	1.57	1.46
1	B	271	ARG	CZ-NH2	-5.58	1.25	1.33
2	C	285	TRP	CB-CG	5.58	1.60	1.50
1	A	499	LYS	CA-CB	5.58	1.66	1.53
2	C	80	TYR	CE1-CZ	5.56	1.45	1.38
2	D	248	MSE	SE-CE	5.54	2.28	1.95
2	C	117	LYS	CD-CE	5.53	1.65	1.51
1	A	194	ILE	CA-CB	-5.51	1.42	1.54
1	A	391	TYR	CD1-CE1	5.51	1.47	1.39
2	C	318	SER	CA-CB	5.50	1.61	1.52
2	C	117	LYS	CE-NZ	5.50	1.62	1.49
3	E	106	VAL	CB-CG1	-5.49	1.41	1.52
1	A	81	GLN	CG-CD	5.47	1.63	1.51
2	D	114	GLU	CG-CD	5.46	1.60	1.51
1	B	363	GLU	CD-OE2	5.45	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	474	TYR	CD2-CE2	5.45	1.47	1.39
2	C	96	GLU	CG-CD	5.43	1.60	1.51
3	F	83	GLU	CG-CD	5.43	1.60	1.51
1	B	313	TYR	CD2-CE2	5.42	1.47	1.39
1	A	67	GLU	CD-OE1	5.40	1.31	1.25
2	C	54	GLU	CB-CG	5.38	1.62	1.52
1	B	493	LYS	CD-CE	5.36	1.64	1.51
1	A	27	TYR	CB-CG	-5.35	1.43	1.51
3	E	95	GLU	CD-OE1	5.34	1.31	1.25
1	B	296	GLU	CG-CD	5.34	1.59	1.51
1	B	216	TYR	CE1-CZ	5.32	1.45	1.38
1	B	468	GLU	CG-CD	5.29	1.59	1.51
2	C	166	TYR	CE2-CZ	5.28	1.45	1.38
1	B	24	GLU	CG-CD	5.26	1.59	1.51
1	B	473	LYS	CD-CE	5.26	1.64	1.51
1	A	225	PHE	CE2-CZ	5.26	1.47	1.37
1	B	220	MSE	SE-CE	5.25	2.26	1.95
1	B	40	GLU	CD-OE1	5.25	1.31	1.25
1	A	211	MSE	CG-SE	5.23	2.13	1.95
2	C	257	TYR	CE1-CZ	5.21	1.45	1.38
2	D	193	GLU	CB-CG	5.20	1.62	1.52
2	D	64	ALA	CA-CB	-5.20	1.41	1.52
2	D	244	GLU	CD-OE1	5.17	1.31	1.25
1	A	311	GLU	CG-CD	5.15	1.59	1.51
1	B	16	TYR	CD2-CE2	5.15	1.47	1.39
1	A	110	ALA	CA-CB	-5.14	1.41	1.52
2	D	271	VAL	CB-CG2	-5.12	1.42	1.52
1	B	170	TRP	CB-CG	-5.11	1.41	1.50
2	C	280	GLU	CG-CD	5.11	1.59	1.51
1	B	249	GLU	CG-CD	5.10	1.59	1.51
2	C	73	VAL	CB-CG1	-5.10	1.42	1.52
1	A	486	TYR	CD1-CE1	5.10	1.47	1.39
1	A	266	PHE	CE1-CZ	5.08	1.47	1.37
2	D	285	TRP	CE3-CZ3	5.08	1.47	1.38
1	B	64	TYR	CD2-CE2	5.07	1.47	1.39
1	A	16	TYR	CG-CD1	5.05	1.45	1.39
2	D	294	TYR	CE1-CZ	5.04	1.45	1.38
1	A	79	PHE	CE2-CZ	5.03	1.47	1.37
1	B	221	ALA	CA-CB	-5.03	1.41	1.52

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	LEU	CA-CB-CG	-12.75	85.98	115.30
2	C	66	ARG	NE-CZ-NH1	12.32	126.46	120.30
2	D	77	ARG	NE-CZ-NH1	-11.38	114.61	120.30
2	D	88	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	B	99	LEU	CB-CG-CD1	-10.52	93.12	111.00
1	A	180	ASP	CB-CG-OD1	10.32	127.58	118.30
2	C	26	ASP	CB-CG-OD1	9.82	127.14	118.30
2	C	26	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	A	491	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	B	56	LEU	CB-CG-CD1	-9.39	95.03	111.00
3	E	6	LEU	CA-CB-CG	9.39	136.90	115.30
1	A	491	ASP	CB-CG-OD1	9.35	126.72	118.30
1	B	388	ARG	NE-CZ-NH1	9.18	124.89	120.30
2	D	131	LEU	CA-CB-CG	-9.13	94.29	115.30
1	B	271	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	B	99	LEU	CB-CG-CD2	8.92	126.16	111.00
2	C	48	ARG	NE-CZ-NH2	-8.79	115.91	120.30
2	D	88	ARG	NE-CZ-NH2	-8.77	115.92	120.30
2	D	107	LEU	CB-CG-CD1	-8.63	96.33	111.00
1	A	428	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	C	169	ARG	NE-CZ-NH2	-8.31	116.14	120.30
2	D	22	ARG	NE-CZ-NH1	-8.23	116.18	120.30
2	C	127	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	235	ARG	NE-CZ-NH2	-7.87	116.37	120.30
2	C	66	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	D	77	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	A	55	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	B	140	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	191	LEU	CB-CG-CD2	-7.45	98.33	111.00
1	A	68	LYS	CD-CE-NZ	-7.40	94.68	111.70
1	B	205	LEU	CA-CB-CG	-7.38	98.32	115.30
1	B	268	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	C	88	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	C	121	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	56	LEU	CA-CB-CG	7.19	131.85	115.30
1	A	180	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	B	67	GLU	CB-CA-C	7.08	124.55	110.40
1	B	55	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	12	ASP	CB-CG-OD1	7.06	124.65	118.30
1	B	120	ARG	NE-CZ-NH2	6.95	123.77	120.30
1	A	264	LYS	CD-CE-NZ	6.90	127.58	111.70
2	C	127	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	C	75	ASP	CB-CG-OD1	6.81	124.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	TYR	CB-CA-C	-6.76	96.88	110.40
1	B	445	GLU	OE1-CD-OE2	-6.70	115.27	123.30
1	B	63	LYS	CD-CE-NZ	-6.68	96.32	111.70
1	A	29	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	140	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	308	LYS	CD-CE-NZ	6.63	126.95	111.70
1	B	273	LEU	CB-CG-CD1	6.62	122.26	111.00
2	D	262	ARG	NE-CZ-NH1	-6.58	117.01	120.30
3	E	59	LYS	CD-CE-NZ	6.41	126.45	111.70
1	A	412	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	A	335	LEU	CB-CG-CD1	-6.38	100.16	111.00
1	A	312	ARG	NE-CZ-NH1	6.37	123.48	120.30
2	D	27	LYS	CD-CE-NZ	-6.36	97.07	111.70
2	D	254	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	331	LEU	CB-CG-CD2	6.34	121.78	111.00
2	D	26	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	205	LEU	CA-CB-CG	-6.34	100.73	115.30
1	A	412	ASP	CB-CG-OD2	6.30	123.97	118.30
2	D	160	ARG	NE-CZ-NH2	-6.28	117.16	120.30
4	L	4	LEU	CA-CB-CG	6.18	129.52	115.30
1	B	335	LEU	CB-CG-CD1	-6.16	100.53	111.00
1	A	237	MSE	CG-SE-CE	6.06	112.24	98.90
1	A	120	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	A	300	GLU	OE1-CD-OE2	-5.93	116.19	123.30
1	A	102	SER	CB-CA-C	-5.91	98.88	110.10
1	A	335	LEU	CA-CB-CG	-5.89	101.74	115.30
4	L	45	ARG	NE-CZ-NH1	-5.89	117.35	120.30
2	C	314	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	159	LEU	CA-CB-CG	5.89	128.84	115.30
2	D	39	ILE	CG1-CB-CG2	-5.88	98.46	111.40
4	L	67	LEU	CA-CB-CG	5.84	128.73	115.30
2	C	71	CYS	CA-CB-SG	-5.83	103.50	114.00
2	D	121	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	C	102	CYS	CA-CB-SG	-5.81	103.53	114.00
1	B	319	LYS	CD-CE-NZ	5.78	125.00	111.70
2	D	59	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	228	SER	N-CA-CB	-5.77	101.85	110.50
1	B	388	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	C	131	LEU	CA-CB-CG	-5.73	102.12	115.30
2	D	59	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	176	LYS	CD-CE-NZ	-5.71	98.56	111.70
3	E	35	LEU	CB-CG-CD2	5.67	120.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	MSE	CG-SE-CE	-5.67	86.43	98.90
1	B	219	ASP	CB-CG-OD1	5.66	123.39	118.30
2	C	310	LEU	CA-CB-CG	-5.63	102.35	115.30
2	D	271	VAL	CG1-CB-CG2	-5.61	101.93	110.90
2	D	48	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	D	246	VAL	CG1-CB-CG2	-5.59	101.95	110.90
1	B	275	LEU	CA-CB-CG	-5.55	102.52	115.30
1	B	216	TYR	N-CA-C	5.53	125.94	111.00
1	B	483	ASN	N-CA-CB	-5.52	100.67	110.60
3	F	23	MSE	CG-SE-CE	5.50	110.99	98.90
1	B	271	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	326	ASP	CB-CG-OD2	-5.49	113.36	118.30
2	C	223	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	D	26	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	A	178	PHE	CB-CA-C	-5.44	99.52	110.40
3	F	23	MSE	CA-CB-CG	-5.42	104.09	113.30
2	C	209	ASP	CB-CG-OD1	5.41	123.17	118.30
3	E	70	LYS	CD-CE-NZ	5.38	124.08	111.70
1	A	199	GLU	OE1-CD-OE2	-5.36	116.86	123.30
1	A	479	ILE	CG1-CB-CG2	-5.35	99.63	111.40
2	C	276	GLU	CB-CA-C	5.35	121.10	110.40
1	A	140	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	237	MSE	CG-SE-CE	5.33	110.62	98.90
3	E	5	ALA	N-CA-C	-5.32	96.63	111.00
1	B	171	TYR	CB-CG-CD1	-5.31	117.81	121.00
2	C	322	LYS	CD-CE-NZ	5.30	123.90	111.70
1	B	404	ILE	CG1-CB-CG2	-5.29	99.75	111.40
2	C	104	LYS	CB-CA-C	5.28	120.97	110.40
1	A	263	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	A	310	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	263	ASP	CB-CG-OD2	5.21	122.99	118.30
2	C	66	ARG	CD-NE-CZ	5.19	130.87	123.60
2	D	48	ARG	CG-CD-NE	-5.19	100.89	111.80
3	F	102	SER	N-CA-CB	5.18	118.28	110.50
1	B	207	PHE	N-CA-CB	5.17	119.92	110.60
1	A	493	LYS	CD-CE-NZ	5.15	123.55	111.70
1	B	216	TYR	CB-CG-CD1	-5.14	117.91	121.00
2	D	102	CYS	CA-CB-SG	-5.10	104.81	114.00
2	C	62	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	395	LEU	CB-CG-CD1	-5.10	102.34	111.00
2	C	246	VAL	CB-CA-C	-5.09	101.72	111.40
4	L	71	ILE	N-CA-C	-5.09	97.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	MSE	CA-CB-CG	-5.08	104.67	113.30
3	F	24	GLN	N-CA-CB	-5.07	101.47	110.60
2	D	71	CYS	CA-CB-SG	-5.01	104.98	114.00
2	D	221	LEU	CB-CG-CD1	-5.00	102.50	111.00

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 (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	4129	0	3860	228	0
1	B	4140	0	3863	334	0
2	C	2593	0	2504	209	0
2	D	2643	0	2557	123	0
3	E	925	0	898	28	0
3	F	925	0	898	66	0
4	L	719	0	677	158	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	1052	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 34.

All (1052) 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:CG	1:B:99:LEU:CD2	1.80	1.57
4:L:34:GLN:HB3	4:L:35:PRO:CD	1.22	1.52
2:C:190:MSE:CE	2:C:190:MSE:SE	2.14	1.46
1:A:289:MSE:SE	1:A:289:MSE:CE	2.16	1.44
2:D:135:MSE:CE	2:D:135:MSE:SE	2.15	1.44
2:C:234:MSE:CE	2:C:234:MSE:SE	2.15	1.44
1:A:58:MSE:HE1	1:A:133:MSE:CE	1.47	1.44
4:L:66:MSE:SE	4:L:66:MSE:CE	2.15	1.44
2:C:268:MSE:SE	2:C:268:MSE:CE	2.15	1.44
2:C:67:MSE:CE	2:C:67:MSE:SE	2.17	1.43
4:L:8:VAL:HG11	4:L:37:MSE:CE	1.48	1.43
2:D:67:MSE:CE	2:D:67:MSE:SE	2.17	1.42
1:B:416:MSE:CE	1:B:416:MSE:SE	2.17	1.42
4:L:31:MSE:CE	4:L:31:MSE:SE	2.16	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:CE	2:C:253:MSE:SE	2.22	1.38
2:C:248:MSE:CE	2:C:248:MSE:SE	2.21	1.37
2:C:198:MSE:CE	2:C:198:MSE:SE	2.20	1.37
3:F:48:MSE:CE	3:F:48:MSE:SE	2.22	1.37
4:L:34:GLN:CB	4:L:35:PRO:HD2	1.28	1.36
2:C:226:MSE:SE	2:C:226:MSE:CE	2.23	1.36
1:B:361:MSE:HE3	1:B:369:PHE:CE1	1.58	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:CE	2:D:248:MSE:SE	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
4:L:48:ILE:CG2	4:L:84:PHE:HB3	1.69	1.23
4:L:65:GLU:O	4:L:68:ILE:HG22	1.07	1.21
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
4:L:65:GLU:O	4:L:68:ILE:CG2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:L:73:ILE:HG12	4:L:86:LEU:HD11	1.15	1.14
4:L:35:PRO:HG2	4:L:37:MSE:SE	1.96	1.13
4:L:48:ILE:HD11	4:L:53:MSE:HE1	1.13	1.13
4:L:8:VAL:HG11	4:L:37:MSE:HE2	1.17	1.13
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
4:L:8:VAL:HG11	4:L:37:MSE:HE3	1.27	1.10
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
4:L:48:ILE:HD11	4:L:53:MSE:CE	1.84	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
2:C:190:MSE:HA	2:C:190:MSE:HE2	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
4:L:8:VAL:CG1	4:L:37:MSE:HE2	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
4:L:48:ILE:HG22	4:L:84:PHE:HB3	1.08	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
4:L:19:ALA:O	4:L:22:VAL:HG12	1.59	1.02
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
4:L:48:ILE:CG2	4:L:84:PHE:CB	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:L:8:VAL:CG1	4:L:37:MSE:CE	2.40	0.98
4:L:48:ILE:HG22	4:L:84:PHE:CB	1.94	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
4:L:34:GLN:HB2	4:L:35:PRO:HD2	1.46	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:HE21	1:B:344:GLN:H	0.97	0.93
4:L:34:GLN:HB3	4:L:35:PRO:HD3	1.51	0.93
4:L:20:GLU:HG2	4:L:56:LYS:NZ	1.84	0.92
4:L:35:PRO:CG	4:L:37:MSE:SE	2.66	0.92
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
4:L:66:MSE:HE2	4:L:67:LEU:N	1.86	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
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
4:L:52:THR:HG22	4:L:53:MSE:N	1.87	0.89
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:O3	7:B:515:MOO:MO	1.43	0.88
7:B:515:MOO:MO	7:B:515:MOO:O2	1.43	0.88
1:B:312:ARG:HH11	1:B:312:ARG:CB	1.86	0.88
2:C:190:MSE:HE1	2:C:199:ARG:NE	1.88	0.88
1:B:244:ILE:HD12	1:B:245:LYS:N	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:515:MOO:O1	7:B:515:MOO:MO	1.45	0.87
1:B:99:LEU:CD2	1:B:99:LEU:HG	2.04	0.87
1:A:397:GLN:OE1	3:F:103:MSE:HE1	1.73	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
4:L:66:MSE:CE	4:L:67:LEU: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:O4	7:B:515:MOO:MO	1.45	0.85
4:L:73:ILE:CG1	4:L:86:LEU:HD11	2.03	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
4:L:80:ASP:HB3	4:L:82:ASP:H	1.40	0.84
1:B:361:MSE:CE	1:B:369:PHE:HZ	1.90	0.84
1:B:302[A]:ASN:HD22	1:B:302[A]:ASN:N	1.71	0.84
4:L:29:ALA:HA	4:L:42:ALA:HB2	1.59	0.84
4:L:50:ARG:NH1	4:L:82:ASP:OD2	2.09	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:312:ARG:HB3	1:B:312:ARG:HH11	1.41	0.83
1:B:120:ARG:HG2	2:D:139:LYS:HB2	1.58	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
4:L:48:ILE:CD1	4:L:53:MSE:HE1	2.03	0.83
1:B:206:LEU:HD22	1:B:206:LEU:C	1.99	0.83
4:L:74:ALA:O	4:L:86:LEU:HD22	1.78	0.82
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
2:C:290:GLU:CG	2:C:291:PRO:HD2	2.10	0.81
1:B:212:SER:HB3	4:L:35:PRO:CG	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:225[B]:PHE:CD1	1:B:226:GLY:HA2	2.16	0.81
1:A:58:MSE:H	2:C:165:GLN:HE22	1.26	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:B:302[A]:ASN:ND2	1:B:302[A]:ASN:N	2.27	0.80
1:A:26:THR:CB	2:C:199:ARG:NH2	2.45	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
4:L:73:ILE:HG23	4:L:74:ALA:N	1.97	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
1:A:206:LEU:HD12	1:A:206:LEU:C	2.04	0.78
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:300:LEU:O	2:D:304:SER:HB2	1.83	0.78
2:D:75:ASP:HA	2:D:152:MSE:CE	2.14	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
4:L:23:MSE:HG3	4:L:31:MSE:HE1	1.66	0.77
1:B:225[B]:PHE:CZ	1:B:229:ALA:HB1	2.19	0.77
1:B:312:ARG:NH1	1:B:312:ARG:CB	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
1:B:203:THR:HG23	1:B:204:ASN:N	1.99	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:HG3	1:B:55:ARG:NH2	1.99	0.76
1:B:49:GLN:HE21	1:B:49:GLN:HA	1.49	0.76
4:L:34:GLN:CB	4:L:35:PRO:CD	2.08	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	1:B:344:GLN:H	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:413:ALA:N	1:B:414:PRO:HD3	2.02	0.73
4:L:64:GLN:O	4:L:67:LEU:HG	1.88	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
4:L:20:GLU:HG2	4:L:56:LYS:HZ1	1.51	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
4:L:21:ALA:HB1	4:L:52:THR:HG21	1.72	0.72
1:A:220:MSE:HE2	1:B:78:ALA:CB	2.20	0.72
1:A:344:GLN:N	1:A:344:GLN:HE21	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
4:L:66:MSE:HE2	4:L:67:LEU:CA	2.20	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
1:A:402:CYS:HG	6:A:514:ZN:ZN	1.01	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:HB2	1:B:312:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:117:LYS:HE2	2:C:184:GLU:OE1	1.92	0.69
4:L:20:GLU:HG2	4:L:56:LYS:HZ2	1.58	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: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:397:GLN:HE22	3:F:103:MSE:CE	2.06	0.69
1:A:132:GLN:OE1	2:C:158:MSE:HE1	1.92	0.69
2:C:311:ASN:O	2:C:313:ALA:N	2.25	0.69
4:L:23:MSE:HG3	4:L:31:MSE:CE	2.22	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
4:L:80:ASP:HB2	4:L:83:HIS:H	1.58	0.68
1:B:149:MSE:HE3	1:B:225[A]:PHE:HE2	1.58	0.68
1:A:211:MSE:N	1:A:211:MSE:HE2	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: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
4:L:6:PHE:CE1	4:L:74:ALA:HB2	2.28	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
4:L:35:PRO:HG2	4:L:37:MSE:CG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:ASN:HB2	8:C:340:HOH:O	1.95	0.66
1:B:49:GLN:NE2	1:B:49:GLN:HA	2.11	0.66
1:A:122:PHE:CE2	1:A:191:LEU:HD22	2.31	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:455:HIS:CE1	3:F:27:TYR:OH	2.48	0.66
4:L:25:ASP:OD1	4:L:52:THR:OG1	2.14	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
4:L:66:MSE:HE3	4:L:70:VAL:CG1	2.26	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
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:B:200:TYR:CD1	1:B:200:TYR:C	2.68	0.65
1:A:319:LYS:O	1:A:320:TYR:HB2	1.96	0.65
4:L:5:VAL:HG11	4:L:87:GLU:HA	1.78	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
4:L:66:MSE:CE	4:L:67:LEU:CA	2.75	0.65
1:A:397:GLN:CD	3:F:103:MSE:HE1	2.17	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
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
4:L:7:ILE:CG2	4:L:46:LEU:CD1	2.76	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
4:L:48:ILE:CD1	4:L:53:MSE:CE	2.71	0.64
1:B:353:PRO:CB	1:B:358:MSE:HE2	2.23	0.64
1:B:65:GLN:HE22	1:B:68:LYS:NZ	1.96	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
2:D:194:MSE:HG2	2:D:194:MSE:O	1.94	0.63
1:B:279:MSE:SE	1:B:279:MSE:C	2.86	0.63
1:A:403:GLN:HE22	2:C:46:HIS:CD2	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLN:HE22	2:C:151:GLN:HE22	1.45	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
4:L:66:MSE:HE3	4:L:67:LEU:HA	1.80	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: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
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
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
2:C:93:GLU:OE1	2:C:93:GLU:HA	1.99	0.62
1:B:67:GLU:HG3	4:L:68:ILE:HD13	1.82	0.62
4:L:4:LEU:CD1	4:L:41:GLN:OE1	2.47	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
1:B:230:GLN:C	1:B:232:ASP:N	2.52	0.61
2:C:194:MSE:HG2	2:C:299:PRO:HB2	1.82	0.61
1:B:271:ARG:CZ	1:B:408:PHE:CD1	2.83	0.61
4:L:48:ILE:CG2	4:L:84:PHE:HB2	2.29	0.61
1:A:374:ARG:N	1:A:375:PRO:HD2	2.15	0.61
1:B:344:GLN:N	1:B:344:GLN:HE21	1.83	0.61
1:B:356:GLU:CD	1:B:356:GLU:H	2.04	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
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:164:HIS:HE1	1:B:474:TYR:O	1.83	0.61
1:B:98:LYS:HE2	1:B:157:ASN:O	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:MSE:HE2	2:D:263:TRP:HB2	1.82	0.60
2:D:75:ASP:CA	2:D:152:MSE:HE3	2.30	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
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
4:L:66:MSE:HE3	4:L:70:VAL:HG12	1.83	0.60
2:C:87:ASN:HD22	2:C:87:ASN:C	2.05	0.60
1:B:92:ARG:HG3	1:B:486:TYR:CE2	2.36	0.60
1:A:27:TYR:HH	2:C:196:GLN:HG3	1.62	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
4:L:7:ILE:HG22	4:L:46:LEU:CD1	2.33	0.59
1:A:164:HIS:HE1	1:A:474:TYR:O	1.84	0.59
1:A:6:LYS:HE2	1:A:6:LYS:HA	1.82	0.59
1:A:81:GLN:HG3	4:L:36:ALA:HB1	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:458:TYR:C	1:B:460:GLY:H	2.05	0.59
1:A:293:GLU:OE2	1:A:364:LYS:HE3	2.03	0.59
2:C:318:SER:O	2:C:322:LYS:HG3	2.03	0.59
2:C:95:ALA:O	2:C:98:SER:HB2	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:206:LEU:HD13	1:B:207:PHE:N	2.18	0.58
1:B:88:ILE:HA	1:B:217:ASN:O	2.03	0.58
2:C:102:CYS:SG	2:C:249:LEU:HD21	2.42	0.58
2:D:49:PRO:HG2	2:D:55:HIS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:477:ILE:HG22	1:A:477:ILE:O	2.03	0.58
2:D:207:VAL:O	2:D:207:VAL:CG1	2.52	0.58
4:L:6:PHE:CD1	4:L:74:ALA:CB	2.87	0.58
1:A:241:LEU:CD1	1:A:245:LYS:CE	2.76	0.58
1:B:308:LYS:C	1:B:310:LEU:H	2.07	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
2:D:160:ARG:HH22	2:D:223:ASP:CG	2.07	0.57
3:F:30:TRP:NE1	3:F:108:THR:HG22	2.17	0.57
4:L:66:MSE:CE	4:L:67:LEU:N	2.64	0.57
1:B:194:ILE:O	1:B:199:GLU:HB2	2.04	0.57
1:B:253:ASP:O	1:B:256:PRO:HD2	2.04	0.57
1:B:68:LYS:HG2	4:L:68:ILE:HD12	1.86	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: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
1:B:26:THR:HB	2:D:199:ARG:NH2	2.19	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:B:494:HIS:HD2	8:B:585:HOH:O	1.87	0.57
1:A:397:GLN:HE22	3:F:103:MSE:HE3	1.70	0.57
4:L:8:VAL:CG1	4:L:37:MSE:HE3	2.15	0.57
2:D:171:ALA:HB3	2:D:182:LEU:HD13	1.85	0.57
4:L:21:ALA:CB	4:L:52:THR:HG21	2.34	0.57
4:L:67:LEU:HD12	4:L:68:ILE:N	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:67:ASP:O	3:F:68:SER:C	2.41	0.57
4:L:28:ASP:O	4:L:29:ALA:C	2.43	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
4:L:34:GLN:HB3	4:L:35:PRO:HD2	0.62	0.56
1:B:342:TYR:C	1:B:344:GLN:NE2	2.59	0.56
1:B:200:TYR:C	1:B:200:TYR:HD1	2.09	0.56
1:B:206:LEU:CD1	1:B:207:PHE:HD2	2.18	0.56
4:L:66:MSE:HE2	4:L:67:LEU:HA	1.81	0.56
1:B:228:SER:H	4:L:10:GLN:HE22	1.54	0.56
4:L:8:VAL:HA	4:L:38:ILE:O	2.06	0.56
4:L:63:VAL:O	4:L:66:MSE:HB3	2.06	0.56
1:B:122:PHE:CE1	1:B:187:PRO:HB2	2.41	0.56
1:B:206:LEU:HB2	1:B:273:LEU:HD21	1.87	0.56
2:C:52:ASP:OD1	2:C:52:ASP:C	2.42	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:226:MSE:O	2:D:230:VAL:HG23	2.07	0.55
2:D:220:ILE:CD1	2:D:264:THR:HB	2.36	0.55
4:L:25:ASP:OD1	4:L:49:ASN:ND2	2.39	0.55
1:B:206:LEU:CD2	1:B:206:LEU:C	2.72	0.55
2:D:91:MSE:HE2	2:D:252:PHE:CE1	2.42	0.55
4:L:22:VAL:CG1	4:L:23:MSE:N	2.69	0.55
4:L:35:PRO:HG3	4:L:37:MSE:SE	2.55	0.55
1:A:259:GLN:NE2	1:A:316:ARG:CG	2.70	0.55
2:C:311:ASN:O	2:C:312:GLU:C	2.44	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:278:MSE:HG2	1:A:283:MSE:HE3	1.87	0.55
1:A:259:GLN:NE2	1:A:316:ARG:H	2.05	0.55
1:B:251:HIS:ND1	1:B:253:ASP:HB2	2.21	0.55
4:L:4:LEU:HA	4:L:42:ALA:O	2.07	0.55
4:L:54:GLU:HG2	4:L:60:ASP:HA	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:121:ARG:CZ	2:C:194:MSE:CE	2.85	0.54
2:C:75:ASP:HB2	2:C:152:MSE:SE	2.57	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
4:L:6:PHE:CE1	4:L:74:ALA:CB	2.91	0.54
4:L:35:PRO:HG2	4:L:37:MSE:HG2	1.89	0.54
4:L:61:TRP:HZ2	4:L:66:MSE:HB2	1.72	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
4:L:33:HIS:O	4:L:34:GLN:CG	2.54	0.54
4:L:52:THR:CG2	4:L:53:MSE:N	2.54	0.54
1:B:95:ASN:CB	1:B:283:MSE:HE2	2.38	0.54
4:L:71:ILE:HG22	4:L:72:SER:N	2.22	0.54
4:L:73:ILE:CG2	4:L:74:ALA:N	2.65	0.54
1:A:101:ILE:O	1:A:101:ILE:HG12	2.08	0.54
1:A:327:ALA:O	1:A:328:LYS:C	2.45	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:10:LEU:HD21	4:L:81:ASP:CG	2.27	0.53
2:D:75:ASP:CG	2:D:152:MSE:HE3	2.27	0.53
4:L:4:LEU:HD11	4:L:41:GLN:OE1	2.07	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: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: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
3:E:106:VAL:O	3:E:106:VAL:HG13	2.09	0.53
1:B:227:PHE:CB	4:L:10:GLN:HE22	2.01	0.53
1:A:410:GLU:CG	1:A:416:MSE:HE2	2.25	0.53
1:B:248:LEU:HD22	1:B:315:ILE:CD1	2.39	0.53
1:B:95:ASN:HB3	1:B:283:MSE:CE	2.38	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
4:L:7:ILE:HG21	4:L:46:LEU:HD13	1.90	0.53
1:A:122:PHE:O	1:A:128:ARG:NH2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:225[A]:PHE:C	1:B:225[A]:PHE:CD1	2.82	0.53
1:B:273:LEU:O	1:B:274:SER:C	2.46	0.53
4:L:80:ASP:CB	4:L:83:HIS:H	2.21	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:C:126:LEU:C	2:C:128:HIS:N	2.63	0.53
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: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
1:A:87:ASN:HB3	1:B:87:ASN:ND2	2.24	0.52
1:A:259:GLN:HE22	1:A:316:ARG:H	1.55	0.52
1:B:294:ALA:O	1:B:298:TYR:HB2	2.09	0.52
4:L:73:ILE:HG12	4:L:86:LEU:CD1	2.10	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
1:A:27:TYR:CD2	2:C:200:LYS:HB2	2.45	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
2:C:329:ARG:HD3	2:C:329:ARG:C	2.29	0.52
4:L:24:GLU:OE2	4:L:56:LYS:HE3	2.09	0.52
1:A:167:ASP:OD1	1:A:176:LYS:CE	2.58	0.52
1:A:138:GLU:OE1	1:A:199:GLU:OE1	2.26	0.52
1:B:225[B]:PHE:CE2	1:B:229:ALA:HB2	2.45	0.52
2:C:188:TYR:O	2:C:189:TRP:C	2.48	0.52
3:F:3:VAL:HG13	3:F:4:ASN:N	2.25	0.52
4:L:44:LYS:O	4:L:87:GLU:HB2	2.09	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
2:D:121:ARG:CZ	2:D:194:MSE:HE3	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:59:LYS:HB3	3:F:60:PRO:HD3	1.92	0.51
4:L:44:LYS:O	4:L:45:ARG:HB2	2.10	0.51
1:A:241:LEU:HD11	1:A:245:LYS:NZ	2.25	0.51
2:C:87:ASN:ND2	2:C:87:ASN:C	2.64	0.51
2:D:123:LEU:O	2:D:124:VAL:C	2.49	0.51
2:D:249:LEU:HD23	2:D:249:LEU:N	2.24	0.51
4:L:6:PHE:CZ	4:L:74:ALA:HB2	2.45	0.51
2:C:322:LYS:HA	2:C:326:LEU:O	2.10	0.51
2:D:118:GLN:HE22	2:D:241:GLN:CG	2.23	0.51
2:D:29:ALA:HB1	2:D:33:GLN:OE1	2.10	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:309:GLY:O	2:C:310:LEU:C	2.48	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
4:L:22:VAL:HG11	4:L:40:ILE:HD13	1.93	0.51
4:L:7:ILE:CG2	4:L:46:LEU:HD13	2.41	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
4:L:10:GLN:HB2	4:L:12:ASN:HD22	1.75	0.51
1:B:342:TYR:HA	1:B:344:GLN:HE22	1.76	0.51
1:B:164:HIS:CE1	1:B:474:TYR:O	2.64	0.51
4:L:4:LEU:HD12	4:L:41:GLN:OE1	2.10	0.51
1:A:143:GLN:HE22	2:C:151:GLN:NE2	2.09	0.50
2:C:157:GLY:C	2:C:158:MSE:HE2	2.31	0.50
2:C:229:LEU:HD22	2:C:310:LEU:HD13	1.91	0.50
1:A:210:PHE:HB3	1:A:211:MSE:CE	2.40	0.50
1:A:68:LYS:NZ	8:A:516:HOH:O	2.43	0.50
1:B:230:GLN:C	1:B:232:ASP:H	2.13	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:198:MSE:CA	2:C:296:ALA:HB1	2.40	0.50
4:L:48:ILE:HG23	4:L:84:PHE:CB	2.38	0.50
1:A:244:ILE:HD12	1:A:245:LYS:N	2.27	0.50
2:C:126:LEU:O	2:C:128:HIS:N	2.44	0.50
2:C:121:ARG:NH2	2:C:194:MSE:HE3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:SER:HB3	3:F:7:TYR:CE2	2.45	0.50
1:A:145:GLN:O	1:A:149:MSE:HG2	2.11	0.50
4:L:11:ASP:HB2	4:L:37:MSE:N	2.26	0.50
4:L:4:LEU:HD12	4:L:41:GLN:HB2	1.94	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
4:L:66:MSE:HE3	4:L:70:VAL:HG11	1.91	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
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:26:THR:CB	2:D:199:ARG:NH2	2.76	0.49
2:C:121:ARG:CZ	2:C:194:MSE:HE3	2.42	0.49
2:D:75:ASP:CG	2:D:77:ARG:HE	2.16	0.49
1:B:462:CYS:O	1:B:470:VAL:HG22	2.12	0.49
2:C:283:GLN:CA	2:C:283:GLN:NE2	2.75	0.49
4:L:45:ARG:HA	4:L:86:LEU:O	2.12	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
2:C:289:TRP:O	2:C:290:GLU:C	2.51	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:D:217:VAL:HA	2:D:221:LEU:HD12	1.93	0.49
4:L:23:MSE:SE	4:L:31:MSE:HE2	2.62	0.49
1:B:129:VAL:HG23	1:B:130:ALA:N	2.27	0.49
7:B:515:MOO:O4	7:B:515:MOO:O2	2.31	0.49
2:D:171:ALA:CB	2:D:182:LEU:HD13	2.43	0.49
2:C:171:ALA:HB3	2:C:182:LEU:CD1	2.41	0.49
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:O1	7:B:515:MOO:O3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:HB1	1:A:239:LEU:HD13	1.95	0.48
1:A:287:LYS:N	1:A:287:LYS:HD3	2.27	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
4:L:5:VAL:O	4:L:41:GLN:HA	2.12	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
7:B:515:MOO:O3	7:B:515:MOO:O2	2.32	0.48
2:C:126:LEU:C	2:C:128:HIS:H	2.17	0.48
2:D:286:ILE:HD13	2:D:321:LEU:HD13	1.95	0.48
1:A:446:LYS:NZ	2:C:50:GLN:HE22	2.12	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
2:D:147:THR:O	2:D:148:THR:C	2.50	0.48
1:B:26:THR:HB	2:D:199:ARG:HH22	1.78	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
4:L:34:GLN:O	4:L:35:PRO:C	2.52	0.48
1:A:220:MSE:HE1	1:B:79:PHE:N	2.29	0.48
1:B:225[A]:PHE:O	1:B:227:PHE:N	2.47	0.48
1:B:92:ARG:HG2	1:B:486:TYR:CD2	2.49	0.48
2:C:63:THR:O	2:C:66:ARG:NH2	2.46	0.48
1:A:483:ASN:HA	1:A:483:ASN:HD22	1.18	0.47
1:B:122:PHE:CZ	1:B:187:PRO:HB2	2.48	0.47
1:B:59:ASP:N	1:B:59:ASP:OD1	2.47	0.47
1:A:342:TYR:HA	1:A:344:GLN:NE2	2.28	0.47
1:B:204:ASN:HD22	1:B:204:ASN:N	2.13	0.47
1:B:68:LYS:CG	4:L:68:ILE:HD12	2.44	0.47
2:C:310:LEU:HA	2:C:310:LEU:HD12	1.49	0.47
2:C:69:ASP:O	2:C:70:TRP:C	2.52	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: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:C:329:ARG:CD	2:C:329:ARG:C	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:22:VAL:HG13	4:L:23:MSE:N	2.29	0.47
1:A:356:GLU:N	1:A:356:GLU:OE2	2.38	0.47
1:B:290:SER:O	1:B:291:TRP:C	2.53	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
2:C:310:LEU:O	2:C:313:ALA:HB3	2.14	0.47
4:L:41:GLN:HG3	4:L:41:GLN:H	1.62	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
4:L:22:VAL:HG11	4:L:40:ILE:CD1	2.44	0.47
1:B:89:SER:N	1:B:217:ASN:O	2.44	0.47
1:B:71:LYS:O	1:B:75:ILE:HG13	2.15	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:B:212:SER:HA	4:L:35:PRO:CB	2.38	0.47
1:B:192:THR:O	1:B:192:THR:HG22	2.15	0.46
1:B:95:ASN:HB2	1:B:283:MSE:CE	2.45	0.46
1:B:283:MSE:O	1:B:285:PRO:HD3	2.14	0.46
1:A:330:HIS:O	1:A:331:LEU:C	2.53	0.46
1:B:104:ILE:O	1:B:105:SER:C	2.48	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:328:SER:O	2:C:329:ARG:HB2	2.14	0.46
2:C:92:GLN:C	2:C:92:GLN:OE1	2.54	0.46
4:L:52:THR:CG2	4:L:53:MSE:H	2.27	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:HG2	1:B:13:LYS:O	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
4:L:75:GLY:HA3	4:L:86:LEU:CD2	2.45	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:171:ALA:O	2:D:172:LEU:C	2.54	0.46
2:D:189:TRP:CZ2	2:D:199:ARG:HG3	2.50	0.46

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:LYS:HB3	2:D:305:VAL:HG11	1.98	0.46
3:F:47:GLY:O	3:F:48:MSE:C	2.54	0.46
4:L:58:GLY:O	4:L:59:ARG:HB3	2.15	0.46
1:B:203:THR:CG2	1:B:204:ASN:N	2.68	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:A:33:ILE:HG22	1:A:34:PHE:CG	2.51	0.46
1:B:341:GLN:NE2	1:B:392:ASN:HD22	2.11	0.46
1:B:168:ARG:HB3	1:B:474:TYR:CE1	2.51	0.46
1:A:97:LEU:CB	1:A:149:MSE:HE1	2.33	0.46
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.82	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:341:GLN:HE22	3:E:37:CYS:N	2.01	0.45
1:B:355:LYS:HG3	1:B:355:LYS:H	1.57	0.45
4:L:45:ARG:HD2	4:L:87:GLU:OE2	2.16	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:206:LEU:HD13	1:B:207:PHE:CD2	2.48	0.45
1:B:99:LEU:HD21	1:B:210:PHE:HZ	1.81	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
1:B:458:TYR:C	1:B:460:GLY:N	2.67	0.45
1:B:494:HIS:O	1:B:495:TRP:C	2.55	0.45
2:C:57:LEU:O	2:C:58:ASN:C	2.54	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
4:L:50:ARG:HB3	4:L:50:ARG:CZ	2.47	0.45
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.67	0.45
1:B:303:GLY:C	1:B:305:ALA:N	2.69	0.45
1:B:348:PHE:CD1	1:B:348:PHE:C	2.89	0.45
1:B:358:MSE:O	1:B:362:SER:N	2.48	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
3:F:34:LEU:O	3:F:35:LEU:C	2.55	0.45
1:B:308:LYS:C	1:B:310:LEU:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:VAL:O	2:D:247:SER:C	2.55	0.45
4:L:23:MSE:CG	4:L:31:MSE:CE	2.94	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
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:B:455:HIS:CD2	3:E:15:ASP:OD2	2.61	0.45
4:L:6:PHE:CD2	4:L:7:ILE:N	2.85	0.45
1:A:160:HIS:CE1	1:A:482:ASP:OD1	2.70	0.45
1:A:50:TRP:HZ3	1:A:243:VAL:HG23	1.81	0.45
1:B:244:ILE:C	1:B:244:ILE:HD12	2.37	0.45
1:B:169:VAL:HG22	1:B:475:TYR:CG	2.52	0.45
2:C:234:MSE:HE3	2:C:234:MSE:HB2	1.96	0.45
2:C:194:MSE:CG	2:C:299:PRO:HB2	2.47	0.45
1:B:312:ARG:NE	4:L:89:ASN:HD22	2.15	0.45
1:A:172:LEU:C	1:A:175:PRO:HD2	2.37	0.45
1:A:85:HIS:O	1:A:88:ILE:HG12	2.16	0.45
1:B:101:ILE:HA	1:B:105:SER:OG	2.16	0.45
2:C:115:THR:O	2:C:116:GLN:C	2.54	0.45
2:C:190:MSE:CA	2:C:190:MSE:CE	2.89	0.45
2:C:108:LEU:HD21	2:C:246:VAL:HG13	1.99	0.45
2:C:59:ASP:HA	2:C:60:PRO:HD3	1.79	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
3:F:117:ALA:O	3:F:118:GLY:C	2.55	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
1:A:224:THR:O	1:A:225:PHE:C	2.53	0.44
1:B:382:LYS:O	1:B:383:GLU:C	2.55	0.44
2:C:151:GLN:HG3	2:C:155:TYR:CE1	2.52	0.44
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:C:311:ASN:C	2:C:313:ALA:N	2.70	0.44
2:D:227:TYR:CD2	2:D:231:TYR:HD1	2.34	0.44
2:D:301:ALA:O	2:D:302:GLU:C	2.54	0.44
2:C:246:VAL:O	2:C:247:SER:C	2.53	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:B:230:GLN:CD	1:B:233:GLU:HG3	2.37	0.44
1:B:65:GLN:NE2	1:B:68:LYS:HE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:GLU:O	2:C:118:GLN:HG3	2.18	0.44
2:C:73:VAL:CG1	2:C:267:MSE:HB2	2.48	0.44
2:C:53:SER:HA	3:F:7:TYR:CE2	2.53	0.44
1:A:455:HIS:HE1	3:F:27:TYR:OH	1.96	0.44
1:A:276:VAL:O	1:A:277:SER:C	2.54	0.44
1:A:407:ILE:HG21	1:A:407:ILE:HD13	1.72	0.44
4:L:25:ASP:OD2	4:L:25:ASP:N	2.50	0.44
2:C:93:GLU:OE1	2:C:93:GLU:CA	2.66	0.44
2:D:75:ASP:CB	2:D:152:MSE:CE	2.83	0.44
1:A:134:GLN:O	1:A:135:ALA:C	2.56	0.44
1:B:129:VAL:CG2	1:B:130:ALA:N	2.81	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
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:C:243:ALA:O	2:C:244:GLU:C	2.56	0.44
2:D:45:PHE:CZ	2:D:58:ASN:HB2	2.52	0.44
4:L:66:MSE:CE	4:L:70:VAL:HG11	2.48	0.44
1:A:374:ARG:HB3	1:A:375:PRO:HD3	1.99	0.43
2:C:131:LEU:HG	2:C:131:LEU:O	2.17	0.43
3:F:81:ASN:HD21	3:F:102:SER:HB3	1.82	0.43
1:A:144:THR:CG2	1:A:225:PHE:CE1	3.02	0.43
1:A:233:GLU:O	1:A:234:ALA:C	2.56	0.43
1:A:36:GLU:HB2	8:A:544:HOH:O	2.18	0.43
1:B:388:ARG:O	1:B:389:ARG:C	2.53	0.43
2:C:40:GLU:HG3	2:C:40:GLU:H	1.45	0.43
3:E:74:LEU:O	3:E:74:LEU:HD22	2.18	0.43
4:L:6:PHE:C	4:L:7:ILE:HG22	2.38	0.43
1:A:27:TYR:N	1:A:27:TYR:CD1	2.86	0.43
1:A:319:LYS:O	1:A:320:TYR:CB	2.62	0.43
1:B:204:ASN:HD22	1:B:204:ASN:H	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
4:L:19:ALA:O	4:L:20:GLU:C	2.57	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
4:L:6:PHE:HD2	4:L:7:ILE:N	2.16	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: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: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:309:GLY:O	2:C:312:GLU:N	2.51	0.43
1:A:66:ALA:CB	2:C:89:ALA:HB2	2.48	0.43
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.50	0.43
1:B:210:PHE:CZ	1:B:279:MSE:HG2	2.53	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:D:182:LEU:HA	2:D:182:LEU:HD12	1.80	0.43
4:L:6:PHE:CD2	4:L:6:PHE:C	2.91	0.43
1:A:214:ALA:CB	1:A:219:ASP:HB3	2.47	0.43
1:A:25:PRO:HA	2:C:203:GLU:OE1	2.19	0.43
4:L:48:ILE:HG23	4:L:84:PHE:HB2	1.96	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:A:44:ILE:HG23	1:A:44:ILE:HD12	1.73	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
4:L:41:GLN:O	4:L:42:ALA:HB2	2.19	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:C:311:ASN:C	2:C:313:ALA:H	2.21	0.43
2:C:81:TYR:C	2:C:81:TYR:CD2	2.92	0.43
2:D:120:LEU:O	2:D:125:PRO:HD3	2.18	0.43
2:D:261:LEU:HA	2:D:261:LEU:HD12	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
4:L:52:THR:O	4:L:55:GLU:HG3	2.19	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:O1	7:B:515:MOO:O2	2.37	0.42
2:C:329:ARG:HD3	2:C:330:GLY:H	1.76	0.42
4:L:47:VAL:HG22	4:L:48:ILE:N	2.34	0.42
1:B:271:ARG:NH1	1:B:408:PHE:CD1	2.87	0.42
1:B:11:LYS:HE3	1:B:51:GLU:OE2	2.20	0.42
2:C:225:MSE:HE1	2:C:294:TYR:CB	2.46	0.42
2:D:71:CYS:C	2:D:73:VAL:N	2.70	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:280:MSE:HE3	1:B:280:MSE:HB2	1.95	0.42
1:B:311:GLU:O	1:B:312:ARG:C	2.56	0.42
1:B:70:LYS:HB2	1:B:70:LYS:HE2	1.55	0.42
4:L:16:ARG:O	4:L:20:GLU:HB2	2.19	0.42
1:B:188:PHE:O	1:B:189:GLU:C	2.56	0.42
1:B:225[B]:PHE:C	1:B:225[B]:PHE:CD1	2.92	0.42
2:C:190:MSE:CE	2:C:199:ARG:CZ	2.98	0.42
2:C:91:MSE:HE2	2:C:252:PHE:CD1	2.54	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
4:L:54:GLU:C	4:L:56:LYS:H	2.22	0.42
1:B:231:SER:CB	4:L:70:VAL:O	2.68	0.42
1:B:274:SER:HB2	1:B:335:LEU:CD1	2.30	0.42
1:B:49:GLN:NE2	1:B:49:GLN:CA	2.80	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:398:LEU:HD11	1:B:454:VAL:HG23	2.02	0.42
1:B:57:THR:O	1:B:58:MSE:C	2.56	0.42
2:C:65:ILE:HG22	2:C:66:ARG:N	2.35	0.42
1:B:289:MSE:CE	4:L:34:GLN:HE22	2.32	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
4:L:21:ALA:O	4:L:25:ASP:OD2	2.38	0.42
4:L:6:PHE:H	4:L:74:ALA:HB3	1.84	0.42
1:A:44:ILE:HG21	1:A:47:TRP:NE1	2.35	0.42
1:A:497:SER:O	1:A:498:ILE:C	2.58	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
8:A:533:HOH:O	2:C:41:ALA:HA	2.20	0.42
2:D:39:ILE:HA	2:D:39:ILE:HD13	1.80	0.42
3:F:22:GLY:N	8:F:120:HOH:O	2.52	0.42
4:L:31:MSE:HE2	4:L:31:MSE:HB2	2.01	0.42
4:L:61:TRP:CZ2	4:L:66:MSE:HB2	2.52	0.42
1:B:143:GLN:O	1:B:146:GLN:HB2	2.20	0.42
1:B:203:THR:O	1:B:204:ASN:C	2.57	0.42
1:B:225[B]:PHE:C	1:B:227:PHE:N	2.71	0.42
2:C:14:ARG:NH1	8:C:357:HOH:O	2.53	0.42
2:D:315:ALA:O	2:D:316:GLU:C	2.56	0.42
2:D:59:ASP:HA	2:D:60:PRO:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:HB2	4:L:88:TRP:CH2	2.55	0.42
1:B:268:ARG:O	1:B:269:GLY:C	2.58	0.42
2:C:201:LEU:HD12	2:C:201:LEU:O	2.20	0.42
2:C:49:PRO:HB3	2:C:51:TRP:CE2	2.55	0.42
1:A:181:ASP:OD1	1:A:264:LYS:NZ	2.53	0.41
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
2:C:146:ALA:O	2:C:147:THR:C	2.57	0.41
2:C:233:LYS:O	2:C:234:MSE:C	2.56	0.41
2:D:166:TYR:O	2:D:167:LEU:C	2.56	0.41
1:A:161:ASP:CB	1:A:165:MSE:HE3	2.50	0.41
1:A:72:LEU:HD12	1:A:224:THR:HG22	2.01	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: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
1:A:169:VAL:O	1:A:170:TRP:C	2.58	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
4:L:43:GLU:HA	4:L:43:GLU:OE1	2.20	0.41
4:L:43:GLU:O	4:L:45:ARG:N	2.53	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
1:B:65:GLN:HE22	1:B:68:LYS:HZ3	1.68	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
4:L:31:MSE:HG2	4:L:33:HIS:CE1	2.55	0.41
4:L:52:THR:HG22	4:L:53:MSE:H	1.75	0.41
1:A:121:GLN:HB3	8:A:544:HOH:O	2.21	0.41
1:A:88:ILE:HG13	1:A:495:TRP:CH2	2.56	0.41
1:B:199:GLU:HG2	1:B:236:HIS:HB3	2.02	0.41
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.88	0.41
1:B:117:LYS:HE2	2:D:51:TRP:CZ3	2.55	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:HB2	2:D:234:MSE:CE	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:B:78:ALA:O	1:B:79:PHE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:O	1:B:89:SER:C	2.58	0.41
1:B:301:GLN:O	1:B:302[A]:ASN:C	2.59	0.41
2:C:298:LYS:O	2:C:301:ALA:HB3	2.20	0.41
1:A:66:ALA:HB2	2:C:89:ALA:HB2	2.03	0.41
3:E:83:GLU:HA	3:E:84:PRO:HD3	1.90	0.41
1:B:339:PHE:O	1:B:340:TYR:C	2.59	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:C:27:LYS:HB2	2:C:28:PRO:CD	2.43	0.41
2:C:40:GLU:CG	2:C:147:THR:OG1	2.69	0.41
2:D:52:ASP:OD2	2:D:55:HIS:CD2	2.73	0.41
1:A:379:TYR:HD1	3:F:114:MSE:HE1	1.86	0.41
1:B:238:THR:HG21	4:L:77:VAL:HG21	2.02	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:452:LEU:CD1	1:A:452:LEU:N	2.84	0.41
2:C:158:MSE:HE2	2:C:158:MSE:N	2.35	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
2:D:73:VAL:HG11	2:D:149:VAL:HG22	2.02	0.41
3:F:59:LYS:HB3	3:F:60:PRO:CD	2.51	0.41
4:L:33:HIS:O	4:L:34:GLN:HG2	2.19	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:478:ASN:O	1:A:479:ILE:C	2.57	0.40
1:A:446:LYS:HE3	2:C:50:GLN:NE2	2.36	0.40
2:D:281:LEU:HD23	2:D:281:LEU:HA	1.78	0.40
1:A:107:LEU:O	1:A:108:GLU:C	2.59	0.40
1:A:112:PHE:CD1	1:A:139:LEU:HB2	2.56	0.40
1:B:277:SER:O	1:B:278:MSE:C	2.58	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: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:244:ILE:O	1:B:245:LYS:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:THR:O	2:D:151:GLN:HB3	2.20	0.40
2:D:103:GLU:HG3	2:D:173:MSE:SE	2.72	0.40
2:D:304:SER:HB3	2:D:305:VAL:H	1.44	0.40
2:D:53:SER:HB3	3:E:7:TYR:CD2	2.56	0.40
3:E:15:ASP:O	3:E:16:LYS:C	2.60	0.40
3:F:8:ASP:OD2	3:F:10:LYS:HD2	2.21	0.40
3:F:33:HIS:HD2	3:F:65:HIS:CE1	2.40	0.40
4:L:5:VAL:HG22	4:L:45:ARG:N	2.36	0.40
1:A:292:SER:O	1:A:296:GLU:HB2	2.21	0.40
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.41	0.40
1:A:349:HIS:HB3	1:A:486:TYR:N	2.36	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
1:B:24:GLU:HA	1:B:25:PRO:HD2	1.85	0.40
2:C:12:PRO:HD2	8:C:379:HOH:O	2.19	0.40
2:C:17:TYR:O	2:C:18:GLY:C	2.59	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
4:L:80:ASP:OD1	4:L:83:HIS:CE1	2.74	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:225[A]:PHE:CD1	1:B:226:GLY:HA2	2.56	0.40
1:B:408:PHE:HD1	1:B:432:CYS:HB2	1.86	0.40
1:B:44:ILE:HD12	1:B:250:GLN:HG2	2.04	0.40
3:E:111:LEU:HA	3:E:111:LEU:HD23	1.80	0.40
3:F:54:VAL:HG12	3:F:54:VAL:O	2.21	0.40
4:L:31:MSE:CE	4:L:31:MSE:HB2	2.52	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%)	15	37
1	B	494/511 (97%)	416 (84%)	60 (12%)	18 (4%)	3	7
2	C	317/333 (95%)	271 (86%)	38 (12%)	8 (2%)	5	14
2	D	323/333 (97%)	298 (92%)	21 (6%)	4 (1%)	13	32
3	E	116/119 (98%)	107 (92%)	8 (7%)	1 (1%)	17	40
3	F	116/119 (98%)	95 (82%)	18 (16%)	3 (3%)	5	13
4	L	85/89 (96%)	55 (65%)	15 (18%)	15 (18%)	0	0
All	All	1945/2015 (96%)	1686 (87%)	205 (10%)	54 (3%)	5	11

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

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Mol	Chain	Res	Type
2	C	315	ALA
2	D	72	ALA
2	D	325	GLU
3	E	16	LYS
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 (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	433/431 (100%)	389 (90%)	44 (10%)	7	17
1	B	435/431 (101%)	386 (89%)	49 (11%)	6	13
2	C	272/268 (102%)	230 (85%)	42 (15%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	D	279/268 (104%)	250 (90%)	29 (10%)	7	16	
3	E	98/94 (104%)	87 (89%)	11 (11%)	6	13	
3	F	98/94 (104%)	82 (84%)	16 (16%)	2	6	
4	L	79/75 (105%)	58 (73%)	21 (27%)	0	1	
All	All	1694/1661 (102%)	1482 (88%)	212 (12%)	4	10	

All (212) 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	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	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	277	SER
1	A	289	MSE
1	A	296	GLU
1	A	308	LYS
1	A	312	ARG
1	A	335	LEU

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Mol	Chain	Res	Type
1	A	344	GLN
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	425	GLU
1	A	445	GLU
1	A	463	GLU
1	A	483	ASN
1	B	7	LYS
1	B	10	LEU
1	B	15	GLN
1	B	16	TYR
1	B	17	LEU
1	B	18	THR
1	B	19	ARG
1	B	30	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	118	VAL
1	B	146	GLN
1	B	159	LEU
1	B	179	PHE
1	B	199	GLU
1	B	200	TYR
1	B	204	ASN
1	B	206	LEU
1	B	208	VAL
1	B	225[A]	PHE
1	B	225[B]	PHE
1	B	237	MSE
1	B	238	THR

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Mol	Chain	Res	Type
1	B	241	LEU
1	B	242	GLU
1	B	277	SER
1	B	278	MSE
1	B	279	MSE
1	B	302[A]	ASN
1	B	302[B]	ASN
1	B	306	LEU
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	412	ASP
1	B	417	LEU
1	B	445	GLU
1	B	493	LYS
1	B	498	ILE
2	C	14	ARG
2	C	27	LYS
2	C	40	GLU
2	C	47	TYR
2	C	57	LEU
2	C	87	ASN
2	C	92	GLN
2	C	93	GLU
2	C	104	LYS
2	C	112	SER
2	C	117	LYS
2	C	122	LEU
2	C	127	ARG
2	C	131	LEU
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

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Mol	Chain	Res	Type
2	C	207	VAL
2	C	241	GLN
2	C	246	VAL
2	C	253	MSE
2	C	261	LEU
2	C	267	MSE
2	C	276	GLU
2	C	277	THR
2	C	279	ARG
2	C	280	GLU
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	C	329	ARG
2	D	6	LYS
2	D	7	THR
2	D	14	ARG
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	177	SER
2	D	182	LEU
2	D	193	GLU
2	D	207	VAL
2	D	215	THR
2	D	234	MSE
2	D	238	PHE
2	D	253	MSE
2	D	261	LEU
2	D	269	LYS
2	D	277	THR
2	D	279	ARG

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Mol	Chain	Res	Type
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	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	6	LEU
3	F	26	LEU
3	F	35	LEU
3	F	44	VAL
3	F	48	MSE
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	12	ASN
4	L	20	GLU
4	L	25	ASP
4	L	30	GLU
4	L	31	MSE
4	L	32	GLN
4	L	41	GLN
4	L	50	ARG

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Mol	Chain	Res	Type
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	73	ILE
4	L	86	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	49	GLN
1	A	81	GLN
1	A	153	ASN
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	87	ASN
1	B	160	HIS
1	B	164	HIS
1	B	204	ASN
1	B	330	HIS
1	B	341	GLN
1	B	344	GLN
1	B	400	GLN

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Mol	Chain	Res	Type
1	B	455	HIS
1	B	476	HIS
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
2	C	219	ASN
2	C	241	GLN
2	C	288	HIS
2	C	292	GLN
2	D	8	ASN
2	D	46	HIS
2	D	50	GLN
2	D	55	HIS
2	D	136	ASN
2	D	137	ASN
2	D	151	GLN
2	D	165	GLN
2	D	219	ASN
2	D	327	GLN
3	F	4	ASN
3	F	96	GLN
4	L	10	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 carbohydrates 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	14.03	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	-14.51	1.43	1.73
7	B	515	MOO	O1-MO	-13.52	1.45	1.73

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%)	-0.61	2 (0%)	92	93	17, 32, 47, 61	0
1	B	477/511 (93%)	-0.57	3 (0%)	89	91	18, 32, 57, 69	0
2	C	303/333 (90%)	-0.54	2 (0%)	87	89	17, 34, 55, 74	0
2	D	309/333 (92%)	-0.60	1 (0%)	94	95	18, 34, 52, 73	0
3	E	114/119 (95%)	-0.44	0	100	100	20, 34, 45, 50	0
3	F	114/119 (95%)	-0.34	0	100	100	30, 48, 62, 64	0
4	L	82/89 (92%)	1.02	13 (15%)	1	1	23, 39, 48, 50	82 (100%)
All	All	1879/2015 (93%)	-0.49	21 (1%)	80	82	17, 34, 55, 74	82 (4%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	81	ASP	3.1
4	L	27	PRO	3.0
4	L	54	GLU	2.9
4	L	4	LEU	2.9
4	L	60	ASP	2.9
4	L	89	ASN	2.9
4	L	55	GLU	2.8
4	L	51	GLU	2.7
1	B	493	LYS	2.7
1	A	5	ASN	2.7
4	L	68	ILE	2.5
4	L	62	ASP	2.5
1	B	496	LEU	2.4
2	C	129	VAL	2.4
2	D	10	VAL	2.3
4	L	80	ASP	2.3
4	L	71	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	6	LYS	2.1
1	A	4	LYS	2.1
2	C	133	ALA	2.1
4	L	69	ASN	2.1

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 carbohydrates 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
7	MOO	B	515	5/5	0.84	0.60	84,86,87,88	0
5	FE	A	513	1/1	0.98	0.11	37,37,37,37	0
5	FE	B	512	1/1	0.99	0.10	28,28,28,28	0
5	FE	A	512	1/1	0.99	0.07	35,35,35,35	0
6	ZN	B	514	1/1	1.00	0.10	36,36,36,36	0
6	ZN	A	514	1/1	1.00	0.09	32,32,32,32	0
5	FE	B	513	1/1	1.00	0.08	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.