



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:57 PM GMT

PDB ID : 1DCL
Title : MCG, A LAMBDA V TYPE LIGHT-CHAIN DIMER (BENCE-JONES PROTEIN), CRYSTALLIZED FROM AMMONIUM SULFATE
Authors : Schiffer, M.; Xu, Z.B.
Deposited on : 1995-10-16
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

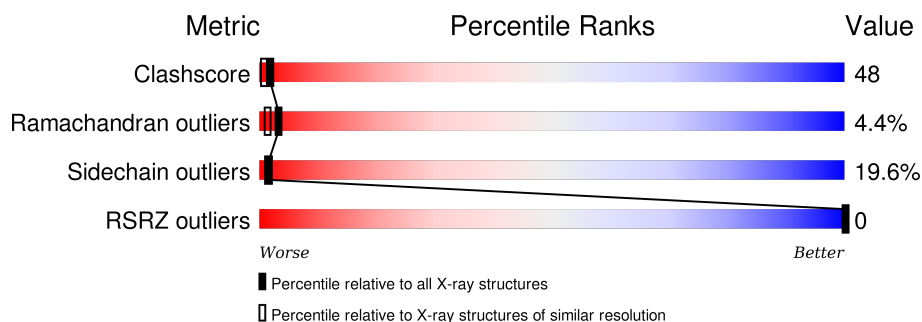
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	216	
1	B	216	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3621 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 MCG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1604	1000	267	332	5			
1	B	216	Total	C	N	O	S	0	0	0
			1604	1000	267	332	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	PHE	CONFLICT	UNP P01709
A	23	THR	SER	CONFLICT	UNP P01709
A	28	ASN	ASP	CONFLICT	UNP P01709
A	29	VAL	ILE	CONFLICT	UNP P01709
A	31	GLY	ASN	CONFLICT	UNP P01709
A	39	GLN	ARG	CONFLICT	UNP P01709
A	42	ALA	PRO	CONFLICT	UNP P01709
A	48	VAL	LEU	CONFLICT	UNP P01709
A	49	ILE	MET	CONFLICT	UNP P01709
A	54	ASN	THR	CONFLICT	UNP P01709
A	62	ASP	ASN	CONFLICT	UNP P01709
A	94	GLU	ALA	CONFLICT	UNP P01709
A	97	ASP	ASN	CONFLICT	UNP P01709
A	98	ASN	SER	CONFLICT	UNP P01709
A	99	PHE	LEU	CONFLICT	UNP P01709
A	100	VAL	ILE	CONFLICT	UNP P01709
A	103	THR	GLY	CONFLICT	UNP P01709
A	106	LYS	ARG	CONFLICT	UNP P01709
A	107	VAL	LEU	CONFLICT	UNP P01709
A	116	ASN	ALA	CONFLICT	UNP P01709
A	118	THR	SER	CONFLICT	UNP P01709
A	156	GLY	SER	CONFLICT	UNP P01709
A	167	LYS	THR	CONFLICT	UNP P01709
B	20	ILE	PHE	CONFLICT	UNP P01709
B	23	THR	SER	CONFLICT	UNP P01709

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Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASN	ASP	CONFLICT	UNP P01709
B	29	VAL	ILE	CONFLICT	UNP P01709
B	31	GLY	ASN	CONFLICT	UNP P01709
B	39	GLN	ARG	CONFLICT	UNP P01709
B	42	ALA	PRO	CONFLICT	UNP P01709
B	48	VAL	LEU	CONFLICT	UNP P01709
B	49	ILE	MET	CONFLICT	UNP P01709
B	54	ASN	THR	CONFLICT	UNP P01709
B	62	ASP	ASN	CONFLICT	UNP P01709
B	94	GLU	ALA	CONFLICT	UNP P01709
B	97	ASP	ASN	CONFLICT	UNP P01709
B	98	ASN	SER	CONFLICT	UNP P01709
B	99	PHE	LEU	CONFLICT	UNP P01709
B	100	VAL	ILE	CONFLICT	UNP P01709
B	103	THR	GLY	CONFLICT	UNP P01709
B	106	LYS	ARG	CONFLICT	UNP P01709
B	107	VAL	LEU	CONFLICT	UNP P01709
B	116	ASN	ALA	CONFLICT	UNP P01709
B	118	THR	SER	CONFLICT	UNP P01709
B	156	GLY	SER	CONFLICT	UNP P01709
B	167	LYS	THR	CONFLICT	UNP P01709

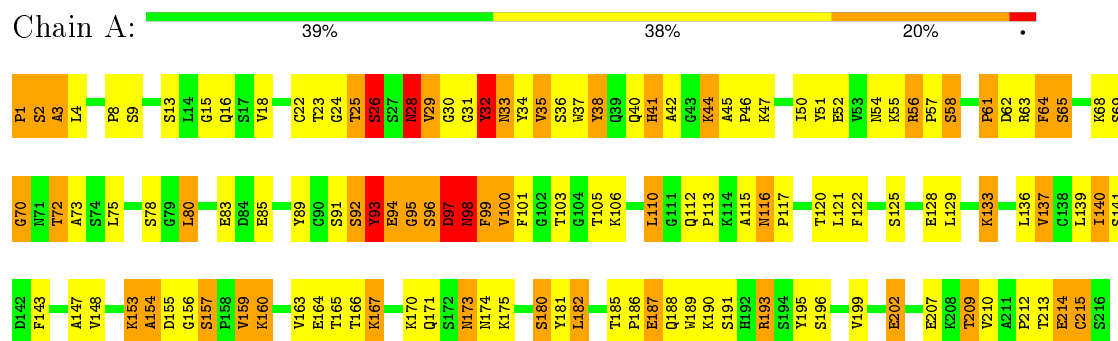
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	195	Total O 195 195	0	0
2	B	218	Total O 218 218	0	0

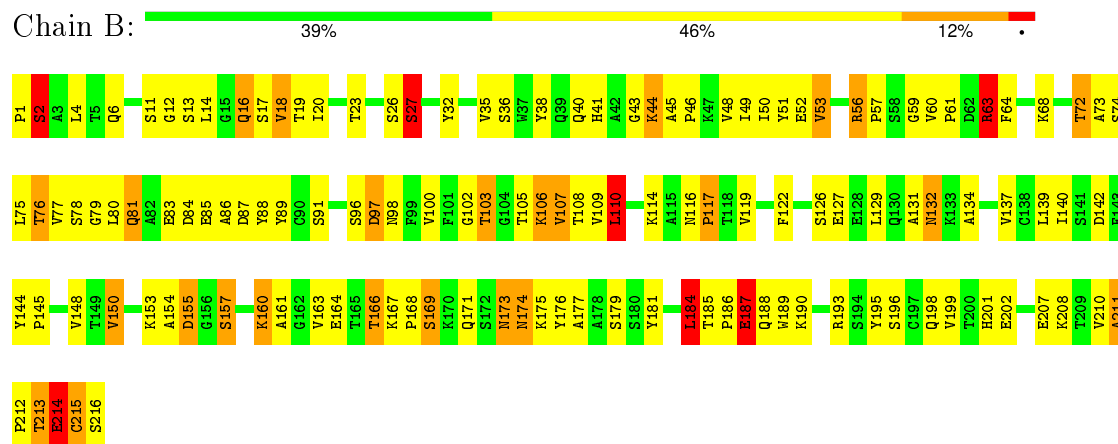
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: MCG



• Molecule 1: MCG



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.30 Å 72.30 Å 185.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30 9.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 34.7 (9.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.140 , (Not available) 0.152 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 12.6	EDS
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 13383 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3621	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.07	1/1643 (0.1%)	1.98	39/2241 (1.7%)
1	B	1.05	0/1643	1.95	40/2241 (1.8%)
All	All	1.06	1/3286 (0.0%)	1.97	79/4482 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	CD-OE1	-5.12	1.20	1.25

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PRO	C-N-CA	10.75	148.58	121.70
1	A	180	SER	N-CA-CB	10.23	125.84	110.50
1	A	202	GLU	OE1-CD-OE2	-9.31	112.13	123.30
1	B	110	LEU	CA-CB-CG	9.09	136.21	115.30
1	A	92	SER	C-N-CA	8.48	142.89	121.70
1	B	56	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	A	63	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	80	LEU	CA-CB-CG	7.96	133.61	115.30
1	B	142	ASP	CB-CG-OD2	-7.85	111.24	118.30
1	B	76	THR	N-CA-CB	7.65	124.84	110.30
1	B	63	ARG	CD-NE-CZ	-7.63	112.92	123.60
1	A	38	TYR	CB-CG-CD1	7.59	125.55	121.00
1	A	97	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	181	TYR	CB-CG-CD1	7.29	125.37	121.00
1	A	159	VAL	CB-CA-C	7.28	125.24	111.40
1	B	187	GLU	CA-CB-CG	7.07	128.95	113.40
1	A	42	ALA	N-CA-CB	-7.01	100.28	110.10
1	B	75	LEU	CA-CB-CG	6.97	131.34	115.30
1	B	27	SER	N-CA-CB	-6.95	100.07	110.50
1	A	193	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	B	187	GLU	OE1-CD-OE2	-6.84	115.10	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	SER	CB-CA-C	6.79	123.00	110.10
1	A	75	LEU	CA-CB-CG	6.74	130.81	115.30
1	B	169	SER	N-CA-CB	-6.72	100.41	110.50
1	B	87	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	56	ARG	NE-CZ-NH2	6.47	123.54	120.30
1	B	2	SER	N-CA-CB	6.29	119.94	110.50
1	B	174	ASN	CA-CB-CG	-6.29	99.57	113.40
1	B	129	LEU	CB-CA-C	6.26	122.09	110.20
1	B	127	GLU	CG-CD-OE1	6.21	130.71	118.30
1	B	144	TYR	CA-CB-CG	-6.18	101.67	113.40
1	B	187	GLU	CG-CD-OE1	6.18	130.65	118.30
1	A	56	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	A	181	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	A	155	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	B	187	GLU	CB-CG-CD	5.99	130.37	114.20
1	B	177	ALA	N-CA-CB	5.94	118.41	110.10
1	A	180	SER	O-C-N	5.91	132.15	122.70
1	A	63	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	28	ASN	N-CA-CB	5.90	121.22	110.60
1	B	103	THR	CA-C-N	5.87	127.94	116.20
1	A	159	VAL	CA-CB-CG1	5.86	119.69	110.90
1	A	116	ASN	N-CA-CB	5.84	121.11	110.60
1	B	105	THR	N-CA-CB	5.75	121.23	110.30
1	A	209	THR	CA-CB-OG1	-5.75	96.93	109.00
1	B	127	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	97	ASP	CB-CG-OD1	5.68	123.42	118.30
1	A	202	GLU	CG-CD-OE1	5.67	129.64	118.30
1	B	129	LEU	CA-CB-CG	5.67	128.33	115.30
1	B	193	ARG	CD-NE-CZ	-5.67	115.67	123.60
1	A	105	THR	O-C-N	5.66	131.75	122.70
1	B	155	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	107	VAL	O-C-N	5.63	131.71	122.70
1	A	52	GLU	CA-C-O	5.57	131.80	120.10
1	B	202	GLU	CG-CD-OE2	5.55	129.40	118.30
1	B	211	ALA	N-CA-CB	-5.54	102.34	110.10
1	A	32	TYR	C-N-CA	5.51	135.47	121.70
1	B	91	SER	N-CA-CB	5.50	118.75	110.50
1	B	91	SER	O-C-N	5.46	131.44	122.70
1	A	65	SER	CB-CA-C	5.43	120.42	110.10
1	B	122	PHE	O-C-N	5.42	131.40	121.10
1	A	41	HIS	CA-CB-CG	-5.41	104.40	113.60
1	A	106	LYS	O-C-N	5.41	131.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	THR	O-C-N	5.34	131.25	122.70
1	B	184	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	154	ALA	O-C-N	5.31	131.20	122.70
1	A	54	ASN	CA-CB-CG	-5.28	101.79	113.40
1	B	117	PRO	O-C-N	5.18	130.99	122.70
1	A	52	GLU	CA-C-N	-5.17	105.83	117.20
1	A	61	PRO	C-N-CA	5.15	134.57	121.70
1	A	98	ASN	CB-CA-C	5.14	120.68	110.40
1	A	64	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	A	125	SER	CA-C-N	-5.10	105.99	117.20
1	B	150	VAL	CA-C-O	5.08	130.77	120.10
1	A	193	ARG	CD-NE-CZ	-5.06	116.51	123.60
1	B	150	VAL	CA-CB-CG1	5.05	118.48	110.90
1	B	97	ASP	C-N-CA	5.04	134.30	121.70
1	A	94	GLU	CA-C-N	-5.04	106.13	116.20
1	B	103	THR	O-C-N	-5.00	114.69	123.20

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	1604	0	1541	175	0
1	B	1604	0	1541	136	1
2	A	195	0	0	24	4
2	B	218	0	0	15	2
All	All	3621	0	3082	298	4

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 48.

All (298) 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:31:GLY:O	1:A:32:TYR:HB2	1.42	1.14
1:A:93:TYR:CE1	1:A:96:SER:HB3	1.84	1.12
1:B:23:THR:HG23	1:B:72:THR:HG22	1.36	1.07
1:A:213:THR:O	1:A:214:GLU:HB2	1.55	1.06
1:B:160:LYS:HD3	1:B:160:LYS:H	1.11	1.05
1:A:25:THR:HG22	2:A:730:HOH:O	1.59	1.00
1:B:19:THR:HG23	1:B:76:THR:HG23	1.46	0.97
1:A:93:TYR:HE1	1:A:96:SER:HB3	1.25	0.94
1:A:29:VAL:HG13	1:A:30:GLY:H	1.31	0.94
1:B:64:PHE:CD1	1:B:77:VAL:HG22	2.04	0.92
1:A:24:GLY:CA	1:A:29:VAL:HG23	2.00	0.90
1:B:160:LYS:HD3	1:B:160:LYS:N	1.79	0.89
1:B:166:THR:HG22	1:B:179:SER:H	1.37	0.89
1:A:160:LYS:HD3	1:A:160:LYS:H	1.35	0.89
1:A:24:GLY:HA3	1:A:29:VAL:HG23	1.55	0.89
1:A:95:GLY:O	1:A:96:SER:CB	2.21	0.88
1:A:128:GLU:HG2	1:A:133:LYS:HB2	1.55	0.87
1:A:32:TYR:CD1	1:A:33:ASN:ND2	2.44	0.86
1:B:38:TYR:CE2	1:B:48:VAL:HG22	2.10	0.85
1:A:171:GLN:HE21	1:A:173:ASN:HD21	1.23	0.84
1:A:214:GLU:O	1:A:215:CYS:SG	2.36	0.84
1:B:160:LYS:CD	1:B:160:LYS:H	1.91	0.84
1:A:159:VAL:HG11	1:A:182:LEU:HD11	1.59	0.84
1:B:36:SER:HB3	1:B:51:TYR:HA	1.60	0.83
1:A:213:THR:O	1:A:214:GLU:CB	2.27	0.81
1:A:32:TYR:HD1	1:A:33:ASN:HD22	1.24	0.81
1:A:34:TYR:CD1	1:A:34:TYR:C	2.51	0.81
1:B:171:GLN:HE21	1:B:173:ASN:HD21	1.29	0.81
1:A:95:GLY:O	1:A:96:SER:HB3	1.79	0.80
1:B:52:GLU:C	1:B:53:VAL:HG23	2.01	0.79
1:B:64:PHE:CE1	1:B:77:VAL:HG22	2.17	0.79
1:A:112:GLN:HB2	1:A:113:PRO:CD	2.13	0.77
1:A:31:GLY:O	1:A:32:TYR:CB	2.25	0.77
1:B:186:PRO:O	1:B:190:LYS:HG2	1.85	0.77
1:A:69:SER:HB3	1:A:72:THR:HG23	1.66	0.76
1:A:122:PHE:O	1:A:136:LEU:HD23	1.86	0.75
1:A:34:TYR:HD1	1:A:34:TYR:C	1.89	0.75
1:B:212:PRO:HG3	2:B:589:HOH:O	1.83	0.75
1:B:175:LYS:HE2	2:B:575:HOH:O	1.85	0.75
1:A:4:LEU:HD23	1:A:22:CYS:SG	2.27	0.74
1:A:26:SER:HB3	2:A:674:HOH:O	1.87	0.74
1:A:214:GLU:HB3	2:A:932:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:CB	2:A:932:HOH:O	2.37	0.72
1:B:171:GLN:NE2	1:B:173:ASN:HD21	1.87	0.71
1:A:4:LEU:HD11	1:A:29:VAL:HG22	1.73	0.71
1:A:2:SER:O	1:A:3:ALA:O	2.08	0.71
1:B:185:THR:OG1	1:B:188:GLN:HG3	1.91	0.70
1:B:81:GLN:O	1:B:109:VAL:HG21	1.91	0.70
1:B:51:TYR:O	1:B:52:GLU:HB2	1.90	0.70
1:A:57:PRO:O	1:A:58:SER:HB2	1.92	0.70
1:B:154:ALA:HB2	1:B:195:TYR:CE1	2.27	0.69
1:A:26:SER:HB2	1:A:29:VAL:O	1.93	0.69
1:B:213:THR:HG23	2:B:895:HOH:O	1.93	0.69
1:B:52:GLU:O	1:B:53:VAL:HG23	1.93	0.69
1:A:24:GLY:HA2	1:A:29:VAL:HG23	1.74	0.68
1:A:29:VAL:HG22	1:A:30:GLY:N	2.08	0.68
1:A:173:ASN:ND2	1:A:175:LYS:H	1.92	0.68
1:A:121:LEU:O	2:A:610:HOH:O	2.11	0.68
1:A:30:GLY:CA	2:A:593:HOH:O	2.41	0.68
1:A:45:ALA:HB2	1:B:89:TYR:CD2	2.29	0.68
1:A:30:GLY:HA3	2:A:593:HOH:O	1.95	0.67
1:A:89:TYR:CE2	1:B:45:ALA:HA	2.29	0.67
1:A:69:SER:CB	1:A:72:THR:HG23	2.24	0.67
1:A:15:GLY:O	2:A:712:HOH:O	2.13	0.67
1:B:131:ALA:O	1:B:132:ASN:CB	2.41	0.67
1:A:65:SER:HA	2:A:783:HOH:O	1.95	0.66
1:B:57:PRO:HD2	1:B:60:VAL:HG21	1.76	0.66
1:A:93:TYR:CE1	1:A:98:ASN:O	2.49	0.66
1:A:34:TYR:O	1:A:34:TYR:CD1	2.48	0.66
1:A:98:ASN:ND2	1:A:100:VAL:CG1	2.59	0.65
1:B:160:LYS:CD	1:B:160:LYS:N	2.52	0.65
1:A:29:VAL:HG13	1:A:30:GLY:N	2.09	0.65
1:B:131:ALA:O	1:B:132:ASN:HB3	1.95	0.65
1:A:24:GLY:HA3	1:A:29:VAL:CG2	2.26	0.65
1:A:99:PHE:CD1	1:A:99:PHE:N	2.64	0.64
1:A:120:THR:HG22	1:A:122:PHE:CE1	2.32	0.64
1:A:115:ALA:O	1:A:143:PHE:HA	1.98	0.64
1:A:95:GLY:O	1:A:96:SER:HB2	1.95	0.64
1:A:25:THR:CG2	2:A:730:HOH:O	2.31	0.64
1:A:32:TYR:CE1	1:A:33:ASN:ND2	2.66	0.63
1:B:52:GLU:C	1:B:53:VAL:CG2	2.67	0.63
1:A:68:LYS:HE2	1:A:70:GLY:O	1.98	0.63
1:B:134:ALA:O	1:B:184:LEU:HD23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:TRP:O	1:B:212:PRO:HG3	1.99	0.62
1:A:196:SER:OG	1:A:209:THR:HG22	1.99	0.62
1:A:171:GLN:NE2	1:A:173:ASN:HD21	1.95	0.62
1:A:173:ASN:HD22	1:A:174:ASN:N	1.97	0.62
1:B:13:SER:H	1:B:16:GLN:HB3	1.64	0.62
1:B:174:ASN:OD1	1:B:174:ASN:N	2.28	0.61
1:A:97:ASP:O	1:B:57:PRO:HB2	2.00	0.61
1:A:136:LEU:HD21	1:A:210:VAL:HG21	1.83	0.61
1:B:36:SER:HB2	1:B:50:ILE:O	2.01	0.60
1:A:9:SER:HB2	1:A:147:ALA:HB3	1.82	0.60
1:A:1:PRO:HB3	1:A:100:VAL:CG1	2.30	0.60
1:A:171:GLN:HE21	1:A:173:ASN:ND2	1.96	0.60
1:A:140:ILE:HD13	1:A:199:VAL:HG21	1.82	0.60
1:B:119:VAL:HG22	1:B:208:LYS:HG3	1.83	0.60
1:A:4:LEU:HD11	1:A:29:VAL:CG2	2.30	0.60
1:A:153:LYS:CG	1:A:196:SER:HB2	2.32	0.60
1:B:49:ILE:HG22	1:B:60:VAL:HG13	1.84	0.60
1:B:4:LEU:N	1:B:4:LEU:HD23	2.16	0.60
1:B:18:VAL:O	1:B:76:THR:HG23	2.01	0.59
1:B:98:ASN:HA	2:B:604:HOH:O	2.02	0.59
1:A:154:ALA:HB2	1:A:159:VAL:HG21	1.84	0.59
1:B:106:LYS:HD2	2:B:912:HOH:O	2.02	0.59
1:A:167:LYS:HE2	1:B:43:GLY:HA3	1.85	0.59
1:A:98:ASN:ND2	1:A:100:VAL:HG12	2.18	0.59
1:A:112:GLN:HB2	1:A:113:PRO:HD3	1.85	0.59
1:A:93:TYR:CE1	1:A:95:GLY:O	2.56	0.59
1:A:213:THR:HG22	2:A:809:HOH:O	2.02	0.58
1:A:173:ASN:HD22	1:A:173:ASN:C	2.06	0.58
1:B:166:THR:HG22	1:B:179:SER:N	2.12	0.58
1:B:4:LEU:HB2	1:B:102:GLY:HA2	1.84	0.58
1:A:154:ALA:HB2	1:A:159:VAL:CG2	2.34	0.58
1:B:171:GLN:HE21	1:B:173:ASN:ND2	2.01	0.58
1:A:93:TYR:CE1	1:A:96:SER:CB	2.74	0.58
1:B:189:TRP:CZ2	1:B:212:PRO:HA	2.39	0.58
1:B:59:GLY:O	1:B:60:VAL:C	2.42	0.57
1:B:64:PHE:HD1	1:B:77:VAL:HG22	1.68	0.57
1:A:166:THR:CG2	1:A:167:LYS:H	2.17	0.57
1:B:40:GLN:NE2	1:B:44:LYS:O	2.36	0.57
1:A:38:TYR:HE1	1:A:91:SER:HB3	1.70	0.57
1:A:45:ALA:HB2	1:B:89:TYR:CE2	2.39	0.57
1:A:69:SER:N	1:A:72:THR:O	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:O	1:B:88:TYR:HA	2.05	0.56
1:A:4:LEU:HD13	1:A:100:VAL:CG2	2.36	0.56
1:A:153:LYS:HG2	1:A:196:SER:HB2	1.89	0.55
1:A:4:LEU:CD1	1:A:29:VAL:HG22	2.37	0.55
1:B:63:ARG:O	1:B:77:VAL:HA	2.07	0.55
1:A:154:ALA:HB2	1:A:195:TYR:CE1	2.43	0.54
1:A:99:PHE:HZ	1:B:51:TYR:CG	2.25	0.54
1:B:2:SER:O	1:B:100:VAL:HG23	2.06	0.54
1:B:4:LEU:HB2	1:B:102:GLY:CA	2.37	0.54
1:A:29:VAL:CG1	1:A:30:GLY:H	2.00	0.54
1:B:40:GLN:HB2	1:B:46:PRO:HA	1.90	0.54
1:B:12:GLY:HA3	1:B:80:LEU:CD1	2.37	0.54
1:B:36:SER:CB	1:B:50:ILE:O	2.56	0.53
1:B:213:THR:HG22	1:B:213:THR:O	2.08	0.53
1:A:35:VAL:HA	1:A:91:SER:O	2.08	0.53
1:A:22:CYS:HB3	1:A:73:ALA:HB3	1.90	0.53
1:A:93:TYR:CZ	1:A:98:ASN:O	2.62	0.53
1:A:4:LEU:CD1	1:A:29:VAL:CG2	2.87	0.53
1:A:24:GLY:HA3	1:A:29:VAL:CB	2.40	0.52
1:B:85:GLU:HA	1:B:107:VAL:O	2.09	0.52
1:B:57:PRO:HD2	1:B:60:VAL:CG2	2.40	0.52
1:B:57:PRO:HG2	1:B:60:VAL:CG2	2.39	0.52
1:A:31:GLY:HA3	2:A:918:HOH:O	2.09	0.52
1:B:157:SER:CB	2:B:735:HOH:O	2.57	0.52
1:A:98:ASN:HD21	1:A:100:VAL:CG1	2.22	0.52
1:B:48:VAL:N	2:B:719:HOH:O	2.11	0.52
1:A:166:THR:CG2	1:A:167:LYS:N	2.73	0.52
1:A:140:ILE:HD13	1:A:199:VAL:CG2	2.39	0.52
1:A:164:GLU:O	1:A:180:SER:CB	2.58	0.51
1:A:32:TYR:HD2	2:A:685:HOH:O	1.91	0.51
1:A:32:TYR:CD2	2:A:685:HOH:O	2.53	0.51
1:B:14:LEU:HD22	2:B:585:HOH:O	2.11	0.51
1:A:18:VAL:CG1	1:A:80:LEU:HD22	2.40	0.51
1:A:68:LYS:HA	1:A:73:ALA:HA	1.92	0.51
1:B:211:ALA:C	1:B:213:THR:H	2.14	0.51
1:A:45:ALA:CB	1:B:89:TYR:CD2	2.94	0.51
1:B:63:ARG:NH1	1:B:84:ASP:OD2	2.44	0.50
1:B:114:LYS:HG2	1:B:145:PRO:HD3	1.94	0.50
1:A:173:ASN:ND2	1:A:173:ASN:C	2.64	0.50
1:A:24:GLY:HA3	1:A:29:VAL:HA	1.93	0.50
1:A:214:GLU:HB2	2:A:932:HOH:O	2.05	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:HA	1:A:47:LYS:O	2.11	0.50
1:B:53:VAL:CG1	1:B:68:LYS:HB2	2.42	0.50
1:B:13:SER:O	1:B:14:LEU:C	2.48	0.50
1:A:28:ASN:O	1:A:29:VAL:HB	2.10	0.50
1:A:164:GLU:O	1:A:180:SER:HA	2.12	0.50
1:A:4:LEU:HD13	1:A:100:VAL:HG23	1.93	0.50
1:A:214:GLU:O	1:A:215:CYS:CB	2.60	0.50
1:B:41:HIS:CD2	1:B:86:ALA:HB2	2.47	0.50
1:A:34:TYR:CD2	1:A:94:GLU:HG2	2.47	0.49
1:B:214:GLU:CG	1:B:215:CYS:H	2.25	0.49
1:A:160:LYS:N	1:A:160:LYS:HD3	2.17	0.49
1:A:121:LEU:HD11	1:A:136:LEU:HD22	1.93	0.49
1:A:185:THR:OG1	1:A:188:GLN:N	2.30	0.49
1:A:22:CYS:O	1:A:72:THR:HA	2.12	0.49
1:A:56:ARG:NE	1:A:64:PHE:O	2.44	0.49
1:B:116:ASN:HB3	1:B:117:PRO:HD2	1.95	0.49
1:B:49:ILE:O	1:B:57:PRO:HD2	2.13	0.49
1:B:196:SER:CB	1:B:208:LYS:O	2.60	0.49
1:A:4:LEU:HG	1:A:29:VAL:CG2	2.43	0.49
1:B:160:LYS:HD3	1:B:161:ALA:N	2.28	0.49
1:A:99:PHE:HB3	2:A:885:HOH:O	2.12	0.48
1:A:128:GLU:HG2	1:A:133:LYS:CB	2.36	0.48
1:A:97:ASP:O	1:B:57:PRO:CB	2.62	0.48
1:A:166:THR:HG22	1:A:167:LYS:N	2.29	0.48
1:B:148:VAL:HG12	1:B:201:HIS:HB2	1.96	0.48
1:B:13:SER:H	1:B:16:GLN:CB	2.27	0.47
1:B:96:SER:O	1:B:97:ASP:HB2	2.14	0.47
1:B:176:TYR:N	1:B:176:TYR:CD1	2.83	0.47
1:B:56:ARG:HG2	1:B:60:VAL:HB	1.95	0.47
1:B:60:VAL:HA	1:B:61:PRO:HD3	1.73	0.47
1:B:35:VAL:HG11	1:B:73:ALA:HB1	1.96	0.47
1:B:27:SER:O	1:B:32:TYR:HE1	1.98	0.47
1:B:19:THR:HG23	1:B:76:THR:CG2	2.32	0.47
1:A:153:LYS:HG3	1:A:196:SER:HB2	1.96	0.47
1:B:57:PRO:HG2	1:B:60:VAL:HG23	1.95	0.47
1:B:154:ALA:O	1:B:155:ASP:HB2	2.13	0.47
1:A:139:LEU:HD22	1:B:137:VAL:HG22	1.97	0.47
1:A:45:ALA:HB1	1:A:46:PRO:HD2	1.96	0.47
1:B:213:THR:CG2	2:B:895:HOH:O	2.58	0.47
1:B:18:VAL:O	1:B:76:THR:CG2	2.63	0.47
1:B:13:SER:O	1:B:16:GLN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLN:HB2	1:A:113:PRO:HD2	1.94	0.47
1:A:185:THR:C	1:A:187:GLU:N	2.64	0.47
1:A:40:GLN:C	1:A:41:HIS:O	2.53	0.47
1:A:121:LEU:HD12	1:A:137:VAL:O	2.14	0.46
1:B:16:GLN:O	1:B:79:GLY:N	2.46	0.46
1:B:214:GLU:HG2	2:B:758:HOH:O	2.15	0.46
1:A:189:TRP:CZ2	1:A:212:PRO:HA	2.50	0.46
1:B:60:VAL:HG12	1:B:61:PRO:HD2	1.97	0.46
1:B:171:GLN:HE21	1:B:171:GLN:HB2	1.38	0.46
1:A:122:PHE:CZ	1:B:137:VAL:HG23	2.50	0.46
1:A:185:THR:O	1:A:186:PRO:C	2.53	0.46
1:B:20:ILE:O	1:B:74:SER:HA	2.16	0.46
1:B:157:SER:HB2	2:B:735:HOH:O	2.15	0.45
1:A:8:PRO:HD2	2:A:625:HOH:O	2.16	0.45
1:B:63:ARG:HH12	1:B:84:ASP:CG	2.20	0.45
1:A:159:VAL:HG13	2:A:776:HOH:O	2.17	0.45
1:B:214:GLU:CG	1:B:215:CYS:N	2.79	0.45
1:A:139:LEU:HD11	1:B:181:TYR:CD2	2.50	0.45
1:A:154:ALA:CB	1:A:195:TYR:CE1	3.00	0.45
1:B:212:PRO:HD3	2:B:589:HOH:O	2.16	0.45
1:B:187:GLU:HG2	2:B:767:HOH:O	2.17	0.45
1:A:1:PRO:HB3	1:A:100:VAL:HB	1.98	0.45
1:A:1:PRO:HB3	1:A:100:VAL:CB	2.47	0.45
1:A:98:ASN:HD22	1:A:100:VAL:HG12	1.82	0.45
1:A:32:TYR:O	1:A:34:TYR:N	2.49	0.45
1:A:154:ALA:N	1:A:157:SER:O	2.39	0.45
1:B:6:GLN:OE1	1:B:103:THR:O	2.35	0.45
1:B:154:ALA:N	1:B:157:SER:O	2.50	0.45
1:A:89:TYR:HE2	1:B:45:ALA:HA	1.82	0.44
1:B:16:GLN:CG	1:B:17:SER:H	2.30	0.44
1:A:193:ARG:HD3	1:A:193:ARG:C	2.38	0.44
1:B:107:VAL:HG22	1:B:107:VAL:O	2.17	0.44
1:A:51:TYR:O	1:A:55:LYS:HB2	2.17	0.44
1:A:30:GLY:HA2	2:A:768:HOH:O	2.18	0.44
1:A:18:VAL:HG13	1:A:80:LEU:HD22	2.00	0.44
1:B:49:ILE:O	1:B:57:PRO:CD	2.66	0.44
1:A:98:ASN:C	1:A:98:ASN:HD22	2.21	0.44
1:B:196:SER:HB2	1:B:208:LYS:O	2.18	0.44
1:B:35:VAL:HG11	1:B:73:ALA:CB	2.47	0.44
1:A:93:TYR:CD1	1:A:95:GLY:O	2.72	0.43
1:B:189:TRP:HA	1:B:189:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:HH11	1:B:63:ARG:HD2	1.40	0.43
1:B:81:GLN:NE2	1:B:81:GLN:HA	2.32	0.43
1:B:119:VAL:CG2	1:B:208:LYS:HG3	2.48	0.43
1:A:32:TYR:HD1	1:A:33:ASN:ND2	1.97	0.43
1:A:143:PHE:CE2	1:A:148:VAL:HG13	2.54	0.43
1:A:45:ALA:HB1	1:A:46:PRO:CD	2.48	0.43
1:B:214:GLU:O	1:B:215:CYS:HB3	2.18	0.43
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.86	0.43
1:A:98:ASN:C	1:A:98:ASN:ND2	2.71	0.43
1:B:56:ARG:HD3	1:B:64:PHE:O	2.19	0.43
1:A:3:ALA:HA	2:A:607:HOH:O	2.18	0.43
1:B:173:ASN:O	1:B:174:ASN:C	2.56	0.42
1:A:40:GLN:O	1:A:41:HIS:C	2.55	0.42
1:B:173:ASN:H	1:B:173:ASN:ND2	2.17	0.42
1:B:26:SER:HB2	2:B:632:HOH:O	2.18	0.42
1:B:160:LYS:HD3	1:B:161:ALA:H	1.83	0.42
1:B:64:PHE:CE1	1:B:77:VAL:CG2	2.97	0.42
1:B:56:ARG:CD	1:B:64:PHE:O	2.68	0.42
1:B:140:ILE:CD1	1:B:150:VAL:HG11	2.49	0.42
1:A:32:TYR:HD1	1:A:33:ASN:H	1.67	0.42
1:A:34:TYR:O	1:A:34:TYR:CG	2.72	0.42
1:A:154:ALA:CB	1:A:159:VAL:CG2	2.98	0.42
1:A:45:ALA:HA	1:A:46:PRO:HD3	1.82	0.42
1:A:36:SER:HB3	1:A:51:TYR:HA	2.01	0.42
1:A:116:ASN:HB3	1:A:117:PRO:HD2	2.01	0.42
1:A:101:PHE:CD2	1:B:46:PRO:HD2	2.55	0.41
1:A:44:LYS:HE2	2:A:818:HOH:O	2.20	0.41
1:A:214:GLU:C	1:A:215:CYS:SG	2.95	0.41
1:A:165:THR:OG1	1:A:180:SER:HB3	2.20	0.41
1:B:140:ILE:HG21	1:B:199:VAL:HG11	2.02	0.41
1:A:1:PRO:HG3	1:A:98:ASN:ND2	2.35	0.41
1:B:12:GLY:O	1:B:110:LEU:HB2	2.20	0.41
1:B:49:ILE:HB	1:B:60:VAL:HG11	2.02	0.41
1:B:61:PRO:HD2	1:B:64:PHE:HD2	1.85	0.41
1:A:136:LEU:HD21	1:A:210:VAL:CG2	2.49	0.41
1:B:168:PRO:HB3	1:B:176:TYR:HB3	2.03	0.41
1:B:48:VAL:HB	2:B:719:HOH:O	2.20	0.41
1:A:16:GLN:HG2	2:A:766:HOH:O	2.20	0.41
1:A:37:TRP:HB2	1:A:50:ILE:HB	2.02	0.41
1:B:198:GLN:HG3	1:B:207:GLU:HB2	2.02	0.41
1:A:24:GLY:HA3	1:A:29:VAL:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLY:C	2:A:593:HOH:O	2.56	0.41
1:A:99:PHE:HD1	1:A:99:PHE:H	1.67	0.41
1:A:2:SER:O	1:A:3:ALA:C	2.60	0.41
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.89	0.40
1:B:107:VAL:O	1:B:107:VAL:CG2	2.66	0.40
1:A:187:GLU:OE1	1:A:187:GLU:HA	2.20	0.40
1:B:80:LEU:HA	1:B:80:LEU:HD23	1.87	0.40
1:A:160:LYS:NZ	2:A:775:HOH:O	1.91	0.40
1:A:18:VAL:HG11	1:A:80:LEU:HD22	2.03	0.40
1:A:56:ARG:HA	1:A:57:PRO:HD3	1.87	0.40

All (4) 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)
2:A:769:HOH:O	2:B:820:HOH:O[6_656]	0.99	1.21
2:A:597:HOH:O	2:A:903:HOH:O[6_656]	1.69	0.51
2:A:647:HOH:O	2:B:901:HOH:O[6_656]	1.76	0.44
1:B:216:SER:O	2:A:526:HOH:O[2_545]	1.94	0.26

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	214/216 (99%)	183 (86%)	16 (8%)	15 (7%)		
1	B	214/216 (99%)	189 (88%)	21 (10%)	4 (2%)		
All	All	428/432 (99%)	372 (87%)	37 (9%)	19 (4%)		

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	29	VAL
1	A	32	TYR
1	A	33	ASN
1	A	96	SER
1	A	214	GLU
1	A	215	CYS
1	A	26	SER
1	A	28	ASN
1	A	95	GLY
1	B	132	ASN
1	B	215	CYS
1	A	58	SER
1	B	2	SER
1	A	93	TYR
1	B	214	GLU
1	A	70	GLY
1	A	156	GLY
1	A	61	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/181 (100%)	141 (78%)	40 (22%)	1	1
1	B	181/181 (100%)	150 (83%)	31 (17%)	2	2
All	All	362/362 (100%)	291 (80%)	71 (20%)	1	1

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	2	SER
1	A	13	SER
1	A	23	THR
1	A	25	THR

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Mol	Chain	Res	Type
1	A	26	SER
1	A	28	ASN
1	A	32	TYR
1	A	35	VAL
1	A	44	LYS
1	A	62	ASP
1	A	72	THR
1	A	78	SER
1	A	83	GLU
1	A	92	SER
1	A	93	TYR
1	A	97	ASP
1	A	98	ASN
1	A	99	PHE
1	A	100	VAL
1	A	103	THR
1	A	110	LEU
1	A	129	LEU
1	A	133	LYS
1	A	137	VAL
1	A	140	ILE
1	A	141	SER
1	A	153	LYS
1	A	157	SER
1	A	160	LYS
1	A	163	VAL
1	A	167	LYS
1	A	170	LYS
1	A	173	ASN
1	A	182	LEU
1	A	187	GLU
1	A	190	LYS
1	A	191	SER
1	A	202	GLU
1	A	207	GLU
1	B	2	SER
1	B	11	SER
1	B	16	GLN
1	B	18	VAL
1	B	27	SER
1	B	44	LYS
1	B	53	VAL

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Mol	Chain	Res	Type
1	B	63	ARG
1	B	72	THR
1	B	78	SER
1	B	81	GLN
1	B	83	GLU
1	B	106	LYS
1	B	108	THR
1	B	110	LEU
1	B	126	SER
1	B	139	LEU
1	B	153	LYS
1	B	157	SER
1	B	160	LYS
1	B	163	VAL
1	B	164	GLU
1	B	166	THR
1	B	167	LYS
1	B	169	SER
1	B	173	ASN
1	B	184	LEU
1	B	187	GLU
1	B	210	VAL
1	B	213	THR
1	B	214	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	54	ASN
1	A	71	ASN
1	A	98	ASN
1	A	173	ASN
1	A	192	HIS
1	B	81	GLN
1	B	112	GLN
1	B	132	ASN
1	B	173	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	216/216 (100%)	-1.11	0 100 100	8, 19, 47, 53	0
1	B	216/216 (100%)	-1.12	0 100 100	8, 21, 38, 55	0
All	All	432/432 (100%)	-1.12	0 100 100	8, 20, 45, 55	0

There are no RSRZ outliers to report.

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 carbohydrates 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.