Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:28 am BST

PDB ID	:	4HFO
Title	:	Biogenic amine-binding protein selenomethionine derivative
Authors	:	Andersen, J.F.; Xu, X.; Chang, B.; Mans, B.J.; Ribeiro, J.M.
Deposited on	:	2012-10-05
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

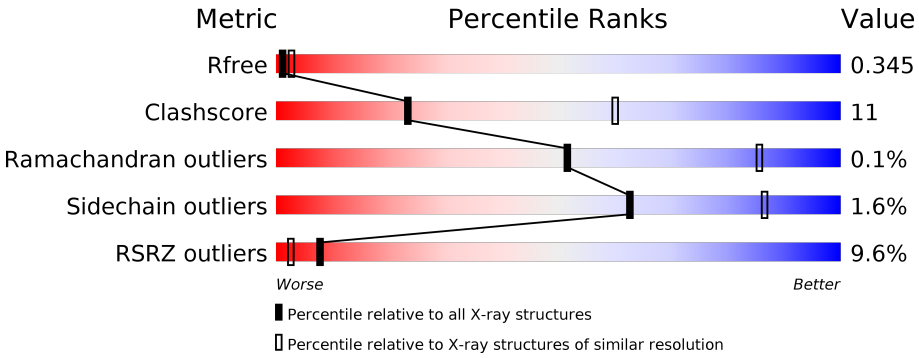
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	195	5% 77% 22% ·
1	B	195	6% 72% 27% ··
1	C	195	9% 75% 24% ·
1	D	195	8% 81% 17% ··
1	I	195	8% 78% 21% ·
1	J	195	7% 71% 28% ··

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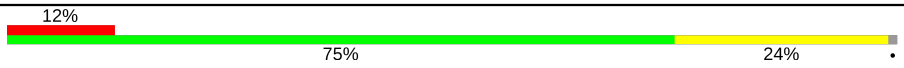
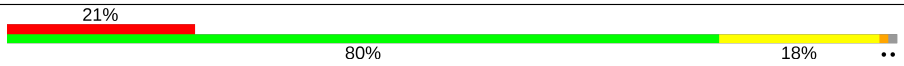
Mol	Chain	Length	Quality of chain
1	K	195	
1	L	195	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12360 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 Biogenic amine-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	0	0
			1552	980	253	313	4	2			
1	B	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			
1	C	193	Total	C	N	O	S	Se	0	0	0
			1542	975	251	310	4	2			
1	D	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			
1	I	195	Total	C	N	O	S	Se	0	0	0
			1552	980	253	313	4	2			
1	J	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			
1	K	193	Total	C	N	O	S	Se	0	0	0
			1542	975	251	310	4	2			
1	L	194	Total	C	N	O	S	Se	0	0	0
			1543	974	251	312	4	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MSE	ILE	CONFLICT	UNP Q86PT9
A	134	MSE	LEU	CONFLICT	UNP Q86PT9
B	25	MSE	ILE	CONFLICT	UNP Q86PT9
B	134	MSE	LEU	CONFLICT	UNP Q86PT9
C	25	MSE	ILE	CONFLICT	UNP Q86PT9
C	134	MSE	LEU	CONFLICT	UNP Q86PT9
D	25	MSE	ILE	CONFLICT	UNP Q86PT9
D	134	MSE	LEU	CONFLICT	UNP Q86PT9
I	25	MSE	ILE	CONFLICT	UNP Q86PT9
I	134	MSE	LEU	CONFLICT	UNP Q86PT9
J	25	MSE	ILE	CONFLICT	UNP Q86PT9
J	134	MSE	LEU	CONFLICT	UNP Q86PT9
K	25	MSE	ILE	CONFLICT	UNP Q86PT9

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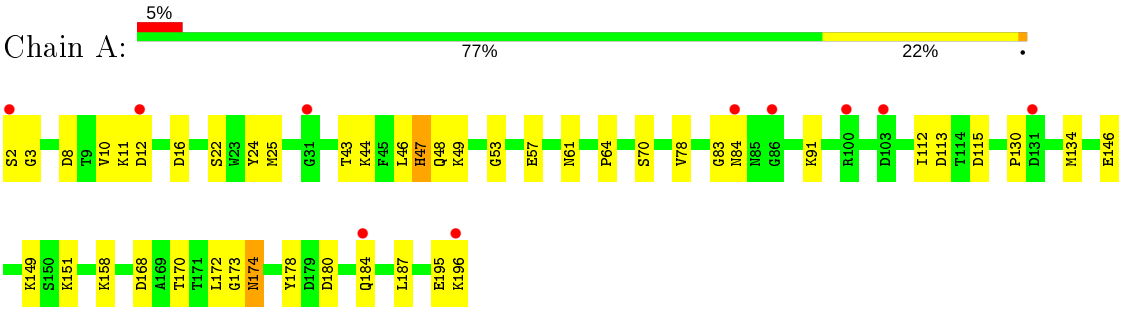
Chain	Residue	Modelled	Actual	Comment	Reference
K	134	MSE	LEU	CONFLICT	UNP Q86PT9
L	25	MSE	ILE	CONFLICT	UNP Q86PT9
L	134	MSE	LEU	CONFLICT	UNP Q86PT9

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

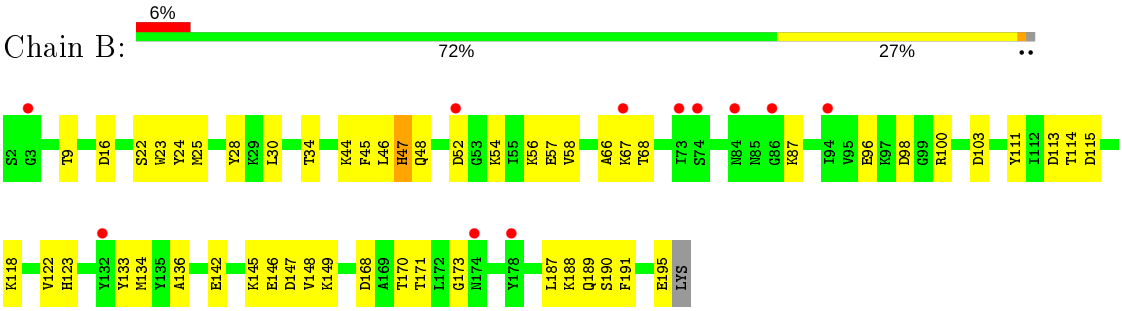
- Molecule 1: Biogenic amine-binding protein

Chain A:



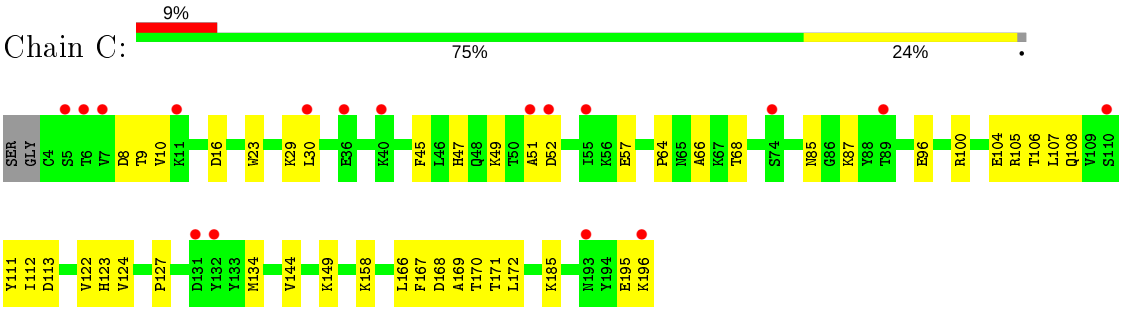
- Molecule 1: Biogenic amine-binding protein

Chain B:



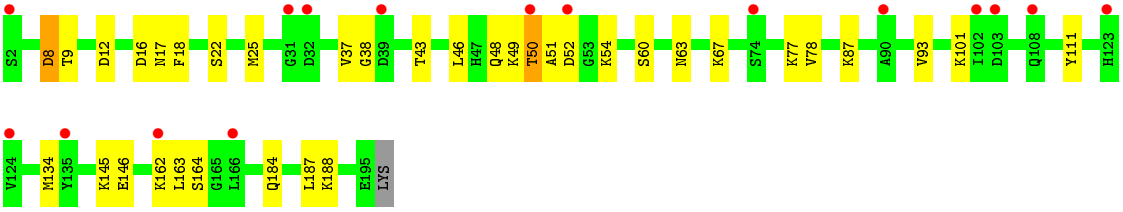
- Molecule 1: Biogenic amine-binding protein

Chain C:

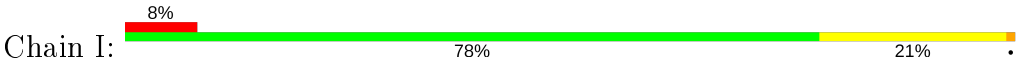


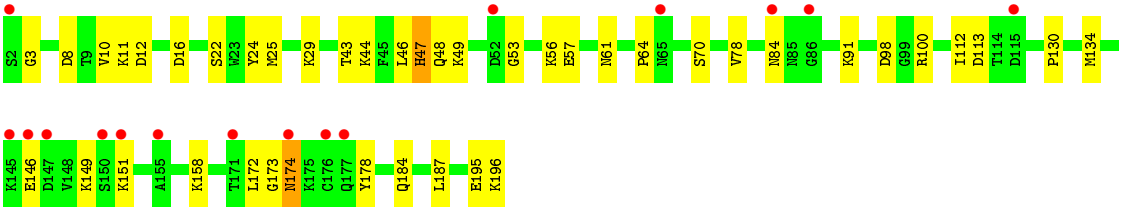
- Molecule 1: Biogenic amine-binding protein

Chain D:

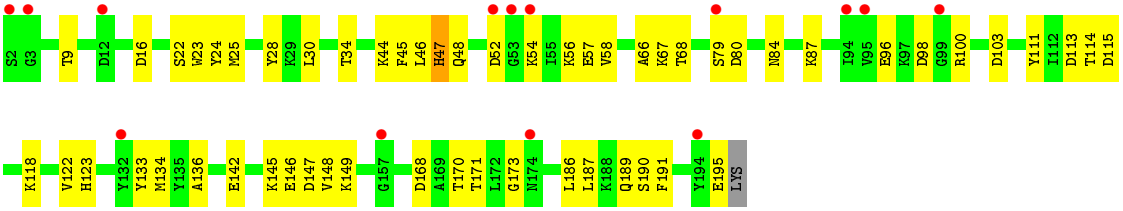


• Molecule 1: Biogenic amine-binding protein

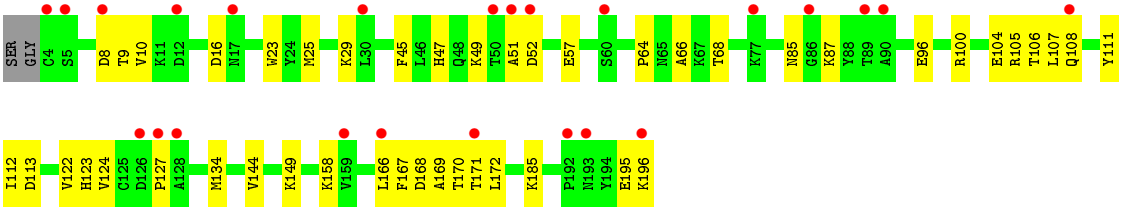




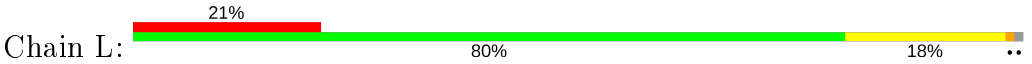
• Molecule 1: Biogenic amine-binding protein

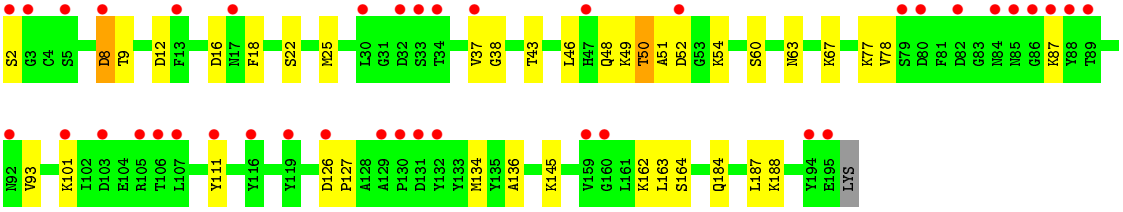


• Molecule 1: Biogenic amine-binding protein



• Molecule 1: Biogenic amine-binding protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.16Å 70.66Å 108.41Å 90.00° 99.16° 90.00°	Depositor
Resolution (Å)	42.66 – 3.00 42.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.66-3.00) 99.5 (42.66-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.321 , 0.349 0.320 , 0.345	Depositor DCC
R_{free} test set	1541 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.3	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	0.84	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4577e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.32	0/1581	0.50	0/2129
1	B	0.30	0/1572	0.48	0/2118
1	C	0.32	0/1571	0.48	0/2116
1	D	0.35	0/1572	0.49	0/2118
1	I	0.32	0/1581	0.51	0/2129
1	J	0.30	0/1572	0.48	0/2118
1	K	0.32	0/1571	0.48	0/2116
1	L	0.35	0/1572	0.50	0/2118
All	All	0.32	0/12592	0.49	0/16962

There are no bond length outliers.

There are no bond angle outliers.

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	1552	0	1497	49	6
1	B	1543	0	1484	39	10
1	C	1542	0	1489	41	1
1	D	1543	0	1484	33	0
1	I	1552	0	1497	38	8
1	J	1543	0	1484	47	2
1	K	1542	0	1489	34	6
1	L	1543	0	1484	29	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12360	0	11908	274	19

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 11.

All (274) 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:11:LYS:NZ	1:J:80:ASP:HA	1.59	1.17
1:C:112:ILE:HG23	1:C:158:LYS:HE3	1.23	1.16
1:L:25:MSE:HE1	1:L:134:MSE:SE	2.00	1.11
1:K:112:ILE:HG23	1:K:158:LYS:HE3	1.23	1.11
1:A:11:LYS:NZ	1:J:80:ASP:OD1	1.88	1.06
1:C:168:ASP:O	1:C:171:THR:HG22	1.63	0.99
1:K:168:ASP:O	1:K:171:THR:HG22	1.63	0.98
1:L:162:LYS:HZ2	1:L:164:SER:H	1.07	0.96
1:A:83:GLY:HA2	1:I:98:ASP:OD2	1.64	0.96
1:A:11:LYS:HZ1	1:J:80:ASP:CA	1.80	0.95
1:A:11:LYS:HZ1	1:J:80:ASP:HA	1.26	0.95
1:A:11:LYS:CE	1:J:80:ASP:HA	1.97	0.94
1:D:162:LYS:HZ2	1:D:164:SER:H	1.09	0.92
1:A:11:LYS:HZ3	1:J:80:ASP:CG	1.77	0.88
1:K:112:ILE:CG2	1:K:158:LYS:HE3	2.06	0.86
1:A:25:MSE:HE1	1:A:134:MSE:SE	2.25	0.85
1:A:11:LYS:NZ	1:J:80:ASP:CA	2.35	0.85
1:B:25:MSE:HE1	1:B:134:MSE:SE	2.26	0.85
1:K:112:ILE:HG23	1:K:158:LYS:CE	2.07	0.84
1:C:112:ILE:HG23	1:C:158:LYS:CE	2.08	0.84
1:J:25:MSE:HE1	1:J:134:MSE:SE	2.28	0.83
1:C:112:ILE:CG2	1:C:158:LYS:HE3	2.06	0.83
1:I:25:MSE:HE1	1:I:134:MSE:SE	2.32	0.78
1:A:11:LYS:HE2	1:J:80:ASP:HA	1.66	0.77
1:L:16:ASP:OD1	1:L:49:LYS:HE2	1.83	0.77
1:D:16:ASP:OD1	1:D:49:LYS:HE2	1.83	0.77
1:B:24:TYR:CE1	1:B:44:LYS:HD2	2.20	0.76
1:J:24:TYR:CE1	1:J:44:LYS:HD2	2.20	0.75
1:J:9:THR:HG21	1:J:87:LYS:HB2	1.69	0.73
1:D:25:MSE:HE1	1:D:134:MSE:SE	2.38	0.73
1:B:9:THR:HG21	1:B:87:LYS:HB2	1.69	0.71
1:L:50:THR:HG21	1:L:52:ASP:OD2	1.91	0.71
1:A:11:LYS:NZ	1:J:80:ASP:CB	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:SER:HB3	1:I:46:LEU:HD23	1.73	0.70
1:A:83:GLY:CA	1:I:98:ASP:OD2	2.37	0.70
1:D:50:THR:HG21	1:D:52:ASP:OD2	1.91	0.70
1:A:22:SER:HB3	1:A:46:LEU:HD23	1.73	0.69
1:L:52:ASP:OD1	1:L:54:LYS:HG3	1.93	0.69
1:J:66:ALA:O	1:J:68:THR:HG23	1.92	0.69
1:K:29:LYS:HB2	1:K:166:LEU:CD2	2.22	0.69
1:D:52:ASP:OD1	1:D:54:LYS:HG3	1.92	0.69
1:B:34:THR:HG21	1:C:185:LYS:NZ	2.08	0.69
1:L:162:LYS:HZ2	1:L:164:SER:N	1.87	0.69
1:B:66:ALA:O	1:B:68:THR:HG23	1.92	0.69
1:C:29:LYS:HB2	1:C:166:LEU:CD2	2.22	0.69
1:D:50:THR:HG21	1:D:52:ASP:CG	2.13	0.68
1:L:50:THR:HG21	1:L:52:ASP:CG	2.13	0.68
1:A:11:LYS:HZ1	1:J:80:ASP:CB	2.08	0.67
1:D:50:THR:CG2	1:D:52:ASP:CG	2.63	0.67
1:A:11:LYS:HE3	1:A:12:ASP:OD2	1.96	0.66
1:L:50:THR:CG2	1:L:52:ASP:CG	2.64	0.66
1:B:25:MSE:HE2	1:B:136:ALA:CB	2.25	0.66
1:C:51:ALA:HB2	1:I:184:GLN:HG2	1.78	0.66
1:B:34:THR:HG21	1:C:185:LYS:HZ3	1.60	0.65
1:D:162:LYS:HD2	1:D:163:LEU:N	2.12	0.65
1:I:11:LYS:HE3	1:I:12:ASP:OD2	1.96	0.65
1:L:162:LYS:HD2	1:L:163:LEU:N	2.12	0.64
1:B:147:ASP:OD1	1:B:148:VAL:HG13	1.97	0.64
1:J:147:ASP:OD1	1:J:148:VAL:HG13	1.97	0.64
1:J:145:LYS:O	1:J:148:VAL:HG22	1.98	0.63
1:K:105:ARG:HG3	1:K:107:LEU:CD1	2.29	0.63
1:D:162:LYS:HZ2	1:D:164:SER:N	1.89	0.63
1:B:145:LYS:O	1:B:148:VAL:HG22	1.98	0.63
1:C:52:ASP:OD2	1:I:44:LYS:NZ	2.30	0.63
1:J:191:PHE:O	1:J:195:GLU:HG2	1.98	0.63
1:C:105:ARG:HG3	1:C:107:LEU:CD1	2.29	0.62
1:L:8:ASP:N	1:L:8:ASP:OD1	2.24	0.62
1:B:191:PHE:O	1:B:195:GLU:HG2	1.99	0.62
1:A:195:GLU:O	1:A:196:LYS:HB2	2.00	0.62
1:I:195:GLU:O	1:I:196:LYS:HB2	2.00	0.62
1:C:106:THR:O	1:C:127:PRO:HD2	2.01	0.61
1:I:8:ASP:H	1:I:158:LYS:HZ1	1.48	0.61
1:K:106:THR:O	1:K:127:PRO:HD2	2.01	0.61
1:K:111:TYR:CE2	1:K:122:VAL:HB	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:TYR:CE2	1:C:122:VAL:HB	2.35	0.60
1:J:54:LYS:HE2	1:J:195:GLU:HA	1.84	0.60
1:B:142:GLU:O	1:B:170:THR:HG21	2.02	0.60
1:I:8:ASP:O	1:I:158:LYS:HE2	2.02	0.59
1:J:142:GLU:O	1:J:170:THR:HG21	2.02	0.59
1:A:8:ASP:O	1:A:158:LYS:HE2	2.02	0.59
1:B:54:LYS:HE2	1:B:195:GLU:HA	1.84	0.59
1:A:83:GLY:O	1:I:100:ARG:CZ	2.50	0.59
1:A:174:ASN:N	1:A:174:ASN:OD1	2.36	0.59
1:J:25:MSE:CE	1:J:134:MSE:SE	3.01	0.58
1:J:25:MSE:HE2	1:J:136:ALA:CB	2.34	0.58
1:A:115:ASP:HB2	1:J:84:ASN:ND2	2.18	0.58
1:K:25:MSE:HE1	1:K:134:MSE:SE	2.52	0.58
1:I:174:ASN:OD1	1:I:174:ASN:N	2.36	0.58
1:C:29:LYS:HB2	1:C:166:LEU:HD22	1.86	0.57
1:I:3:GLY:HA2	1:I:130:PRO:CB	2.34	0.57
1:L:22:SER:HB3	1:L:46:LEU:HD23	1.86	0.57
1:A:11:LYS:HE2	1:J:79:SER:O	2.05	0.57
1:A:47:HIS:HB3	1:A:57:GLU:HA	1.86	0.57
1:B:25:MSE:CE	1:B:134:MSE:SE	3.01	0.57
1:D:8:ASP:N	1:D:8:ASP:OD1	2.24	0.57
1:A:195:GLU:O	1:A:196:LYS:CB	2.53	0.57
1:I:47:HIS:HB3	1:I:57:GLU:HA	1.86	0.57
1:D:50:THR:HG23	1:D:52:ASP:H	1.70	0.57
1:I:10:VAL:HG22	1:I:113:ASP:HA	1.87	0.57
1:L:162:LYS:HD2	1:L:163:LEU:H	1.68	0.57
1:A:10:VAL:HG22	1:A:113:ASP:HA	1.87	0.56
1:D:22:SER:HB3	1:D:46:LEU:HD23	1.86	0.56
1:K:29:LYS:HB2	1:K:166:LEU:HD22	1.86	0.56
1:C:8:ASP:HB2	1:C:158:LYS:NZ	2.20	0.56
1:K:8:ASP:HB2	1:K:158:LYS:NZ	2.20	0.56
1:A:3:GLY:HA2	1:A:130:PRO:CB	2.34	0.56
1:A:83:GLY:C	1:I:100:ARG:CZ	2.73	0.56
1:I:195:GLU:O	1:I:196:LYS:CB	2.53	0.56
1:D:162:LYS:HD2	1:D:163:LEU:H	1.69	0.56
1:L:25:MSE:CE	1:L:134:MSE:SE	2.92	0.56
1:C:9:THR:HG21	1:C:87:LYS:HB2	1.89	0.55
1:K:9:THR:HG21	1:K:87:LYS:HB2	1.89	0.55
1:L:50:THR:HG23	1:L:52:ASP:H	1.70	0.54
1:B:98:ASP:OD2	1:B:100:ARG:NH2	2.32	0.54
1:A:12:ASP:HA	1:A:84:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:GLU:HG2	1:K:105:ARG:N	2.23	0.53
1:I:12:ASP:HA	1:I:84:ASN:ND2	2.23	0.53
1:J:146:GLU:HA	1:J:149:LYS:HG3	1.90	0.53
1:C:104:GLU:HG2	1:C:105:ARG:N	2.23	0.53
1:A:8:ASP:H	1:A:158:LYS:HZ1	1.57	0.53
1:B:96:GLU:HB2	1:B:98:ASP:OD1	2.08	0.53
1:J:115:ASP:OD2	1:J:118:LYS:HB2	2.09	0.53
1:B:146:GLU:HA	1:B:149:LYS:HG3	1.90	0.53
1:K:158:LYS:HG3	1:K:158:LYS:O	2.09	0.53
1:C:158:LYS:HG3	1:C:158:LYS:O	2.09	0.53
1:K:64:PRO:HG2	1:K:172:LEU:HD13	1.92	0.52
1:B:115:ASP:OD2	1:B:118:LYS:HB2	2.09	0.52
1:J:96:GLU:HB2	1:J:98:ASP:OD1	2.09	0.52
1:A:2:SER:CB	1:D:17:ASN:OD1	2.58	0.52
1:I:48:GLN:HG2	1:I:187:LEU:HD11	1.92	0.52
1:C:64:PRO:HG2	1:C:172:LEU:HD13	1.92	0.52
1:C:104:GLU:CG	1:C:105:ARG:N	2.73	0.52
1:K:104:GLU:CG	1:K:105:ARG:N	2.73	0.51
1:A:48:GLN:HG2	1:A:187:LEU:HD11	1.92	0.51
1:K:167:PHE:CE2	1:K:169:ALA:HA	2.46	0.51
1:J:98:ASP:OD2	1:J:100:ARG:NH2	2.32	0.51
1:I:146:GLU:HA	1:I:149:LYS:HG3	1.92	0.51
1:D:48:GLN:HG2	1:D:187:LEU:HD11	1.93	0.51
1:C:167:PHE:CE2	1:C:169:ALA:HA	2.46	0.51
1:J:48:GLN:HG2	1:J:187:LEU:HD11	1.94	0.50
1:A:146:GLU:HA	1:A:149:LYS:HG3	1.92	0.50
1:B:48:GLN:HG2	1:B:187:LEU:HD11	1.94	0.50
1:D:63:ASN:O	1:D:67:LYS:N	2.44	0.50
1:B:47:HIS:HB3	1:B:57:GLU:HA	1.93	0.50
1:I:25:MSE:HE1	1:I:134:MSE:CE	2.41	0.50
1:L:50:THR:CG2	1:L:52:ASP:OD1	2.60	0.50
1:L:9:THR:HG21	1:L:87:LYS:HB2	1.93	0.50
1:D:50:THR:CG2	1:D:52:ASP:OD1	2.60	0.50
1:J:47:HIS:HB3	1:J:57:GLU:HA	1.93	0.50
1:L:48:GLN:HG2	1:L:187:LEU:HD11	1.93	0.49
1:D:9:THR:HG21	1:D:87:LYS:HB2	1.93	0.49
1:K:9:THR:OG1	1:K:85:ASN:HB3	2.12	0.49
1:C:23:TRP:HB2	1:C:45:PHE:CZ	2.47	0.49
1:K:23:TRP:HB2	1:K:45:PHE:CZ	2.47	0.49
1:B:52:ASP:OD2	1:B:54:LYS:HB2	2.13	0.49
1:B:111:TYR:CE2	1:B:122:VAL:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:ASP:OD2	1:J:54:LYS:HB2	2.13	0.49
1:B:190:SER:HA	1:B:195:GLU:OE2	2.12	0.49
1:J:111:TYR:CE2	1:J:122:VAL:HB	2.47	0.48
1:A:53:GLY:O	1:A:78:VAL:HG23	2.13	0.48
1:J:25:MSE:SE	1:J:28:TYR:CD2	3.16	0.48
1:D:25:MSE:CE	1:D:134:MSE:SE	3.11	0.48
1:L:63:ASN:O	1:L:67:LYS:N	2.44	0.48
1:J:190:SER:HA	1:J:195:GLU:OE2	2.12	0.48
1:A:8:ASP:H	1:A:158:LYS:NZ	2.11	0.48
1:I:53:GLY:O	1:I:78:VAL:HG23	2.14	0.48
1:C:9:THR:OG1	1:C:85:ASN:HB3	2.12	0.48
1:I:25:MSE:SE	1:I:43:THR:HG21	2.63	0.48
1:K:167:PHE:CZ	1:K:169:ALA:HA	2.50	0.47
1:B:34:THR:HG21	1:C:185:LYS:HD3	1.97	0.47
1:I:24:TYR:CE2	1:I:44:LYS:HD2	2.49	0.47
1:B:133:TYR:CZ	1:D:146:GLU:HB2	2.50	0.47
1:A:24:TYR:CE2	1:A:44:LYS:HD2	2.50	0.47
1:C:144:VAL:O	1:C:149:LYS:HE3	2.15	0.46
1:I:112:ILE:HG23	1:I:158:LYS:HD3	1.98	0.46
1:C:167:PHE:CZ	1:C:169:ALA:HA	2.50	0.46
1:K:144:VAL:O	1:K:149:LYS:HE3	2.15	0.46
1:C:16:ASP:OD1	1:C:49:LYS:HE2	2.16	0.46
1:C:66:ALA:O	1:C:68:THR:HG23	2.16	0.46
1:C:195:GLU:O	1:C:196:LYS:HB2	2.16	0.46
1:K:16:ASP:OD1	1:K:49:LYS:HE2	2.16	0.46
1:A:112:ILE:HG23	1:A:158:LYS:HD3	1.98	0.46
1:J:34:THR:HG21	1:K:185:LYS:HZ3	1.81	0.46
1:K:195:GLU:O	1:K:196:LYS:HB2	2.16	0.46
1:B:23:TRP:HB2	1:B:45:PHE:CZ	2.50	0.46
1:C:30:LEU:HD13	1:C:134:MSE:HE3	1.96	0.46
1:C:10:VAL:CG2	1:C:113:ASP:HA	2.46	0.45
1:I:8:ASP:H	1:I:158:LYS:NZ	2.11	0.45
1:K:10:VAL:CG2	1:K:113:ASP:HA	2.46	0.45
1:K:66:ALA:O	1:K:68:THR:HG23	2.16	0.45
1:I:16:ASP:OD1	1:I:49:LYS:CE	2.64	0.45
1:L:184:GLN:O	1:L:188:LYS:HG2	2.17	0.45
1:B:25:MSE:HE2	1:B:136:ALA:HB2	1.98	0.45
1:C:52:ASP:CG	1:I:44:LYS:HZ1	2.19	0.45
1:J:23:TRP:HB2	1:J:45:PHE:CZ	2.50	0.45
1:A:11:LYS:NZ	1:J:80:ASP:CG	2.50	0.45
1:D:184:GLN:O	1:D:188:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASP:OD1	1:A:49:LYS:CE	2.64	0.45
1:J:168:ASP:O	1:J:171:THR:HG22	2.16	0.45
1:B:168:ASP:O	1:B:171:THR:HG22	2.16	0.45
1:A:2:SER:HB2	1:D:17:ASN:OD1	2.17	0.45
1:B:25:MSE:SE	1:B:28:TYR:CD2	3.20	0.44
1:J:30:LEU:HD12	1:J:133:TYR:O	2.17	0.44
1:J:34:THR:HG21	1:K:185:LYS:HD3	1.99	0.44
1:C:122:VAL:HG22	1:C:123:HIS:N	2.32	0.44
1:K:108:GLN:CG	1:K:127:PRO:HG3	2.47	0.44
1:K:122:VAL:HG22	1:K:123:HIS:N	2.32	0.44
1:B:30:LEU:HD12	1:B:133:TYR:O	2.17	0.44
1:J:56:LYS:NZ	1:J:189:GLN:O	2.51	0.44
1:C:108:GLN:CG	1:C:127:PRO:HG3	2.48	0.44
1:B:56:LYS:NZ	1:B:189:GLN:O	2.51	0.44
1:L:145:LYS:HE2	1:L:145:LYS:HB3	1.79	0.44
1:L:37:VAL:HG13	1:L:38:GLY:N	2.33	0.44
1:B:113:ASP:O	1:B:114:THR:HB	2.18	0.43
1:J:113:ASP:O	1:J:114:THR:HB	2.18	0.43
1:A:11:LYS:HZ3	1:J:80:ASP:CB	2.24	0.43
1:A:61:ASN:HB2	1:A:70:SER:OG	2.19	0.43
1:B:34:THR:HG21	1:C:185:LYS:CE	2.48	0.43
1:A:2:SER:HB3	1:D:17:ASN:OD1	2.18	0.43
1:L:25:MSE:HE3	1:L:136:ALA:CB	2.49	0.43
1:A:151:LYS:HB2	1:A:151:LYS:HE3	1.87	0.43
1:I:61:ASN:HB2	1:I:70:SER:OG	2.19	0.43
1:B:22:SER:HB3	1:B:46:LEU:CD2	2.49	0.43
1:C:96:GLU:OE2	1:C:100:ARG:NH2	2.47	0.43
1:D:37:VAL:HG13	1:D:38:GLY:N	2.33	0.43
1:B:133:TYR:CE1	1:D:146:GLU:HB2	2.54	0.43
1:J:22:SER:HB3	1:J:46:LEU:CD2	2.49	0.43
1:I:151:LYS:HE3	1:I:151:LYS:HB2	1.87	0.42
1:A:10:VAL:CG2	1:A:113:ASP:HA	2.49	0.42
1:I:10:VAL:CG2	1:I:113:ASP:HA	2.49	0.42
1:I:64:PRO:HG2	1:I:172:LEU:HD22	2.01	0.42
1:L:43:THR:HA	1:L:60:SER:O	2.19	0.42
1:C:51:ALA:HB2	1:I:184:GLN:CG	2.48	0.42
1:D:43:THR:HA	1:D:60:SER:O	2.19	0.42
1:J:122:VAL:HG22	1:J:123:HIS:N	2.35	0.42
1:C:8:ASP:HB2	1:C:158:LYS:HZ3	1.84	0.42
1:K:96:GLU:OE2	1:K:100:ARG:NH2	2.47	0.41
1:A:64:PRO:HG2	1:A:172:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:THR:CG2	1:C:185:LYS:NZ	2.82	0.41
1:L:50:THR:HG21	1:L:52:ASP:OD1	2.21	0.41
1:A:25:MSE:SE	1:A:43:THR:HG21	2.70	0.41
1:A:83:GLY:O	1:I:100:ARG:NH2	2.54	0.41
1:D:93:VAL:CG1	1:D:101:LYS:HG3	2.51	0.41
1:A:44:LYS:HB2	1:A:178:TYR:CD1	2.55	0.41
1:D:50:THR:HG22	1:D:52:ASP:OD1	2.21	0.41
1:I:44:LYS:HB2	1:I:178:TYR:CD1	2.55	0.41
1:L:93:VAL:CG1	1:L:101:LYS:HG3	2.50	0.41
1:B:122:VAL:HG22	1:B:123:HIS:N	2.35	0.41
1:I:29:LYS:O	1:I:134:MSE:HA	2.21	0.41
1:B:171:THR:C	1:B:173:GLY:H	2.24	0.41
1:C:107:LEU:HD23	1:C:124:VAL:HG11	2.02	0.41
1:D:18:PHE:CZ	1:D:111:TYR:CZ	3.08	0.41
1:L:50:THR:HG23	1:L:51:ALA:N	2.35	0.41
1:D:50:THR:HG23	1:D:51:ALA:N	2.35	0.41
1:B:45:PHE:CB	1:B:58:VAL:O	2.69	0.41
1:D:50:THR:HG21	1:D:52:ASP:OD1	2.21	0.41
1:L:18:PHE:CZ	1:L:111:TYR:CZ	3.08	0.40
1:I:47:HIS:CB	1:I:56:LYS:O	2.70	0.40
1:J:58:VAL:HG11	1:J:186:LEU:HB2	2.03	0.40
1:B:100:ARG:HE	1:B:100:ARG:HB2	1.69	0.40
1:C:47:HIS:CD2	1:C:57:GLU:HG2	2.57	0.40
1:J:171:THR:C	1:J:173:GLY:H	2.24	0.40
1:K:47:HIS:CD2	1:K:57:GLU:HG2	2.57	0.40
1:C:107:LEU:HD23	1:C:124:VAL:CG1	2.52	0.40
1:D:162:LYS:NZ	1:D:164:SER:H	1.95	0.40
1:J:45:PHE:CB	1:J:58:VAL:O	2.70	0.40
1:K:8:ASP:HB2	1:K:158:LYS:HZ3	1.86	0.40
1:L:50:THR:HG22	1:L:52:ASP:OD1	2.21	0.40
1:A:168:ASP:OD1	1:A:170:THR:OG1	2.33	0.40
1:D:145:LYS:HE2	1:D:145:LYS:HB3	1.80	0.40
1:A:83:GLY:HA2	1:I:100:ARG:NE	2.36	0.40
1:K:107:LEU:HD23	1:K:124:VAL:HG11	2.02	0.40
1:K:124:VAL:O	1:K:134:MSE:N	2.51	0.40
1:L:126:ASP:HA	1:L:127:PRO:HD2	1.84	0.40

All (19) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:ASP:O	1:J:67:LYS:NZ[2_546]	1.00	1.20
1:B:142:GLU:CD	1:I:146:GLU:OE2[2_645]	1.08	1.12
1:B:142:GLU:OE2	1:I:146:GLU:OE1[2_645]	1.26	0.94
1:A:184:GLN:CG	1:K:51:ALA:CB[1_545]	1.32	0.88
1:B:142:GLU:OE2	1:I:146:GLU:CD[2_645]	1.35	0.85
1:B:142:GLU:OE2	1:I:146:GLU:OE2[2_645]	1.41	0.79
1:B:142:GLU:CG	1:I:146:GLU:OE2[2_645]	1.65	0.55
1:B:188:LYS:NZ	1:C:106:THR:OG1[2_645]	1.78	0.42
1:A:184:GLN:CD	1:K:51:ALA:CB[1_545]	1.81	0.39
1:A:44:LYS:NZ	1:K:52:ASP:OD2[1_545]	1.87	0.33
1:A:184:GLN:NE2	1:K:51:ALA:CB[1_545]	1.92	0.28
1:A:180:ASP:OD1	1:K:52:ASP:OD2[1_545]	1.95	0.25
1:J:16:ASP:C	1:J:67:LYS:NZ[2_546]	1.96	0.24
1:I:8:ASP:OD1	1:L:2:SER:O[2_656]	1.96	0.24
1:B:142:GLU:CD	1:I:146:GLU:CD[2_645]	1.97	0.23
1:B:142:GLU:OE1	1:I:146:GLU:OE2[2_645]	2.02	0.18
1:B:16:ASP:CA	1:B:67:LYS:NZ[2_645]	2.09	0.11
1:A:44:LYS:NZ	1:K:52:ASP:CG[1_545]	2.16	0.04
1:B:16:ASP:CB	1:B:67:LYS:NZ[2_645]	2.18	0.02

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	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	29 68
1	B	192/195 (98%)	184 (96%)	8 (4%)	0	100 100
1	C	191/195 (98%)	185 (97%)	6 (3%)	0	100 100
1	D	192/195 (98%)	187 (97%)	5 (3%)	0	100 100
1	I	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	29 68
1	J	192/195 (98%)	184 (96%)	8 (4%)	0	100 100
1	K	191/195 (98%)	185 (97%)	6 (3%)	0	100 100
1	L	192/195 (98%)	187 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1536/1560 (98%)	1484 (97%)	50 (3%)	2 (0%)	51 85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLY
1	I	173	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	173/171 (101%)	170 (98%)	3 (2%)	60 85
1	B	172/171 (101%)	170 (99%)	2 (1%)	71 90
1	C	172/171 (101%)	171 (99%)	1 (1%)	86 95
1	D	172/171 (101%)	167 (97%)	5 (3%)	42 76
1	I	173/171 (101%)	170 (98%)	3 (2%)	60 85
1	J	172/171 (101%)	170 (99%)	2 (1%)	71 90
1	K	172/171 (101%)	171 (99%)	1 (1%)	86 95
1	L	172/171 (101%)	167 (97%)	5 (3%)	42 76
All	All	1378/1368 (101%)	1356 (98%)	22 (2%)	62 86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	91	LYS
1	A	174	ASN
1	B	47	HIS
1	B	103	ASP
1	C	170	THR
1	D	8	ASP
1	D	12	ASP

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Mol	Chain	Res	Type
1	D	50	THR
1	D	77	LYS
1	D	78	VAL
1	I	47	HIS
1	I	91	LYS
1	I	174	ASN
1	J	47	HIS
1	J	103	ASP
1	K	170	THR
1	L	8	ASP
1	L	12	ASP
1	L	50	THR
1	L	77	LYS
1	L	78	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	B	123	HIS
1	I	123	HIS
1	I	184	GLN
1	J	84	ASN
1	J	123	HIS
1	L	17	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	193/195 (98%)	0.29	10 (5%) 27 10	16, 56, 166, 320	0
1	B	192/195 (98%)	0.51	11 (5%) 23 8	21, 72, 172, 556	0
1	C	191/195 (97%)	0.57	17 (8%) 9 3	15, 69, 185, 315	0
1	D	192/195 (98%)	0.55	16 (8%) 11 3	19, 62, 181, 342	0
1	I	193/195 (98%)	0.62	16 (8%) 11 3	18, 66, 185, 392	0
1	J	192/195 (98%)	0.53	14 (7%) 15 4	12, 57, 207, 522	0
1	K	191/195 (97%)	0.91	24 (12%) 3 1	17, 62, 241, 558	0
1	L	192/195 (98%)	1.18	40 (20%) 1 0	19, 77, 244, 554	0
All	All	1536/1560 (98%)	0.65	148 (9%) 8 2	12, 65, 199, 558	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	51	ALA	6.7
1	I	2	SER	6.4
1	K	12	ASP	5.7
1	K	50	THR	5.7
1	K	89	THR	5.6
1	K	127	PRO	5.5
1	L	52	ASP	4.8
1	L	129	ALA	4.8
1	C	132	TYR	4.7
1	B	52	ASP	4.7
1	A	2	SER	4.5
1	L	92	ASN	4.3
1	L	33	SER	4.3
1	K	166	LEU	4.2
1	K	52	ASP	4.1
1	I	146	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	J	2	SER	4.1
1	L	85	ASN	4.1
1	L	116	TYR	4.0
1	I	147	ASP	4.0
1	J	94	ILE	3.9
1	D	74	SER	3.9
1	D	124	VAL	3.9
1	L	2	SER	3.9
1	J	12	ASP	3.8
1	K	5	SER	3.7
1	K	60	SER	3.7
1	J	52	ASP	3.7
1	K	128	ALA	3.7
1	I	145	LYS	3.6
1	B	174	ASN	3.6
1	K	126	ASP	3.6
1	L	131	ASP	3.5
1	I	177	GLN	3.5
1	K	108	GLN	3.5
1	L	82	ASP	3.5
1	C	5	SER	3.5
1	L	89	THR	3.5
1	J	53	GLY	3.5
1	L	79	SER	3.4
1	L	107	LEU	3.4
1	L	132	TYR	3.3
1	L	103	ASP	3.3
1	L	86	GLY	3.2
1	K	196	LYS	3.2
1	K	159	VAL	3.1
1	L	159	VAL	3.1
1	D	2	SER	3.1
1	L	126	ASP	3.1
1	K	86	GLY	3.0
1	K	90	ALA	3.0
1	K	4	CYS	3.0
1	D	52	ASP	3.0
1	B	73	ILE	2.9
1	I	115	ASP	2.9
1	C	196	LYS	2.9
1	K	30	LEU	2.9
1	D	90	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	37	VAL	2.8
1	B	178	TYR	2.8
1	L	130	PRO	2.8
1	C	131	ASP	2.8
1	L	3	GLY	2.8
1	L	106	THR	2.8
1	J	79	SER	2.8
1	D	31	GLY	2.8
1	J	95	VAL	2.8
1	K	171	THR	2.8
1	L	8	ASP	2.7
1	B	86	GLY	2.7
1	A	84	ASN	2.7
1	D	166	LEU	2.7
1	I	52	ASP	2.7
1	A	31	GLY	2.7
1	L	111	TYR	2.7
1	L	17	ASN	2.6
1	I	86	GLY	2.6
1	I	84	ASN	2.6
1	L	80	ASP	2.6
1	J	132	TYR	2.6
1	L	119	TYR	2.6
1	B	3	GLY	2.6
1	K	193	ASN	2.6
1	C	7	VAL	2.6
1	K	17	ASN	2.6
1	A	12	ASP	2.6
1	J	3	GLY	2.6
1	A	100	ARG	2.5
1	C	51	ALA	2.5
1	A	184	GLN	2.5
1	B	67	LYS	2.5
1	A	196	LYS	2.5
1	B	94	ILE	2.5
1	L	194	TYR	2.5
1	I	176	CYS	2.5
1	L	87	LYS	2.5
1	L	5	SER	2.5
1	I	174	ASN	2.4
1	J	99	GLY	2.4
1	C	110	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	39	ASP	2.4
1	L	195	GLU	2.4
1	C	36	GLU	2.4
1	I	155	ALA	2.4
1	I	65	ASN	2.4
1	D	123	HIS	2.4
1	K	77	LYS	2.4
1	B	84	ASN	2.4
1	A	103	ASP	2.3
1	I	150	SER	2.3
1	K	192	PRO	2.3
1	A	86	GLY	2.3
1	D	103	ASP	2.3
1	I	171	THR	2.3
1	L	160	GLY	2.3
1	D	108	GLN	2.3
1	L	88	TYR	2.3
1	D	135	TYR	2.3
1	C	6	THR	2.3
1	L	101	LYS	2.3
1	J	174	ASN	2.2
1	L	84	ASN	2.2
1	C	193	ASN	2.2
1	J	157	GLY	2.2
1	D	162	LYS	2.2
1	K	8	ASP	2.2
1	B	132	TYR	2.2
1	L	47	HIS	2.2
1	L	34	THR	2.2
1	D	102	ILE	2.2
1	J	54	LYS	2.2
1	C	11	LYS	2.2
1	C	89	THR	2.2
1	C	40	LYS	2.2
1	J	194	TYR	2.2
1	I	151	LYS	2.1
1	C	30	LEU	2.1
1	L	30	LEU	2.1
1	C	52	ASP	2.1
1	C	55	ILE	2.1
1	B	74	SER	2.1
1	L	105	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	13	PHE	2.1
1	D	50	THR	2.1
1	L	32	ASP	2.1
1	C	74	SER	2.1
1	D	32	ASP	2.1
1	A	131	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.