Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 04:51 PM EST

PDB ID	:	3GB8
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:

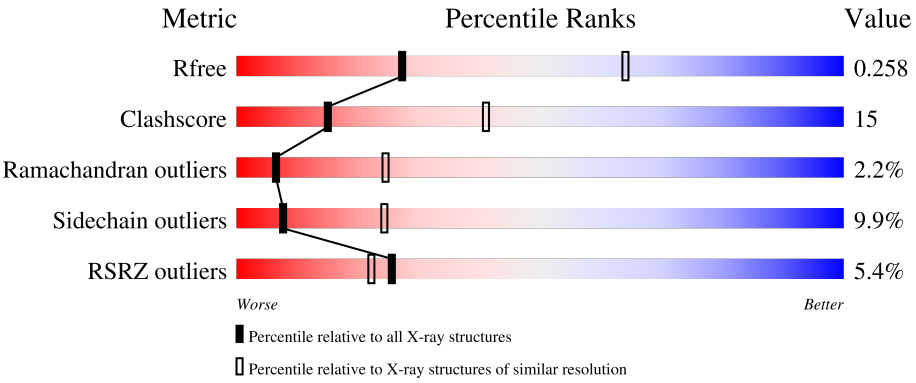
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	5% 60% 25% • 10%
2	B	329	2% 47% 28% 5% • 19%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	959	7624	4896	1278	1401	49	0	0	1

- Molecule 2 is a protein called Snurportin-1.

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

There is a discrepancy between the modelled and reference sequences:

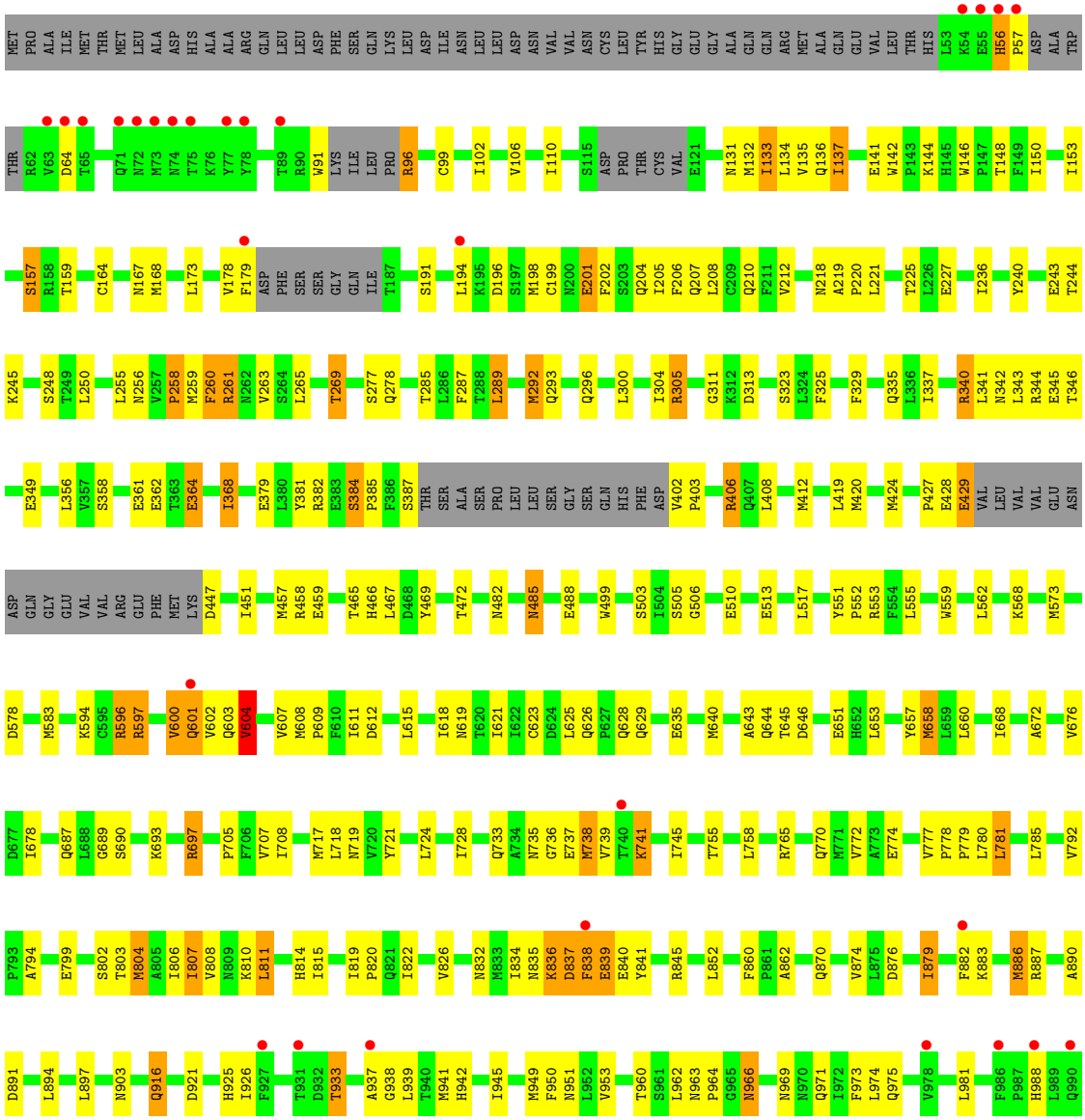
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP O95149

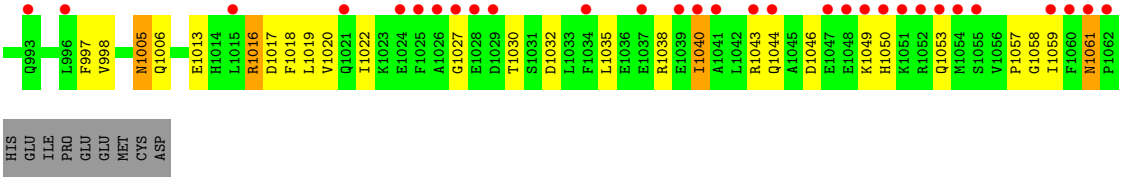
3 Residue-property plots (i)

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: Exportin-1

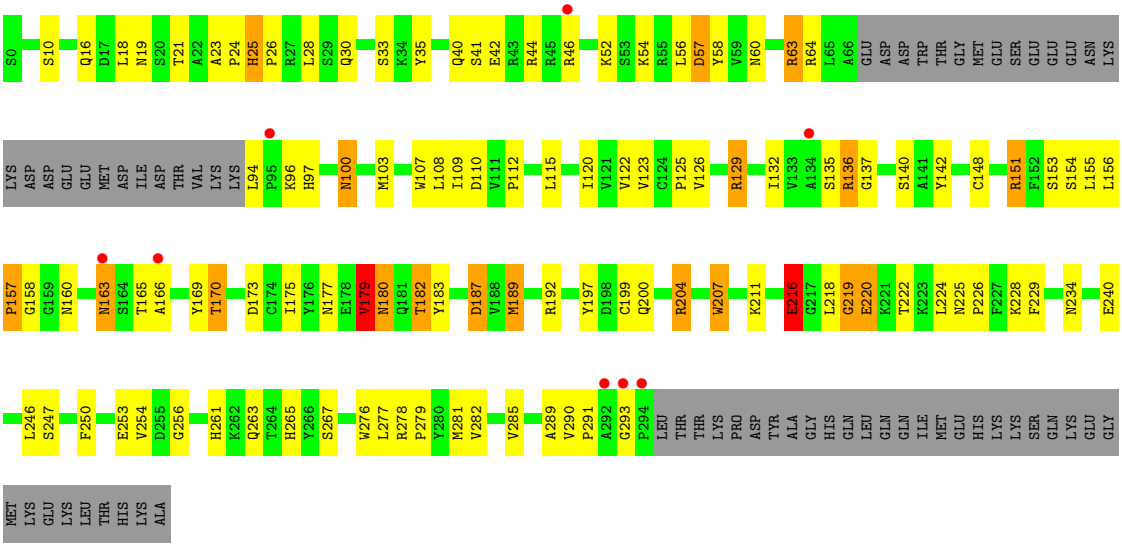
Chain A:





• Molecule 2: Snurportin-1

Chain B:



4 Data and refinement statistics (i)

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 48.13 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.67-2.90) 97.0 (48.13-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.267 0.229 , 0.258	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 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.61	1/7777 (0.0%)	0.68	3/10551 (0.0%)
2	B	0.88	11/2183 (0.5%)	0.82	3/2966 (0.1%)
All	All	0.68	12/9960 (0.1%)	0.71	6/13517 (0.0%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	GLU	CD-OE1	14.23	1.41	1.25
2	B	179	VAL	CB-CG1	10.51	1.75	1.52
2	B	216	GLU	CD-OE2	8.58	1.35	1.25
2	B	216	GLU	CG-CD	7.53	1.63	1.51
2	B	179	VAL	CB-CG2	6.83	1.67	1.52
2	B	216	GLU	CB-CG	6.21	1.64	1.52
2	B	180	ASN	CG-ND2	5.86	1.47	1.32
2	B	199	CYS	CB-SG	-5.73	1.72	1.81
2	B	224	LEU	CG-CD1	5.64	1.72	1.51
2	B	293	GLY	C-N	-5.46	1.23	1.34
2	B	180	ASN	CG-OD1	5.17	1.35	1.24
1	A	1061	ASN	C-N	-5.13	1.24	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CB-CA-C	-5.98	98.44	110.40
2	B	179	VAL	CG1-CB-CG2	5.85	120.26	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	28	LEU	CA-CB-CG	5.55	128.07	115.30
2	B	204	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	604	VAL	CB-CA-C	5.37	121.60	111.40
1	A	811	LEU	CA-CB-CG	5.04	126.89	115.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7624	0	7524	217	0
2	B	2126	0	2060	75	0
All	All	9750	0	9584	292	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 15.

All (292) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:HD11	1:A:925:HIS:HB3	1.59	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
2:B:137:GLY:HA2	2:B:160:ASN:C	2.00	0.82
1:A:804:MET:HA	1:A:804:MET:CE	2.09	0.81
1:A:384:SER:HB3	1:A:406:ARG:NH2	1.98	0.79
1:A:628:GLN:CD	1:A:628:GLN:H	1.86	0.78
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
2:B:165:THR:HG22	2:B:166:ALA:N	2.00	0.76
1:A:552:PRO:HG3	1:A:594:LYS:HD3	1.66	0.75
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:717:MET:HE3	1:A:758:LEU:HD23	1.72	0.72
1:A:651:GLU:HG2	1:A:708:ILE:HD13	1.72	0.72
2:B:173:ASP:CB	2:B:189:MET:HE1	2.21	0.70
2:B:165:THR:CG2	2:B:166:ALA:H	2.04	0.70
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
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:278:ARG:HG2	2:B:281:MET:HE3	1.75	0.67
1:A:420:MET:HE1	1:A:457:MET:HA	1.77	0.66
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: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:804:MET:HA	1:A:804:MET:HE2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:GLN:HA	1:A:609:PRO:CB	2.28	0.64
2:B:103:MET:HE3	2:B:267:SER:H	1.62	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:966:ASN:CG	1:A:966:ASN:O	2.37	0.62
1:A:202:PHE:HA	1:A:205:ILE:HD12	1.79	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: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
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
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: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: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
1:A:573:MET:HE1	1:A:621:ILE:HG22	1.86	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
2:B:103:MET:CE	2:B:267:SER:H	2.17	0.57
1:A:420:MET:CE	1:A:457:MET:HA	2.34	0.57
2:B:173:ASP:HB3	2:B:189:MET:HE1	1.86	0.57
1:A:717:MET:CE	1:A:758:LEU:HD23	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:O	1:A:137:ILE:HG22	2.04	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
1:A:837:ASP:O	1:A:838:PHE:C	2.43	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: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: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: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
2:B:240:GLU:H	2:B:240:GLU:CD	2.10	0.54
1:A:611:ILE:HD13	1:A:640:MET:CE	2.38	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: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:804:MET:HA	1:A:804:MET:HE3	1.90	0.52
1:A:966:ASN:O	1:A:966:ASN:ND2	2.43	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:705:PRO:C	1:A:707:VAL:H	2.14	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:838:PHE:O	1:A:839:GLU:C	2.49	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:803:THR:O	1:A:807:ILE:HG23	2.11	0.51

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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	0.51
1:A:131:ASN:O	1:A:135:VAL:HG23	2.11	0.51
2:B:173:ASP:HB2	2:B:189:MET:HE1	1.92	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: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
1:A:559:TRP:CE2	1:A:604:VAL:HG21	2.47	0.50
1:A:835:ASN:OD1	1:A:836:LYS:HD3	2.11	0.50
1:A:836:LYS:O	1:A:837:ASP:C	2.49	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
2:B:63:ARG:HB3	2:B:169:TYR:OH	2.12	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
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:60:ASN:HB3	2:B:64:ARG:NH1	2.28	0.49
1:A:657:TYR:CD2	1:A:658:MET:HE1	2.46	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
1:A:482:ASN:HD22	1:A:488:GLU:CD	2.17	0.48
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: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
2:B:207:TRP:CZ2	2:B:211:LYS:HE3	2.49	0.48
1:A:615:LEU:HD22	1:A:657:TYR:HA	1.96	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:657:TYR:CE2	1:A:658:MET:HE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:CD	1:A:364:GLU:H	2.16	0.47
1:A:379:GLU:OE2	1:A:382:ARG:NH2	2.46	0.47
1:A:555:LEU:HB3	1:A:562:LEU:HD13	1.97	0.47
1:A:717:MET:HE2	1:A:755:THR:HA	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
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
1:A:600:VAL:C	1:A:602:VAL:N	2.66	0.46
2:B:261:HIS:HD2	2:B:263:GLN:N	2.08	0.46
1:A:573:MET:HE3	1:A:625:LEU:HD11	1.96	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:168:MET:HE3	1:A:225:THR:HG23	1.97	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:705:PRO:C	1:A:707:VAL:N	2.70	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:513:GLU:CD	1:A:553:ARG:HH11	2.19	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
1:A:601:GLN:HE22	1:A:612:ASP:CG	2.19	0.45
1:A:950:PHE:O	1:A:953:VAL:HG22	2.17	0.45
2:B:103:MET:HE3	2:B:267:SER:N	2.28	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
2:B:218:LEU:C	2:B:220:GLU:H	2.19	0.45
1:A:611:ILE:HD13	1:A:640:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:573:MET:CE	1:A:621:ILE:HG22	2.46	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
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
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:56:HIS:H	1:A:57:PRO:CD	2.26	0.43
1:A:412:MET:SD	1:A:412:MET:C	2.96	0.43
1:A:191:SER:HA	1:A:194:LEU:HD12	1.99	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:424:MET:CE	1:A:457:MET:HB2	2.48	0.43
1:A:278:GLN:OE1	1:A:278:GLN:N	2.45	0.43
1:A:344:ARG:O	1:A:345:GLU:C	2.57	0.43
1:A:292:MET:HE3	1:A:293:GLN:HG2	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:VAL:H	2:B:179:VAL:HG12	1.85	0.42
2:B:256:GLY:HA3	2:B:276:TRP:CH2	2.55	0.42
1:A:781:LEU:HD11	1:A:804:MET:HE1	2.01	0.42
1:A:358:SER:HB3	1:A:419:LEU:CD2	2.50	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:573:MET:HE1	1:A:621:ILE:CG2	2.49	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:292:MET:CE	1:A:293:GLN:HG2	2.50	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:198:MET:HE3	1:A:198:MET:HB3	1.75	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: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:142:TRP:CH2	1:A:198:MET:HE1	2.56	0.41
1:A:573:MET:CE	1:A:625:LEU:HD11	2.50	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: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:717:MET:CE	1:A:755:THR:HA	2.51	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: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 (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	945/1071 (88%)	849 (90%)	78 (8%)	18 (2%)	8 28
2	B	264/329 (80%)	240 (91%)	15 (6%)	9 (3%)	3 15
All	All	1209/1400 (86%)	1089 (90%)	93 (8%)	27 (2%)	6 24

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	834/976 (86%)	756 (91%)	78 (9%)	8 26
2	B	235/296 (79%)	207 (88%)	28 (12%)	5 15
All	All	1069/1272 (84%)	963 (90%)	106 (10%)	8 24

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	91	TRP
1	A	96	ARG
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	179	PHE
1	A	201	GLU
1	A	227	GLU
1	A	236	ILE
1	A	243	GLU
1	A	248	SER
1	A	250	LEU
1	A	260	PHE
1	A	261	ARG
1	A	263	VAL

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Mol	Chain	Res	Type
1	A	269	THR
1	A	277	SER
1	A	289	LEU
1	A	292	MET
1	A	296	GLN
1	A	305	ARG
1	A	313	ASP
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	510	GLU
1	A	568	LYS
1	A	583	MET
1	A	597	ARG
1	A	600	VAL
1	A	604	VAL
1	A	645	THR
1	A	658	MET
1	A	676	VAL
1	A	690	SER
1	A	697	ARG
1	A	719	ASN
1	A	733	GLN
1	A	738	MET
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	804	MET
1	A	807	ILE
1	A	810	LYS
1	A	836	LYS
1	A	870	GLN
1	A	879	ILE

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Mol	Chain	Res	Type
1	A	886	MET
1	A	891	ASP
1	A	916	GLN
1	A	921	ASP
1	A	933	THR
1	A	960	THR
1	A	966	ASN
1	A	981	LEU
1	A	988	HIS
1	A	1005	ASN
1	A	1006	GLN
1	A	1016	ARG
1	A	1032	ASP
1	A	1040	ILE
1	A	1043	ARG
2	B	25	HIS
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	120	ILE
2	B	129	ARG
2	B	135	SER
2	B	136	ARG
2	B	151	ARG
2	B	163	ASN
2	B	170	THR
2	B	179	VAL
2	B	182	THR
2	B	187	ASP
2	B	189	MET
2	B	207	TRP
2	B	220	GLU
2	B	222	THR
2	B	253	GLU
2	B	254	VAL
2	B	285	VAL

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Mol	Chain	Res	Type
2	B	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	218	ASN
1	A	234	ASN
1	A	296	GLN
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	626	GLN
1	A	629	GLN
1	A	644	GLN
1	A	767	ASN
1	A	770	GLN
1	A	853	GLN
1	A	895	GLN
1	A	916	GLN
1	A	942	HIS
1	A	951	ASN
1	A	966	ASN
1	A	969	ASN
1	A	1005	ASN
2	B	100	ASN
2	B	160	ASN
2	B	163	ASN
2	B	261	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 monosaccharides 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, 95^{th} 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%)	0.13	58 (6%)	21	18	8, 42, 110, 125	0
2	B	268/329 (81%)	0.18	8 (2%)	50	45	9, 29, 61, 75	0
All	All	1227/1400 (87%)	0.14	66 (5%)	25	22	8, 38, 108, 125	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	294	PRO	5.3
1	A	601	GLN	4.8
1	A	78	TYR	4.6
1	A	1040	ILE	4.6
1	A	1052	ARG	4.5
1	A	72	ASN	4.5
1	A	1060	PHE	4.5
1	A	1054	MET	4.4
2	B	292	ALA	4.2
2	B	166	ALA	3.9
1	A	1059	ILE	3.9
1	A	73	MET	3.9
1	A	1055	SER	3.9
1	A	63	VAL	3.9
1	A	1062	PRO	3.9
1	A	1050	HIS	3.8
1	A	996	LEU	3.7
1	A	1025	PHE	3.6
1	A	75	THR	3.5
1	A	1027	GLY	3.5
1	A	1026	ALA	3.4
1	A	55	GLU	3.4
1	A	65	THR	3.4
1	A	179	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	986	PHE	3.3
2	B	95	PRO	3.3
1	A	1061	ASN	3.3
1	A	1028	GLU	3.3
1	A	988	HIS	3.2
1	A	1021	GLN	3.2
1	A	57	PRO	3.2
1	A	1015	LEU	3.2
1	A	978	VAL	3.1
2	B	293	GLY	3.0
1	A	64	ASP	3.0
1	A	993	GLN	3.0
1	A	1053	GLN	3.0
2	B	163	ASN	2.8
1	A	54	LYS	2.8
1	A	740	THR	2.7
2	B	46	ARG	2.7
1	A	1043	ARG	2.7
1	A	1034	PHE	2.6
1	A	1051	LYS	2.6
1	A	1047	GLU	2.6
1	A	1049	LYS	2.6
1	A	937	ALA	2.4
1	A	1044	GLN	2.4
1	A	1048	GLU	2.3
1	A	1029	ASP	2.3
1	A	89	THR	2.3
1	A	74	ASN	2.3
1	A	882	PHE	2.3
2	B	134	ALA	2.3
1	A	931	THR	2.2
1	A	990	GLN	2.2
1	A	838	PHE	2.2
1	A	1037	GLU	2.2
1	A	56	HIS	2.2
1	A	927	PHE	2.2
1	A	1039	GLU	2.1
1	A	1041	ALA	2.1
1	A	71	GLN	2.1
1	A	77	TYR	2.1
1	A	194	LEU	2.0
1	A	1024	GLU	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 monosaccharides 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.