



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:51 PM UTC

PDB ID : 6L8D / pdb_00006l8d
Title : Hexameric structure of the ATPase subunit of magnesium chelatase
Authors : Gao, Y.; Liu, L.
Deposited on : 2019-11-05
Resolution : 2.91 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

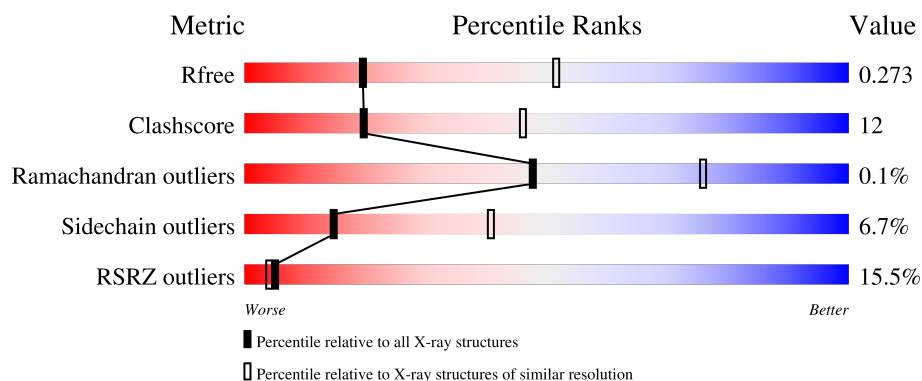
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	365	9% 56% 15% • 27%
1	B	365	9% 59% 12% • 25%
1	C	365	12% 56% 11% • 30%
1	D	365	13% 51% 16% • 31%
1	E	365	13% 57% 15% • 27%

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Mol	Chain	Length	Quality of chain
1	F	365	11% 58% 13% 27%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12112 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 Magnesium-chelatase subunit ChII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2035	1284	349	394	8			
1	B	273	Total	C	N	O	S	0	0	0
			2060	1311	358	383	8			
1	C	256	Total	C	N	O	S	0	0	0
			1943	1229	340	366	8			
1	D	253	Total	C	N	O	S	0	0	0
			1937	1227	339	363	8			
1	E	266	Total	C	N	O	S	0	0	0
			2002	1264	351	379	8			
1	F	267	Total	C	N	O	S	0	0	0
			2023	1277	354	384	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	LEU	-	expression tag	UNP P51634
A	359	GLU	-	expression tag	UNP P51634
A	360	HIS	-	expression tag	UNP P51634
A	361	HIS	-	expression tag	UNP P51634
A	362	HIS	-	expression tag	UNP P51634
A	363	HIS	-	expression tag	UNP P51634
A	364	HIS	-	expression tag	UNP P51634
A	365	HIS	-	expression tag	UNP P51634
B	358	LEU	-	expression tag	UNP P51634
B	359	GLU	-	expression tag	UNP P51634
B	360	HIS	-	expression tag	UNP P51634
B	361	HIS	-	expression tag	UNP P51634
B	362	HIS	-	expression tag	UNP P51634
B	363	HIS	-	expression tag	UNP P51634
B	364	HIS	-	expression tag	UNP P51634
B	365	HIS	-	expression tag	UNP P51634
C	358	LEU	-	expression tag	UNP P51634

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Chain	Residue	Modelled	Actual	Comment	Reference
C	359	GLU	-	expression tag	UNP P51634
C	360	HIS	-	expression tag	UNP P51634
C	361	HIS	-	expression tag	UNP P51634
C	362	HIS	-	expression tag	UNP P51634
C	363	HIS	-	expression tag	UNP P51634
C	364	HIS	-	expression tag	UNP P51634
C	365	HIS	-	expression tag	UNP P51634
D	358	LEU	-	expression tag	UNP P51634
D	359	GLU	-	expression tag	UNP P51634
D	360	HIS	-	expression tag	UNP P51634
D	361	HIS	-	expression tag	UNP P51634
D	362	HIS	-	expression tag	UNP P51634
D	363	HIS	-	expression tag	UNP P51634
D	364	HIS	-	expression tag	UNP P51634
D	365	HIS	-	expression tag	UNP P51634
E	358	LEU	-	expression tag	UNP P51634
E	359	GLU	-	expression tag	UNP P51634
E	360	HIS	-	expression tag	UNP P51634
E	361	HIS	-	expression tag	UNP P51634
E	362	HIS	-	expression tag	UNP P51634
E	363	HIS	-	expression tag	UNP P51634
E	364	HIS	-	expression tag	UNP P51634
E	365	HIS	-	expression tag	UNP P51634
F	358	LEU	-	expression tag	UNP P51634
F	359	GLU	-	expression tag	UNP P51634
F	360	HIS	-	expression tag	UNP P51634
F	361	HIS	-	expression tag	UNP P51634
F	362	HIS	-	expression tag	UNP P51634
F	363	HIS	-	expression tag	UNP P51634
F	364	HIS	-	expression tag	UNP P51634
F	365	HIS	-	expression tag	UNP P51634

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	22	Total O 22 22	0	0
2	C	19	Total O 19 19	0	0
2	D	19	Total O 19 19	0	0

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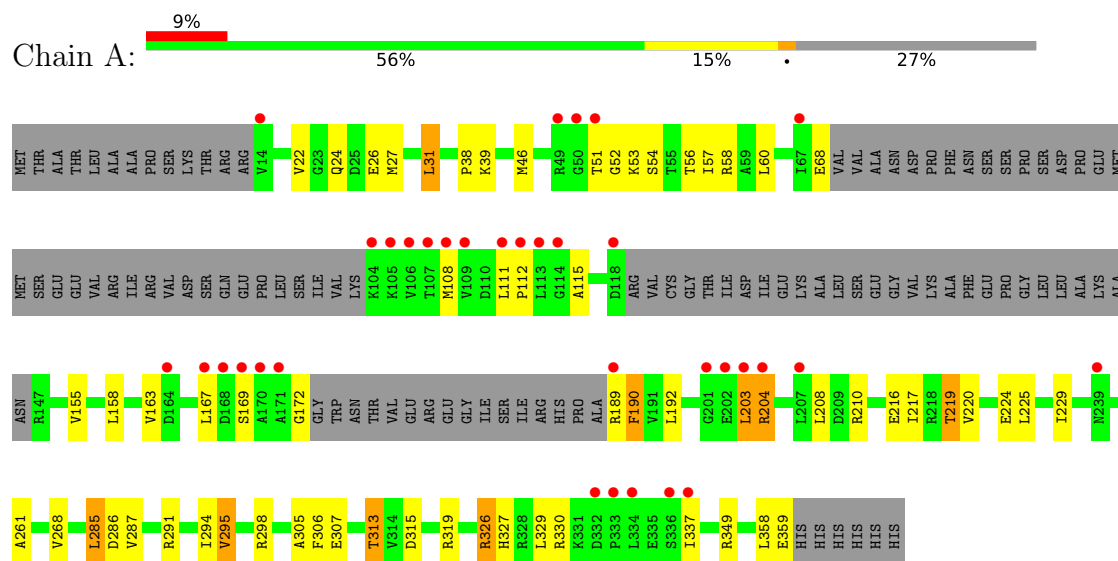
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	14	Total	O	0	0
			14	14		
2	F	18	Total	O	0	0
			18	18		

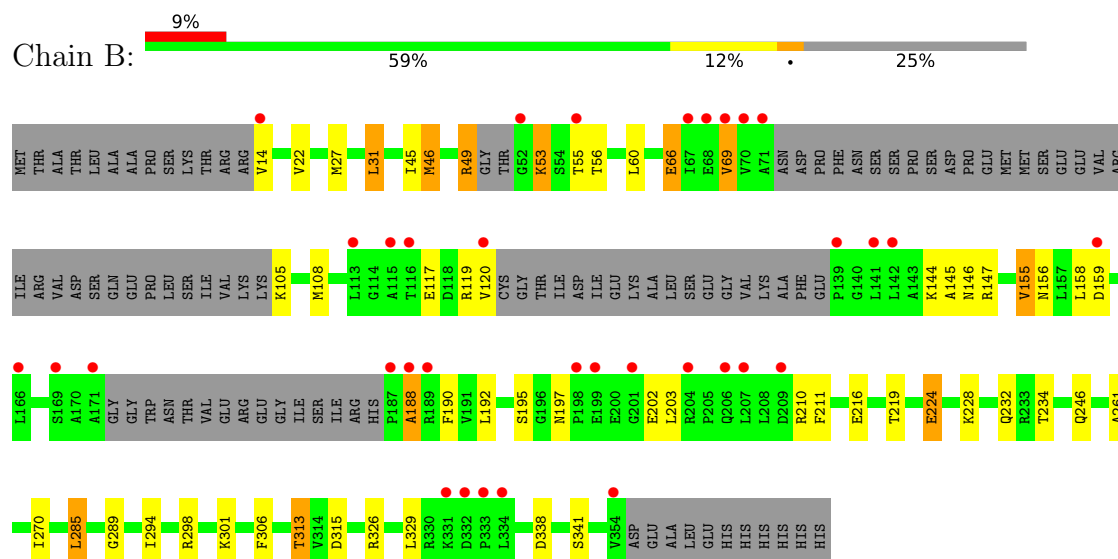
3 Residue-property plots [i](#)

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

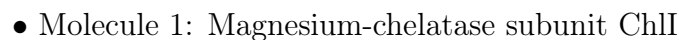
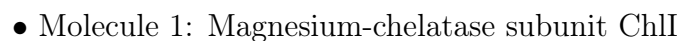
• Molecule 1: Magnesium-chelatase subunit ChII



• Molecule 1: Magnesium-chelatase subunit ChII

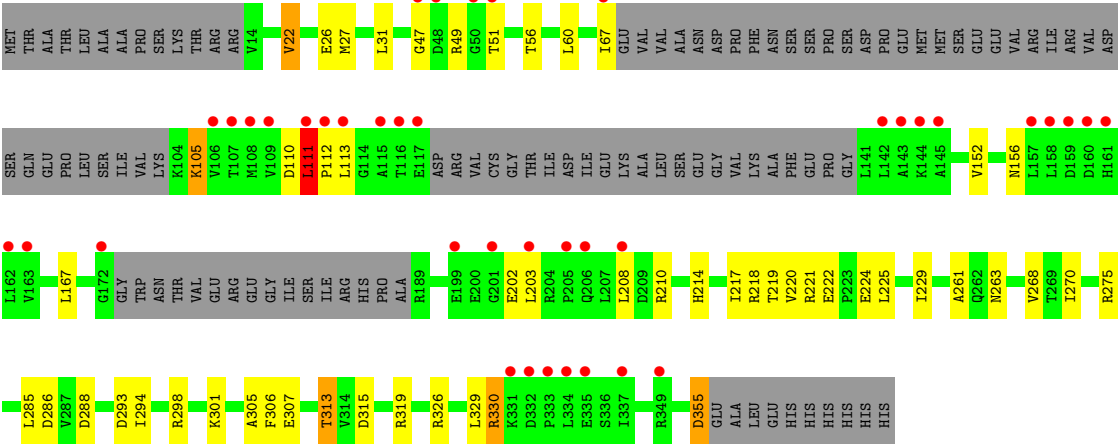


• Molecule 1: Magnesium-chelatase subunit ChII





● Molecule 1: Magnesium-chelatase subunit ChII



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.03Å 121.15Å 119.42Å 90.00° 99.06° 90.00°	Depositor
Resolution (Å)	49.33 – 2.91 49.33 – 2.91	Depositor EDS
% Data completeness (in resolution range)	80.7 (49.33-2.91) 81.0 (49.33-2.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.233 , 0.252 (Not available) , 0.273	Depositor DCC
R_{free} test set	2725 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12112	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 ⓘ

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	0.24	0/2058	0.50	1/2788 (0.0%)
1	B	0.26	0/2085	0.58	4/2826 (0.1%)
1	C	0.29	0/1965	0.56	1/2662 (0.0%)
1	D	0.27	0/1959	0.48	0/2653
1	E	0.26	0/2026	0.49	0/2747
1	F	0.28	0/2047	0.52	2/2773 (0.1%)
All	All	0.27	0/12140	0.52	8/16449 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	VAL	N-CA-C	9.19	119.24	110.42
1	B	66	GLU	N-CA-C	7.13	121.19	110.64
1	B	66	GLU	CB-CA-C	-6.72	101.53	109.80
1	F	111	LEU	CA-C-N	-5.99	114.38	120.85
1	F	111	LEU	C-N-CA	-5.99	114.38	120.85
1	C	66	GLU	N-CA-C	5.26	125.74	111.00
1	A	337	ILE	N-CA-C	5.16	116.23	109.21
1	B	188	ALA	CB-CA-C	5.13	119.10	109.86

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	2035	0	2034	50	0
1	B	2060	0	2083	27	0
1	C	1943	0	1943	42	0
1	D	1937	0	1958	70	0
1	E	2002	0	1992	36	0
1	F	2023	0	2025	59	0
2	A	20	0	0	1	0
2	B	22	0	0	2	0
2	C	19	0	0	2	0
2	D	19	0	0	2	0
2	E	14	0	0	1	0
2	F	18	0	0	0	0
All	All	12112	0	12035	277	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 12.

All (277) 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:F:111:LEU:HD13	1:F:152:VAL:CG2	1.58	1.33
1:A:51:THR:HG21	1:A:217:ILE:CG2	1.69	1.23
1:F:111:LEU:CD1	1:F:152:VAL:HG22	1.73	1.15
1:D:44:MET:HE2	1:D:203:LEU:HD23	1.28	1.14
1:D:169:SER:HB3	1:D:190:PHE:HE2	1.07	1.13
1:D:44:MET:HE2	1:D:203:LEU:CD2	1.78	1.11
1:F:111:LEU:HD22	1:F:152:VAL:HG13	1.14	1.10
1:C:106:VAL:CG1	1:C:107:THR:H	1.67	1.07
1:F:111:LEU:CD2	1:F:152:VAL:HG13	1.84	1.06
1:C:106:VAL:HG12	1:C:107:THR:H	0.89	1.06
1:F:111:LEU:CD1	1:F:152:VAL:CG2	2.27	1.06
1:F:110:ASP:O	1:F:112:PRO:HD3	1.54	1.05
1:D:204:ARG:HE	1:D:206:GLN:CG	1.70	1.05
1:D:203:LEU:HD13	1:D:208:LEU:HB2	1.08	1.04
1:C:106:VAL:HG12	1:C:107:THR:N	1.56	1.04
1:A:39:LYS:HD2	1:A:172:GLY:HA2	1.40	1.03
1:F:111:LEU:HD23	1:F:111:LEU:O	1.58	1.02
1:F:111:LEU:HD13	1:F:152:VAL:CG1	1.90	1.00
1:A:51:THR:HG21	1:A:217:ILE:HG21	1.00	0.98
1:D:169:SER:CB	1:D:190:PHE:HE2	1.76	0.97
1:D:169:SER:HB3	1:D:190:PHE:CE2	1.99	0.97
1:D:204:ARG:NE	1:D:206:GLN:HG3	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ARG:NE	1:D:206:GLN:CG	2.28	0.97
1:D:204:ARG:CD	1:D:206:GLN:HE21	1.78	0.96
1:D:204:ARG:HE	1:D:206:GLN:HG3	1.29	0.95
1:A:54:SER:O	1:A:58:ARG:HG3	1.65	0.95
1:D:203:LEU:HD13	1:D:208:LEU:CB	1.97	0.94
1:F:111:LEU:HD22	1:F:152:VAL:CG1	1.97	0.94
1:F:111:LEU:HD13	1:F:152:VAL:HG21	1.50	0.92
1:A:51:THR:CG2	1:A:217:ILE:HG21	1.96	0.90
1:F:111:LEU:HB3	1:F:152:VAL:HA	1.53	0.90
1:D:204:ARG:HG2	1:D:206:GLN:HG2	1.56	0.87
1:D:63:LEU:HD21	1:D:254:LEU:HD22	1.55	0.87
1:D:157:LEU:HD11	1:D:200:GLU:OE2	1.75	0.86
1:C:113:LEU:HD23	1:C:114:GLY:H	1.40	0.86
1:D:44:MET:CE	1:D:203:LEU:HD23	2.08	0.83
1:F:111:LEU:HD13	1:F:152:VAL:CB	2.08	0.83
1:F:111:LEU:HD12	1:F:152:VAL:HG22	1.59	0.83
1:C:66:GLU:O	1:C:66:GLU:HG2	1.77	0.82
1:D:39:LYS:HD3	1:D:172:GLY:HA2	1.60	0.82
1:D:169:SER:CB	1:D:190:PHE:CE2	2.63	0.78
1:F:111:LEU:CG	1:F:152:VAL:HG13	2.15	0.76
1:E:348:LYS:HG3	1:E:353:VAL:HB	1.67	0.76
1:D:204:ARG:CZ	1:D:206:GLN:HG3	2.15	0.76
1:D:203:LEU:HD12	1:D:203:LEU:O	1.85	0.75
1:F:167:LEU:HD13	1:F:210:ARG:HB2	1.69	0.75
1:D:204:ARG:NE	1:D:206:GLN:HE21	1.84	0.74
1:E:24:GLN:HE21	1:E:51:THR:HG22	1.51	0.74
1:C:66:GLU:O	1:C:66:GLU:CG	2.35	0.73
1:D:204:ARG:HE	1:D:206:GLN:NE2	1.87	0.72
1:F:111:LEU:HB2	1:F:152:VAL:HG22	1.71	0.72
1:A:219:THR:HG21	1:B:289:GLY:HA2	1.72	0.71
1:D:204:ARG:HE	1:D:206:GLN:CD	1.97	0.71
1:B:69:VAL:O	1:B:147:ARG:NH2	2.24	0.70
1:C:26:GLU:OE2	1:C:326:ARG:NH2	2.27	0.68
1:F:111:LEU:CD1	1:F:152:VAL:CG1	2.69	0.68
1:D:204:ARG:HD2	1:D:206:GLN:HE21	1.60	0.67
1:A:51:THR:CG2	1:A:217:ILE:CG2	2.63	0.67
1:D:204:ARG:NH2	1:D:206:GLN:HG3	2.09	0.67
1:F:111:LEU:HD13	1:F:152:VAL:HG13	1.76	0.67
1:B:14:VAL:N	2:B:402:HOH:O	2.30	0.65
1:C:57:ILE:HB	1:C:108:MET:HE1	1.79	0.65
1:F:111:LEU:CD1	1:F:152:VAL:HG13	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:ARG:N	2:E:401:HOH:O	2.30	0.64
1:C:106:VAL:CG1	1:C:107:THR:N	2.30	0.64
1:F:111:LEU:CB	1:F:152:VAL:HG22	2.28	0.64
1:C:64:LEU:HB2	1:C:106:VAL:HG21	1.80	0.64
1:D:204:ARG:NE	1:D:206:GLN:NE2	2.46	0.63
1:F:111:LEU:CD1	1:F:152:VAL:HG21	2.15	0.63
1:F:111:LEU:CD2	1:F:111:LEU:O	2.40	0.62
1:C:270:ILE:HG22	1:C:301:LYS:HE3	1.81	0.62
1:D:111:LEU:HG	1:D:150:LEU:HD11	1.80	0.62
1:D:348:LYS:HG3	1:D:353:VAL:HB	1.82	0.62
1:F:110:ASP:C	1:F:112:PRO:HD3	2.24	0.62
1:E:291:ARG:O	1:E:295:VAL:HG23	2.00	0.61
1:A:39:LYS:HD2	1:A:172:GLY:CA	2.24	0.61
1:D:62:ASP:OD1	1:D:105:LYS:NZ	2.29	0.61
1:A:26:GLU:OE2	1:A:326:ARG:NH2	2.34	0.61
1:F:285:LEU:HG	1:F:329:LEU:HD21	1.83	0.60
1:D:203:LEU:CD1	1:D:208:LEU:HB2	2.04	0.60
1:A:285:LEU:HG	1:A:329:LEU:HD21	1.84	0.60
1:F:111:LEU:CB	1:F:152:VAL:HA	2.30	0.59
1:C:47:GLY:HA3	1:C:217:ILE:HB	1.83	0.59
1:F:110:ASP:O	1:F:112:PRO:CD	2.39	0.58
1:C:57:ILE:HG22	1:C:108:MET:SD	2.43	0.58
1:D:203:LEU:HD11	1:D:208:LEU:HD22	1.84	0.58
1:F:31:LEU:HB3	1:F:60:LEU:HD22	1.86	0.58
1:E:48:ASP:OD2	1:E:219:THR:HB	2.02	0.58
1:F:105:LYS:H	1:F:105:LYS:HD2	1.69	0.58
1:A:38:PRO:HD2	1:A:189:ARG:HH21	1.69	0.57
1:D:189:ARG:N	2:D:401:HOH:O	2.37	0.57
1:F:27:MET:HE3	1:F:56:THR:HG21	1.86	0.57
1:A:349:ARG:NH1	2:A:401:HOH:O	2.27	0.57
1:E:192:LEU:HD22	1:E:211:PHE:HE2	1.70	0.57
1:F:47:GLY:HA3	1:F:217:ILE:HB	1.87	0.57
1:C:49:ARG:HA	1:D:288:ASP:OD2	2.05	0.56
1:A:31:LEU:HB3	1:A:60:LEU:HD22	1.87	0.56
1:A:203:LEU:HB2	1:A:208:LEU:HD22	1.87	0.56
1:C:44:MET:HE3	1:C:46:MET:SD	2.46	0.56
1:D:204:ARG:NE	1:D:206:GLN:HG2	2.18	0.56
1:D:204:ARG:HH21	1:D:206:GLN:HG3	1.70	0.56
1:F:307:GLU:CD	1:F:319:ARG:HH22	2.14	0.56
1:D:167:LEU:HD13	1:D:210:ARG:CB	2.36	0.55
1:B:313:THR:HG22	1:B:315:ASP:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ALA:HB2	1:A:306:PHE:HA	1.88	0.55
1:C:285:LEU:HG	1:C:329:LEU:HD21	1.89	0.55
1:E:313:THR:HG22	1:E:316:ASP:CG	2.33	0.54
1:D:204:ARG:CG	1:D:206:GLN:HE21	2.20	0.53
1:A:53:LYS:O	1:A:57:ILE:HD12	2.08	0.53
1:B:46:MET:O	1:B:216:GLU:HA	2.08	0.53
1:A:208:LEU:HD21	1:A:327:HIS:HB2	1.90	0.53
1:F:261:ALA:HB2	1:F:306:PHE:HA	1.90	0.53
1:B:285:LEU:HG	1:B:329:LEU:HD21	1.90	0.53
1:A:268:VAL:HG21	1:A:305:ALA:HB2	1.89	0.53
1:F:26:GLU:OE2	1:F:326:ARG:NH2	2.40	0.53
1:A:313:THR:HG22	1:A:315:ASP:H	1.73	0.52
1:A:313:THR:HG22	1:A:315:ASP:N	2.25	0.52
1:C:113:LEU:HD23	1:C:114:GLY:N	2.16	0.52
1:E:261:ALA:HB2	1:E:306:PHE:HA	1.92	0.52
1:D:169:SER:HB2	1:D:190:PHE:CE2	2.43	0.51
1:D:51:THR:O	1:D:51:THR:HG22	2.10	0.51
1:D:307:GLU:OE1	1:D:319:ARG:NH2	2.43	0.51
1:A:167:LEU:HD13	1:A:210:ARG:HB2	1.92	0.51
1:A:204:ARG:H	1:A:204:ARG:CZ	2.24	0.51
1:B:224:GLU:CD	1:B:224:GLU:H	2.19	0.51
1:D:26:GLU:OE2	1:D:326:ARG:NH2	2.43	0.51
1:F:111:LEU:HD13	1:F:152:VAL:HG11	1.82	0.51
1:C:313:THR:HG22	1:C:315:ASP:H	1.75	0.51
1:E:307:GLU:CD	1:E:319:ARG:HH22	2.19	0.51
1:F:268:VAL:HG21	1:F:305:ALA:HB2	1.92	0.51
1:D:31:LEU:HB3	1:D:60:LEU:HD22	1.93	0.51
1:A:286:ASP:OD2	1:F:49:ARG:NH1	2.45	0.50
1:A:330:ARG:HH22	1:F:49:ARG:CG	2.24	0.50
1:C:261:ALA:HB2	1:C:306:PHE:HA	1.92	0.50
1:C:268:VAL:HG21	1:C:305:ALA:HB2	1.92	0.50
1:D:307:GLU:CD	1:D:319:ARG:HH22	2.19	0.49
1:B:313:THR:HG22	1:B:315:ASP:N	2.27	0.49
1:C:49:ARG:HE	1:C:219:THR:HB	1.77	0.49
1:E:26:GLU:OE2	1:E:326:ARG:NH2	2.44	0.49
1:D:167:LEU:HD13	1:D:210:ARG:HB2	1.94	0.49
1:C:27:MET:HE3	1:C:56:THR:HG21	1.95	0.49
1:A:204:ARG:H	1:A:204:ARG:NE	2.11	0.49
1:D:151:TYR:HA	1:D:193:VAL:O	2.13	0.48
1:E:202:GLU:C	1:E:204:ARG:H	2.20	0.48
1:A:307:GLU:CD	1:A:319:ARG:HH22	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HB3	1:B:60:LEU:HD22	1.95	0.48
1:D:291:ARG:HD2	1:D:295:VAL:HG23	1.96	0.48
1:C:53:LYS:NZ	2:C:405:HOH:O	2.47	0.48
1:C:113:LEU:HD23	1:C:113:LEU:N	2.28	0.48
1:F:270:ILE:HG22	1:F:301:LYS:HE3	1.96	0.48
1:F:294:ILE:O	1:F:298:ARG:HG3	2.13	0.48
1:B:156:ASN:HD21	1:B:197:ASN:HB3	1.78	0.47
1:F:286:ASP:OD1	1:F:330:ARG:NH1	2.47	0.47
1:B:246:GLN:NE2	2:B:404:HOH:O	2.47	0.47
1:C:65:PRO:O	1:C:66:GLU:HB3	2.15	0.47
1:D:39:LYS:HD3	1:D:172:GLY:CA	2.37	0.47
1:A:220:VAL:HG11	1:A:225:LEU:HB3	1.96	0.47
1:B:261:ALA:HB2	1:B:306:PHE:HA	1.96	0.47
1:C:313:THR:HG22	1:C:315:ASP:N	2.29	0.47
1:F:329:LEU:HD23	1:F:329:LEU:HA	1.73	0.47
1:A:112:PRO:HD2	1:A:115:ALA:HB2	1.97	0.47
1:E:225:LEU:O	1:E:229:ILE:HG13	2.15	0.47
1:B:219:THR:HG21	1:C:289:GLY:HA2	1.97	0.46
1:C:47:GLY:C	1:C:49:ARG:H	2.22	0.46
1:F:111:LEU:HD12	1:F:152:VAL:CG2	2.24	0.46
1:B:228:LYS:HE2	1:B:232:GLN:NE2	2.30	0.46
1:D:220:VAL:HG11	1:D:225:LEU:HB3	1.96	0.46
1:A:291:ARG:O	1:A:295:VAL:HG13	2.14	0.46
1:A:294:ILE:O	1:A:298:ARG:HG3	2.15	0.46
1:E:24:GLN:HE21	1:E:51:THR:CG2	2.26	0.46
1:D:268:VAL:HG21	1:D:305:ALA:HB2	1.97	0.46
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.78	0.46
1:A:27:MET:HE3	1:A:56:THR:HG21	1.98	0.46
1:B:117:GLU:C	1:B:119:ARG:H	2.24	0.46
1:A:24:GLN:OE1	1:A:51:THR:HB	2.16	0.46
1:C:113:LEU:N	1:C:113:LEU:CD2	2.78	0.46
1:D:204:ARG:HG2	1:D:206:GLN:CG	2.37	0.46
1:F:220:VAL:HG11	1:F:225:LEU:HB3	1.98	0.46
1:B:49:ARG:HE	1:B:49:ARG:HB2	1.63	0.45
1:E:24:GLN:NE2	1:E:51:THR:HG22	2.25	0.45
1:F:113:LEU:HD23	1:F:113:LEU:HA	1.80	0.45
1:E:44:MET:HB2	1:E:211:PHE:CD1	2.51	0.45
1:F:307:GLU:OE2	1:F:319:ARG:NH2	2.42	0.45
1:B:27:MET:HE3	1:B:56:THR:HG21	1.99	0.45
1:C:224:GLU:CD	1:C:224:GLU:H	2.25	0.45
1:D:160:ASP:CB	1:D:204:ARG:HH12	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:LEU:HD11	1:F:214:HIS:HD2	1.82	0.45
1:E:285:LEU:HG	1:E:329:LEU:HD21	1.98	0.45
1:F:202:GLU:O	1:F:203:LEU:C	2.59	0.45
1:C:31:LEU:HB3	1:C:60:LEU:HD22	1.97	0.45
1:D:109:VAL:HG21	1:D:145:ALA:HB2	1.99	0.45
1:D:204:ARG:CG	1:D:206:GLN:NE2	2.80	0.45
1:E:27:MET:HE3	1:E:56:THR:HG21	1.99	0.45
1:D:201:GLY:O	1:D:202:GLU:C	2.59	0.45
1:E:307:GLU:OE2	1:E:319:ARG:NH2	2.49	0.45
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.73	0.44
1:D:294:ILE:O	1:D:298:ARG:HG3	2.17	0.44
1:A:46:MET:O	1:A:216:GLU:HA	2.18	0.44
1:E:46:MET:O	1:E:216:GLU:HA	2.18	0.44
1:E:27:MET:HE2	1:E:27:MET:HB3	1.81	0.44
1:D:204:ARG:CD	1:D:206:GLN:NE2	2.63	0.44
1:C:161:HIS:O	1:C:165:VAL:HG23	2.18	0.44
1:C:225:LEU:HD23	1:C:225:LEU:HA	1.76	0.44
1:B:192:LEU:HD22	1:B:211:PHE:HE2	1.82	0.43
1:D:108:MET:HB2	1:D:108:MET:HE3	1.67	0.43
1:E:226:ARG:NH2	1:F:293:ASP:OD1	2.52	0.43
1:D:225:LEU:O	1:D:229:ILE:HG13	2.19	0.43
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.68	0.43
1:E:66:GLU:HG2	1:E:105:LYS:HA	2.00	0.43
1:B:338:ASP:HB3	1:B:341:SER:HB3	2.01	0.43
1:C:31:LEU:HD12	1:C:43:VAL:HG21	2.01	0.43
1:C:189:ARG:NH1	2:C:403:HOH:O	2.40	0.43
1:E:202:GLU:C	1:E:204:ARG:N	2.76	0.43
1:F:49:ARG:HD2	1:F:218:ARG:HA	2.01	0.43
1:F:355:ASP:OD1	1:F:355:ASP:N	2.51	0.43
1:F:22:VAL:HG13	1:F:229:ILE:HG12	2.01	0.42
1:A:203:LEU:CB	1:A:208:LEU:HD22	2.49	0.42
1:A:51:THR:HG21	1:A:217:ILE:HG22	1.84	0.42
1:A:158:LEU:O	1:A:163:VAL:HG23	2.20	0.42
1:D:285:LEU:HG	1:D:329:LEU:HD21	2.01	0.42
1:E:225:LEU:HD23	1:E:225:LEU:HA	1.90	0.42
1:F:225:LEU:HD23	1:F:225:LEU:HA	1.90	0.42
1:C:33:LEU:HD12	1:C:213:MET:HE1	2.01	0.42
1:D:326:ARG:NH1	2:D:404:HOH:O	2.52	0.42
1:F:313:THR:HG22	1:F:315:ASP:H	1.84	0.42
1:B:66:GLU:HA	1:B:105:LYS:HA	2.01	0.42
1:D:158:LEU:O	1:D:163:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:VAL:HG11	1:D:207:LEU:HD21	2.01	0.42
1:A:169:SER:HB2	1:A:190:PHE:CE2	2.54	0.42
1:C:27:MET:SD	1:C:217:ILE:HD11	2.60	0.42
1:E:309:ARG:HH22	1:E:316:ASP:CG	2.25	0.42
1:B:145:ALA:O	1:B:190:PHE:HB3	2.20	0.42
1:C:329:LEU:HD23	1:C:329:LEU:HA	1.79	0.42
1:A:330:ARG:HH22	1:F:49:ARG:HG3	1.84	0.42
1:E:220:VAL:HG11	1:E:225:LEU:HB3	2.02	0.42
1:B:270:ILE:HG22	1:B:301:LYS:HE3	2.02	0.42
1:E:161:HIS:O	1:E:165:VAL:HG23	2.19	0.42
1:E:275:ARG:HE	1:E:275:ARG:HB2	1.65	0.42
1:A:27:MET:HE2	1:A:27:MET:HB3	1.76	0.41
1:A:53:LYS:O	1:A:57:ILE:CD1	2.68	0.41
1:A:285:LEU:HG	1:A:329:LEU:CD2	2.48	0.41
1:B:27:MET:HE2	1:B:27:MET:HB3	1.82	0.41
1:C:277:LYS:O	1:C:281:VAL:HG23	2.20	0.41
1:E:31:LEU:HB3	1:E:60:LEU:HD22	2.02	0.41
1:A:38:PRO:HG2	1:A:189:ARG:HE	1.85	0.41
1:B:146:ASN:HA	1:B:188:ALA:HB1	2.02	0.41
1:F:22:VAL:HG21	1:F:225:LEU:HD22	2.02	0.41
1:A:52:GLY:C	1:A:54:SER:N	2.77	0.41
1:C:285:LEU:HG	1:C:329:LEU:CD2	2.50	0.41
1:E:24:GLN:HB3	1:E:27:MET:HE2	2.03	0.41
1:F:288:ASP:HA	1:F:330:ARG:NH2	2.36	0.41
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.89	0.41
1:F:49:ARG:CD	1:F:218:ARG:HA	2.50	0.41
1:A:52:GLY:C	1:A:54:SER:H	2.28	0.41
1:D:35:VAL:HG11	1:D:64:LEU:HD21	2.03	0.41
1:D:204:ARG:CG	1:D:206:GLN:HG2	2.39	0.41
1:A:53:LYS:H	1:A:53:LYS:HG3	1.74	0.41
1:E:207:LEU:HD12	1:E:207:LEU:HA	1.81	0.41
1:E:281:VAL:HG11	1:E:321:ILE:HD11	2.03	0.41
1:A:220:VAL:HG21	1:A:229:ILE:HD11	2.02	0.41
1:C:159:ASP:HA	1:C:163:VAL:CG2	2.51	0.41
1:C:204:ARG:C	1:C:206:GLN:N	2.77	0.41
1:D:285:LEU:HG	1:D:329:LEU:CD2	2.51	0.41
1:E:169:SER:OG	1:E:210:ARG:NH2	2.54	0.41
1:E:294:ILE:O	1:E:298:ARG:HG3	2.21	0.41
1:A:169:SER:HB2	1:A:190:PHE:CZ	2.56	0.40
1:B:155:VAL:HG23	1:B:195:SER:O	2.21	0.40
1:D:53:LYS:O	1:D:57:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:VAL:CG1	1:D:207:LEU:HD21	2.51	0.40
1:F:222:GLU:HB3	1:F:225:LEU:HB2	2.03	0.40
1:B:45:ILE:CG2	1:B:53:LYS:HD3	2.51	0.40
1:B:294:ILE:O	1:B:298:ARG:HG3	2.22	0.40
1:D:291:ARG:O	1:D:295:VAL:HG23	2.22	0.40
1:F:27:MET:HE2	1:F:27:MET:HB3	1.92	0.40
1:D:277:LYS:O	1:D:281:VAL:HG23	2.22	0.40
1:E:49:ARG:HA	1:E:53:LYS:NZ	2.37	0.40
1:E:277:LYS:O	1:E:281:VAL:HG23	2.22	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	259/365 (71%)	243 (94%)	16 (6%)	0	100	100
1	B	263/365 (72%)	252 (96%)	11 (4%)	0	100	100
1	C	246/365 (67%)	235 (96%)	11 (4%)	0	100	100
1	D	243/365 (67%)	230 (95%)	13 (5%)	0	100	100
1	E	258/365 (71%)	246 (95%)	12 (5%)	0	100	100
1	F	259/365 (71%)	242 (93%)	16 (6%)	1 (0%)	30	58
All	All	1528/2190 (70%)	1448 (95%)	79 (5%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	111	LEU

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	219/315 (70%)	201 (92%)	18 (8%)	10	31
1	B	218/315 (69%)	198 (91%)	20 (9%)	8	26
1	C	206/315 (65%)	195 (95%)	11 (5%)	20	50
1	D	209/315 (66%)	195 (93%)	14 (7%)	15	41
1	E	210/315 (67%)	200 (95%)	10 (5%)	23	54
1	F	215/315 (68%)	202 (94%)	13 (6%)	17	45
All	All	1277/1890 (68%)	1191 (93%)	86 (7%)	15	41

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	31	LEU
1	A	68	GLU
1	A	108	MET
1	A	155	VAL
1	A	190	PHE
1	A	192	LEU
1	A	203	LEU
1	A	204	ARG
1	A	219	THR
1	A	224	GLU
1	A	285	LEU
1	A	287	VAL
1	A	295	VAL
1	A	313	THR
1	A	326	ARG
1	A	358	LEU
1	A	359	GLU
1	B	22	VAL
1	B	31	LEU
1	B	46	MET
1	B	49	ARG

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Mol	Chain	Res	Type
1	B	53	LYS
1	B	55	THR
1	B	108	MET
1	B	120	VAL
1	B	144	LYS
1	B	155	VAL
1	B	158	LEU
1	B	159	ASP
1	B	202	GLU
1	B	203	LEU
1	B	210	ARG
1	B	224	GLU
1	B	234	THR
1	B	285	LEU
1	B	313	THR
1	B	326	ARG
1	C	22	VAL
1	C	49	ARG
1	C	108	MET
1	C	113	LEU
1	C	157	LEU
1	C	189	ARG
1	C	207	LEU
1	C	219	THR
1	C	224	GLU
1	C	313	THR
1	C	326	ARG
1	D	14	VAL
1	D	22	VAL
1	D	53	LYS
1	D	54	SER
1	D	107	THR
1	D	108	MET
1	D	113	LEU
1	D	155	VAL
1	D	192	LEU
1	D	203	LEU
1	D	206	GLN
1	D	224	GLU
1	D	291	ARG
1	D	348	LYS
1	E	22	VAL

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Mol	Chain	Res	Type
1	E	51	THR
1	E	111	LEU
1	E	147	ARG
1	E	158	LEU
1	E	221	ARG
1	E	224	GLU
1	E	249	THR
1	E	295	VAL
1	E	348	LYS
1	F	22	VAL
1	F	51	THR
1	F	67	ILE
1	F	105	LYS
1	F	156	ASN
1	F	219	THR
1	F	221	ARG
1	F	224	GLU
1	F	263	ASN
1	F	275	ARG
1	F	313	THR
1	F	330	ARG
1	F	355	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	232	GLN
1	B	232	GLN
1	C	241	HIS
1	D	206	GLN
1	D	241	HIS
1	E	24	GLN
1	E	255	GLN
1	F	232	GLN
1	F	239	ASN
1	F	241	HIS

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](#)

There are no ligands in this entry.

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	267/365 (73%)	0.43	34 (12%) 8 6	17, 37, 85, 92	0
1	B	273/365 (74%)	0.53	34 (12%) 8 7	22, 41, 83, 93	0
1	C	256/365 (70%)	0.67	42 (16%) 4 3	24, 44, 87, 95	0
1	D	253/365 (69%)	0.78	49 (19%) 3 3	22, 42, 81, 91	0
1	E	266/365 (72%)	0.78	46 (17%) 4 3	25, 48, 86, 100	0
1	F	267/365 (73%)	0.60	40 (14%) 5 4	19, 43, 85, 97	0
All	All	1582/2190 (72%)	0.63	245 (15%) 5 4	17, 43, 85, 100	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	GLU	8.1
1	E	203	LEU	7.8
1	D	169	SER	6.0
1	B	71	ALA	5.7
1	E	202	GLU	5.7
1	E	332	ASP	5.5
1	F	115	ALA	5.5
1	F	160	ASP	5.3
1	C	207	LEU	5.2
1	E	158	LEU	5.2
1	E	142	LEU	5.1
1	A	203	LEU	5.1
1	F	112	PRO	4.8
1	B	52	GLY	4.7
1	E	157	LEU	4.7
1	D	166	LEU	4.7
1	D	198	PRO	4.7
1	C	113	LEU	4.6
1	F	113	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	48	ASP	4.6
1	C	107	THR	4.5
1	D	168	ASP	4.5
1	B	116	THR	4.5
1	B	69	VAL	4.4
1	C	159	ASP	4.4
1	E	67	ILE	4.3
1	C	198	PRO	4.3
1	E	112	PRO	4.3
1	C	204	ARG	4.3
1	B	334	LEU	4.2
1	F	172	GLY	4.2
1	D	113	LEU	4.1
1	D	158	LEU	4.0
1	B	332	ASP	4.0
1	C	168	ASP	4.0
1	E	333	PRO	4.0
1	B	171	ALA	4.0
1	F	117	GLU	4.0
1	F	158	LEU	4.0
1	A	204	ARG	3.9
1	E	207	LEU	3.9
1	A	113	LEU	3.9
1	C	116	THR	3.9
1	E	49	ARG	3.9
1	A	189	ARG	3.9
1	F	51	THR	3.9
1	F	332	ASP	3.8
1	C	160	ASP	3.8
1	D	155	VAL	3.8
1	A	112	PRO	3.8
1	D	203	LEU	3.8
1	E	198	PRO	3.8
1	D	171	ALA	3.8
1	E	50	GLY	3.7
1	C	332	ASP	3.7
1	F	111	LEU	3.7
1	E	189	ARG	3.7
1	B	166	LEU	3.6
1	D	207	LEU	3.6
1	F	203	LEU	3.6
1	A	105	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	145	ALA	3.6
1	A	337	ILE	3.6
1	D	162	LEU	3.6
1	D	147	ARG	3.5
1	D	152	VAL	3.5
1	E	165	VAL	3.5
1	D	200	GLU	3.5
1	B	206	GLN	3.4
1	C	206	GLN	3.4
1	E	51	THR	3.4
1	E	113	LEU	3.3
1	C	145	ALA	3.3
1	C	164	ASP	3.2
1	E	197	ASN	3.2
1	B	189	ARG	3.2
1	D	172	GLY	3.2
1	D	107	THR	3.2
1	E	199	GLU	3.2
1	E	175	ASN	3.2
1	D	206	GLN	3.2
1	A	51	THR	3.2
1	B	187	PRO	3.2
1	A	170	ALA	3.1
1	C	161	HIS	3.1
1	D	161	HIS	3.1
1	E	205	PRO	3.1
1	E	161	HIS	3.1
1	C	197	ASN	3.1
1	A	336	SER	3.1
1	F	337	ILE	3.1
1	B	204	ARG	3.1
1	C	51	THR	3.1
1	E	162	LEU	3.1
1	A	104	LYS	3.1
1	D	160	ASP	3.1
1	F	335	GLU	3.1
1	A	169	SER	3.0
1	F	48	ASP	3.0
1	F	159	ASP	3.0
1	E	166	LEU	3.0
1	A	171	ALA	3.0
1	F	143	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	334	LEU	3.0
1	D	167	LEU	3.0
1	E	334	LEU	3.0
1	B	68	GLU	3.0
1	B	67	ILE	3.0
1	A	207	LEU	3.0
1	E	238	GLN	3.0
1	B	199	GLU	3.0
1	B	209	ASP	2.9
1	D	156	ASN	2.9
1	A	167	LEU	2.9
1	F	162	LEU	2.9
1	D	148	GLY	2.9
1	F	47	GLY	2.9
1	C	146	ASN	2.9
1	D	165	VAL	2.9
1	E	159	ASP	2.9
1	F	208	LEU	2.9
1	D	199	GLU	2.8
1	A	118	ASP	2.8
1	D	208	LEU	2.8
1	C	163	VAL	2.8
1	D	201	GLY	2.8
1	E	173	GLY	2.8
1	C	333	PRO	2.8
1	F	67	ILE	2.8
1	D	153	ASP	2.8
1	F	201	GLY	2.8
1	E	109	VAL	2.8
1	F	106	VAL	2.8
1	A	332	ASP	2.8
1	D	159	ASP	2.8
1	E	169	SER	2.8
1	B	70	VAL	2.7
1	E	46	MET	2.7
1	E	116	THR	2.7
1	E	164	ASP	2.7
1	C	334	LEU	2.7
1	C	47	GLY	2.7
1	C	49	ARG	2.7
1	C	189	ARG	2.7
1	D	332	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	164	ASP	2.6
1	D	163	VAL	2.6
1	D	204	ARG	2.6
1	F	50	GLY	2.6
1	E	156	ASN	2.6
1	E	170	ALA	2.6
1	C	169	SER	2.6
1	C	112	PRO	2.6
1	F	199	GLU	2.6
1	C	105	LYS	2.5
1	F	142	LEU	2.5
1	C	14	VAL	2.5
1	A	109	VAL	2.5
1	E	218	ARG	2.5
1	C	205	PRO	2.5
1	A	49	ARG	2.5
1	B	207	LEU	2.5
1	C	166	LEU	2.5
1	E	190	PHE	2.5
1	D	170	ALA	2.5
1	A	164	ASP	2.4
1	B	333	PRO	2.4
1	D	112	PRO	2.4
1	D	354	VAL	2.4
1	F	334	LEU	2.4
1	E	160	ASP	2.4
1	F	206	GLN	2.4
1	F	116	THR	2.4
1	A	239	ASN	2.4
1	B	201	GLY	2.4
1	C	50	GLY	2.4
1	D	52	GLY	2.4
1	B	188	ALA	2.4
1	F	107	THR	2.4
1	E	108	MET	2.4
1	A	201	GLY	2.4
1	F	331	LYS	2.4
1	D	54	SER	2.4
1	F	157	LEU	2.4
1	A	14	VAL	2.3
1	E	48	ASP	2.3
1	B	142	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	198	PRO	2.3
1	E	330	ARG	2.3
1	D	151	TYR	2.3
1	C	155	VAL	2.3
1	A	168	ASP	2.3
1	F	333	PRO	2.3
1	D	46	MET	2.3
1	C	337	ILE	2.3
1	D	51	THR	2.3
1	A	202	GLU	2.2
1	F	349	ARG	2.2
1	B	14	VAL	2.2
1	C	65	PRO	2.2
1	F	163	VAL	2.2
1	F	161	HIS	2.2
1	D	205	PRO	2.2
1	B	113	LEU	2.2
1	E	174	TRP	2.2
1	A	111	LEU	2.2
1	E	111	LEU	2.2
1	B	115	ALA	2.2
1	C	66	GLU	2.2
1	D	335	GLU	2.2
1	F	145	ALA	2.2
1	A	67	ILE	2.2
1	D	110	ASP	2.2
1	C	55	THR	2.2
1	A	114	GLY	2.2
1	B	169	SER	2.2
1	D	154	GLU	2.2
1	E	239	ASN	2.1
1	A	333	PRO	2.1
1	F	205	PRO	2.1
1	B	159	ASP	2.1
1	B	55	THR	2.1
1	F	144	LYS	2.1
1	B	141	LEU	2.1
1	D	202	GLU	2.1
1	B	139	PRO	2.1
1	F	108	MET	2.1
1	A	107	THR	2.1
1	C	272	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	147	ARG	2.1
1	A	106	VAL	2.1
1	B	331	LYS	2.1
1	C	154	GLU	2.1
1	E	219	THR	2.1
1	B	120	VAL	2.0
1	F	109	VAL	2.0
1	D	111	LEU	2.0
1	A	50	GLY	2.0
1	D	338	ASP	2.0
1	A	108	MET	2.0
1	C	106	VAL	2.0
1	C	115	ALA	2.0
1	D	209	ASP	2.0
1	C	108	MET	2.0
1	B	354	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.