



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:07 AM UTC

PDB ID : 3GB8 / pdb_00003gb8
Title : Crystal structure of CRM1/Snurportin-1 complex
Authors : Dong, X.; Biswas, A.; Suel, K.E.; Jackson, L.K.; Martinez, R.; Gu, H.; Chook, Y.M.
Deposited on : 2009-02-19
Resolution : 2.90 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

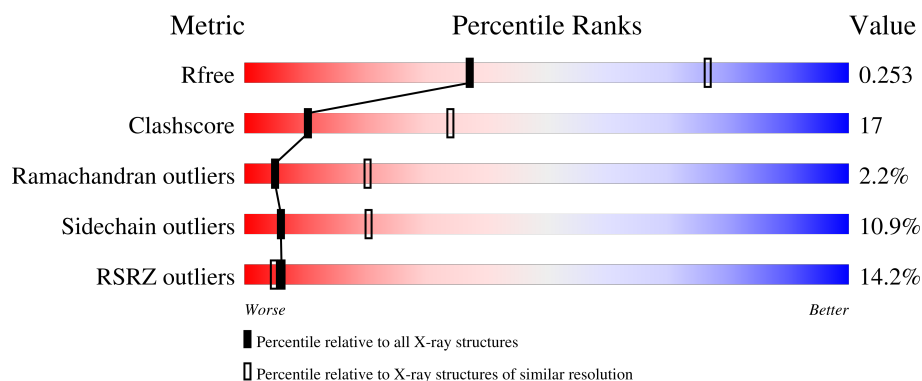
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1071	12% 57% 28% • 10%
2	B	329	13% 45% 31% 5% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9750 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 Exportin-1.

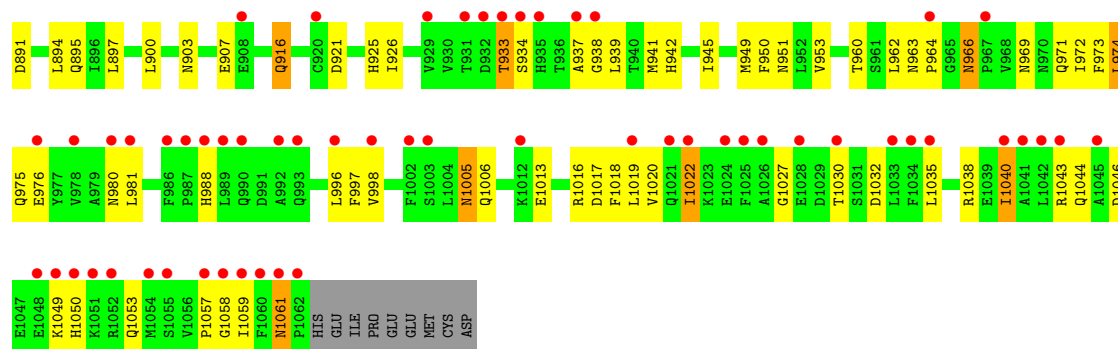
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	959	Total	C	N	O	S	0	0	1
			7624	4896	1278	1401	49			

- Molecule 2 is a protein called Snurportin-1.

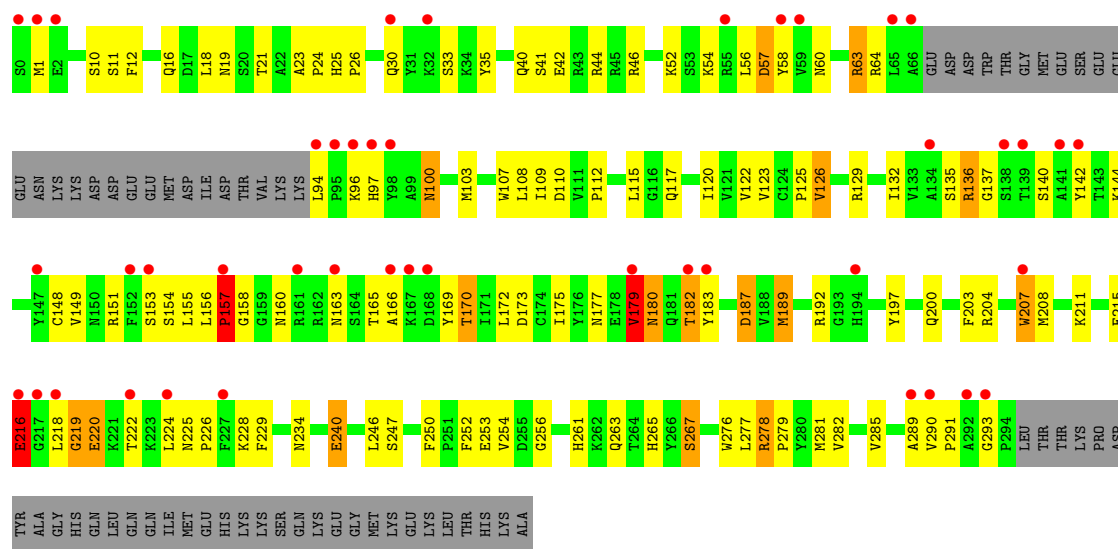
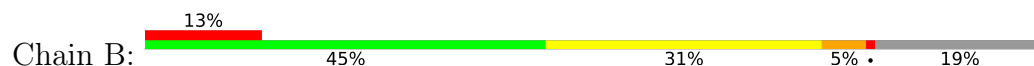
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	268	Total	C	N	O	S	0	0	1
			2126	1355	363	395	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP O95149



• Molecule 2: Snurportin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	250.40Å 250.40Å 190.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.67 – 2.90 47.67 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.67-2.90) 94.3 (47.67-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.267 0.223 , 0.253	Depositor DCC
R_{free} test set	7330 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.6	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	0.90	EDS
Total number of atoms	9750	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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	0.74	1/7777 (0.0%)	1.02	14/10551 (0.1%)
2	B	0.92	7/2183 (0.3%)	1.08	5/2966 (0.2%)
All	All	0.79	8/9960 (0.1%)	1.03	19/13517 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	GLU	CD-OE1	8.40	1.41	1.25
2	B	180	ASN	CG-ND2	6.79	1.47	1.33
2	B	179	VAL	CB-CG1	6.78	1.75	1.52
2	B	293	GLY	C-N	-6.67	1.23	1.34
1	A	1061	ASN	C-N	-6.28	1.24	1.34
2	B	180	ASN	CG-OD1	6.19	1.35	1.23
2	B	224	LEU	CG-CD1	6.12	1.72	1.52
2	B	216	GLU	CD-OE2	5.12	1.35	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CB-CA-C	-7.20	98.44	110.68
1	A	827	PHE	N-CA-C	6.96	118.76	111.03
1	A	607	VAL	N-CA-C	6.90	118.53	111.00
1	A	257	VAL	CA-C-N	6.78	128.31	119.84
1	A	257	VAL	C-N-CA	6.78	128.31	119.84
1	A	604	VAL	CB-CA-C	6.29	121.60	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	SER	N-CA-C	6.00	123.57	110.80
1	A	606	GLU	N-CA-C	5.78	115.47	107.73
1	A	519	THR	N-CA-CB	5.70	118.59	110.16
1	A	534	LYS	N-CA-C	-5.55	105.31	111.36
2	B	278	ARG	N-CA-C	-5.53	102.95	110.36
2	B	11	SER	N-CA-C	5.43	116.95	110.44
1	A	934	SER	N-CA-C	5.40	117.51	109.25
1	A	659	LEU	N-CA-C	5.40	116.85	111.07
1	A	533	GLY	N-CA-C	5.28	118.13	112.33
2	B	267	SER	CA-C-N	5.14	124.90	119.76
2	B	267	SER	C-N-CA	5.14	124.90	119.76
2	B	180	ASN	OD1-CG-ND2	5.11	127.71	122.60
1	A	867	PRO	O-C-N	5.07	123.64	121.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	384	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7624	0	7524	239	0
2	B	2126	0	2060	91	0
All	All	9750	0	9584	326	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 (326) 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:B:179:VAL:CB	2:B:179:VAL:CG1	1.74	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:MET:HE3	1:A:804:MET:HA	1.27	1.10
1:A:244:THR:HG22	1:A:245:LYS:H	1.09	1.09
1:A:600:VAL:O	1:A:602:VAL:N	1.88	1.06
1:A:459:GLU:HG3	1:A:1059:ILE:HD11	1.41	0.99
1:A:345:GLU:O	1:A:349:GLU:HG3	1.69	0.92
2:B:165:THR:HG22	2:B:166:ALA:H	1.37	0.90
1:A:323:SER:OG	1:A:368:ILE:HD11	1.72	0.90
2:B:103:MET:HE3	2:B:267:SER:H	1.38	0.88
2:B:137:GLY:HA2	2:B:160:ASN:C	2.00	0.86
1:A:997:PHE:CZ	1:A:1018:PHE:HB2	2.10	0.86
1:A:244:THR:HG22	1:A:245:LYS:N	1.91	0.84
1:A:739:VAL:HG12	1:A:745:ILE:HG13	1.58	0.83
1:A:879:ILE:HD11	1:A:925:HIS:HB3	1.59	0.83
1:A:424:MET:HE1	1:A:457:MET:HB2	1.61	0.83
1:A:628:GLN:CD	1:A:628:GLN:H	1.86	0.83
2:B:218:LEU:HD22	2:B:229:PHE:HB2	1.61	0.82
1:A:808:VAL:HA	1:A:815:ILE:HD11	1.61	0.82
1:A:804:MET:HA	1:A:804:MET:CE	2.09	0.81
1:A:292:MET:HE3	1:A:293:GLN:HG2	1.63	0.81
1:A:573:MET:HE3	1:A:625:LEU:HD11	1.63	0.80
1:A:420:MET:HE1	1:A:457:MET:HA	1.62	0.80
1:A:384:SER:HB3	1:A:406:ARG:NH2	1.98	0.79
1:A:601:GLN:HB2	1:A:644:GLN:OE1	1.83	0.78
1:A:56:HIS:H	1:A:57:PRO:HD2	1.49	0.78
2:B:261:HIS:HD2	2:B:263:GLN:H	1.32	0.77
1:A:384:SER:CB	1:A:406:ARG:NH2	2.48	0.77
1:A:644:GLN:HE21	1:A:646:ASP:H	1.32	0.76
1:A:168:MET:HE3	1:A:225:THR:HG23	1.68	0.76
2:B:165:THR:HG22	2:B:166:ALA:N	2.00	0.76
1:A:420:MET:HE2	1:A:460:THR:HB	1.66	0.76
1:A:552:PRO:HG3	1:A:594:LYS:HD3	1.66	0.75
1:A:717:MET:HE1	1:A:758:LEU:HD23	1.69	0.74
1:A:614:ILE:HD12	1:A:640:MET:HE1	1.70	0.74
2:B:132:ILE:HD11	2:B:183:TYR:CE1	2.23	0.73
1:A:465:THR:HG23	1:A:472:THR:HG21	1.68	0.73
1:A:601:GLN:HA	1:A:609:PRO:HB3	1.70	0.73
1:A:651:GLU:HG2	1:A:708:ILE:HD13	1.72	0.72
1:A:424:MET:HE3	1:A:425:ALA:H	1.56	0.70
2:B:189:MET:N	2:B:189:MET:HE3	2.06	0.70
2:B:165:THR:CG2	2:B:166:ALA:H	2.04	0.70
1:A:717:MET:HE2	1:A:755:THR:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLN:HB2	2:B:110:ASP:HB3	1.74	0.70
1:A:244:THR:CG2	1:A:245:LYS:H	1.93	0.69
2:B:180:ASN:O	2:B:182:THR:HG22	1.93	0.68
1:A:951:ASN:HB2	1:A:1005:ASN:HD21	1.58	0.68
2:B:179:VAL:CG1	2:B:179:VAL:CA	2.71	0.68
1:A:876:ASP:O	1:A:879:ILE:HG22	1.95	0.67
1:A:966:ASN:CG	1:A:966:ASN:O	2.37	0.67
2:B:21:THR:HA	2:B:107:TRP:NE1	2.10	0.67
2:B:155:LEU:HD13	2:B:216:GLU:O	1.94	0.67
1:A:99:CYS:HA	1:A:102:ILE:HD12	1.77	0.67
2:B:261:HIS:CD2	2:B:263:GLN:H	2.10	0.67
2:B:219:GLY:O	2:B:228:LYS:HD2	1.94	0.66
1:A:879:ILE:HD11	1:A:925:HIS:CB	2.26	0.66
1:A:142:TRP:CH2	1:A:198:MET:HE1	2.31	0.66
1:A:975:GLN:HG3	1:A:998:VAL:HG12	1.77	0.65
1:A:157:SER:HB3	1:A:167:ASN:HD22	1.61	0.65
1:A:406:ARG:HH21	1:A:467:LEU:HD22	1.62	0.65
1:A:969:ASN:HD21	1:A:971:GLN:HB3	1.62	0.64
1:A:897:LEU:HD21	1:A:926:ILE:HD11	1.80	0.64
1:A:601:GLN:HA	1:A:609:PRO:CB	2.28	0.64
1:A:428:GLU:HG3	1:A:451:ILE:HD12	1.80	0.63
1:A:886:MET:SD	1:A:886:MET:N	2.69	0.63
2:B:279:PRO:O	2:B:282:VAL:HG22	1.99	0.63
2:B:247:SER:OG	2:B:291:PRO:HG3	1.99	0.63
1:A:340:ARG:HH11	1:A:340:ARG:HG2	1.63	0.62
2:B:129:ARG:NH2	2:B:173:ASP:OD1	2.32	0.62
2:B:140:SER:HB3	2:B:151:ARG:HG3	1.81	0.62
1:A:304:ILE:HG13	1:A:356:LEU:HB3	1.80	0.62
1:A:202:PHE:HA	1:A:205:ILE:HD12	1.79	0.62
1:A:518:VAL:CG2	2:B:1:MET:HE1	2.30	0.62
1:A:657:TYR:CD2	1:A:658:MET:HE2	2.35	0.62
1:A:626:GLN:H	1:A:629:GLN:NE2	1.98	0.62
1:A:724:LEU:O	1:A:728:ILE:HG13	2.00	0.61
2:B:60:ASN:HB3	2:B:64:ARG:HH11	1.66	0.61
1:A:651:GLU:HG2	1:A:708:ILE:CD1	2.30	0.61
1:A:837:ASP:O	1:A:838:PHE:C	2.43	0.61
1:A:102:ILE:O	1:A:106:VAL:HG23	2.01	0.61
1:A:834:ILE:HG21	1:A:845:ARG:HB3	1.84	0.60
2:B:189:MET:HE3	2:B:189:MET:H	1.66	0.60
1:A:259:MET:HG3	1:A:260:PHE:CD2	2.36	0.60
2:B:148:CYS:SG	2:B:151:ARG:NH2	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ILE:O	1:A:826:VAL:HB	2.02	0.59
1:A:1019:LEU:HA	1:A:1022:ILE:HG22	1.83	0.59
1:A:611:ILE:HD13	1:A:640:MET:HE2	1.84	0.59
1:A:657:TYR:CD2	1:A:658:MET:CE	2.84	0.59
1:A:469:TYR:O	1:A:472:THR:HG22	2.03	0.59
2:B:173:ASP:N	2:B:189:MET:HE1	2.18	0.59
1:A:424:MET:HE1	1:A:457:MET:CB	2.32	0.58
2:B:126:VAL:O	2:B:177:ASN:ND2	2.35	0.58
1:A:963:ASN:HB2	1:A:973:PHE:CE1	2.37	0.58
2:B:240:GLU:H	2:B:240:GLU:CD	2.10	0.58
2:B:25:HIS:CE1	2:B:109:ILE:HG12	2.39	0.58
2:B:179:VAL:CG1	2:B:179:VAL:H	2.16	0.58
1:A:626:GLN:H	1:A:629:GLN:HE21	1.52	0.58
1:A:258:PRO:O	1:A:261:ARG:HD2	2.03	0.58
1:A:778:PRO:HB2	1:A:779:PRO:HD3	1.86	0.58
1:A:852:LEU:HD11	1:A:874:VAL:HG13	1.86	0.57
1:A:717:MET:CE	1:A:758:LEU:HD23	2.33	0.57
2:B:103:MET:HE3	2:B:267:SER:N	2.15	0.57
1:A:219:ALA:HB3	1:A:220:PRO:HD3	1.87	0.57
1:A:997:PHE:CE1	1:A:1018:PHE:HB2	2.39	0.57
1:A:420:MET:CE	1:A:457:MET:HA	2.34	0.57
1:A:269:THR:HB	1:A:325:PHE:HA	1.85	0.57
1:A:792:VAL:HG23	1:A:794:ALA:H	1.70	0.57
1:A:133:ILE:O	1:A:137:ILE:HG22	2.04	0.56
1:A:573:MET:HE2	1:A:621:ILE:HG22	1.87	0.56
1:A:384:SER:HB3	1:A:406:ARG:HH22	1.67	0.56
1:A:811:LEU:HB3	1:A:814:HIS:HB2	1.88	0.56
2:B:33:SER:HB3	2:B:35:TYR:H	1.69	0.56
1:A:208:LEU:O	1:A:212:VAL:HG23	2.05	0.56
1:A:705:PRO:C	1:A:707:VAL:H	2.14	0.56
2:B:278:ARG:HG2	2:B:281:MET:HE3	1.86	0.56
1:A:838:PHE:O	1:A:839:GLU:C	2.49	0.56
1:A:218:ASN:HD22	1:A:221:LEU:HB2	1.71	0.55
1:A:406:ARG:NH2	1:A:467:LEU:HD22	2.21	0.55
2:B:278:ARG:CG	2:B:281:MET:HE3	2.36	0.55
2:B:246:LEU:HD11	2:B:282:VAL:HG21	1.87	0.55
1:A:132:MET:HG3	1:A:136:GLN:HE21	1.71	0.55
1:A:459:GLU:CG	1:A:1059:ILE:HD11	2.28	0.55
1:A:657:TYR:CE2	1:A:658:MET:CE	2.89	0.55
1:A:559:TRP:CD2	1:A:604:VAL:HG21	2.42	0.55
1:A:657:TYR:CE2	1:A:658:MET:HE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:LYS:O	1:A:837:ASP:C	2.49	0.54
1:A:157:SER:HB3	1:A:164:CYS:HA	1.89	0.54
1:A:447:ASP:O	1:A:451:ILE:HG12	2.06	0.54
1:A:802:SER:O	1:A:806:ILE:HG13	2.07	0.54
2:B:157:PRO:HB2	2:B:170:THR:CG2	2.38	0.54
2:B:218:LEU:HD23	2:B:225:ASN:HD21	1.73	0.54
1:A:1040:ILE:O	1:A:1044:GLN:HG2	2.08	0.54
1:A:611:ILE:HD13	1:A:640:MET:CE	2.38	0.53
1:A:482:ASN:HD22	1:A:488:GLU:CD	2.17	0.53
2:B:16:GLN:HB3	2:B:35:TYR:CE1	2.44	0.53
2:B:137:GLY:HA2	2:B:160:ASN:O	2.07	0.53
1:A:518:VAL:HG21	2:B:1:MET:HE1	1.91	0.53
1:A:601:GLN:HA	1:A:609:PRO:HG3	1.91	0.53
2:B:153:SER:O	2:B:226:PRO:HD2	2.09	0.52
1:A:364:GLU:CD	1:A:364:GLU:H	2.16	0.52
1:A:966:ASN:O	1:A:966:ASN:ND2	2.43	0.52
2:B:103:MET:CE	2:B:267:SER:H	2.17	0.52
1:A:305:ARG:HG2	1:A:305:ARG:HH11	1.75	0.52
2:B:25:HIS:ND1	2:B:26:PRO:HD2	2.25	0.52
1:A:644:GLN:HE21	1:A:646:ASP:N	2.03	0.52
2:B:179:VAL:CG1	2:B:179:VAL:N	2.73	0.52
1:A:466:HIS:HE1	1:A:1057:PRO:O	1.92	0.52
2:B:30:GLN:OE1	2:B:30:GLN:HA	2.09	0.52
1:A:939:LEU:HA	1:A:942:HIS:HD2	1.75	0.51
1:A:218:ASN:HD22	1:A:221:LEU:CB	2.23	0.51
1:A:458:ARG:HG3	1:A:503:SER:HB2	1.91	0.51
1:A:736:GLY:O	1:A:738:MET:N	2.43	0.51
1:A:887:ARG:HG3	1:A:937:ALA:HB1	1.92	0.51
1:A:600:VAL:C	1:A:602:VAL:N	2.66	0.51
1:A:803:THR:O	1:A:807:ILE:HG23	2.11	0.51
2:B:107:TRP:CZ3	2:B:281:MET:HE1	2.45	0.51
1:A:131:ASN:O	1:A:135:VAL:HG23	2.11	0.51
1:A:424:MET:HE3	1:A:425:ALA:N	2.24	0.51
1:A:427:PRO:O	1:A:429:GLU:HG3	2.11	0.51
1:A:777:VAL:HG22	1:A:807:ILE:HD12	1.93	0.51
1:A:265:LEU:O	1:A:269:THR:HG22	2.11	0.50
1:A:340:ARG:HB2	1:A:343:LEU:HD12	1.94	0.50
1:A:255:LEU:O	1:A:261:ARG:HB2	2.11	0.50
1:A:424:MET:HE2	1:A:454:TYR:CD1	2.45	0.50
1:A:735:ASN:HB2	1:A:739:VAL:CG2	2.41	0.50
2:B:10:SER:HB2	2:B:33:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HE2	2:B:1:MET:HE3	1.94	0.50
1:A:559:TRP:CE2	1:A:604:VAL:HG21	2.47	0.50
1:A:573:MET:HE1	1:A:633:PHE:CD1	2.45	0.50
1:A:513:GLU:CD	1:A:553:ARG:HH11	2.19	0.50
1:A:835:ASN:OD1	1:A:836:LYS:HD3	2.11	0.50
1:A:1049:LYS:O	1:A:1053:GLN:HG2	2.12	0.50
1:A:56:HIS:N	1:A:57:PRO:HD2	2.21	0.50
1:A:601:GLN:HE22	1:A:612:ASP:CG	2.19	0.50
2:B:63:ARG:HB3	2:B:169:TYR:OH	2.12	0.49
2:B:218:LEU:C	2:B:220:GLU:H	2.19	0.49
1:A:133:ILE:HG13	1:A:134:LEU:N	2.27	0.49
1:A:141:GLU:HG3	1:A:146:TRP:HB2	1.94	0.49
1:A:833:MET:HE1	1:A:844:HIS:ND1	2.27	0.49
2:B:16:GLN:HG2	2:B:35:TYR:CZ	2.48	0.49
2:B:25:HIS:HE1	2:B:109:ILE:HG12	1.76	0.49
2:B:172:LEU:C	2:B:189:MET:HE1	2.38	0.49
2:B:60:ASN:HB3	2:B:64:ARG:NH1	2.28	0.49
1:A:705:PRO:C	1:A:707:VAL:N	2.70	0.49
2:B:40:GLN:O	2:B:44:ARG:HG3	2.13	0.49
2:B:179:VAL:CG1	2:B:179:VAL:HB	2.17	0.49
2:B:182:THR:HB	2:B:228:LYS:HB2	1.95	0.48
1:A:736:GLY:O	1:A:739:VAL:HG23	2.14	0.48
1:A:832:ASN:HA	1:A:835:ASN:ND2	2.27	0.48
1:A:412:MET:SD	1:A:412:MET:C	2.96	0.48
1:A:781:LEU:HG	1:A:785:LEU:HD11	1.93	0.48
1:A:618:ILE:HG23	1:A:660:LEU:HD11	1.96	0.48
2:B:156:LEU:O	2:B:158:GLY:N	2.46	0.48
2:B:218:LEU:O	2:B:220:GLU:N	2.47	0.48
1:A:811:LEU:HB2	1:A:815:ILE:HG12	1.96	0.48
1:A:96:ARG:HE	1:A:96:ARG:HA	1.78	0.48
1:A:300:LEU:HD11	1:A:349:GLU:HB3	1.95	0.48
1:A:424:MET:HE2	1:A:454:TYR:HD1	1.79	0.48
2:B:207:TRP:CZ2	2:B:211:LYS:HE3	2.49	0.48
1:A:344:ARG:O	1:A:345:GLU:C	2.57	0.47
1:A:615:LEU:HD22	1:A:657:TYR:HA	1.96	0.47
2:B:208:MET:HB2	2:B:208:MET:HE3	1.69	0.47
1:A:259:MET:HG3	1:A:260:PHE:CE2	2.50	0.47
1:A:345:GLU:OE1	1:A:345:GLU:HA	2.14	0.47
1:A:381:TYR:CE1	1:A:385:PRO:HB2	2.49	0.47
1:A:692:LEU:HD22	1:A:717:MET:HE3	1.96	0.47
1:A:379:GLU:OE2	1:A:382:ARG:NH2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:MET:CE	1:A:225:THR:HG23	2.41	0.47
1:A:555:LEU:HB3	1:A:562:LEU:HD13	1.97	0.47
1:A:879:ILE:HA	1:A:882:PHE:CE1	2.49	0.47
1:A:153:ILE:O	1:A:157:SER:OG	2.33	0.47
1:A:635:GLU:OE1	1:A:697:ARG:NH1	2.48	0.47
1:A:717:MET:HE2	1:A:755:THR:HG23	1.95	0.47
2:B:112:PRO:HD2	2:B:115:LEU:HD13	1.95	0.47
1:A:916:GLN:HE22	1:A:962:LEU:HD23	1.80	0.47
1:A:945:ILE:O	1:A:949:MET:HG3	2.14	0.47
1:A:835:ASN:OD1	1:A:836:LYS:N	2.48	0.46
2:B:261:HIS:HD2	2:B:263:GLN:N	2.08	0.46
1:A:1016:ARG:O	1:A:1020:VAL:N	2.48	0.46
1:A:150:ILE:HG21	1:A:201:GLU:HG3	1.97	0.46
2:B:211:LYS:HA	2:B:211:LYS:HD3	1.69	0.46
1:A:245:LYS:HD3	1:A:245:LYS:HA	1.81	0.46
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.98	0.46
1:A:513:GLU:OE1	1:A:553:ARG:HD2	2.16	0.46
1:A:926:ILE:HD13	1:A:945:ILE:HG21	1.97	0.46
1:A:668:ILE:HD11	1:A:687:GLN:NE2	2.32	0.45
1:A:1040:ILE:O	1:A:1040:ILE:HG23	2.15	0.45
2:B:187:ASP:OD1	2:B:204:ARG:HD2	2.16	0.45
1:A:718:LEU:O	1:A:721:TYR:HB3	2.15	0.45
1:A:807:ILE:HG13	1:A:815:ILE:HD13	1.99	0.45
1:A:1035:LEU:HA	1:A:1038:ARG:HD3	1.98	0.45
1:A:1046:ASP:O	1:A:1050:HIS:HB2	2.16	0.45
1:A:1016:ARG:O	1:A:1020:VAL:HG23	2.16	0.45
1:A:601:GLN:NE2	1:A:612:ASP:OD1	2.49	0.45
2:B:103:MET:HE1	2:B:265:HIS:O	2.15	0.45
2:B:187:ASP:HB3	2:B:189:MET:HE2	1.99	0.45
1:A:950:PHE:O	1:A:953:VAL:HG22	2.17	0.45
1:A:601:GLN:NE2	1:A:653:LEU:HD21	2.32	0.45
2:B:122:VAL:HG22	2:B:234:ASN:HB3	1.99	0.45
2:B:200:GLN:HB3	2:B:263:GLN:HA	1.98	0.45
1:A:573:MET:CE	1:A:621:ILE:HG22	2.46	0.45
1:A:644:GLN:NE2	1:A:646:ASP:H	2.06	0.44
1:A:1017:ASP:HA	1:A:1020:VAL:HB	1.98	0.44
2:B:108:LEU:HB3	2:B:277:LEU:HD21	1.99	0.44
1:A:601:GLN:HA	1:A:609:PRO:CG	2.46	0.44
2:B:58:TYR:CE2	2:B:94:LEU:HD11	2.51	0.44
1:A:210:GLN:NE2	1:A:244:THR:HG21	2.32	0.44
1:A:482:ASN:HA	1:A:485:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:VAL:HG22	1:A:608:MET:HG2	2.00	0.44
1:A:625:LEU:HB3	1:A:629:GLN:HB2	1.99	0.44
1:A:938:GLY:O	1:A:942:HIS:CD2	2.71	0.44
2:B:154:SER:HA	2:B:225:ASN:OD1	2.17	0.44
2:B:197:TYR:O	2:B:265:HIS:HB3	2.17	0.44
2:B:250:PHE:C	2:B:252:PHE:H	2.26	0.44
1:A:206:PHE:CE2	1:A:240:TYR:HB3	2.52	0.44
1:A:362:GLU:N	1:A:362:GLU:OE1	2.50	0.44
1:A:950:PHE:O	1:A:951:ASN:C	2.61	0.44
1:A:56:HIS:H	1:A:57:PRO:CD	2.26	0.43
1:A:191:SER:HA	1:A:194:LEU:HD12	1.99	0.43
2:B:173:ASP:OD1	2:B:173:ASP:C	2.61	0.43
2:B:170:THR:HG22	2:B:192:ARG:H	1.83	0.43
1:A:506:GLY:HA3	1:A:1058:GLY:HA2	2.00	0.43
1:A:402:VAL:HA	1:A:403:PRO:HD2	1.87	0.43
1:A:278:GLN:OE1	1:A:278:GLN:N	2.45	0.43
1:A:294:LEU:C	1:A:296:GLN:H	2.27	0.43
2:B:129:ARG:NH2	2:B:173:ASP:CG	2.77	0.43
1:A:545:MET:HG3	1:A:583:MET:HE1	2.01	0.43
1:A:344:ARG:CZ	1:A:408:LEU:CD2	2.97	0.43
1:A:860:PHE:CE1	1:A:903:ASN:HB3	2.53	0.43
2:B:123:VAL:HG21	2:B:250:PHE:CZ	2.53	0.43
1:A:545:MET:HE3	2:B:12:PHE:HE2	1.84	0.42
1:A:838:PHE:O	1:A:838:PHE:CG	2.72	0.42
1:A:619:ASN:O	1:A:623:CYS:HB3	2.20	0.42
1:A:879:ILE:O	1:A:883:LYS:HB2	2.18	0.42
2:B:218:LEU:C	2:B:220:GLU:N	2.78	0.42
1:A:294:LEU:C	1:A:296:GLN:N	2.78	0.42
2:B:57:ASP:OD2	2:B:60:ASN:HB2	2.20	0.42
2:B:157:PRO:O	2:B:163:ASN:ND2	2.53	0.42
1:A:799:GLU:HA	1:A:802:SER:OG	2.20	0.42
2:B:142:TYR:CD2	2:B:142:TYR:N	2.88	0.42
2:B:240:GLU:OE1	2:B:240:GLU:N	2.34	0.42
1:A:287:PHE:HB2	1:A:329:PHE:CZ	2.55	0.42
1:A:204:GLN:HA	1:A:207:GLN:HE21	1.84	0.42
1:A:596:ARG:HB3	1:A:643:ALA:HB2	2.01	0.42
2:B:203:PHE:C	2:B:203:PHE:CD2	2.97	0.42
1:A:689:GLY:O	1:A:693:LYS:HG3	2.19	0.42
1:A:882:PHE:HA	1:A:890:ALA:HA	2.01	0.42
2:B:173:ASP:CB	2:B:189:MET:HE1	2.50	0.42
2:B:179:VAL:H	2:B:179:VAL:HG12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:GLY:HA3	2:B:276:TRP:CH2	2.55	0.42
1:A:552:PRO:O	1:A:553:ARG:C	2.62	0.42
1:A:358:SER:HB3	1:A:419:LEU:CD2	2.50	0.41
1:A:963:ASN:CG	1:A:966:ASN:HD22	2.28	0.41
1:A:265:LEU:O	1:A:269:THR:CG2	2.68	0.41
1:A:285:THR:HG22	1:A:289:LEU:HD22	2.02	0.41
1:A:777:VAL:HG12	1:A:781:LEU:HD22	2.02	0.41
1:A:879:ILE:HD11	1:A:925:HIS:CG	2.55	0.41
1:A:132:MET:O	1:A:136:GLN:HG3	2.20	0.41
1:A:305:ARG:NH2	1:A:361:GLU:OE1	2.53	0.41
1:A:603:GLN:HG3	1:A:609:PRO:HD3	2.01	0.41
1:A:962:LEU:O	1:A:964:PRO:HD3	2.19	0.41
2:B:18:LEU:HD23	2:B:18:LEU:HA	1.77	0.41
1:A:157:SER:C	1:A:159:THR:H	2.28	0.41
1:A:559:TRP:O	1:A:560:LYS:C	2.62	0.41
1:A:672:ALA:HA	1:A:678:ILE:HG22	2.01	0.41
1:A:819:ILE:N	1:A:820:PRO:CD	2.84	0.41
1:A:196:ASP:O	1:A:199:CYS:HB2	2.20	0.41
1:A:424:MET:HE3	1:A:424:MET:HA	2.02	0.41
1:A:427:PRO:HD3	1:A:499:TRP:CD2	2.56	0.41
1:A:860:PHE:O	1:A:862:ALA:N	2.53	0.41
1:A:74:ASN:C	1:A:76:LYS:H	2.29	0.41
1:A:666:ASP:CG	1:A:712:ARG:HH22	2.27	0.41
1:A:894:LEU:HD13	1:A:941:MET:CB	2.51	0.41
1:A:772:VAL:O	1:A:777:VAL:HG23	2.21	0.41
1:A:847:ASN:O	1:A:848:PHE:C	2.64	0.41
1:A:287:PHE:CE2	1:A:337:ILE:HG21	2.56	0.40
1:A:597:ARG:H	1:A:597:ARG:HG2	1.64	0.40
1:A:953:VAL:HG21	1:A:974:LEU:HD22	2.02	0.40
1:A:178:VAL:O	1:A:178:VAL:HG12	2.21	0.40
1:A:840:GLU:HB3	1:A:841:TYR:CD2	2.56	0.40
1:A:358:SER:HB3	1:A:419:LEU:HD21	2.03	0.40
1:A:517:LEU:HD11	1:A:551:TYR:CD1	2.55	0.40
1:A:628:GLN:CD	1:A:628:GLN:N	2.65	0.40
1:A:351:LEU:O	1:A:352:HIS:C	2.64	0.40
1:A:738:MET:O	1:A:741:LYS:HB2	2.21	0.40
1:A:1013:GLU:HA	1:A:1016:ARG:HG2	2.04	0.40
2:B:125:PRO:HD2	2:B:175:ILE:HD12	2.03	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	945/1071 (88%)	849 (90%)	78 (8%)	18 (2%)	6	23
2	B	264/329 (80%)	240 (91%)	15 (6%)	9 (3%)	3	12
All	All	1209/1400 (86%)	1089 (90%)	93 (8%)	27 (2%)	5	20

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	601	GLN
1	A	737	GLU
1	A	1030	THR
1	A	256	ASN
1	A	341	LEU
1	A	837	ASP
1	A	933	THR
2	B	96	LYS
2	B	216	GLU
2	B	219	GLY
1	A	596	ARG
1	A	604	VAL
1	A	839	GLU
2	B	97	HIS
2	B	157	PRO
1	A	258	PRO
1	A	505	SER
1	A	578	ASP
1	A	838	PHE
2	B	19	ASN
2	B	136	ARG
2	B	289	ALA
1	A	56	HIS
2	B	100	ASN
1	A	1061	ASN

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Mol	Chain	Res	Type
1	A	311	GLY
1	A	1027	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	834/976 (86%)	748 (90%)	86 (10%)	7	23
2	B	235/296 (79%)	204 (87%)	31 (13%)	4	13
All	All	1069/1272 (84%)	952 (89%)	117 (11%)	6	20

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	64	ASP
1	A	91	TRP
1	A	110	ILE
1	A	133	ILE
1	A	137	ILE
1	A	144	LYS
1	A	148	THR
1	A	157	SER
1	A	159	THR
1	A	173	LEU
1	A	201	GLU
1	A	227	GLU
1	A	236	ILE
1	A	248	SER
1	A	250	LEU
1	A	261	ARG
1	A	263	VAL
1	A	269	THR
1	A	277	SER
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	292	MET
1	A	296	GLN
1	A	304	ILE
1	A	335	GLN
1	A	340	ARG
1	A	342	ASN
1	A	346	THR
1	A	364	GLU
1	A	368	ILE
1	A	387	SER
1	A	406	ARG
1	A	429	GLU
1	A	448	THR
1	A	510	GLU
1	A	539	ILE
1	A	568	LYS
1	A	580	VAL
1	A	597	ARG
1	A	600	VAL
1	A	604	VAL
1	A	607	VAL
1	A	645	THR
1	A	658	MET
1	A	668	ILE
1	A	676	VAL
1	A	690	SER
1	A	697	ARG
1	A	719	ASN
1	A	733	GLN
1	A	741	LYS
1	A	765	ARG
1	A	770	GLN
1	A	774	GLU
1	A	780	LEU
1	A	781	LEU
1	A	792	VAL
1	A	804	MET
1	A	807	ILE
1	A	810	LYS
1	A	826	VAL
1	A	836	LYS
1	A	879	ILE

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Mol	Chain	Res	Type
1	A	886	MET
1	A	891	ASP
1	A	895	GLN
1	A	900	LEU
1	A	907	GLU
1	A	916	GLN
1	A	921	ASP
1	A	933	THR
1	A	960	THR
1	A	966	ASN
1	A	972	ILE
1	A	974	LEU
1	A	976	GLU
1	A	980	ASN
1	A	981	LEU
1	A	988	HIS
1	A	996	LEU
1	A	1005	ASN
1	A	1006	GLN
1	A	1022	ILE
1	A	1032	ASP
1	A	1040	ILE
1	A	1043	ARG
2	B	41	SER
2	B	42	GLU
2	B	46	ARG
2	B	52	LYS
2	B	54	LYS
2	B	56	LEU
2	B	57	ASP
2	B	63	ARG
2	B	100	ASN
2	B	117	GLN
2	B	120	ILE
2	B	126	VAL
2	B	135	SER
2	B	136	ARG
2	B	144	LYS
2	B	149	VAL
2	B	157	PRO
2	B	170	THR
2	B	179	VAL

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Mol	Chain	Res	Type
2	B	182	THR
2	B	187	ASP
2	B	189	MET
2	B	207	TRP
2	B	215	GLU
2	B	220	GLU
2	B	222	THR
2	B	240	GLU
2	B	253	GLU
2	B	254	VAL
2	B	285	VAL
2	B	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	136	GLN
1	A	167	ASN
1	A	207	GLN
1	A	210	GLN
1	A	215	ASN
1	A	218	ASN
1	A	234	ASN
1	A	296	GLN
1	A	374	ASN
1	A	456	ASN
1	A	466	HIS
1	A	482	ASN
1	A	485	ASN
1	A	558	HIS
1	A	581	GLN
1	A	601	GLN
1	A	629	GLN
1	A	644	GLN
1	A	767	ASN
1	A	770	GLN
1	A	895	GLN
1	A	902	GLN
1	A	903	ASN
1	A	916	GLN
1	A	942	HIS

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Mol	Chain	Res	Type
1	A	951	ASN
1	A	966	ASN
1	A	969	ASN
1	A	1005	ASN
1	A	1014	HIS
1	A	1044	GLN
2	B	16	GLN
2	B	60	ASN
2	B	100	ASN
2	B	160	ASN
2	B	163	ASN
2	B	200	GLN
2	B	234	ASN
2	B	261	HIS
2	B	263	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	959/1071 (89%)	0.67	130 (13%) 7 5	8, 42, 110, 125	0
2	B	268/329 (81%)	0.92	44 (16%) 4 3	9, 29, 61, 75	0
All	All	1227/1400 (87%)	0.73	174 (14%) 6 5	8, 38, 108, 125	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	ASN	7.8
1	A	62	ARG	7.3
1	A	63	VAL	6.8
1	A	187	THR	6.7
1	A	1042	LEU	6.4
1	A	1062	PRO	6.4
1	A	179	PHE	6.2
1	A	66	ILE	6.1
2	B	292	ALA	5.9
1	A	67	LEU	5.7
1	A	57	PRO	5.6
2	B	166	ALA	5.6
2	B	95	PRO	5.3
1	A	115	SER	5.3
1	A	1030	THR	5.2
1	A	601	GLN	5.1
1	A	53	LEU	5.1
1	A	1060	PHE	5.0
1	A	91	TRP	5.0
1	A	71	GLN	4.9
1	A	605	GLY	4.8
2	B	293	GLY	4.7
1	A	1049	LYS	4.4
2	B	96	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	73	MET	4.3
1	A	75	THR	4.3
1	A	1052	ARG	4.3
1	A	1058	GLY	4.3
1	A	1054	MET	4.2
1	A	886	MET	4.2
1	A	931	THR	4.1
1	A	933	THR	4.1
1	A	604	VAL	4.0
1	A	90	ARG	4.0
1	A	838	PHE	4.0
2	B	94	LEU	3.9
1	A	178	VAL	3.9
1	A	1025	PHE	3.8
1	A	1034	PHE	3.8
1	A	603	GLN	3.7
2	B	55	ARG	3.7
1	A	77	TYR	3.7
1	A	987	PRO	3.6
1	A	883	LYS	3.6
1	A	125	VAL	3.6
2	B	207	TRP	3.5
1	A	1057	PRO	3.5
1	A	1050	HIS	3.4
2	B	141	ALA	3.4
1	A	150	ILE	3.4
1	A	935	HIS	3.4
1	A	976	GLU	3.4
1	A	1040	ILE	3.4
1	A	602	VAL	3.3
2	B	58	TYR	3.3
1	A	1035	LEU	3.3
1	A	996	LEU	3.2
1	A	144	LYS	3.2
2	B	227	PHE	3.2
1	A	937	ALA	3.1
1	A	54	LYS	3.1
1	A	978	VAL	3.1
1	A	65	THR	3.1
1	A	908	GLU	3.1
1	A	1048	GLU	3.1
1	A	387	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	ASN	3.0
1	A	81	GLN	3.0
2	B	0	SER	3.0
1	A	1026	ALA	3.0
1	A	240	TYR	3.0
1	A	157	SER	3.0
1	A	72	ASN	2.9
2	B	152	PHE	2.9
1	A	932	ASP	2.9
1	A	96	ARG	2.9
1	A	1055	SER	2.9
2	B	153	SER	2.9
1	A	142	TRP	2.8
2	B	289	ALA	2.8
2	B	1	MET	2.8
1	A	1024	GLU	2.8
1	A	163	LEU	2.8
1	A	124	LYS	2.8
2	B	161	ARG	2.7
1	A	112	LYS	2.7
1	A	68	GLU	2.7
1	A	129	LYS	2.7
2	B	216	GLU	2.7
1	A	986	PHE	2.6
1	A	988	HIS	2.6
2	B	147	TYR	2.6
1	A	55	GLU	2.6
2	B	163	ASN	2.6
2	B	222	THR	2.6
2	B	290	VAL	2.6
1	A	447	ASP	2.6
1	A	193	HIS	2.5
1	A	143	PRO	2.5
1	A	880	TRP	2.5
1	A	1022	ILE	2.5
1	A	361	GLU	2.5
1	A	992	ALA	2.5
1	A	981	LEU	2.5
1	A	78	TYR	2.5
2	B	134	ALA	2.5
2	B	157	PRO	2.5
1	A	428	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1041	ALA	2.5
1	A	1002	PHE	2.4
1	A	1045	ALA	2.4
2	B	97	HIS	2.4
1	A	967	PRO	2.4
1	A	114	SER	2.4
1	A	993	GLN	2.4
2	B	139	THR	2.4
2	B	183	TYR	2.4
1	A	190	LYS	2.3
1	A	1043	ARG	2.3
1	A	578	ASP	2.3
1	A	82	ILE	2.3
2	B	66	ALA	2.3
1	A	1021	GLN	2.3
1	A	1033	LEU	2.3
2	B	138	SER	2.3
1	A	113	THR	2.3
1	A	76	LYS	2.3
2	B	168	ASP	2.3
1	A	989	LEU	2.3
1	A	934	SER	2.3
2	B	182	THR	2.3
1	A	845	ARG	2.3
1	A	929	VAL	2.3
2	B	179	VAL	2.3
1	A	80	LEU	2.3
2	B	65	LEU	2.3
2	B	32	LYS	2.3
1	A	137	ILE	2.3
1	A	429	GLU	2.2
2	B	167	LYS	2.2
1	A	102	ILE	2.2
1	A	884	HIS	2.2
1	A	980	ASN	2.2
1	A	1019	LEU	2.2
1	A	56	HIS	2.2
1	A	1003	SER	2.2
2	B	142	TYR	2.2
2	B	59	VAL	2.2
1	A	990	GLN	2.2
2	B	194	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	259	MET	2.2
1	A	938	GLY	2.2
1	A	1051	LYS	2.2
2	B	217	GLY	2.2
1	A	175	SER	2.2
1	A	964	PRO	2.1
1	A	998	VAL	2.1
1	A	132	MET	2.1
1	A	920	CYS	2.1
1	A	1059	ILE	2.1
1	A	189	VAL	2.1
2	B	224	LEU	2.1
2	B	2	GLU	2.1
2	B	218	LEU	2.1
1	A	260	PHE	2.1
1	A	83	LEU	2.1
1	A	110	ILE	2.1
1	A	1012	LYS	2.0
2	B	30	GLN	2.0
1	A	1028	GLU	2.0
1	A	139	LYS	2.0
2	B	98	TYR	2.0
1	A	844	HIS	2.0
1	A	122	LYS	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.