



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:13 AM UTC

PDB ID : 3CVG / pdb_00003cvg
Title : Crystal structure of a periplasmic putative metal binding protein
Authors : Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2008-04-18
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (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

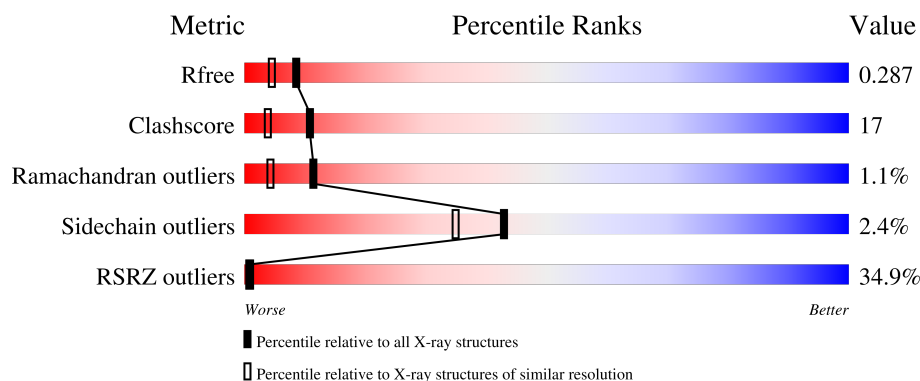
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	294	18% 70% 20% • 8%
1	B	294	36% 65% 24% • 8%
1	C	294	21% 45% 24% •• 30%
1	D	294	43% 60% 29% •• 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8486 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 Putative metal binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	Se	0	0	0
			2113	1356	353	399	5			
1	B	270	Total	C	N	O	Se	0	0	0
			2113	1356	353	399	5			
1	C	207	Total	C	N	O	Se	0	0	0
			1640	1055	276	304	5			
1	D	268	Total	C	N	O	Se	0	0	0
			2096	1347	351	393	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MSE	-	expression tag	UNP Q1DXA6
A	20	SER	-	expression tag	UNP Q1DXA6
A	21	LEU	-	expression tag	UNP Q1DXA6
A	305	GLU	-	expression tag	UNP Q1DXA6
A	306	GLY	-	expression tag	UNP Q1DXA6
A	307	HIS	-	expression tag	UNP Q1DXA6
A	308	HIS	-	expression tag	UNP Q1DXA6
A	309	HIS	-	expression tag	UNP Q1DXA6
A	310	HIS	-	expression tag	UNP Q1DXA6
A	311	HIS	-	expression tag	UNP Q1DXA6
A	312	HIS	-	expression tag	UNP Q1DXA6
B	19	MSE	-	expression tag	UNP Q1DXA6
B	20	SER	-	expression tag	UNP Q1DXA6
B	21	LEU	-	expression tag	UNP Q1DXA6
B	305	GLU	-	expression tag	UNP Q1DXA6
B	306	GLY	-	expression tag	UNP Q1DXA6
B	307	HIS	-	expression tag	UNP Q1DXA6
B	308	HIS	-	expression tag	UNP Q1DXA6
B	309	HIS	-	expression tag	UNP Q1DXA6
B	310	HIS	-	expression tag	UNP Q1DXA6
B	311	HIS	-	expression tag	UNP Q1DXA6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	312	HIS	-	expression tag	UNP Q1DXA6
C	19	MSE	-	expression tag	UNP Q1DXA6
C	20	SER	-	expression tag	UNP Q1DXA6
C	21	LEU	-	expression tag	UNP Q1DXA6
C	305	GLU	-	expression tag	UNP Q1DXA6
C	306	GLY	-	expression tag	UNP Q1DXA6
C	307	HIS	-	expression tag	UNP Q1DXA6
C	308	HIS	-	expression tag	UNP Q1DXA6
C	309	HIS	-	expression tag	UNP Q1DXA6
C	310	HIS	-	expression tag	UNP Q1DXA6
C	311	HIS	-	expression tag	UNP Q1DXA6
C	312	HIS	-	expression tag	UNP Q1DXA6
D	19	MSE	-	expression tag	UNP Q1DXA6
D	20	SER	-	expression tag	UNP Q1DXA6
D	21	LEU	-	expression tag	UNP Q1DXA6
D	305	GLU	-	expression tag	UNP Q1DXA6
D	306	GLY	-	expression tag	UNP Q1DXA6
D	307	HIS	-	expression tag	UNP Q1DXA6
D	308	HIS	-	expression tag	UNP Q1DXA6
D	309	HIS	-	expression tag	UNP Q1DXA6
D	310	HIS	-	expression tag	UNP Q1DXA6
D	311	HIS	-	expression tag	UNP Q1DXA6
D	312	HIS	-	expression tag	UNP Q1DXA6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	159	Total O 159 159	0	0

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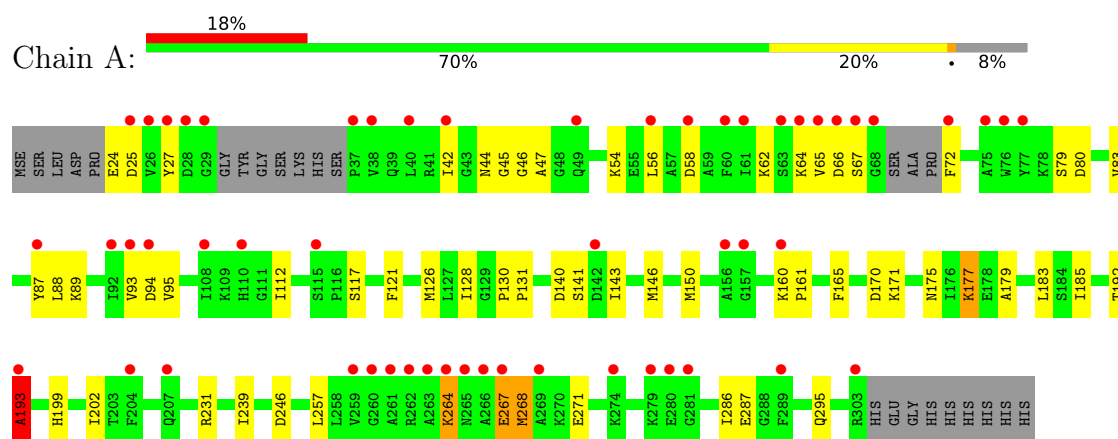
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	113	Total 113	O 113	0	0
3	C	135	Total 135	O 135	0	0
3	D	113	Total 113	O 113	0	0

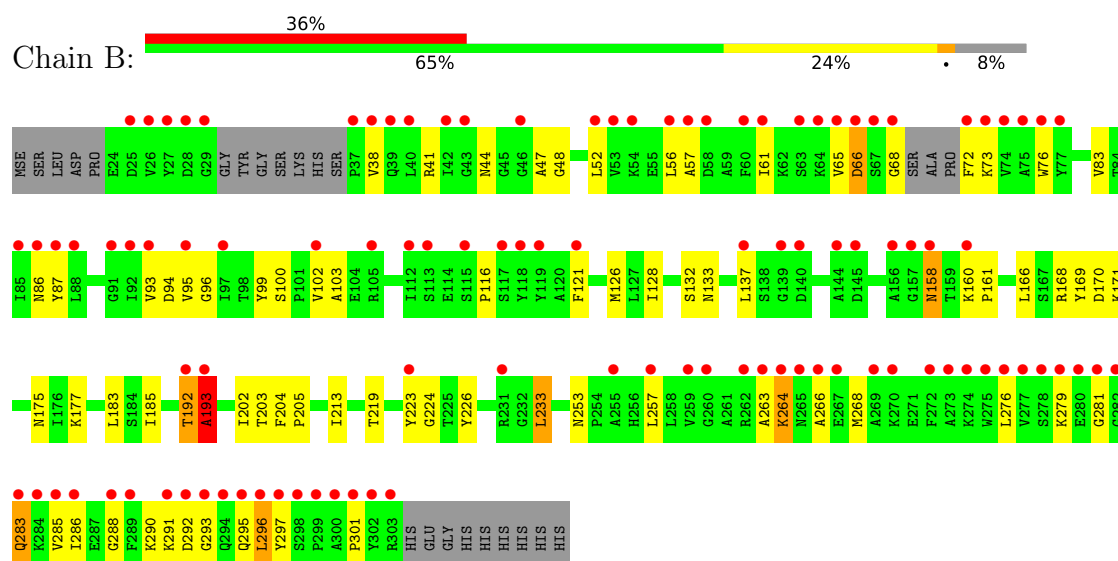
3 Residue-property plots [i](#)

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

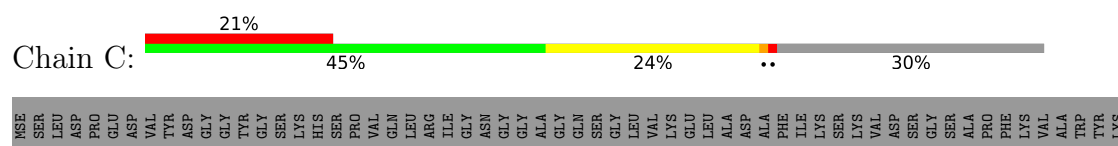
• Molecule 1: Putative metal binding protein

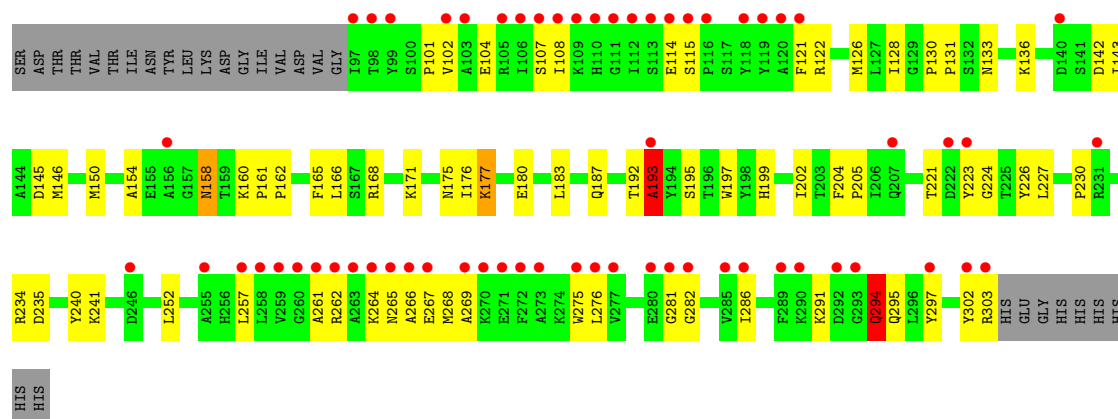


• Molecule 1: Putative metal binding protein

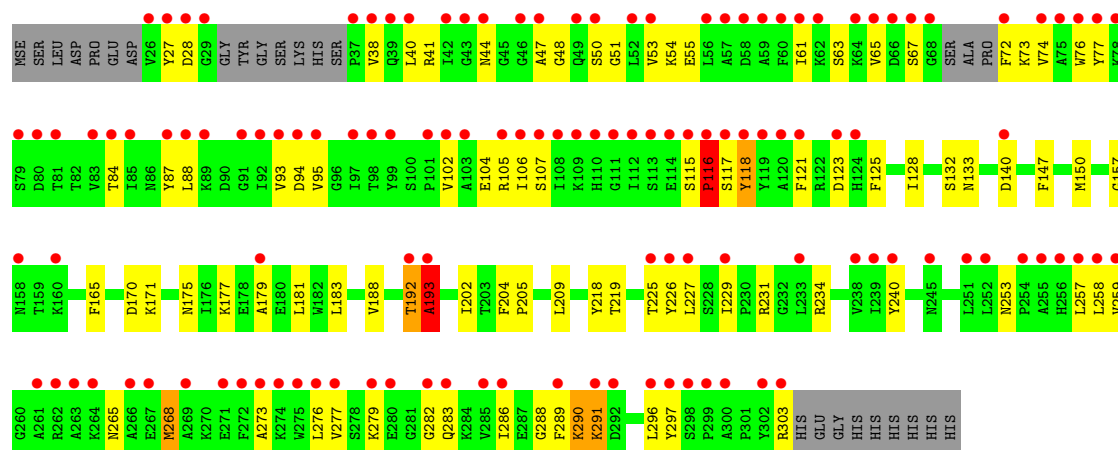
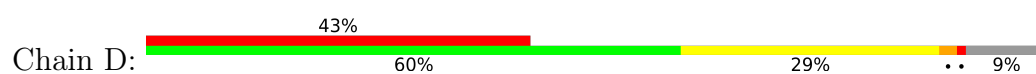


• Molecule 1: Putative metal binding protein





● Molecule 1: Putative metal binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.78Å 150.78Å 116.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.14 – 1.97 44.14 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.14-1.97) 94.4 (44.14-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.289 0.258 , 0.287	Depositor DCC
R_{free} test set	2721 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	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	0.92	EDS
Total number of atoms	8486	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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	0.43	1/2160 (0.0%)	0.94	6/2918 (0.2%)
1	B	0.38	0/2160	0.93	6/2918 (0.2%)
1	C	0.40	0/1681	0.94	5/2274 (0.2%)
1	D	0.40	1/2143 (0.0%)	0.93	7/2895 (0.2%)
All	All	0.40	2/8144 (0.0%)	0.93	24/11005 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	ALA	CA-CB	5.49	1.61	1.53
1	D	179	ALA	CA-CB	5.43	1.61	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	ALA	N-CA-C	-13.39	82.28	110.80
1	A	193	ALA	N-CA-C	-12.91	83.31	110.80
1	B	193	ALA	N-CA-C	-12.68	83.80	110.80
1	C	193	ALA	N-CA-C	-12.42	84.35	110.80
1	B	264	LYS	N-CA-C	-8.09	99.35	110.35
1	B	66	ASP	N-CA-C	-7.23	104.43	113.18
1	D	179	ALA	N-CA-C	-7.20	103.51	111.36
1	A	264	LYS	N-CA-C	-7.08	100.99	110.55
1	A	46	GLY	N-CA-C	6.90	121.01	112.73
1	D	117	SER	N-CA-C	-6.81	99.49	110.32
1	C	294	GLN	N-CA-C	6.67	119.07	109.14
1	C	265	ASN	N-CA-C	-6.44	103.99	112.24
1	A	179	ALA	N-CA-C	-6.26	104.37	111.07
1	B	192	THR	N-CA-C	5.55	118.07	110.24
1	A	199	HIS	N-CA-C	5.33	116.99	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	MSE	N-CA-C	-5.27	105.95	112.38
1	D	290	LYS	N-CA-C	5.27	117.69	109.52
1	C	199	HIS	N-CA-C	5.26	116.83	108.67
1	D	188	VAL	CA-C-N	5.21	125.26	119.32
1	D	188	VAL	C-N-CA	5.21	125.26	119.32
1	D	192	THR	N-CA-C	5.11	117.64	110.23
1	A	117	SER	N-CA-C	-5.07	103.99	110.53
1	B	158	ASN	N-CA-C	5.00	121.46	110.80
1	B	276	LEU	N-CA-C	5.00	116.73	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	2113	0	2087	60	0
1	B	2113	0	2087	75	0
1	C	1640	0	1619	68	0
1	D	2096	0	2077	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	159	0	0	4	0
3	B	113	0	0	6	0
3	C	135	0	0	6	0
3	D	113	0	0	6	0
All	All	8486	0	7870	263	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 17.

All (263) 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:A:183:LEU:HD12	1:C:183:LEU:HD12	1.52	0.92
1:A:143:ILE:HA	1:A:146:MSE:HE3	1.55	0.88
1:C:136:LYS:HE3	3:C:470:HOH:O	1.76	0.85
1:D:277:VAL:HA	1:D:283:GLN:HE21	1.45	0.82
1:D:44:ASN:HD21	1:D:47:ALA:HB3	1.44	0.81
1:C:291:LYS:HD2	3:C:497:HOH:O	1.81	0.80
1:C:221:THR:HB	3:C:491:HOH:O	1.82	0.78
1:B:126:MSE:HE2	1:B:223:TYR:HA	1.65	0.78
1:A:202:ILE:HD13	1:C:192:THR:HG21	1.64	0.77
1:B:202:ILE:HD13	1:D:192:THR:HG21	1.67	0.76
1:D:118:TYR:HB2	1:D:257:LEU:HB3	1.65	0.76
1:B:160:LYS:HD2	1:B:161:PRO:HA	1.68	0.75
1:B:102:VAL:HG23	3:B:440:HOH:O	1.88	0.73
1:A:72:PHE:CE2	1:A:268:MSE:HE1	2.24	0.72
1:A:171:LYS:H	1:A:175:ASN:HD22	1.38	0.72
1:C:126:MSE:HE1	1:C:226:TYR:HB2	1.70	0.72
1:A:192:THR:HG21	1:C:202:ILE:HD13	1.70	0.71
1:C:158:ASN:HD22	1:C:158:ASN:H	1.38	0.71
1:A:171:LYS:HD2	1:C:193:ALA:HB3	1.73	0.70
1:A:231:ARG:HH11	1:A:231:ARG:HG2	1.55	0.70
1:B:171:LYS:H	1:B:175:ASN:HD22	1.39	0.70
1:D:44:ASN:ND2	1:D:47:ALA:HB3	2.06	0.70
1:A:185:ILE:HA	1:C:102:VAL:HG11	1.73	0.70
1:B:192:THR:HG21	1:D:202:ILE:HD13	1.71	0.70
1:B:283:GLN:HE21	1:B:283:GLN:HA	1.54	0.70
1:C:143:ILE:HD12	1:C:146:MSE:HE3	1.72	0.69
1:B:121:PHE:HB3	1:B:286:ILE:HD13	1.73	0.69
1:D:38:VAL:HG22	1:D:73:LYS:HB2	1.72	0.69
1:D:77:TYR:CD2	1:D:93:VAL:HG12	2.28	0.69
1:D:171:LYS:H	1:D:175:ASN:HD22	1.38	0.69
1:C:143:ILE:HA	1:C:146:MSE:HE3	1.73	0.68
1:C:150:MSE:HE1	1:C:165:PHE:HD1	1.58	0.68
1:C:266:ALA:HA	1:C:269:ALA:HB3	1.75	0.68
1:B:183:LEU:HD12	1:D:183:LEU:HD12	1.76	0.68
1:C:121:PHE:HB3	1:C:286:ILE:HD13	1.77	0.67
1:A:150:MSE:HE1	1:A:165:PHE:HD1	1.59	0.66
1:D:227:LEU:HD12	1:D:296:LEU:HD13	1.78	0.66
1:D:258:LEU:HG	3:D:446:HOH:O	1.96	0.65
1:A:89:LYS:HD2	1:A:112:ILE:HD11	1.77	0.65
1:D:72:PHE:CE2	1:D:268:MSE:HE1	2.33	0.64
1:B:295:GLN:HG3	3:B:481:HOH:O	1.98	0.63
1:C:171:LYS:H	1:C:175:ASN:HD22	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ALA:HA	3:B:487:HOH:O	1.97	0.63
1:D:128:ILE:C	1:D:128:ILE:HD12	2.24	0.63
1:B:296:LEU:HG	1:B:297:TYR:CE1	2.34	0.62
1:A:80:ASP:OD1	1:A:83:VAL:HG23	1.99	0.62
1:D:288:GLY:O	1:D:290:LYS:HG3	1.99	0.62
1:A:177:LYS:HE3	1:A:177:LYS:HA	1.82	0.61
1:C:146:MSE:HE1	1:C:241:LYS:CG	2.30	0.61
1:D:28:ASP:O	1:D:61:ILE:HG21	2.00	0.61
1:D:303:ARG:HD3	3:D:461:HOH:O	1.99	0.61
1:C:158:ASN:H	1:C:158:ASN:ND2	1.99	0.61
1:C:224:GLY:HA2	3:C:497:HOH:O	2.01	0.60
1:B:95:VAL:HB	1:B:257:LEU:HD11	1.83	0.60
1:A:121:PHE:HB3	1:A:286:ILE:HD13	1.83	0.60
1:B:296:LEU:HD12	1:B:297:TYR:N	2.16	0.60
1:D:28:ASP:OD1	1:D:73:LYS:HG2	2.00	0.60
1:C:294:GLN:HG2	3:C:446:HOH:O	2.01	0.60
1:C:276:LEU:HD12	1:C:282:GLY:HA3	1.83	0.59
1:A:79:SER:HB2	1:A:83:VAL:HB	1.83	0.59
1:B:183:LEU:HD12	1:D:183:LEU:CD1	2.32	0.59
1:A:72:PHE:CZ	1:A:268:MSE:HE1	2.38	0.59
1:A:140:ASP:HB2	3:A:532:HOH:O	2.02	0.59
1:B:44:ASN:ND2	1:B:47:ALA:HB3	2.18	0.58
1:C:146:MSE:HE1	1:C:241:LYS:HG2	1.84	0.58
1:D:282:GLY:O	1:D:286:ILE:HG13	2.02	0.58
1:A:95:VAL:HB	1:A:257:LEU:HD11	1.86	0.58
1:D:48:GLY:HA3	1:D:76:TRP:CZ2	2.37	0.58
1:A:44:ASN:ND2	1:A:47:ALA:HB3	2.19	0.58
1:D:63:SER:O	1:D:67:SER:HB3	2.04	0.58
1:B:171:LYS:HD2	1:D:193:ALA:HB3	1.86	0.57
1:C:235:ASP:HB3	3:C:496:HOH:O	2.04	0.57
1:D:150:MSE:HE1	1:D:165:PHE:HD1	1.68	0.57
1:A:231:ARG:HG2	1:A:231:ARG:NH1	2.20	0.57
1:A:246:ASP:HB3	3:A:444:HOH:O	2.05	0.56
1:B:290:LYS:HG2	1:B:295:GLN:HA	1.87	0.56
1:D:55:GLU:HG2	3:D:431:HOH:O	2.06	0.56
1:B:183:LEU:CD1	1:D:183:LEU:HD12	2.35	0.56
1:B:213:ILE:HG21	1:B:233:LEU:HD22	1.87	0.56
1:B:192:THR:O	1:B:193:ALA:CB	2.54	0.56
1:A:72:PHE:CD2	1:A:268:MSE:HE1	2.41	0.56
1:B:292:ASP:CG	1:B:293:GLY:H	2.13	0.56
1:C:158:ASN:HD22	1:C:158:ASN:N	2.00	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:HG22	1:B:73:LYS:HB2	1.87	0.56
1:C:143:ILE:HA	1:C:146:MSE:CE	2.35	0.55
1:B:52:LEU:HD22	1:B:297:TYR:CD1	2.41	0.55
1:D:88:LEU:HD23	1:D:93:VAL:HG23	1.88	0.55
1:B:263:ALA:O	1:B:266:ALA:HB2	2.07	0.54
1:B:203:THR:HB	3:B:502:HOH:O	2.07	0.54
1:B:292:ASP:OD2	1:B:293:GLY:N	2.41	0.53
1:C:223:TYR:CE2	1:C:227:LEU:HD11	2.43	0.53
1:C:158:ASN:ND2	1:C:158:ASN:N	2.52	0.53
1:D:227:LEU:HB3	1:D:291:LYS:HG2	1.89	0.53
1:A:65:VAL:C	1:A:67:SER:N	2.62	0.53
1:D:257:LEU:CD2	1:D:273:ALA:HA	2.38	0.53
1:D:27:TYR:HE1	1:D:53:VAL:HG12	1.74	0.53
1:C:176:ILE:O	1:C:180:GLU:HG3	2.09	0.53
1:D:289:PHE:HB3	3:D:458:HOH:O	2.08	0.53
1:D:171:LYS:H	1:D:175:ASN:ND2	2.07	0.52
1:D:72:PHE:CD2	1:D:268:MSE:HE1	2.45	0.52
1:A:58:ASP:O	1:A:62:LYS:HB2	2.09	0.52
1:C:108:ILE:HG23	1:C:115:SER:HB2	1.92	0.52
1:C:101:PRO:O	1:C:104:GLU:HB2	2.10	0.52
1:D:40:LEU:HD11	1:D:95:VAL:HG22	1.92	0.52
1:A:44:ASN:HD21	1:A:47:ALA:HB3	1.75	0.52
1:C:128:ILE:HD12	1:C:128:ILE:C	2.35	0.52
1:C:108:ILE:CG2	1:C:115:SER:HB2	2.41	0.51
1:D:303:ARG:HG2	1:D:303:ARG:HH11	1.75	0.51
1:C:166:LEU:HD23	1:C:166:LEU:C	2.36	0.51
1:B:185:ILE:HA	1:D:102:VAL:HG21	1.93	0.51
1:D:95:VAL:HG12	1:D:259:VAL:HG22	1.93	0.51
1:D:121:PHE:HB3	1:D:286:ILE:HD13	1.93	0.51
1:D:61:ILE:HD11	1:D:74:VAL:HG23	1.91	0.51
1:A:27:TYR:CD2	1:A:54:LYS:HG3	2.46	0.51
1:A:64:LYS:HE2	1:A:64:LYS:HA	1.93	0.51
1:C:142:ASP:OD2	1:C:145:ASP:HB2	2.11	0.51
1:D:54:LYS:HB3	3:D:431:HOH:O	2.11	0.51
1:D:171:LYS:N	1:D:175:ASN:HD22	2.06	0.51
1:C:126:MSE:CE	1:C:226:TYR:HB2	2.39	0.50
1:B:192:THR:O	1:B:193:ALA:HB3	2.11	0.50
1:D:226:TYR:O	1:D:229:ILE:HG12	2.11	0.50
1:A:89:LYS:HD2	1:A:112:ILE:CD1	2.40	0.50
1:B:279:LYS:H	1:B:279:LYS:HD2	1.77	0.50
1:A:267:GLU:O	1:A:271:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLY:HA3	1:B:76:TRP:CZ2	2.46	0.50
1:D:88:LEU:CD2	1:D:93:VAL:HG23	2.40	0.50
1:A:65:VAL:C	1:A:67:SER:H	2.20	0.50
1:A:192:THR:O	1:A:193:ALA:CB	2.59	0.50
1:A:171:LYS:H	1:A:175:ASN:ND2	2.06	0.50
1:B:291:LYS:O	1:B:292:ASP:HB3	2.10	0.50
1:C:262:ARG:HA	1:C:262:ARG:NH1	2.27	0.50
1:C:262:ARG:HA	1:C:262:ARG:HH11	1.76	0.50
1:B:126:MSE:CE	1:B:223:TYR:HA	2.41	0.50
1:C:150:MSE:HE1	1:C:165:PHE:CD1	2.42	0.50
1:A:193:ALA:HB3	1:C:171:LYS:HD2	1.93	0.49
1:B:116:PRO:HG2	3:B:486:HOH:O	2.12	0.49
1:D:125:PHE:CE2	1:D:253:ASN:HB2	2.47	0.49
1:A:183:LEU:CD1	1:C:183:LEU:HD12	2.33	0.49
1:D:231:ARG:HG2	1:D:234:ARG:CZ	2.43	0.49
1:B:65:VAL:HA	1:B:68:GLY:O	2.13	0.49
1:B:166:LEU:C	1:B:166:LEU:HD23	2.38	0.49
1:D:61:ILE:O	1:D:65:VAL:HG23	2.13	0.49
1:A:171:LYS:N	1:A:175:ASN:HD22	2.08	0.49
1:B:87:TYR:HB3	1:B:93:VAL:HG22	1.95	0.49
1:B:296:LEU:HG	1:B:297:TYR:CD1	2.47	0.49
1:D:105:ARG:HH11	1:D:105:ARG:HG2	1.78	0.49
1:B:41:ARG:NH2	3:B:487:HOH:O	2.46	0.48
1:D:192:THR:O	1:D:193:ALA:CB	2.61	0.48
1:D:209:LEU:HD23	1:D:225:THR:HG22	1.95	0.48
1:A:88:LEU:HD23	1:A:93:VAL:HG23	1.96	0.48
1:B:83:VAL:HA	1:B:86:ASN:HD22	1.78	0.48
1:B:204:PHE:HB3	1:B:205:PRO:HD2	1.94	0.48
1:C:257:LEU:C	1:C:257:LEU:HD23	2.38	0.48
1:D:41:ARG:HB3	1:D:77:TYR:HE2	1.78	0.48
1:B:126:MSE:HE2	1:B:223:TYR:CA	2.41	0.48
1:D:296:LEU:HG	1:D:297:TYR:CE1	2.48	0.48
1:A:150:MSE:HE1	1:A:165:PHE:CD1	2.46	0.47
1:D:94:ASP:CG	1:D:265:ASN:HD22	2.22	0.47
1:D:257:LEU:HD22	1:D:276:LEU:HD23	1.96	0.47
1:B:52:LEU:HD22	1:B:297:TYR:CE1	2.49	0.47
1:B:193:ALA:HB3	1:D:171:LYS:HD2	1.95	0.47
1:A:94:ASP:OD1	1:A:264:LYS:O	2.33	0.47
1:C:160:LYS:HD2	1:C:161:PRO:HA	1.96	0.47
1:C:161:PRO:HB2	1:C:162:PRO:HD2	1.97	0.47
1:C:183:LEU:HD23	1:C:187:GLN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:LYS:C	1:C:266:ALA:N	2.70	0.47
1:C:204:PHE:HB3	1:C:205:PRO:HD2	1.96	0.47
1:D:257:LEU:HD21	1:D:273:ALA:HA	1.97	0.47
1:D:204:PHE:HB3	1:D:205:PRO:HD2	1.96	0.47
1:C:133:ASN:HB2	1:C:240:TYR:OH	2.15	0.46
1:C:192:THR:O	1:C:193:ALA:CB	2.63	0.46
1:D:150:MSE:CE	1:D:218:TYR:HB2	2.45	0.46
1:B:283:GLN:HA	1:B:283:GLN:NE2	2.27	0.46
1:B:44:ASN:HD21	1:B:47:ALA:H	1.64	0.46
1:A:170:ASP:O	1:A:171:LYS:HB2	2.15	0.46
1:D:48:GLY:HA2	1:D:53:VAL:HB	1.98	0.46
1:A:89:LYS:HD3	3:A:505:HOH:O	2.15	0.46
1:B:57:ALA:O	1:B:61:ILE:HG13	2.16	0.45
1:B:94:ASP:OD1	1:B:264:LYS:O	2.34	0.45
1:C:171:LYS:N	1:C:175:ASN:HD22	2.13	0.45
1:D:102:VAL:O	1:D:106:ILE:HG13	2.16	0.45
1:B:72:PHE:CE1	1:B:268:MSE:HE3	2.51	0.45
1:B:100:SER:HB3	1:B:103:ALA:HB3	1.98	0.45
1:B:170:ASP:O	1:B:171:LYS:HB2	2.16	0.45
1:A:44:ASN:HD21	1:A:47:ALA:H	1.64	0.45
1:A:128:ILE:C	1:A:128:ILE:HD12	2.41	0.45
1:A:62:LYS:O	1:A:66:ASP:HB2	2.17	0.45
1:B:44:ASN:HD21	1:B:47:ALA:HB3	1.81	0.45
1:C:295:GLN:HG2	1:C:297:TYR:O	2.16	0.45
1:A:24:GLU:O	1:A:25:ASP:HB2	2.16	0.45
1:A:177:LYS:HE3	1:A:177:LYS:CA	2.46	0.45
1:B:96:GLY:O	1:B:257:LEU:HA	2.17	0.45
1:B:128:ILE:C	1:B:128:ILE:HD12	2.42	0.45
1:C:122:ARG:HB3	1:C:252:LEU:HD11	1.99	0.44
1:D:132:SER:O	1:D:133:ASN:C	2.60	0.44
1:B:292:ASP:CG	1:B:293:GLY:N	2.75	0.44
1:C:130:PRO:HA	1:C:131:PRO:HD3	1.94	0.44
1:D:104:GLU:O	1:D:107:SER:HB3	2.17	0.44
1:B:204:PHE:HB3	1:B:205:PRO:CD	2.48	0.44
1:B:281:GLY:O	1:B:285:VAL:HG23	2.17	0.44
1:C:204:PHE:HB3	1:C:205:PRO:CD	2.48	0.44
1:A:160:LYS:HA	1:A:161:PRO:HA	1.86	0.44
1:C:275:TRP:O	1:C:281:GLY:HA3	2.18	0.44
1:D:147:PHE:CE1	1:D:181:LEU:HD13	2.53	0.43
1:D:204:PHE:HB3	1:D:205:PRO:CD	2.48	0.43
1:C:160:LYS:HD2	1:C:160:LYS:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:MSE:HE1	1:B:226:TYR:CB	2.48	0.43
1:B:224:GLY:CA	1:B:296:LEU:HD11	2.47	0.43
1:B:279:LYS:HD2	1:B:279:LYS:N	2.33	0.43
1:B:44:ASN:HD22	1:B:48:GLY:H	1.65	0.43
1:A:44:ASN:CG	1:A:45:GLY:N	2.76	0.43
1:A:64:LYS:HE2	3:A:530:HOH:O	2.19	0.43
1:B:133:ASN:HD21	1:B:137:LEU:N	2.17	0.43
1:A:62:LYS:O	1:A:66:ASP:CB	2.67	0.43
1:C:177:LYS:HE3	1:C:177:LYS:HA	2.00	0.43
1:D:227:LEU:HD13	1:D:291:LYS:HB3	2.01	0.43
1:B:213:ILE:HG21	1:B:233:LEU:CD2	2.49	0.43
1:D:44:ASN:HD21	1:D:47:ALA:CB	2.25	0.43
1:A:42:ILE:HG12	1:A:95:VAL:CG2	2.49	0.42
1:A:130:PRO:HA	1:A:131:PRO:HD3	1.93	0.42
1:A:192:THR:O	1:A:193:ALA:HB3	2.18	0.42
1:B:44:ASN:HD21	1:B:47:ALA:N	2.16	0.42
1:D:133:ASN:HB2	1:D:240:TYR:OH	2.20	0.42
1:D:157:GLY:HA2	3:D:428:HOH:O	2.19	0.42
1:B:168:ARG:O	1:B:169:TYR:C	2.62	0.42
1:B:288:GLY:O	1:B:290:LYS:HG3	2.20	0.42
1:C:168:ARG:NH1	1:C:205:PRO:HG3	2.34	0.42
1:C:230:PRO:O	1:C:234:ARG:HG3	2.19	0.42
1:B:192:THR:CG2	1:D:202:ILE:HD13	2.43	0.42
1:A:126:MSE:HE3	1:A:239:ILE:HG12	2.01	0.42
1:B:224:GLY:HA2	1:B:296:LEU:HD11	2.01	0.42
1:B:160:LYS:HA	1:B:161:PRO:HA	1.92	0.42
1:B:44:ASN:ND2	1:B:48:GLY:H	2.18	0.42
1:B:99:TYR:HB3	1:B:253:ASN:OD1	2.20	0.42
1:C:104:GLU:O	1:C:107:SER:HB2	2.19	0.41
1:C:154:ALA:HB1	1:C:197:TRP:CG	2.55	0.41
1:D:118:TYR:CE1	1:D:273:ALA:HB1	2.55	0.41
1:A:160:LYS:HA	1:A:160:LYS:HD2	1.74	0.41
1:B:41:ARG:HE	1:B:41:ARG:HB2	1.73	0.41
1:D:128:ILE:HD11	1:D:219:THR:HG22	2.02	0.41
1:D:150:MSE:HE1	1:D:218:TYR:HB2	2.01	0.41
1:A:192:THR:HG21	1:C:202:ILE:CD1	2.46	0.41
1:B:48:GLY:HA3	1:B:76:TRP:CE2	2.56	0.41
1:D:125:PHE:CD2	1:D:253:ASN:HB2	2.56	0.41
1:D:257:LEU:HD22	1:D:276:LEU:CD2	2.50	0.41
1:A:87:TYR:HB3	1:A:93:VAL:HG22	2.02	0.41
1:C:223:TYR:CZ	1:C:227:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:TYR:N	1:D:118:TYR:CD2	2.88	0.41
1:C:195:SER:HB3	1:C:197:TRP:CE2	2.56	0.41
1:C:171:LYS:H	1:C:175:ASN:ND2	2.15	0.41
1:C:257:LEU:HD23	1:C:257:LEU:O	2.21	0.41
1:C:303:ARG:HG3	1:C:303:ARG:HH11	1.84	0.41
1:D:84:THR:O	1:D:87:TYR:HB2	2.21	0.41
1:A:287:GLU:HA	1:A:295:GLN:NE2	2.35	0.41
1:B:132:SER:O	1:B:133:ASN:C	2.64	0.41
1:C:114:GLU:HG3	1:C:261:ALA:HA	2.03	0.41
1:A:44:ASN:HD21	1:A:47:ALA:N	2.19	0.41
1:A:141:SER:O	1:A:146:MSE:HE2	2.21	0.41
1:D:170:ASP:O	1:D:171:LYS:HB2	2.22	0.40
1:A:202:ILE:CD1	1:C:192:THR:HG21	2.44	0.40
1:D:115:SER:HA	1:D:116:PRO:HA	1.76	0.40
1:B:128:ILE:HD11	1:B:219:THR:HG22	2.04	0.40
1:D:123:ASP:HB3	1:D:253:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/294 (90%)	256 (97%)	7 (3%)	1 (0%)	30	20
1	B	264/294 (90%)	244 (92%)	17 (6%)	3 (1%)	11	4
1	C	205/294 (70%)	191 (93%)	12 (6%)	2 (1%)	12	5
1	D	262/294 (89%)	240 (92%)	17 (6%)	5 (2%)	6	1
All	All	995/1176 (85%)	931 (94%)	53 (5%)	11 (1%)	11	4

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA
1	B	193	ALA
1	C	193	ALA
1	D	193	ALA
1	B	158	ASN
1	D	279	LYS
1	C	302	TYR
1	D	50	SER
1	B	301	PRO
1	D	51	GLY
1	D	116	PRO

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	222/236 (94%)	218 (98%)	4 (2%)	51	46
1	B	222/236 (94%)	216 (97%)	6 (3%)	39	31
1	C	172/236 (73%)	168 (98%)	4 (2%)	44	37
1	D	220/236 (93%)	214 (97%)	6 (3%)	39	31
All	All	836/944 (89%)	816 (98%)	20 (2%)	43	35

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	177	LYS
1	A	267	GLU
1	A	268	MSE
1	B	56	LEU
1	B	66	ASP
1	B	177	LYS
1	B	233	LEU
1	B	283	GLN
1	B	296	LEU
1	C	158	ASN

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Mol	Chain	Res	Type
1	C	177	LYS
1	C	267	GLU
1	C	294	GLN
1	D	116	PRO
1	D	118	TYR
1	D	140	ASP
1	D	177	LYS
1	D	268	MSE
1	D	291	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	44	ASN
1	A	49	GLN
1	A	86	ASN
1	A	175	ASN
1	A	245	ASN
1	A	295	GLN
1	B	44	ASN
1	B	86	ASN
1	B	175	ASN
1	B	245	ASN
1	B	295	GLN
1	C	158	ASN
1	C	175	ASN
1	C	207	GLN
1	C	256	HIS
1	D	49	GLN
1	D	124	HIS
1	D	175	ASN
1	D	256	HIS
1	D	265	ASN
1	D	283	GLN
1	D	295	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 4 ligands modelled in this entry, 4 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	265/294 (90%)	1.04	54 (20%) 3 3	15, 30, 50, 58	0
1	B	265/294 (90%)	1.71	105 (39%) 1 0	17, 39, 55, 59	0
1	C	202/294 (68%)	1.36	61 (30%) 1 1	16, 34, 57, 63	0
1	D	263/294 (89%)	2.04	127 (48%) 0 0	17, 44, 55, 60	0
All	All	995/1176 (84%)	1.55	347 (34%) 1 1	15, 36, 55, 63	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	ALA	6.5
1	C	302	TYR	6.4
1	C	266	ALA	6.1
1	C	112	ILE	6.1
1	B	72	PHE	6.0
1	D	53	VAL	5.8
1	A	262	ARG	5.8
1	B	38	VAL	5.5
1	D	257	LEU	5.4
1	B	118	TYR	5.3
1	B	276	LEU	5.3
1	B	302	TYR	5.3
1	D	65	VAL	5.3
1	A	269	ALA	5.2
1	B	281	GLY	5.1
1	D	56	LEU	5.0
1	A	37	PRO	5.0
1	B	26	VAL	4.9
1	C	263	ALA	4.9
1	C	272	PHE	4.9
1	A	280	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	255	ALA	4.8
1	D	116	PRO	4.8
1	B	68	GLY	4.7
1	D	77	TYR	4.5
1	B	275	TRP	4.5
1	D	118	TYR	4.5
1	B	40	LEU	4.5
1	A	61	ILE	4.5
1	D	113	SER	4.5
1	A	28	ASP	4.4
1	D	119	TYR	4.4
1	C	111	GLY	4.4
1	B	263	ALA	4.4
1	C	103	ALA	4.4
1	B	67	SER	4.4
1	D	76	TRP	4.4
1	B	296	LEU	4.3
1	C	267	GLU	4.3
1	D	296	LEU	4.2
1	C	113	SER	4.2
1	D	42	ILE	4.2
1	A	68	GLY	4.2
1	C	260	GLY	4.2
1	D	39	GLN	4.2
1	B	272	PHE	4.2
1	B	282	GLY	4.1
1	D	61	ILE	4.1
1	B	289	PHE	4.1
1	D	72	PHE	4.1
1	B	266	ALA	4.1
1	C	276	LEU	4.1
1	D	277	VAL	4.1
1	C	261	ALA	4.1
1	D	269	ALA	4.1
1	D	85	ILE	4.0
1	D	259	VAL	4.0
1	D	263	ALA	4.0
1	D	88	LEU	4.0
1	B	193	ALA	4.0
1	D	75	ALA	4.0
1	A	263	ALA	4.0
1	B	92	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	112	ILE	4.0
1	D	275	TRP	3.9
1	D	193	ALA	3.9
1	B	53	VAL	3.9
1	D	108	ILE	3.9
1	C	271	GLU	3.9
1	A	267	GLU	3.9
1	B	270	LYS	3.9
1	C	97	ILE	3.9
1	C	262	ARG	3.8
1	D	74	VAL	3.8
1	C	289	PHE	3.8
1	B	260	GLY	3.8
1	D	273	ALA	3.8
1	B	267	GLU	3.8
1	A	264	LYS	3.8
1	A	289	PHE	3.7
1	D	60	PHE	3.7
1	C	114	GLU	3.7
1	D	117	SER	3.7
1	B	65	VAL	3.7
1	D	38	VAL	3.7
1	B	95	VAL	3.7
1	C	293	GLY	3.7
1	C	303	ARG	3.7
1	B	75	ALA	3.6
1	D	297	TYR	3.6
1	B	42	ILE	3.6
1	D	286	ILE	3.6
1	B	93	VAL	3.6
1	B	76	TRP	3.6
1	A	40	LEU	3.6
1	D	66	ASP	3.6
1	D	40	LEU	3.6
1	D	68	GLY	3.6
1	D	106	ILE	3.6
1	D	285	VAL	3.6
1	D	121	PHE	3.6
1	D	289	PHE	3.6
1	D	78	LYS	3.6
1	D	303	ARG	3.5
1	D	261	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	37	PRO	3.5
1	D	93	VAL	3.5
1	A	204	PHE	3.5
1	B	297	TYR	3.5
1	C	265	ASN	3.5
1	C	106	ILE	3.5
1	B	257	LEU	3.5
1	D	107	SER	3.4
1	A	157	GLY	3.4
1	D	258	LEU	3.4
1	B	279	LYS	3.4
1	B	269	ALA	3.4
1	B	56	LEU	3.4
1	B	292	ASP	3.4
1	D	28	ASP	3.3
1	B	286	ILE	3.3
1	D	97	ILE	3.3
1	B	113	SER	3.3
1	B	158	ASN	3.3
1	B	285	VAL	3.3
1	D	120	ALA	3.3
1	D	264	LYS	3.3
1	C	259	VAL	3.3
1	D	266	ALA	3.3
1	D	227	LEU	3.3
1	D	256	HIS	3.3
1	D	83	VAL	3.3
1	D	50	SER	3.3
1	D	87	TYR	3.2
1	A	193	ALA	3.2
1	C	257	LEU	3.2
1	D	52	LEU	3.2
1	B	265	ASN	3.2
1	B	102	VAL	3.2
1	C	108	ILE	3.2
1	D	37	PRO	3.2
1	A	26	VAL	3.2
1	B	259	VAL	3.2
1	B	57	ALA	3.1
1	A	93	VAL	3.1
1	D	262	ARG	3.1
1	A	265	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	92	ILE	3.1
1	C	99	TYR	3.1
1	D	26	VAL	3.1
1	A	63	SER	3.1
1	D	43	GLY	3.1
1	D	280	GLU	3.1
1	A	38	VAL	3.0
1	B	277	VAL	3.0
1	C	118	TYR	3.0
1	B	293	GLY	3.0
1	C	282	GLY	3.0
1	B	52	LEU	3.0
1	C	280	GLU	3.0
1	A	77	TYR	3.0
1	B	121	PHE	3.0
1	B	303	ARG	3.0
1	B	112	ILE	3.0
1	C	110	HIS	2.9
1	D	252	LEU	2.9
1	B	74	VAL	2.9
1	B	27	TYR	2.9
1	C	107	SER	2.9
1	C	273	ALA	2.9
1	B	278	SER	2.9
1	D	84	THR	2.9
1	B	66	ASP	2.9
1	D	233	LEU	2.9
1	D	254	PRO	2.9
1	A	60	PHE	2.9
1	B	86	ASN	2.8
1	B	273	ALA	2.8
1	D	57	ALA	2.8
1	D	95	VAL	2.8
1	A	27	TYR	2.8
1	C	281	GLY	2.8
1	C	223	TYR	2.8
1	C	193	ALA	2.8
1	B	262	ARG	2.8
1	D	276	LEU	2.8
1	D	239	ILE	2.8
1	B	25	ASP	2.8
1	B	283	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	59	ALA	2.7
1	D	114	GLU	2.7
1	C	98	THR	2.7
1	D	79	SER	2.7
1	B	294	GLN	2.7
1	B	54	LYS	2.7
1	B	91	GLY	2.7
1	B	280	GLU	2.7
1	D	102	VAL	2.7
1	D	110	HIS	2.7
1	A	72	PHE	2.7
1	D	58	ASP	2.7
1	A	42	ILE	2.7
1	B	73	LYS	2.7
1	B	157	GLY	2.6
1	A	94	ASP	2.6
1	D	272	PHE	2.6
1	C	264	LYS	2.6
1	D	62	LYS	2.6
1	A	29	GLY	2.6
1	D	27	TYR	2.6
1	B	105	ARG	2.6
1	B	140	ASP	2.6
1	D	103	ALA	2.6
1	B	264	LYS	2.6
1	D	89	LYS	2.6
1	D	109	LYS	2.6
1	B	298	SER	2.6
1	B	301	PRO	2.6
1	C	275	TRP	2.6
1	B	97	ILE	2.6
1	D	111	GLY	2.6
1	C	290	LYS	2.6
1	B	87	TYR	2.5
1	B	145	ASP	2.5
1	D	123	ASP	2.5
1	B	46	GLY	2.5
1	D	46	GLY	2.5
1	D	158	ASN	2.5
1	D	124	HIS	2.5
1	D	81	THR	2.5
1	D	192	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	105	ARG	2.5
1	B	64	LYS	2.5
1	B	288	GLY	2.5
1	A	67	SER	2.5
1	C	120	ALA	2.5
1	D	271	GLU	2.5
1	B	77	TYR	2.5
1	B	115	SER	2.5
1	D	49	GLN	2.5
1	A	76	TRP	2.5
1	B	300	ALA	2.5
1	D	47	ALA	2.5
1	C	292	ASP	2.5
1	D	91	GLY	2.4
1	D	44	ASN	2.4
1	A	49	GLN	2.4
1	A	207	GLN	2.4
1	A	156	ALA	2.4
1	C	140	ASP	2.4
1	C	102	VAL	2.4
1	B	60	PHE	2.4
1	A	274	LYS	2.4
1	A	25	ASP	2.4
1	B	85	ILE	2.4
1	D	140	ASP	2.4
1	A	261	ALA	2.4
1	C	207	GLN	2.4
1	A	64	LYS	2.4
1	C	258	LEU	2.4
1	C	270	LYS	2.4
1	B	274	LYS	2.4
1	D	105	ARG	2.3
1	D	267	GLU	2.3
1	A	75	ALA	2.3
1	D	229	ILE	2.3
1	C	116	PRO	2.3
1	A	281	GLY	2.3
1	B	29	GLY	2.3
1	D	29	GLY	2.3
1	D	279	LYS	2.3
1	C	277	VAL	2.3
1	C	285	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	67	SER	2.3
1	D	115	SER	2.3
1	D	251	LEU	2.3
1	C	119	TYR	2.3
1	D	99	TYR	2.3
1	C	115	SER	2.3
1	C	246	ASP	2.3
1	D	238	VAL	2.3
1	A	279	LYS	2.3
1	B	291	LYS	2.3
1	B	299	PRO	2.3
1	D	282	GLY	2.3
1	A	110	HIS	2.3
1	A	160	LYS	2.3
1	A	266	ALA	2.2
1	D	299	PRO	2.2
1	D	302	TYR	2.2
1	D	298	SER	2.2
1	B	61	ILE	2.2
1	A	65	VAL	2.2
1	B	160	LYS	2.2
1	D	291	LYS	2.2
1	B	192	THR	2.2
1	D	98	THR	2.2
1	A	58	ASP	2.2
1	B	28	ASP	2.2
1	B	117	SER	2.2
1	D	94	ASP	2.2
1	D	300	ALA	2.2
1	B	223	TYR	2.2
1	B	284	LYS	2.2
1	D	160	LYS	2.2
1	D	274	LYS	2.2
1	B	88	LEU	2.2
1	B	43	GLY	2.2
1	D	292	ASP	2.2
1	B	144	ALA	2.2
1	B	255	ALA	2.2
1	C	121	PHE	2.2
1	C	297	TYR	2.2
1	C	286	ILE	2.2
1	C	109	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	231	ARG	2.2
1	B	39	GLN	2.2
1	A	115	SER	2.2
1	B	63	SER	2.2
1	A	56	LEU	2.2
1	B	137	LEU	2.2
1	B	156	ALA	2.2
1	C	156	ALA	2.2
1	A	87	TYR	2.1
1	B	119	TYR	2.1
1	D	240	TYR	2.1
1	A	92	ILE	2.1
1	A	260	GLY	2.1
1	D	64	LYS	2.1
1	C	255	ALA	2.1
1	D	226	TYR	2.1
1	A	66	ASP	2.1
1	B	139	GLY	2.1
1	A	142	ASP	2.1
1	D	225	THR	2.1
1	A	259	VAL	2.1
1	B	295	GLN	2.1
1	D	283	GLN	2.1
1	D	179	ALA	2.1
1	A	108	ILE	2.0
1	D	245	ASN	2.0
1	D	101	PRO	2.0
1	A	303	ARG	2.0
1	B	58	ASP	2.0
1	C	222	ASP	2.0
1	C	231	ARG	2.0
1	D	80	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	401	1/1	0.94	0.09	49,49,49,49	0
2	CA	D	401	1/1	0.96	0.15	39,39,39,39	0
2	CA	C	401	1/1	0.99	0.11	35,35,35,35	0
2	CA	A	401	1/1	0.99	0.12	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.