



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 1XMG / pdb_00001xmg
Title : Crystal structure of apo methane monooxygenase hydroxylase from *M. capsulatus* (Bath)
Authors : Sazinsky, M.H.; Merckx, M.; Cadieux, E.; Tang, S.; Lippard, S.J.
Deposited on : 2004-10-02
Resolution : 2.10 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

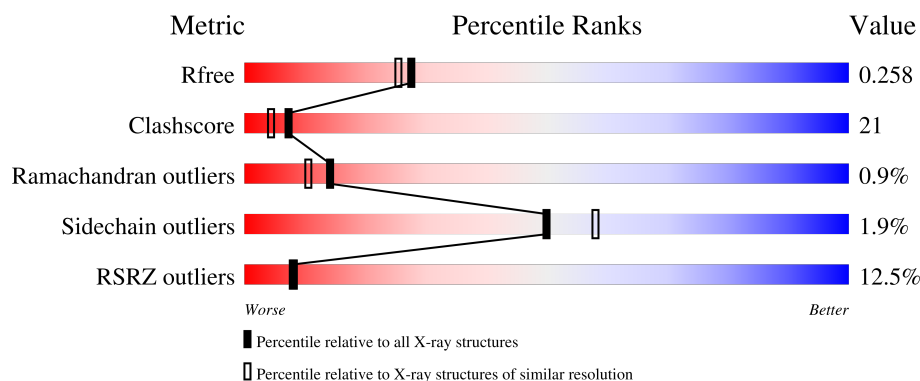
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	527	14% 62% 31% • •
1	B	527	11% 57% 36% • •
2	C	388	0% 71% 27% •
2	D	388	21% 52% 44% •
3	E	169	2% 73% 22% • •

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Mol	Chain	Length	Quality of chain
3	F	169	27% 52% 44% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18102 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4138	2649	709	762	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	18			

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3167	2038	545	576	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLU	ALA	conflict	UNP P18798
C	370	ARG	ALA	conflict	UNP P18798
D	18	GLU	ALA	conflict	UNP P18798
D	370	ARG	ALA	conflict	UNP P18798

- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

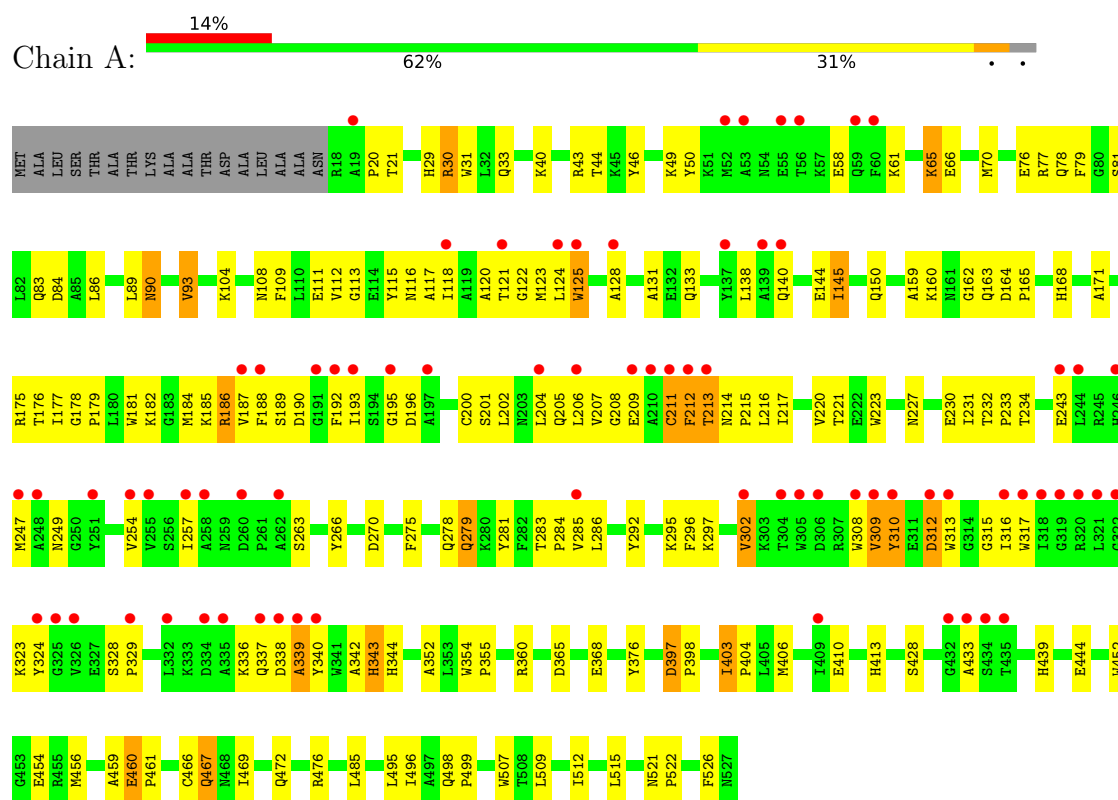
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total 156	O 156	0	0
5	B	170	Total 170	O 170	0	0
5	C	249	Total 249	O 249	0	0
5	D	86	Total 86	O 86	0	0
5	E	106	Total 106	O 106	0	0
5	F	18	Total 18	O 18	0	0

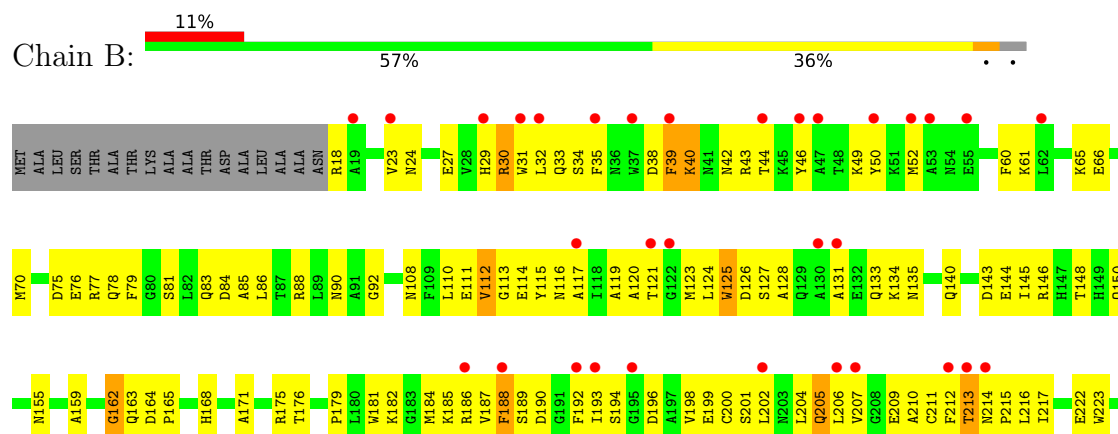
3 Residue-property plots

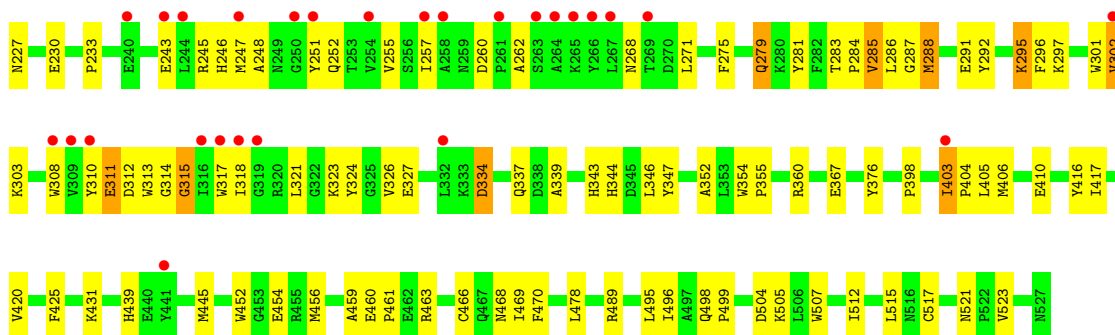
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Methane monooxygenase component A alpha chain

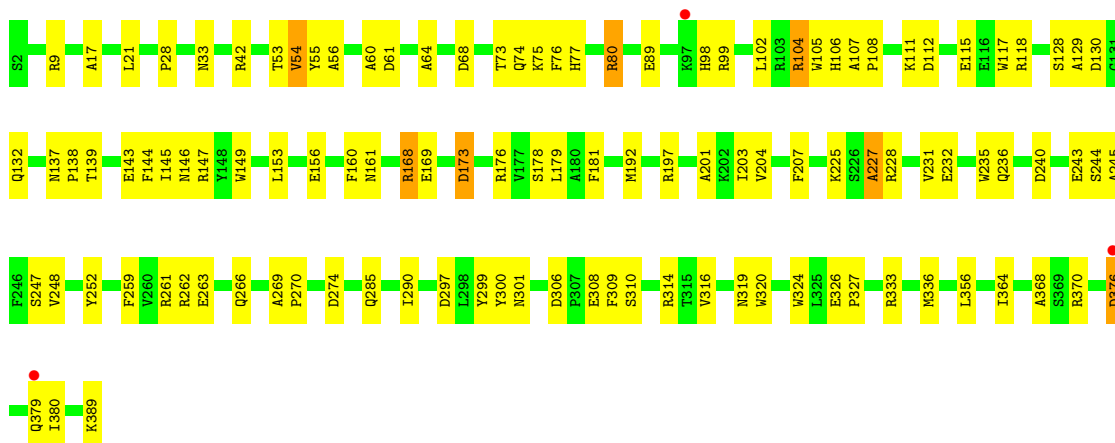


- Molecule 1: Methane monooxygenase component A alpha chain

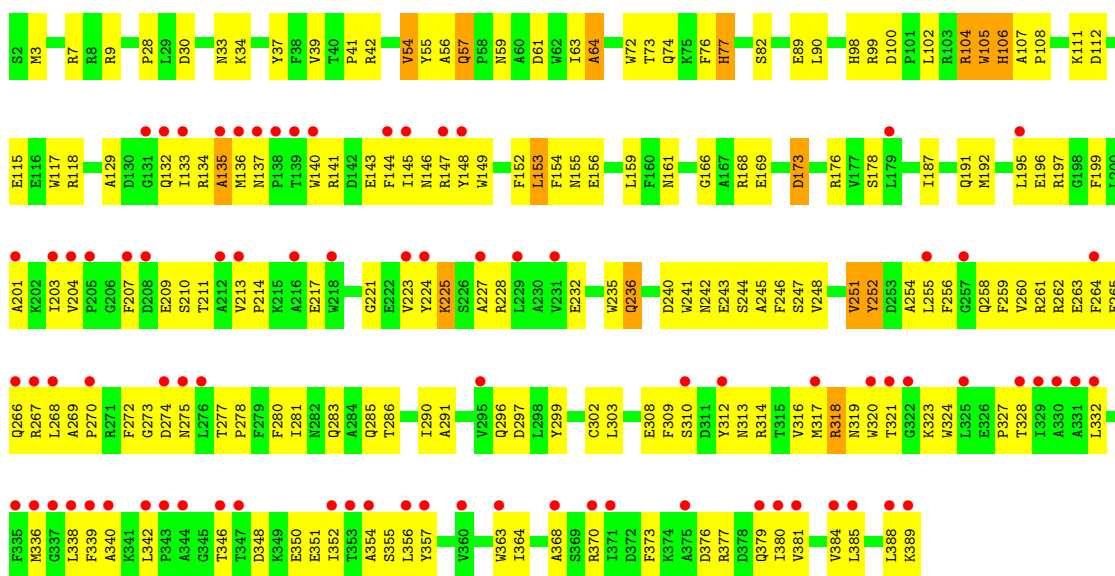




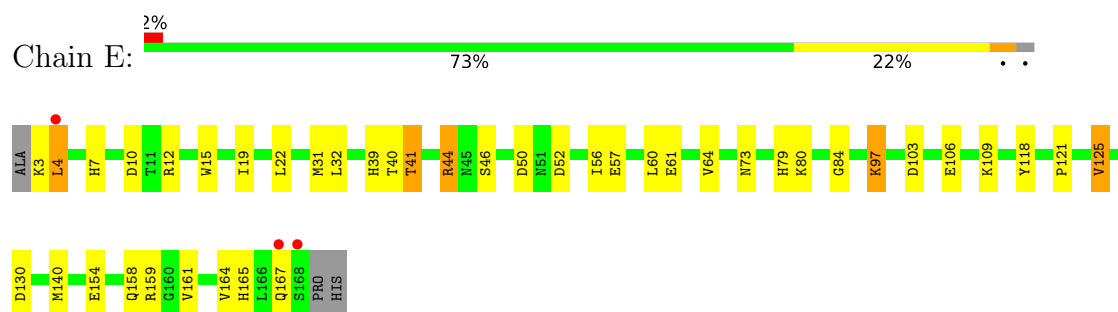
• Molecule 2: Methane monooxygenase component A beta chain



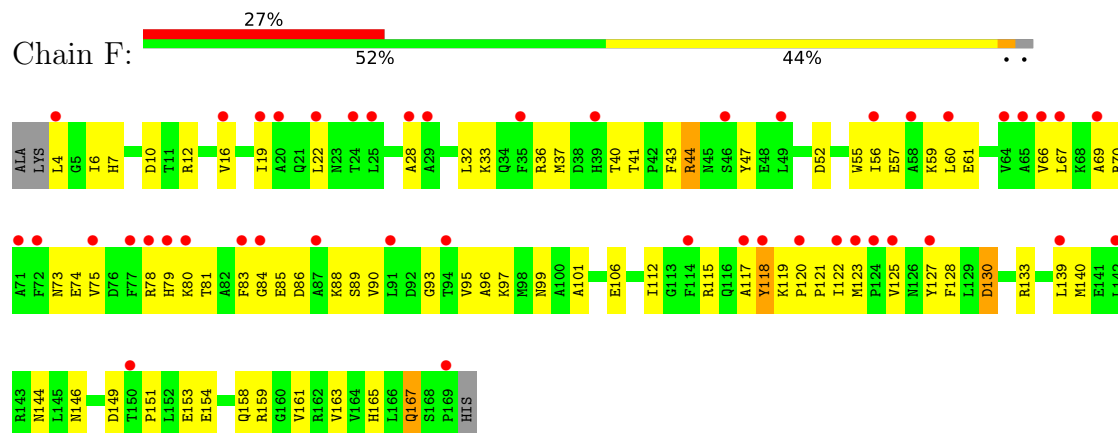
• Molecule 2: Methane monooxygenase component A beta chain



• Molecule 3: Methane monooxygenase component A gamma chain



- Molecule 3: Methane monooxygenase component A gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.35Å 171.63Å 220.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.77 – 2.10 24.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.7 (24.77-2.10) 83.7 (24.77-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.261 0.218 , 0.258	Depositor DCC
R_{free} test set	4360 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18102	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/4263	0.95	22/5797 (0.4%)
1	B	0.39	1/4262 (0.0%)	0.90	14/5796 (0.2%)
2	C	0.44	0/3263	0.91	13/4435 (0.3%)
2	D	0.37	0/3247	0.87	14/4417 (0.3%)
3	E	0.42	0/1392	0.92	7/1876 (0.4%)
3	F	0.33	0/1387	0.84	3/1873 (0.2%)
All	All	0.39	1/17814 (0.0%)	0.90	73/24194 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	MET	SD-CE	-5.92	1.64	1.79

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	7.62	119.37	111.14
1	B	285	VAL	N-CA-C	7.33	117.46	110.42
3	E	130	ASP	N-CA-C	-7.29	103.42	111.36
1	B	431	LYS	N-CA-C	-6.97	104.77	113.28
3	E	118	TYR	N-CA-C	6.96	122.63	113.30
1	B	478	LEU	N-CA-C	6.88	119.37	111.11
3	E	4	LEU	N-CA-C	6.84	118.65	110.44
2	C	149	TRP	N-CA-C	-6.82	103.92	111.36
1	B	164	ASP	CA-C-N	6.80	126.77	119.28
1	B	164	ASP	C-N-CA	6.80	126.77	119.28
3	F	6	ILE	N-CA-C	6.80	116.92	110.53
2	D	236	GLN	N-CA-C	6.69	121.61	113.38
2	D	105	TRP	N-CA-C	-6.60	100.20	110.17
1	A	397	ASP	CA-C-N	6.39	126.07	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ASP	C-N-CA	6.39	126.07	119.56
1	A	496	ILE	N-CA-C	-6.34	104.57	110.53
1	A	145	ILE	N-CA-C	-6.26	104.18	111.00
3	E	73	ASN	N-CA-C	-6.14	102.61	110.53
1	A	309	VAL	N-CA-C	6.08	117.55	110.62
1	A	460	GLU	CA-C-N	6.07	125.55	119.24
1	A	460	GLU	C-N-CA	6.07	125.55	119.24
1	A	164	ASP	CA-C-N	6.06	125.74	119.56
1	A	164	ASP	C-N-CA	6.06	125.74	119.56
1	B	496	ILE	N-CA-C	-6.05	104.84	110.53
3	F	118	TYR	N-CA-C	6.01	120.32	112.92
2	C	106	HIS	N-CA-C	6.00	118.31	111.11
1	A	168	HIS	N-CA-C	-5.98	104.84	111.36
1	A	212	PHE	CA-C-N	5.97	128.20	120.44
1	A	212	PHE	C-N-CA	5.97	128.20	120.44
2	D	56	ALA	N-CA-C	-5.97	104.85	111.36
2	C	105	TRP	N-CA-C	-5.90	101.26	110.17
2	D	252	TYR	N-CA-C	5.89	117.37	111.07
2	C	236	GLN	N-CA-C	5.88	120.61	113.38
2	C	104	ARG	N-CA-C	5.82	117.69	108.67
2	C	56	ALA	N-CA-C	-5.79	105.11	111.82
2	C	169	GLU	N-CA-C	5.75	120.36	113.23
1	A	213	THR	N-CA-C	5.74	117.21	111.07
3	F	130	ASP	N-CA-C	-5.72	105.12	111.36
2	D	169	GLU	N-CA-C	5.71	120.24	113.28
1	A	93	VAL	N-CA-C	5.61	116.64	111.81
2	D	54	VAL	N-CA-C	5.60	116.50	108.93
3	E	39	HIS	N-CA-C	5.60	122.01	113.61
1	B	145	ILE	N-CA-C	-5.55	105.11	110.72
1	A	178	GLY	CA-C-N	5.53	125.05	119.19
1	A	178	GLY	C-N-CA	5.53	125.05	119.19
2	C	252	TYR	N-CA-C	5.49	116.95	110.97
2	D	104	ARG	N-CA-C	5.49	117.24	108.41
2	D	106	HIS	N-CA-C	5.49	117.97	111.33
2	D	57	GLN	CA-C-N	5.48	126.69	119.84
2	D	57	GLN	C-N-CA	5.48	126.69	119.84
2	C	54	VAL	N-CA-C	5.45	116.72	109.37
2	C	53	THR	N-CA-C	5.44	120.16	112.93
1	A	104	LYS	N-CA-C	-5.40	105.39	111.28
1	A	285	VAL	N-CA-C	5.35	116.83	111.00
2	C	227	ALA	N-CA-C	-5.34	105.37	111.14
1	A	65	LYS	N-CA-C	5.19	116.93	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLY	N-CA-C	5.17	120.51	112.60
2	D	149	TRP	N-CA-C	-5.15	105.58	111.14
2	D	286	THR	N-CA-C	-5.14	105.68	111.28
1	A	211	CYS	N-CA-C	5.13	116.68	111.14
3	E	79	HIS	N-CA-C	5.12	121.30	113.61
1	B	310	TYR	N-CA-C	5.12	116.72	111.03
1	B	148	THR	N-CA-C	-5.08	105.64	111.07
2	C	299	TYR	N-CA-C	5.06	118.60	112.23
1	B	295	LYS	N-CA-C	-5.05	105.21	112.13
2	D	77	HIS	N-CA-C	-5.05	102.44	109.96
2	C	144	PHE	N-CA-C	5.04	117.67	111.82
1	B	162	GLY	N-CA-C	5.04	120.84	112.89
1	A	122	GLY	N-CA-C	-5.03	106.63	113.37
1	B	205	GLN	N-CA-C	5.03	117.53	111.40
1	B	188	PHE	N-CA-C	5.02	118.72	112.59
3	E	161	VAL	CB-CA-C	-5.01	106.08	111.59
2	D	318	ARG	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	3897	185	0
1	B	4137	0	3888	219	0
2	C	3167	0	2987	99	0
2	D	3151	0	2957	178	0
3	E	1364	0	1352	35	0
3	F	1358	0	1335	66	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	156	0	0	16	0
5	B	170	0	0	13	0
5	C	249	0	0	15	0
5	D	86	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	106	0	0	1	0
5	F	18	0	0	0	0
All	All	18102	0	16416	695	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 21.

All (695) 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)
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.18	1.11
1:B:44:THR:HG22	1:B:46:TYR:H	1.14	1.05
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.41	1.01
1:A:243:GLU:OE1	5:A:1135:HOH:O	1.79	0.99
2:C:376:ASP:HB3	2:C:379:GLN:NE2	1.79	0.97
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.13	0.96
1:B:288:MET:HE1	1:B:346:LEU:HG	1.49	0.94
3:F:41:THR:O	3:F:44:ARG:HD2	1.69	0.92
1:A:171:ALA:O	1:A:175:ARG:HG2	1.68	0.92
1:A:243:GLU:CD	5:A:1135:HOH:O	2.12	0.91
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.33	0.91
1:A:78:GLN:HE22	1:A:150:GLN:HE21	0.94	0.91
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.51	0.91
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.72	0.88
3:E:80:LYS:HD3	3:E:84:GLY:HA2	1.55	0.88
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.18	0.88
1:B:209:GLU:HA	1:B:213:THR:OG1	1.75	0.86
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.58	0.86
1:B:18:ARG:O	2:D:129:ALA:HA	1.76	0.86
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.41	0.86
2:C:102:LEU:HD13	2:C:290:ILE:HG23	1.58	0.85
1:A:433:ALA:HB2	5:A:1152:HOH:O	1.79	0.83
1:A:243:GLU:OE2	5:A:1135:HOH:O	1.97	0.82
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.61	0.82
1:A:216:LEU:HD13	1:A:286:LEU:HD13	1.59	0.82
1:B:202:LEU:HD22	1:B:206:LEU:HD22	1.62	0.81
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.45	0.81
3:F:153:GLU:H	3:F:153:GLU:CD	1.87	0.80
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.63	0.80
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.80	0.80
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.78	0.79
1:A:175:ARG:HD3	1:A:181:TRP:CE2	2.19	0.78
1:B:175:ARG:HD3	1:B:181:TRP:CE2	2.18	0.78
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.06	0.78
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.31	0.78
1:A:44:THR:HG22	1:A:46:TYR:H	1.50	0.77
1:A:467:GLN:HG3	5:A:1086:HOH:O	1.84	0.77
2:C:333:ARG:NH1	5:C:1245:HOH:O	2.16	0.77
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.77	0.77
2:C:379:GLN:NE2	2:C:379:GLN:H	1.80	0.77
2:D:352:ILE:O	2:D:356:LEU:HD23	1.85	0.76
2:C:376:ASP:HB2	2:C:379:GLN:HB2	1.68	0.75
3:F:101:ALA:HA	3:F:106:GLU:OE2	1.85	0.75
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.69	0.75
2:D:136:MET:HE3	2:D:141:ARG:HB2	1.68	0.75
1:B:288:MET:HE1	1:B:346:LEU:CG	2.16	0.74
1:A:202:LEU:HD23	1:A:206:LEU:HD12	1.69	0.74
2:D:187:ILE:O	2:D:191:GLN:HG3	1.86	0.74
1:B:283:THR:HB	1:B:284:PRO:HD3	1.69	0.74
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.68	0.74
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.33	0.74
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.70	0.74
3:F:80:LYS:HD3	3:F:84:GLY:HA2	1.70	0.73
1:A:342:ALA:HB3	5:A:1147:HOH:O	1.87	0.73
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.86	0.73
2:D:135:ALA:O	2:D:273:GLY:HA3	1.88	0.73
3:E:97:LYS:NZ	3:E:97:LYS:HB3	2.04	0.72
1:A:338:ASP:OD1	1:A:342:ALA:HB2	1.89	0.72
2:D:153:LEU:HD12	2:D:154:PHE:N	2.04	0.71
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.20	0.71
2:C:376:ASP:CB	2:C:379:GLN:NE2	2.54	0.71
2:D:77:HIS:HB3	3:F:139:LEU:HD23	1.72	0.70
2:C:333:ARG:NH2	5:C:1243:HOH:O	2.24	0.70
3:F:151:PRO:HB2	3:F:153:GLU:OE1	1.91	0.70
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.90	0.70
2:C:111:LYS:O	2:C:115:GLU:HG3	1.92	0.70
1:A:336:LYS:C	1:A:338:ASP:H	1.99	0.70
1:B:268:ASN:HD21	1:B:327:GLU:H	1.37	0.70
1:A:113:GLY:HA3	1:A:188:PHE:HD2	1.56	0.69
2:D:377:ARG:O	2:D:381:VAL:HG23	1.91	0.69
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:342:LEU:HD22	2:D:346:THR:HG21	1.73	0.69
1:A:188:PHE:HZ	1:A:213:THR:HG1	1.37	0.69
1:B:119:ALA:HB1	2:D:168:ARG:HD2	1.75	0.69
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.73	0.69
1:B:198:VAL:O	1:B:202:LEU:HG	1.92	0.69
1:B:227:ASN:HD21	1:B:295:LYS:H	1.41	0.69
1:A:86:LEU:HD22	5:A:1140:HOH:O	1.92	0.68
1:B:406:MET:O	1:B:410:GLU:HG3	1.93	0.68
1:A:190:ASP:HB3	2:C:74:GLN:O	1.94	0.68
1:A:206:LEU:HD11	1:A:254:VAL:CG2	2.24	0.68
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.23	0.68
2:C:379:GLN:H	2:C:379:GLN:HE21	1.38	0.68
1:B:88:ARG:NH1	5:B:656:HOH:O	2.26	0.68
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.91	0.68
2:D:376:ASP:CG	2:D:379:GLN:HG2	2.19	0.68
1:A:209:GLU:HA	1:A:213:THR:HB	1.76	0.68
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.23	0.68
1:B:184:MET:HE3	1:B:188:PHE:HB2	1.75	0.67
1:B:44:THR:HG22	1:B:46:TYR:N	1.99	0.67
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.74	0.67
1:B:281:TYR:O	1:B:284:PRO:HD2	1.93	0.67
1:B:337:GLN:C	5:B:692:HOH:O	2.37	0.67
1:A:206:LEU:HD11	1:A:254:VAL:HG22	1.76	0.67
1:B:85:ALA:HA	1:B:88:ARG:NH1	2.10	0.67
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.77	0.67
1:B:403:ILE:HG23	1:B:406:MET:HG3	1.77	0.66
2:D:275:ASN:C	2:D:278:PRO:HD2	2.20	0.66
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.60	0.66
1:A:109:PHE:O	1:A:184:MET:HE2	1.96	0.66
2:C:333:ARG:CZ	5:C:1243:HOH:O	2.42	0.66
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.76	0.66
3:F:119:LYS:HA	3:F:128:PHE:CE1	2.31	0.66
2:D:259:PHE:CE1	2:D:356:LEU:HD22	2.32	0.65
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.31	0.65
1:A:184:MET:HE3	1:A:188:PHE:CB	2.26	0.65
1:A:476:ARG:NH1	5:A:1150:HOH:O	2.17	0.65
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.78	0.65
1:B:52:MET:HG3	5:B:693:HOH:O	1.97	0.65
3:F:165:HIS:HE1	3:F:167:GLN:HE21	1.44	0.65
1:A:231:ILE:HD13	5:A:1140:HOH:O	1.96	0.65
1:A:188:PHE:HZ	1:A:213:THR:OG1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:192:MET:HE2	2:C:192:MET:HA	1.79	0.64
2:D:133:ILE:HD11	2:D:136:MET:HE2	1.80	0.64
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.16	0.64
2:C:376:ASP:CB	2:C:379:GLN:HE21	2.11	0.64
2:C:179:LEU:HD21	2:C:245:ALA:HB2	1.78	0.64
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.80	0.64
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.43	0.64
2:D:269:ALA:HB1	2:D:274:ASP:OD2	1.98	0.64
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.78	0.63
2:C:376:ASP:HB3	2:C:379:GLN:HE21	1.63	0.63
2:D:148:TYR:CE2	2:D:223:VAL:HG21	2.25	0.63
1:B:207:VAL:HG11	1:B:275:PHE:HA	1.80	0.63
1:B:88:ARG:NE	5:B:657:HOH:O	2.31	0.63
1:B:288:MET:HE2	1:B:347:TYR:N	2.14	0.63
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.92	0.63
1:B:185:LYS:O	1:B:189:SER:HB2	1.99	0.63
1:B:186:ARG:HD3	1:B:186:ARG:C	2.23	0.63
3:E:3:LYS:O	3:E:4:LEU:HD12	1.99	0.63
1:B:108:ASN:HD21	1:B:175:ARG:HE	1.45	0.63
1:B:171:ALA:O	1:B:175:ARG:HG2	1.98	0.63
1:B:216:LEU:HD13	1:B:286:LEU:HD13	1.80	0.63
1:A:113:GLY:HA2	1:A:188:PHE:HB3	1.80	0.63
1:A:213:THR:O	1:A:217:ILE:HG12	1.99	0.62
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.34	0.62
3:F:97:LYS:NZ	3:F:97:LYS:HB3	2.14	0.62
1:A:202:LEU:CD2	1:A:206:LEU:HD12	2.28	0.62
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.81	0.62
1:A:33:GLN:HA	1:A:131:ALA:HB3	1.80	0.62
1:B:128:ALA:HB1	1:B:133:GLN:HB3	1.79	0.62
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.35	0.62
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.81	0.62
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.80	0.62
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.82	0.62
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.30	0.62
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.81	0.62
1:B:134:LYS:HD3	2:D:161:ASN:ND2	2.14	0.61
1:A:120:ALA:HA	1:A:193:ILE:HG22	1.83	0.61
1:A:185:LYS:O	1:A:189:SER:HB2	1.99	0.61
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.81	0.61
1:B:110:LEU:O	1:B:114:GLU:HG2	2.00	0.61
1:A:113:GLY:HA2	1:A:188:PHE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.61
1:A:140:GLN:OE1	1:A:249:ASN:OD1	2.17	0.61
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.83	0.61
2:D:9:ARG:NH2	5:D:447:HOH:O	2.34	0.61
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.82	0.61
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.81	0.61
2:C:333:ARG:NE	5:C:1243:HOH:O	2.32	0.61
1:B:44:THR:HG21	5:B:653:HOH:O	1.99	0.61
1:A:185:LYS:HA	1:A:189:SER:HB2	1.82	0.60
1:B:186:ARG:HB3	5:B:685:HOH:O	2.00	0.60
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.98	0.60
2:D:324:TRP:C	2:D:327:PRO:HD2	2.26	0.60
3:E:22:LEU:HD11	3:E:31:MET:SD	2.41	0.60
2:C:61:ASP:OD1	3:E:7:HIS:HD2	1.83	0.60
2:D:332:LEU:HB3	2:D:384:VAL:HG13	1.84	0.60
1:A:338:ASP:C	1:A:340:TYR:H	2.08	0.60
1:B:23:VAL:HG13	1:B:27:GLU:OE2	2.02	0.60
1:B:190:ASP:HB3	2:D:74:GLN:O	2.01	0.60
3:E:57:GLU:O	3:E:61:GLU:HG3	2.02	0.60
2:D:197:ARG:HH12	2:D:209:GLU:C	2.09	0.60
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.36	0.60
2:D:247:SER:HG	2:D:324:TRP:CD1	2.18	0.60
1:B:31:TRP:CZ2	2:D:210:SER:HA	2.37	0.60
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.84	0.60
1:B:209:GLU:HG2	5:B:682:HOH:O	2.02	0.59
1:A:140:GLN:O	1:A:144:GLU:HG2	2.02	0.59
1:B:185:LYS:HA	1:B:189:SER:HB2	1.83	0.59
3:F:12:ARG:O	3:F:16:VAL:HG23	2.03	0.59
2:D:228:ARG:O	2:D:232:GLU:HG3	2.02	0.59
1:B:209:GLU:OE2	1:B:246:HIS:HB3	2.02	0.59
2:D:310:SER:O	2:D:314:ARG:HG3	2.03	0.59
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.36	0.59
2:C:379:GLN:NE2	2:C:379:GLN:N	2.49	0.59
2:C:98:HIS:HE1	2:C:178:SER:OG	1.86	0.58
2:D:340:ALA:HA	2:D:389:LYS:NZ	2.18	0.58
3:E:15:TRP:HB2	3:E:56:ILE:HD12	1.85	0.58
1:A:312:ASP:O	1:A:316:ILE:HB	2.03	0.58
1:B:179:PRO:HD3	5:B:608:HOH:O	2.04	0.58
1:A:186:ARG:HA	2:C:73:THR:OG1	2.04	0.58
1:A:216:LEU:O	1:A:220:VAL:HG23	2.04	0.58
3:F:81:THR:C	3:F:83:PHE:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLU:HB3	5:A:1148:HOH:O	2.03	0.58
1:B:24:ASN:OD1	1:B:27:GLU:HG3	2.04	0.58
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.85	0.58
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.86	0.57
3:E:167:GLN:NE2	5:E:221:HOH:O	2.36	0.57
1:A:336:LYS:O	1:A:338:ASP:N	2.36	0.57
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.86	0.57
1:A:121:THR:HG21	1:A:140:GLN:HG2	1.84	0.57
1:A:227:ASN:HD21	1:A:295:LYS:H	1.52	0.57
2:C:225:LYS:HE2	5:C:1251:HOH:O	2.04	0.57
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.34	0.57
1:A:339:ALA:HA	5:A:1147:HOH:O	2.04	0.57
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.40	0.57
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.39	0.57
1:A:323:LYS:HE2	1:A:324:TYR:CE1	2.40	0.57
1:A:204:LEU:O	1:A:209:GLU:HG3	2.05	0.57
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.40	0.57
1:B:202:LEU:HA	1:B:206:LEU:HB3	1.86	0.56
1:A:66:GLU:O	1:A:70:MET:HG2	2.04	0.56
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.27	0.56
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.35	0.56
1:B:209:GLU:HA	1:B:213:THR:CB	2.35	0.56
3:F:57:GLU:O	3:F:61:GLU:HG3	2.04	0.56
1:B:321:LEU:HB3	1:B:326:VAL:HG21	1.87	0.56
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.41	0.56
1:B:469:ILE:HG21	5:B:608:HOH:O	2.04	0.56
2:C:89:GLU:CD	3:E:125:VAL:HG13	2.30	0.56
2:C:310:SER:O	2:C:314:ARG:HG3	2.05	0.56
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.88	0.56
3:E:41:THR:O	3:E:44:ARG:HD2	2.05	0.56
3:F:4:LEU:HD22	3:F:10:ASP:H	1.70	0.56
1:A:175:ARG:HD3	1:A:181:TRP:CZ2	2.40	0.56
1:A:207:VAL:HG11	1:A:275:PHE:HA	1.88	0.56
2:D:351:GLU:O	2:D:354:ALA:N	2.39	0.56
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.87	0.56
2:D:376:ASP:O	2:D:380:ILE:HG12	2.06	0.56
1:B:175:ARG:HG3	1:B:176:THR:N	2.20	0.56
1:B:213:THR:O	1:B:217:ILE:HG12	2.05	0.56
2:C:266:GLN:NE2	2:D:132:GLN:OE1	2.39	0.56
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.36	0.56
2:C:261:ARG:NE	2:C:285:GLN:HE22	1.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASN:OD1	1:B:243:GLU:HG2	2.06	0.56
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.71	0.56
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.05	0.56
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.41	0.56
2:D:143:GLU:O	2:D:147:ARG:HB3	2.06	0.56
2:C:266:GLN:HE21	2:D:132:GLN:CD	2.14	0.55
3:E:41:THR:O	3:E:44:ARG:CD	2.54	0.55
1:B:403:ILE:HG21	1:B:515:LEU:HD13	1.88	0.55
1:A:84:ASP:HB3	1:B:81:SER:OG	2.07	0.55
1:B:288:MET:CE	1:B:346:LEU:HB3	2.37	0.55
2:D:153:LEU:HD12	2:D:153:LEU:C	2.31	0.55
1:B:466:CYS:HB2	2:D:73:THR:HA	1.88	0.55
3:E:80:LYS:CD	3:E:84:GLY:HA2	2.34	0.55
2:D:296:GLN:NE2	2:D:370:ARG:HH12	2.05	0.55
3:E:44:ARG:NH2	3:E:50:ASP:OD1	2.40	0.55
2:D:269:ALA:O	2:D:274:ASP:HB3	2.07	0.55
1:A:227:ASN:ND2	1:A:295:LYS:H	2.05	0.55
1:A:338:ASP:O	1:A:340:TYR:N	2.40	0.55
1:B:32:LEU:HD12	1:B:35:PHE:CD2	2.42	0.55
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.04	0.55
2:D:224:TYR:O	2:D:227:ALA:HB3	2.07	0.55
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.88	0.54
3:E:12:ARG:HA	3:E:56:ILE:HD11	1.89	0.54
1:A:81:SER:OG	1:B:84:ASP:HB3	2.06	0.54
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.90	0.54
1:B:123:MET:HE1	2:D:76:PHE:CE2	2.42	0.54
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.42	0.54
2:C:244:SER:O	2:C:248:VAL:HG23	2.08	0.54
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.90	0.54
2:D:277:THR:HG22	2:D:281:ILE:HD11	1.89	0.54
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.38	0.54
1:A:243:GLU:O	1:A:247:MET:HG2	2.08	0.54
1:B:186:ARG:HA	2:D:73:THR:OG1	2.08	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.56	0.53
1:A:310:TYR:CE1	1:A:336:LYS:HD2	2.42	0.53
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.43	0.53
3:E:154:GLU:O	3:E:158:GLN:HG3	2.07	0.53
1:B:85:ALA:HA	1:B:88:ARG:HH12	1.72	0.53
1:A:336:LYS:C	1:A:338:ASP:N	2.66	0.53
1:B:196:ASP:HB2	3:F:140:MET:SD	2.49	0.53
2:C:80:ARG:CZ	5:C:1249:HOH:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:CA	1:B:188:PHE:HB3	2.38	0.53
2:D:195:LEU:O	2:D:195:LEU:HD23	2.07	0.53
2:D:240:ASP:OD1	3:F:125:VAL:HG21	2.09	0.53
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.38	0.53
1:A:113:GLY:CA	1:A:188:PHE:HB3	2.38	0.53
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.09	0.53
2:D:312:TYR:O	2:D:316:VAL:HG23	2.09	0.53
2:D:340:ALA:HA	2:D:389:LYS:HZ3	1.72	0.53
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.23	0.53
1:B:360:ARG:HD2	1:B:489:ARG:NH2	2.24	0.53
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.91	0.53
2:C:247:SER:HG	2:C:324:TRP:CD1	2.27	0.52
2:D:147:ARG:NH1	2:D:217:GLU:OE1	2.42	0.52
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.09	0.52
2:C:54:VAL:O	2:C:55:TYR:HB2	2.08	0.52
1:A:186:ARG:HD3	1:A:186:ARG:C	2.34	0.52
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.91	0.52
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.10	0.52
2:D:235:TRP:CD1	2:D:235:TRP:C	2.87	0.52
1:B:23:VAL:HB	2:D:195:LEU:CD2	2.40	0.52
1:B:227:ASN:ND2	1:B:295:LYS:H	2.06	0.52
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.91	0.52
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.38	0.52
1:A:406:MET:O	1:A:410:GLU:HG3	2.09	0.52
1:A:109:PHE:O	1:A:112:VAL:HG12	2.10	0.52
1:A:184:MET:CE	1:A:188:PHE:HB2	2.38	0.52
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.92	0.52
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.91	0.52
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.52
2:D:228:ARG:HG2	2:D:228:ARG:HH11	1.74	0.52
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.90	0.52
2:C:225:LYS:CE	5:C:1251:HOH:O	2.58	0.52
2:D:133:ILE:CD1	2:D:136:MET:HE2	2.40	0.52
1:B:207:VAL:HG22	1:B:313:TRP:HZ2	1.75	0.52
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.93	0.52
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.45	0.51
2:C:306:ASP:O	2:C:310:SER:HB2	2.10	0.51
2:D:291:ALA:HB2	5:D:473:HOH:O	2.09	0.51
1:A:40:LYS:HB3	5:A:1049:HOH:O	2.10	0.51
1:A:121:THR:HG21	1:A:140:GLN:CG	2.40	0.51
3:E:106:GLU:HA	3:E:109:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CE2	1:A:204:LEU:HA	2.46	0.51
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.46	0.51
1:A:230:GLU:C	1:A:233:PRO:HD2	2.36	0.51
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.94	0.51
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.76	0.50
1:A:338:ASP:C	1:A:340:TYR:N	2.70	0.50
1:B:367:GLU:HG3	5:B:638:HOH:O	2.10	0.50
1:A:175:ARG:HG3	1:A:176:THR:N	2.27	0.50
1:A:124:LEU:HD21	1:A:201:SER:HB2	1.93	0.50
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.94	0.50
1:A:175:ARG:HD2	5:C:1159:HOH:O	2.12	0.50
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.11	0.50
1:B:66:GLU:O	1:B:70:MET:HG2	2.12	0.50
1:B:186:ARG:HD3	1:B:186:ARG:O	2.12	0.50
2:D:321:THR:HG21	2:D:373:PHE:CD2	2.47	0.50
1:B:185:LYS:CA	1:B:189:SER:HB2	2.41	0.50
2:D:39:VAL:O	2:D:41:PRO:HD3	2.12	0.50
3:E:40:THR:C	3:E:41:THR:HG23	2.37	0.50
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.47	0.50
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.58	0.50
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.93	0.50
1:A:79:PHE:O	1:A:83:GLN:HG3	2.12	0.50
1:A:283:THR:HB	1:A:284:PRO:CD	2.41	0.50
1:A:413:HIS:HD2	1:A:428:SER:OG	1.95	0.50
1:B:88:ARG:NH2	5:B:657:HOH:O	2.45	0.50
3:F:86:ASP:O	3:F:89:SER:HB2	2.12	0.50
1:B:251:TYR:O	1:B:255:VAL:HG23	2.12	0.50
1:B:337:GLN:O	5:B:692:HOH:O	2.20	0.50
2:D:111:LYS:O	2:D:115:GLU:HG3	2.11	0.50
1:A:116:ASN:CG	1:A:189:SER:HA	2.37	0.49
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.12	0.49
1:B:192:PHE:O	1:B:200:CYS:HB3	2.11	0.49
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:B:44:THR:OG1	1:B:127:SER:HA	2.12	0.49
1:B:115:TYR:OH	2:D:173:ASP:HA	2.12	0.49
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.12	0.49
2:C:263:GLU:OE2	2:C:263:GLU:HA	2.12	0.49
1:A:208:GLY:HA2	1:A:278:GLN:HE21	1.76	0.49
1:B:439:HIS:CD2	3:F:163:VAL:HA	2.32	0.49
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.45	0.49
3:E:165:HIS:HE1	3:E:167:GLN:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:19:ILE:HG12	3:F:60:LEU:HD13	1.94	0.49
1:B:38:ASP:O	1:B:39:PHE:HB3	2.11	0.49
2:C:308:GLU:HB3	2:C:309:PHE:CD1	2.48	0.49
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.47	0.49
2:D:350:GLU:HG3	5:D:425:HOH:O	2.12	0.49
1:A:185:LYS:CA	1:A:189:SER:HB2	2.43	0.49
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.48	0.49
1:B:459:ALA:C	1:B:461:PRO:HD3	2.38	0.49
2:D:159:LEU:HD22	2:D:248:VAL:HG13	1.95	0.49
3:F:75:VAL:O	3:F:79:HIS:HD2	1.96	0.49
1:A:499:PRO:HG3	1:A:507:TRP:NE1	2.28	0.49
1:B:113:GLY:HA2	1:B:188:PHE:O	2.12	0.49
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.45	0.49
1:B:42:ASN:HA	2:D:236:GLN:HG3	1.95	0.48
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.94	0.48
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.94	0.48
2:C:153:LEU:C	2:C:153:LEU:HD12	2.38	0.48
2:C:297:ASP:O	2:C:301:ASN:HB3	2.12	0.48
1:A:108:ASN:O	1:A:111:GLU:HB3	2.13	0.48
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.49	0.48
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.13	0.48
2:D:105:TRP:O	2:D:108:PRO:HD2	2.12	0.48
3:E:3:LYS:HB3	3:E:10:ASP:OD1	2.13	0.48
3:F:33:LYS:O	3:F:37:MET:HG2	2.13	0.48
1:B:116:ASN:CG	1:B:189:SER:HA	2.39	0.48
1:B:212:PHE:O	1:B:215:PRO:HD2	2.13	0.48
1:A:93:VAL:HG11	2:D:3:MET:HG2	1.95	0.48
1:B:75:ASP:OD2	1:B:146:ARG:NH1	2.46	0.48
2:D:37:TYR:CD1	2:D:37:TYR:C	2.92	0.48
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.44	0.48
3:F:61:GLU:O	3:F:121:PRO:HG3	2.13	0.48
2:D:247:SER:O	2:D:251:VAL:HB	2.13	0.48
1:A:343:HIS:CD2	1:A:343:HIS:H	2.31	0.48
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.49	0.48
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.78	0.48
2:D:370:ARG:HH11	2:D:370:ARG:HG3	1.79	0.48
1:A:182:LYS:O	2:C:73:THR:HG21	2.14	0.48
1:A:77:ARG:HH22	1:B:83:GLN:HB3	1.79	0.48
1:B:44:THR:HG23	1:B:126:ASP:OD1	2.14	0.48
2:C:235:TRP:CD1	2:C:235:TRP:C	2.92	0.48
1:A:202:LEU:HD12	1:A:270:ASP:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:HG3	1:A:324:TYR:CE1	2.49	0.47
1:A:338:ASP:HB2	5:A:1152:HOH:O	2.14	0.47
1:B:186:ARG:NH1	1:B:420:VAL:HG12	2.29	0.47
2:C:181:PHE:HD1	5:C:1180:HOH:O	1.97	0.47
1:B:31:TRP:CH2	2:D:210:SER:HA	2.49	0.47
2:D:192:MET:HE2	2:D:283:GLN:OE1	2.14	0.47
2:D:264:PHE:O	2:D:268:LEU:HB2	2.14	0.47
2:D:313:ASN:HB3	2:D:317:MET:HE2	1.96	0.47
2:D:336:MET:C	2:D:338:LEU:H	2.22	0.47
3:E:97:LYS:HB3	3:E:97:LYS:HZ2	1.77	0.47
3:F:120:PRO:HD3	3:F:128:PHE:CD1	2.49	0.47
1:B:469:ILE:HG13	1:B:470:PHE:N	2.28	0.47
3:F:154:GLU:O	3:F:158:GLN:HG3	2.14	0.47
1:B:32:LEU:HD21	1:B:135:ASN:HB2	1.95	0.47
3:F:66:VAL:O	3:F:69:ALA:HB3	2.14	0.47
1:A:459:ALA:C	1:A:461:PRO:HD3	2.40	0.47
2:D:260:VAL:O	2:D:265:PHE:HD1	1.97	0.47
1:A:116:ASN:CB	1:A:189:SER:HA	2.44	0.47
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.45	0.47
1:B:405:LEU:HD23	1:B:517:CYS:SG	2.54	0.47
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.49	0.47
2:D:224:TYR:O	2:D:225:LYS:C	2.58	0.47
3:F:90:VAL:HG11	3:F:118:TYR:CZ	2.49	0.47
2:D:266:GLN:HG3	2:D:266:GLN:O	2.13	0.47
1:A:187:VAL:HG11	1:A:281:TYR:HB3	1.97	0.47
1:B:30:ARG:HD3	1:B:30:ARG:C	2.40	0.47
1:B:88:ARG:CZ	5:B:657:HOH:O	2.62	0.47
1:B:230:GLU:C	1:B:233:PRO:HD2	2.40	0.47
2:D:197:ARG:HB3	2:D:197:ARG:NH1	2.29	0.47
2:D:259:PHE:CD1	2:D:263:GLU:HB2	2.49	0.47
1:B:452:TRP:O	1:B:456:MET:HG3	2.16	0.46
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.97	0.46
2:D:166:GLY:HA2	2:D:241:TRP:HB2	1.96	0.46
3:E:165:HIS:CE1	3:E:167:GLN:HB2	2.51	0.46
1:B:248:ALA:O	1:B:252:GLN:HG2	2.14	0.46
1:B:313:TRP:C	1:B:315:GLY:H	2.23	0.46
1:B:334:ASP:CG	1:B:452:TRP:HE1	2.24	0.46
1:A:313:TRP:HA	1:A:317:TRP:HB3	1.97	0.46
1:B:175:ARG:HD3	1:B:181:TRP:CZ2	2.50	0.46
1:B:313:TRP:HA	1:B:317:TRP:HB3	1.98	0.46
1:B:34:SER:O	2:D:154:PHE:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:VAL:O	1:B:211:CYS:HB3	2.15	0.46
2:D:144:PHE:HA	2:D:148:TYR:HD1	1.81	0.46
3:F:40:THR:C	3:F:41:THR:HG23	2.39	0.46
3:F:81:THR:C	3:F:83:PHE:N	2.73	0.46
3:F:88:LYS:HB2	3:F:127:TYR:HE2	1.81	0.46
3:F:118:TYR:HB3	3:F:123:MET:HB2	1.96	0.46
1:B:125:TRP:CD1	1:B:125:TRP:C	2.94	0.46
2:C:76:PHE:CE2	5:C:1249:HOH:O	2.67	0.46
1:A:128:ALA:CB	1:A:133:GLN:HG2	2.45	0.46
1:A:205:GLN:NE2	1:A:249:ASN:HB3	2.31	0.46
1:A:472:GLN:NE2	5:A:1086:HOH:O	2.48	0.46
1:B:60:PHE:N	1:B:60:PHE:CD1	2.84	0.46
1:B:287:GLY:HA3	1:B:301:TRP:CD1	2.51	0.46
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.50	0.46
1:B:504:ASP:OD2	1:B:505:LYS:HG3	2.15	0.46
2:C:139:THR:O	2:C:143:GLU:HB3	2.16	0.46
3:E:97:LYS:HB3	3:E:97:LYS:HZ3	1.76	0.46
3:F:4:LEU:CD2	3:F:10:ASP:H	2.29	0.46
3:F:4:LEU:HD21	3:F:10:ASP:CG	2.41	0.46
1:A:163:GLN:HG2	5:A:1033:HOH:O	2.15	0.46
1:B:125:TRP:O	1:B:134:LYS:HG2	2.16	0.46
2:C:99:ARG:NH2	5:C:1170:HOH:O	2.23	0.45
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.00	0.45
2:D:376:ASP:OD1	2:D:379:GLN:HG2	2.14	0.45
1:A:83:GLN:HB3	1:B:77:ARG:NH2	2.31	0.45
2:D:98:HIS:HE1	2:D:178:SER:OG	1.99	0.45
1:B:268:ASN:ND2	1:B:327:GLU:H	2.09	0.45
2:D:98:HIS:HA	2:D:302:CYS:SG	2.55	0.45
2:D:192:MET:HE3	2:D:280:PHE:CD2	2.52	0.45
2:D:316:VAL:HG12	2:D:320:TRP:CE2	2.52	0.45
1:B:222:GLU:OE2	2:D:7:ARG:NH1	2.50	0.45
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.52	0.45
3:F:159:ARG:HG3	3:F:161:VAL:HG13	1.99	0.45
1:B:92:GLY:O	1:B:162:GLY:HA2	2.16	0.45
2:D:63:ILE:O	2:D:64:ALA:C	2.59	0.45
1:A:50:TYR:CD2	1:A:257:ILE:HD12	2.52	0.45
1:A:192:PHE:O	1:A:200:CYS:HB3	2.17	0.45
2:D:148:TYR:CE2	2:D:338:LEU:HD13	2.51	0.45
2:D:255:LEU:HB2	2:D:328:THR:HG21	1.98	0.45
1:A:257:ILE:O	1:A:263:SER:HB2	2.17	0.45
1:B:29:HIS:CD2	1:B:61:LYS:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.52	0.45
2:C:168:ARG:HH11	2:C:168:ARG:CG	2.30	0.45
3:F:52:ASP:O	3:F:56:ILE:HG12	2.17	0.45
1:A:212:PHE:O	1:A:216:LEU:CB	2.65	0.45
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.52	0.45
2:D:57:GLN:NE2	2:D:59:ASN:HD21	2.15	0.45
2:D:136:MET:HE3	2:D:141:ARG:CB	2.44	0.45
1:B:216:LEU:HD11	1:B:286:LEU:HD22	1.99	0.45
1:B:159:ALA:O	2:D:33:ASN:HB2	2.18	0.45
2:D:140:TRP:CE2	2:D:269:ALA:HA	2.53	0.45
1:B:190:ASP:OD1	2:D:72:TRP:HB3	2.17	0.44
2:D:357:TYR:CE2	2:D:377:ARG:NH1	2.85	0.44
3:F:146:ASN:HB3	3:F:149:ASP:CG	2.42	0.44
1:A:46:TYR:CD2	1:A:123:MET:HE3	2.53	0.44
2:D:203:ILE:HG13	2:D:204:VAL:HG23	1.99	0.44
3:F:75:VAL:O	3:F:79:HIS:CD2	2.71	0.44
1:A:77:ARG:NH2	1:B:83:GLN:HB3	2.33	0.44
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.18	0.44
2:D:277:THR:HG22	2:D:281:ILE:CD1	2.47	0.44
1:A:207:VAL:HG22	1:A:313:TRP:HZ2	1.82	0.44
2:D:204:VAL:HG12	2:D:204:VAL:O	2.16	0.44
2:D:211:THR:HA	2:D:214:PRO:HG2	1.99	0.44
1:A:234:THR:HG23	1:B:84:ASP:OD1	2.18	0.44
2:D:176:ARG:NH1	2:D:176:ARG:HB2	2.32	0.44
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.80	0.44
1:A:439:HIS:HE1	1:A:454:GLU:OE1	2.01	0.44
1:B:403:ILE:CG2	1:B:515:LEU:HD13	2.47	0.44
3:F:115:ARG:O	3:F:119:LYS:HB2	2.17	0.44
1:A:159:ALA:O	2:C:33:ASN:HB2	2.17	0.44
1:B:114:GLU:O	1:B:117:ALA:HB3	2.18	0.44
2:C:259:PHE:CZ	2:C:336:MET:HE1	2.53	0.44
2:D:34:LYS:O	2:D:37:TYR:HB3	2.18	0.44
3:F:83:PHE:C	3:F:85:GLU:H	2.25	0.44
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.18	0.43
1:B:163:GLN:O	2:D:28:PRO:HA	2.18	0.43
1:B:184:MET:HE3	1:B:188:PHE:CB	2.44	0.43
1:B:209:GLU:CA	1:B:213:THR:OG1	2.58	0.43
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.52	0.43
2:D:54:VAL:O	2:D:55:TYR:HB2	2.18	0.43
2:D:240:ASP:HB3	2:D:243:GLU:HB3	2.00	0.43
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.43
1:A:196:ASP:HB2	3:E:140:MET:SD	2.58	0.43
1:B:146:ARG:HB2	2:D:106:HIS:CD2	2.54	0.43
2:D:318:ARG:O	2:D:321:THR:HB	2.18	0.43
1:A:125:TRP:CD1	1:A:125:TRP:C	2.96	0.43
1:B:120:ALA:O	1:B:124:LEU:HG	2.19	0.43
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.54	0.43
3:F:165:HIS:CE1	3:F:167:GLN:HE21	2.31	0.43
1:A:221:THR:HG22	1:A:233:PRO:HA	2.00	0.43
1:B:108:ASN:O	1:B:111:GLU:HB3	2.18	0.43
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.00	0.43
2:D:242:ASN:O	2:D:243:GLU:C	2.61	0.43
2:D:336:MET:HE3	2:D:385:LEU:HA	2.00	0.43
1:A:120:ALA:CA	1:A:193:ILE:HG22	2.48	0.43
1:B:112:VAL:HG21	1:B:181:TRP:HH2	1.83	0.43
1:B:460:GLU:HB3	1:B:463:ARG:HG3	2.01	0.43
1:A:30:ARG:HD3	1:A:31:TRP:CD1	2.53	0.43
1:A:163:GLN:O	2:C:28:PRO:HA	2.18	0.43
2:C:376:ASP:OD2	2:C:376:ASP:N	2.51	0.43
2:D:244:SER:O	2:D:248:VAL:HG23	2.18	0.43
2:D:270:PRO:O	2:D:273:GLY:N	2.50	0.43
1:B:39:PHE:O	1:B:40:LYS:C	2.61	0.43
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.37	0.43
2:D:82:SER:O	2:D:168:ARG:NH2	2.48	0.43
2:D:89:GLU:OE2	3:F:125:VAL:HG22	2.19	0.43
2:D:102:LEU:HB2	2:D:104:ARG:HD2	2.01	0.43
2:D:197:ARG:NH1	2:D:209:GLU:O	2.48	0.43
2:D:351:GLU:O	2:D:352:ILE:C	2.60	0.43
1:A:21:THR:HG22	2:C:128:SER:CB	2.49	0.43
1:A:211:CYS:SG	1:A:309:VAL:HG22	2.58	0.43
5:C:1040:HOH:O	3:E:121:PRO:HB3	2.19	0.43
2:D:246:PHE:CZ	2:D:317:MET:HB3	2.53	0.43
1:B:32:LEU:HD21	1:B:135:ASN:CB	2.49	0.43
1:B:206:LEU:HD11	1:B:321:LEU:HD11	2.00	0.43
1:B:460:GLU:N	1:B:461:PRO:HD3	2.34	0.43
2:C:104:ARG:NH1	5:C:1180:HOH:O	2.52	0.43
2:C:227:ALA:O	2:C:231:VAL:HG23	2.18	0.43
2:C:228:ARG:O	2:C:232:GLU:HG3	2.19	0.43
2:D:146:ASN:OD1	2:D:146:ASN:O	2.37	0.43
2:D:255:LEU:HD21	2:D:363:TRP:CD2	2.54	0.43
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HE1	2:D:76:PHE:HE2	1.82	0.43
1:B:417:ILE:HG13	1:B:468:ASN:HB2	2.00	0.43
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.48	0.43
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.54	0.43
2:D:277:THR:N	2:D:278:PRO:CD	2.82	0.43
1:A:185:LYS:C	1:A:189:SER:HB2	2.43	0.42
1:B:202:LEU:HA	1:B:206:LEU:CB	2.49	0.42
1:B:227:ASN:HD21	1:B:296:PHE:H	1.67	0.42
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.53	0.42
2:D:140:TRP:HE1	2:D:145:ILE:HD11	1.83	0.42
2:D:348:ASP:OD2	2:D:348:ASP:C	2.61	0.42
1:A:117:ALA:HA	1:A:120:ALA:HB3	2.00	0.42
1:B:79:PHE:O	1:B:83:GLN:HG3	2.19	0.42
1:B:108:ASN:HD21	1:B:175:ARG:NE	2.15	0.42
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.83	0.42
2:C:77:HIS:CG	3:E:140:MET:HG2	2.53	0.42
2:D:134:ARG:C	2:D:136:MET:H	2.27	0.42
1:A:177:ILE:HG12	1:A:485:LEU:HB2	2.01	0.42
1:B:445:MET:HB3	1:B:523:VAL:HG21	2.02	0.42
1:A:165:PRO:HG3	5:A:1155:HOH:O	2.19	0.42
1:A:312:ASP:C	1:A:316:ILE:HB	2.45	0.42
1:A:495:LEU:HD21	1:A:509:LEU:HA	2.00	0.42
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.54	0.42
1:B:186:ARG:HH12	1:B:420:VAL:HG12	1.83	0.42
1:B:288:MET:HE1	1:B:346:LEU:CB	2.49	0.42
2:C:130:ASP:HB3	2:C:132:GLN:HG3	2.01	0.42
2:C:376:ASP:O	2:C:380:ILE:HG12	2.18	0.42
2:D:90:LEU:HD13	2:D:303:LEU:HD13	2.01	0.42
2:D:213:VAL:N	2:D:214:PRO:HD2	2.34	0.42
3:F:86:ASP:HB3	3:F:89:SER:OG	2.19	0.42
1:A:29:HIS:HE2	1:A:58:GLU:CD	2.27	0.42
1:A:279:GLN:HE21	1:A:279:GLN:HB3	1.67	0.42
1:B:302:VAL:HG23	1:B:303:LYS:H	1.85	0.42
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.01	0.42
2:C:389:LYS:HB3	5:C:1123:HOH:O	2.20	0.42
2:C:61:ASP:OD1	3:E:7:HIS:CD2	2.69	0.42
1:B:121:THR:HA	1:B:124:LEU:HD12	2.02	0.42
1:A:466:CYS:HB2	2:C:73:THR:HA	2.01	0.42
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.91	0.42
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.71	0.42
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ILE:HD11	2:C:274:ASP:OD2	2.20	0.42
2:D:277:THR:HB	2:D:278:PRO:HD3	2.01	0.42
1:A:115:TYR:OH	2:C:173:ASP:HA	2.20	0.42
1:A:186:ARG:HD3	1:A:186:ARG:O	2.20	0.42
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.55	0.42
1:B:187:VAL:HG23	1:B:188:PHE:N	2.34	0.42
1:B:196:ASP:HB3	1:B:199:GLU:HB2	2.02	0.42
2:C:143:GLU:O	2:C:147:ARG:HB3	2.19	0.42
2:D:196:GLU:O	2:D:199:PHE:HB3	2.20	0.42
3:F:67:LEU:HD23	3:F:70:ARG:HH21	1.84	0.42
1:A:227:ASN:HD21	1:A:296:PHE:H	1.68	0.42
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.55	0.42
2:C:168:ARG:HH11	2:C:168:ARG:HG2	1.85	0.42
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.20	0.42
2:D:388:LEU:O	2:D:389:LYS:C	2.62	0.42
3:F:36:ARG:NH1	3:F:119:LYS:HB3	2.35	0.42
1:A:76:GLU:CD	1:B:76:GLU:HG2	2.44	0.41
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.18	0.41
1:A:188:PHE:CD1	1:A:192:PHE:CZ	3.08	0.41
1:B:140:GLN:HA	1:B:143:ASP:HB2	2.02	0.41
3:E:32:LEU:HA	3:E:60:LEU:CD2	2.50	0.41
3:F:32:LEU:HD21	3:F:36:ARG:NH2	2.35	0.41
1:A:328:SER:HA	1:A:329:PRO:HD3	1.87	0.41
1:B:193:ILE:O	2:D:76:PHE:CZ	2.73	0.41
1:B:416:TYR:HB2	1:B:425:PHE:CE1	2.54	0.41
3:F:43:PHE:CE2	3:F:112:ILE:HD12	2.55	0.41
1:A:121:THR:HA	1:A:124:LEU:HD12	2.02	0.41
1:A:302:VAL:HG11	1:A:340:TYR:CD1	2.55	0.41
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.55	0.41
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.67	0.41
1:A:20:PRO:HG3	2:C:129:ALA:HB2	2.03	0.41
1:B:123:MET:CE	2:D:168:ARG:NH1	2.84	0.41
1:B:210:ALA:N	1:B:247:MET:HE1	2.35	0.41
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.54	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.66	0.41
1:A:365:ASP:OD2	1:A:365:ASP:C	2.64	0.41
1:A:207:VAL:HG22	1:A:313:TRP:CZ2	2.55	0.41
2:C:17:ALA:O	2:C:21:LEU:HG	2.20	0.41
2:C:75:LYS:HB3	2:C:80:ARG:O	2.20	0.41
2:C:176:ARG:NH1	2:C:176:ARG:HB2	2.36	0.41
2:D:254:ALA:O	2:D:258:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:93:GLY:O	3:F:96:ALA:HB3	2.21	0.41
1:A:83:GLN:HB3	1:B:77:ARG:HH22	1.85	0.41
1:A:128:ALA:HB2	1:A:133:GLN:HG2	2.01	0.41
1:A:521:ASN:HA	1:A:522:PRO:HD2	1.94	0.41
2:C:60:ALA:HA	2:C:68:ASP:HB3	2.02	0.41
3:E:103:ASP:OD2	3:E:103:ASP:C	2.63	0.41
3:F:4:LEU:CD2	3:F:10:ASP:CG	2.94	0.41
1:A:193:ILE:HB	2:C:168:ARG:NE	2.36	0.41
1:A:195:GLY:HA2	5:C:1217:HOH:O	2.20	0.41
1:B:155:ASN:OD1	1:B:168:HIS:HD2	2.04	0.41
1:B:460:GLU:HG2	2:D:77:HIS:CE1	2.56	0.41
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.95	0.41
2:D:308:GLU:HB3	2:D:309:PHE:CD1	2.56	0.41
3:F:73:ASN:O	3:F:74:GLU:C	2.64	0.41
1:A:212:PHE:O	1:A:216:LEU:HB2	2.20	0.41
1:A:460:GLU:N	1:A:461:PRO:HD3	2.35	0.41
1:A:526:PHE:HB3	3:E:164:VAL:HG11	2.02	0.41
1:B:194:SER:HA	2:D:76:PHE:CE1	2.55	0.41
1:B:216:LEU:CD1	1:B:286:LEU:HD22	2.51	0.41
1:B:279:GLN:HE21	1:B:279:GLN:HB2	1.69	0.41
2:D:213:VAL:HB	2:D:214:PRO:CD	2.50	0.41
2:D:332:LEU:HB3	2:D:384:VAL:CG1	2.48	0.41
2:D:339:PHE:O	2:D:342:LEU:HB2	2.21	0.41
3:E:64:VAL:CG1	3:E:121:PRO:HG2	2.51	0.41
1:B:50:TYR:CD1	1:B:50:TYR:N	2.89	0.41
1:B:123:MET:HE1	2:D:76:PHE:CZ	2.56	0.41
1:B:182:LYS:O	2:D:73:THR:HG21	2.21	0.41
2:C:262:ARG:HA	2:C:266:GLN:HB3	2.03	0.41
2:D:195:LEU:HD23	2:D:195:LEU:C	2.45	0.41
2:D:267:ARG:HG2	2:D:267:ARG:HH11	1.85	0.41
1:A:230:GLU:OE2	2:C:9:ARG:NH1	2.54	0.40
2:C:243:GLU:HA	2:C:320:TRP:CZ3	2.57	0.40
2:D:168:ARG:HD2	2:D:168:ARG:HA	1.95	0.40
1:A:43:ARG:C	1:A:43:ARG:HD2	2.45	0.40
1:A:49:LYS:HE3	1:A:266:TYR:HB3	2.04	0.40
1:A:232:THR:HB	1:A:233:PRO:HD3	2.03	0.40
2:C:316:VAL:O	2:C:319:ASN:HB3	2.21	0.40
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.56	0.40
1:B:288:MET:CE	1:B:346:LEU:CB	2.99	0.40
2:C:300:TYR:CD1	2:C:370:ARG:HG3	2.57	0.40
2:D:42:ARG:HB2	2:D:99:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:GLU:HB2	2:D:320:TRP:CE2	2.56	0.40
3:E:52:ASP:O	3:E:56:ILE:HG12	2.21	0.40
3:F:97:LYS:HB3	3:F:97:LYS:HZ3	1.85	0.40
1:A:118:ILE:CG2	2:C:176:ARG:HD3	2.52	0.40
1:A:452:TRP:O	1:A:456:MET:HG3	2.22	0.40
1:B:52:MET:HE2	1:B:133:GLN:HE22	1.87	0.40
1:B:165:PRO:HD2	2:D:30:ASP:HB3	2.03	0.40
2:D:152:PHE:O	2:D:155:ASN:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	508/527 (96%)	476 (94%)	27 (5%)	5 (1%)	12	9
1	B	508/527 (96%)	478 (94%)	24 (5%)	6 (1%)	10	7
2	C	386/388 (100%)	371 (96%)	14 (4%)	1 (0%)	36	36
2	D	386/388 (100%)	344 (89%)	37 (10%)	5 (1%)	9	6
3	E	164/169 (97%)	161 (98%)	3 (2%)	0	100	100
3	F	164/169 (97%)	148 (90%)	15 (9%)	1 (1%)	21	18
All	All	2116/2168 (98%)	1978 (94%)	120 (6%)	18 (1%)	14	10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	B	40	LYS
1	B	311	GLU
1	A	339	ALA

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Mol	Chain	Res	Type
1	B	312	ASP
1	B	315	GLY
2	D	251	VAL
1	A	308	TRP
1	A	315	GLY
2	D	64	ALA
2	D	135	ALA
1	A	312	ASP
1	B	39	PHE
2	C	64	ALA
2	D	225	LYS
2	D	221	GLY
3	F	122	ILE
1	B	314	GLY

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	423/442 (96%)	413 (98%)	10 (2%)	43	49
1	B	422/442 (96%)	412 (98%)	10 (2%)	43	49
2	C	316/323 (98%)	311 (98%)	5 (2%)	55	64
2	D	312/323 (97%)	310 (99%)	2 (1%)	78	86
3	E	143/146 (98%)	138 (96%)	5 (4%)	32	35
3	F	142/146 (97%)	140 (99%)	2 (1%)	59	67
All	All	1758/1822 (96%)	1724 (98%)	34 (2%)	50	58

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	90	ASN
1	A	125	TRP
1	A	186	ARG

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Mol	Chain	Res	Type
1	A	279	GLN
1	A	302	VAL
1	A	310	TYR
1	A	343	HIS
1	A	403	ILE
1	A	467	GLN
1	B	30	ARG
1	B	90	ASN
1	B	112	VAL
1	B	125	TRP
1	B	213	THR
1	B	279	GLN
1	B	302	VAL
1	B	311	GLU
1	B	334	ASP
1	B	403	ILE
2	C	80	ARG
2	C	168	ARG
2	C	173	ASP
2	C	356	LEU
2	C	376	ASP
2	D	153	LEU
2	D	173	ASP
3	E	41	THR
3	E	44	ARG
3	E	46	SER
3	E	97	LYS
3	E	125	VAL
3	F	44	ARG
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	108	ASN
1	A	133	GLN
1	A	147	HIS
1	A	168	HIS
1	A	203	ASN

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Mol	Chain	Res	Type
1	A	227	ASN
1	A	249	ASN
1	A	259	ASN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	33	GLN
1	B	42	ASN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	116	ASN
1	B	168	HIS
1	B	203	ASN
1	B	205	GLN
1	B	227	ASN
1	B	246	HIS
1	B	249	ASN
1	B	252	GLN
1	B	259	ASN
1	B	268	ASN
1	B	273	ASN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	382	HIS
1	B	411	ASN
1	B	413	HIS
1	B	439	HIS
1	B	442	ASN
1	B	451	GLN
1	B	516	ASN

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Mol	Chain	Res	Type
1	B	527	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN
2	C	296	GLN
2	C	301	ASN
2	C	379	GLN
2	D	57	GLN
2	D	59	ASN
2	D	98	HIS
2	D	132	GLN
2	D	155	ASN
2	D	161	ASN
2	D	275	ASN
2	D	285	GLN
2	D	293	GLN
2	D	296	GLN
2	D	301	ASN
3	E	7	HIS
3	E	45	ASN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	F	7	HIS
3	F	34	GLN
3	F	39	HIS
3	F	45	ASN
3	F	99	ASN
3	F	134	GLN
3	F	144	ASN
3	F	158	GLN
3	F	165	HIS
3	F	167	GLN

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	510/527 (96%)	0.68	74 (14%) 6 6	18, 38, 74, 82	0
1	B	510/527 (96%)	0.58	59 (11%) 9 10	22, 37, 70, 77	0
2	C	388/388 (100%)	-0.26	3 (0%) 82 84	17, 26, 39, 50	0
2	D	388/388 (100%)	1.14	82 (21%) 2 2	23, 46, 64, 87	0
3	E	166/169 (98%)	0.01	3 (1%) 67 70	20, 29, 48, 63	0
3	F	166/169 (98%)	1.51	46 (27%) 1 1	36, 54, 64, 70	0
All	All	2128/2168 (98%)	0.58	267 (12%) 8 8	17, 37, 67, 87	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	ALA	6.0
1	A	326	VAL	5.4
1	A	308	TRP	5.2
1	A	316	ILE	5.1
1	A	213	THR	5.0
2	D	139	THR	4.8
3	F	4	LEU	4.7
1	A	433	ALA	4.5
2	D	356	LEU	4.5
2	D	328	THR	4.4
1	A	251	TYR	4.2
1	B	53	ALA	4.0
1	A	212	PHE	3.9
1	B	188	PHE	3.9
2	D	204	VAL	3.9
1	A	310	TYR	3.8
2	D	145	ILE	3.8
1	B	310	TYR	3.8
1	A	434	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	PHE	3.7
1	A	206	LEU	3.7
2	D	354	ALA	3.7
1	A	309	VAL	3.6
1	B	31	TRP	3.6
2	D	203	ILE	3.6
3	F	125	VAL	3.5
1	A	258	ALA	3.5
3	F	72	PHE	3.4
1	A	255	VAL	3.4
1	B	309	VAL	3.4
1	A	329	PRO	3.3
1	A	247	MET	3.3
1	A	306	ASP	3.3
2	D	227	ALA	3.2
2	D	380	ILE	3.2
2	D	337	GLY	3.2
2	D	267	ARG	3.2
2	D	375	ALA	3.2
2	D	148	TYR	3.2
2	D	275	ASN	3.2
1	A	262	ALA	3.2
3	E	168	SER	3.2
1	A	318	ILE	3.1
2	D	274	ASP	3.1
1	B	263	SER	3.1
2	D	310	SER	3.1
1	B	44	THR	3.1
1	B	206	LEU	3.1
3	F	60	LEU	3.1
2	D	335	PHE	3.1
1	A	211	CYS	3.1
1	A	53	ALA	3.1
2	D	385	LEU	3.1
2	D	140	TRP	3.0
2	D	343	PRO	3.0
1	A	244	LEU	3.0
2	D	342	LEU	3.0
3	F	66	VAL	3.0
1	A	435	THR	3.0
1	A	340	TYR	3.0
1	A	335	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	318	ILE	3.0
1	A	193	ILE	2.9
3	F	24	THR	2.9
2	D	317	MET	2.9
1	A	192	PHE	2.9
3	F	118	TYR	2.9
2	D	330	ALA	2.9
1	B	193	ILE	2.9
1	B	257	ILE	2.9
1	B	302	VAL	2.9
2	D	381	VAL	2.9
1	A	257	ILE	2.9
2	D	132	GLN	2.9
2	D	144	PHE	2.9
2	D	207	PHE	2.9
1	B	29	HIS	2.9
1	A	204	LEU	2.8
1	B	316	ILE	2.8
1	B	266	TYR	2.8
1	A	248	ALA	2.8
1	B	32	LEU	2.8
3	E	4	LEU	2.8
1	A	187	VAL	2.8
2	D	295	VAL	2.8
2	D	347	THR	2.8
2	D	137	ASN	2.8
1	A	197	ALA	2.8
2	D	276	LEU	2.8
3	F	150	THR	2.8
1	A	254	VAL	2.8
1	B	317	TRP	2.8
3	E	167	GLN	2.8
1	A	338	ASP	2.8
1	A	324	TYR	2.8
2	D	320	TRP	2.8
1	B	39	PHE	2.7
3	F	77	PHE	2.7
1	A	128	ALA	2.7
2	D	212	ALA	2.7
3	F	69	ALA	2.7
2	D	205	PRO	2.7
1	A	409	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	334	ASP	2.7
1	B	131	ALA	2.7
2	D	352	ILE	2.7
1	A	317	TRP	2.7
3	F	84	GLY	2.7
1	B	19	ALA	2.7
1	B	47	ALA	2.7
2	D	331	ALA	2.7
3	F	83	PHE	2.7
3	F	117	ALA	2.7
3	F	91	LEU	2.7
2	D	213	VAL	2.7
2	D	360	VAL	2.7
3	F	56	ILE	2.7
1	A	243	GLU	2.6
3	F	87	ALA	2.6
2	D	208	ASP	2.6
2	D	389	LYS	2.6
1	A	337	GLN	2.6
2	D	136	MET	2.6
1	B	332	LEU	2.6
2	D	332	LEU	2.6
2	D	339	PHE	2.6
1	A	209	GLU	2.6
1	B	55	GLU	2.6
1	B	243	GLU	2.6
1	A	139	ALA	2.6
2	D	135	ALA	2.6
1	B	267	LEU	2.6
2	D	179	LEU	2.6
2	D	268	LEU	2.6
2	D	270	PRO	2.6
2	D	357	TYR	2.6
2	D	384	VAL	2.6
3	F	127	TYR	2.6
2	C	97	LYS	2.6
1	B	117	ALA	2.6
2	D	363	TRP	2.6
1	B	23	VAL	2.5
1	B	403	ILE	2.5
3	F	64	VAL	2.5
2	D	147	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	210	ALA	2.5
2	D	138	PRO	2.5
1	A	195	GLY	2.5
3	F	79	HIS	2.5
2	D	370	ARG	2.5
1	B	213	THR	2.5
1	B	269	THR	2.5
1	B	264	ALA	2.5
3	F	124	PRO	2.5
2	D	224	TYR	2.5
2	C	376	ASP	2.5
1	A	121	THR	2.5
2	D	321	THR	2.5
3	F	67	LEU	2.5
1	B	319	GLY	2.5
2	D	344	ALA	2.4
1	A	321	LEU	2.4
3	F	80	LYS	2.4
1	A	60	PHE	2.4
1	A	325	GLY	2.4
2	D	231	VAL	2.4
2	D	371	ILE	2.4
1	B	251	TYR	2.4
3	F	29	ALA	2.4
1	A	322	GLY	2.4
3	F	114	PHE	2.4
1	B	247	MET	2.4
1	B	265	LYS	2.4
1	B	261	PRO	2.4
3	F	71	ALA	2.4
1	A	302	VAL	2.4
1	A	313	TRP	2.4
1	B	441	TYR	2.3
2	D	368	ALA	2.3
2	D	229	LEU	2.3
2	D	379	GLN	2.3
1	B	254	VAL	2.3
2	D	353	THR	2.3
1	A	305	TRP	2.3
1	A	19	ALA	2.3
1	A	137	TYR	2.3
2	D	201	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	62	LEU	2.3
1	B	250	GLY	2.3
3	F	78	ARG	2.3
2	D	336	MET	2.3
1	B	35	PHE	2.3
3	F	35	PHE	2.3
2	D	133	ILE	2.3
3	F	19	ILE	2.3
1	A	285	VAL	2.3
2	D	322	GLY	2.3
2	D	338	LEU	2.3
3	F	22	LEU	2.3
3	F	25	LEU	2.3
1	A	52	MET	2.3
3	F	20	ALA	2.3
2	D	257	GLY	2.3
1	B	244	LEU	2.3
3	F	139	LEU	2.3
1	B	37	TRP	2.3
3	F	39	HIS	2.2
3	F	46	SER	2.2
1	B	192	PHE	2.2
1	B	186	ARG	2.2
1	B	214	ASN	2.2
1	A	432	GLY	2.2
2	D	216	ALA	2.2
2	D	340	ALA	2.2
2	D	388	LEU	2.2
1	B	308	TRP	2.2
1	A	319	GLY	2.2
1	B	240	GLU	2.2
2	C	379	GLN	2.2
1	A	118	ILE	2.2
1	B	121	THR	2.2
3	F	94	THR	2.2
3	F	16	VAL	2.2
1	B	130	ALA	2.2
2	D	195	LEU	2.2
3	F	123	MET	2.2
3	F	122	ILE	2.1
3	F	28	ALA	2.1
3	F	65	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	332	LEU	2.1
3	F	142	LEU	2.1
1	B	50	TYR	2.1
1	A	55	GLU	2.1
1	A	312	ASP	2.1
3	F	120	PRO	2.1
1	A	125	TRP	2.1
2	D	218	TRP	2.1
1	B	122	GLY	2.1
1	B	195	GLY	2.1
3	F	58	ALA	2.1
2	D	255	LEU	2.1
1	A	260	ASP	2.1
2	D	312	TYR	2.1
1	A	56	THR	2.1
1	A	304	THR	2.1
2	D	346	THR	2.1
3	F	169	PRO	2.1
1	A	191	GLY	2.1
2	D	131	GLY	2.1
1	B	202	LEU	2.1
1	B	52	MET	2.1
1	A	140	GLN	2.1
2	D	329	ILE	2.1
1	B	212	PHE	2.1
2	D	223	VAL	2.1
2	D	264	PHE	2.1
2	D	266	GLN	2.0
1	A	320	ARG	2.0
1	A	246	HIS	2.0
1	B	207	VAL	2.0
3	F	75	VAL	2.0
1	B	258	ALA	2.0
1	A	59	GLN	2.0
1	A	124	LEU	2.0
2	D	325	LEU	2.0
3	F	49	LEU	2.0
1	B	46	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
4	CA	A	1001	1/1	0.94	0.07	50,50,50,50	0
4	CA	C	1002	1/1	0.98	0.05	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.