Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:41 PM GMT

PDB ID	:	1LIL
Title	:	BENCE JONES PROTEIN CLE, A LAMBDA III IMMUNOGLOBULIN LIGHT-CHAIN DIMER
Authors	:	Schiffer, M.; Huang, D.B.
Deposited on	:	1996-05-13
Resolution	:	2.65 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

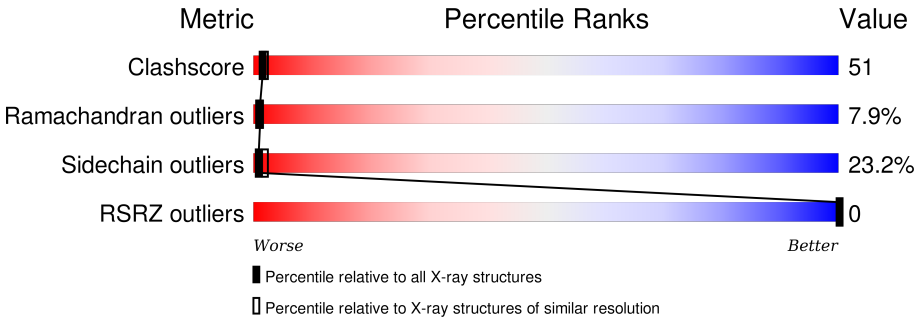
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 <=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	212	32% 48% 17%
1	B	212	25% 47% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3314 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 LAMBDA III BENCE JONES PROTEIN CLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1595	994	267	328	6			
1	B	212	Total	C	N	O	S	0	0	0
			1595	994	267	328	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	VAL	LEU	CONFLICT	UNP P01842
A	11	LEU	VAL	CONFLICT	UNP P01842
A	20	ARG	SER	CONFLICT	UNP P01842
A	26	GLU	ASP	CONFLICT	UNP P01842
A	27	LYS	THR	CONFLICT	UNP P01842
A	31	ALA	LYS	CONFLICT	UNP P01842
A	33	VAL	ALA	CONFLICT	UNP P01842
A	39	ARG	LYS	CONFLICT	UNP P01842
A	42	GLN	HIS	CONFLICT	UNP P01842
A	46	VAL	LEU	CONFLICT	UNP P01842
A	49	TYR	PHE	CONFLICT	UNP P01842
A	52	ASN	SER	CONFLICT	UNP P01842
A	53	ARG	LYS	CONFLICT	UNP P01842
A	66	SER	ASN	CONFLICT	UNP P01842
A	80	THR	ALA	CONFLICT	UNP P01842
A	81	LEU	MET	CONFLICT	UNP P01842
A	90	VAL	ALA	CONFLICT	UNP P01842
A	94	ASN	-	INSERTION	UNP P01842
A	95	ALA	-	INSERTION	UNP P01842
A	?	-	THR	DELETION	UNP P01842
A	96	VAL	ALA	CONFLICT	UNP P01842
B	4	VAL	LEU	CONFLICT	UNP P01842
B	11	LEU	VAL	CONFLICT	UNP P01842
B	20	ARG	SER	CONFLICT	UNP P01842
B	26	GLU	ASP	CONFLICT	UNP P01842

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	LYS	THR	CONFLICT	UNP P01842
B	31	ALA	LYS	CONFLICT	UNP P01842
B	33	VAL	ALA	CONFLICT	UNP P01842
B	39	ARG	LYS	CONFLICT	UNP P01842
B	42	GLN	HIS	CONFLICT	UNP P01842
B	46	VAL	LEU	CONFLICT	UNP P01842
B	49	TYR	PHE	CONFLICT	UNP P01842
B	52	ASN	SER	CONFLICT	UNP P01842
B	53	ARG	LYS	CONFLICT	UNP P01842
B	66	SER	ASN	CONFLICT	UNP P01842
B	80	THR	ALA	CONFLICT	UNP P01842
B	81	LEU	MET	CONFLICT	UNP P01842
B	90	VAL	ALA	CONFLICT	UNP P01842
B	94	ASN	-	INSERTION	UNP P01842
B	95	ALA	-	INSERTION	UNP P01842
B	?	-	THR	DELETION	UNP P01842
B	96	VAL	ALA	CONFLICT	UNP P01842

- Molecule 2 is water.

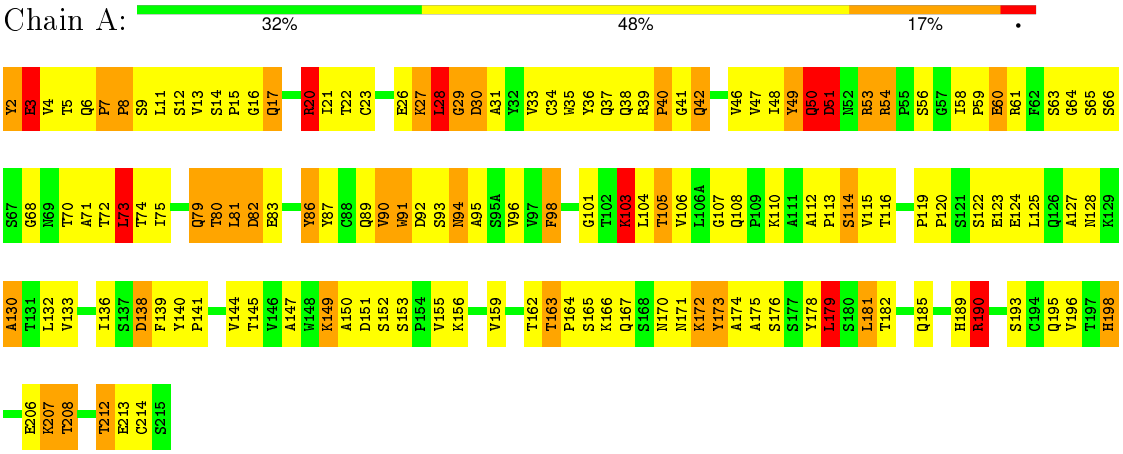
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0
2	B	64	Total O 64 64	0	0

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 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.

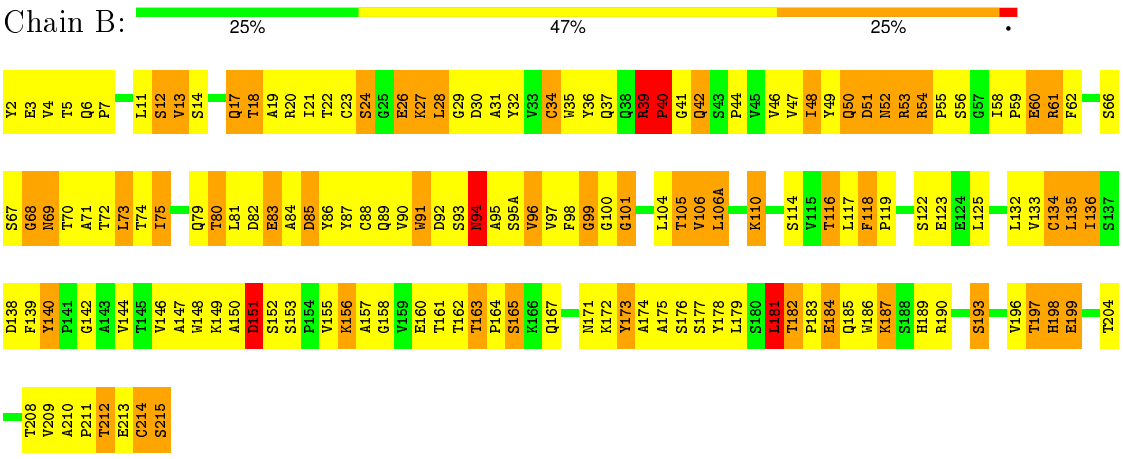
- Molecule 1: LAMBDA III BENCE JONES PROTEIN CLE

Chain A:



- Molecule 1: LAMBDA III BENCE JONES PROTEIN CLE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.17Å 72.54Å 49.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65 9.42 – 2.66	Depositor EDS
% Data completeness (in resolution range)	71.0 (10.00-2.65) 73.0 (9.42-2.66)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.190 , 0.340 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 135.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 8684 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3314	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.98	1/1634 (0.1%)	1.78	27/2234 (1.2%)
1	B	0.98	0/1634	1.87	36/2234 (1.6%)
All	All	0.98	1/3268 (0.0%)	1.83	63/4468 (1.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLN	CB-CG	7.52	1.72	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	54	ARG	NE-CZ-NH1	-12.58	114.01	120.30
1	B	39	ARG	NE-CZ-NH2	11.35	125.97	120.30
1	A	190	ARG	NE-CZ-NH1	-10.25	115.18	120.30
1	A	53	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	B	53	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	B	151	ASP	CA-CB-CG	9.41	134.10	113.40
1	A	190	ARG	NE-CZ-NH2	8.89	124.74	120.30
1	A	79	GLN	CA-CB-CG	8.74	132.63	113.40
1	A	173	TYR	CB-CG-CD1	-7.77	116.33	121.00
1	A	38	GLN	CA-CB-CG	7.75	130.44	113.40
1	B	26	GLU	CA-CB-CG	7.43	129.75	113.40
1	B	181	LEU	CA-CB-CG	7.26	131.99	115.30
1	A	49	TYR	CA-CB-CG	7.20	127.09	113.40
1	B	178	TYR	CA-CB-CG	6.88	126.47	113.40
1	B	18	THR	CA-CB-CG2	6.75	121.85	112.40
1	B	68	GLY	N-CA-C	-6.51	96.82	113.10
1	A	86	TYR	CB-CG-CD2	6.50	124.90	121.00
1	B	178	TYR	N-CA-CB	6.45	122.21	110.60
1	B	34	CYS	CA-CB-SG	-6.44	102.42	114.00
1	A	172	LYS	N-CA-CB	6.39	122.11	110.60
1	A	151	ASP	CB-CA-C	6.36	123.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	106	VAL	CB-CA-C	6.33	123.43	111.40
1	B	54	ARG	CD-NE-CZ	-6.31	114.76	123.60
1	A	86	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	A	20	ARG	CD-NE-CZ	6.20	132.28	123.60
1	B	54	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	82	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	3	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	B	184	GLU	CA-CB-CG	6.04	126.69	113.40
1	A	40	PRO	CA-N-CD	-6.01	103.08	111.50
1	B	92	ASP	CB-CG-OD2	6.01	123.70	118.30
1	A	79	GLN	CG-CD-OE1	-5.97	109.67	121.60
1	B	39	ARG	CB-CA-C	5.90	122.19	110.40
1	A	30	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	73	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	133	VAL	O-C-N	5.78	131.94	122.70
1	A	179	LEU	O-C-N	5.74	131.88	122.70
1	B	173	TYR	CB-CG-CD2	-5.58	117.66	121.00
1	B	190	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	53	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	B	212	THR	C-N-CA	5.51	135.47	121.70
1	B	181	LEU	O-C-N	5.49	131.48	122.70
1	A	29	GLY	N-CA-C	-5.47	99.42	113.10
1	A	175	ALA	CB-CA-C	5.46	118.28	110.10
1	A	30	ASP	N-CA-CB	5.42	120.35	110.60
1	B	163	THR	N-CA-C	-5.37	96.50	111.00
1	B	85	ASP	CB-CA-C	5.36	121.13	110.40
1	A	90	VAL	CA-CB-CG2	5.30	118.85	110.90
1	B	61	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	B	189	HIS	CA-CB-CG	-5.24	104.69	113.60
1	B	99	GLY	N-CA-C	-5.24	100.01	113.10
1	A	156	LYS	O-C-N	5.22	131.05	122.70
1	B	110	LYS	CB-CA-C	5.21	120.83	110.40
1	B	140	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	B	31	ALA	N-CA-CB	-5.14	102.90	110.10
1	B	39	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	B	106	VAL	CA-CB-CG1	5.13	118.60	110.90
1	B	118	PHE	CA-CB-CG	5.11	126.17	113.90
1	A	132	LEU	CA-CB-CG	5.10	127.04	115.30
1	B	83	GLU	CG-CD-OE1	5.09	128.47	118.30
1	B	84	ALA	O-C-N	5.06	130.79	122.70
1	A	173	TYR	CA-CB-CG	-5.06	103.79	113.40
1	A	138	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1595	0	1533	144	0
1	B	1595	0	1533	179	1
2	A	60	0	0	9	2
2	B	64	0	0	12	1
All	All	3314	0	3066	319	2

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 51.

All (319) 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:B:36:TYR:CE1	1:B:46:VAL:HG22	1.69	1.26
1:B:199:GLU:HA	2:B:409:HOH:O	1.35	1.25
1:A:47:VAL:O	1:A:48:ILE:HD13	1.43	1.14
1:A:87:TYR:HB3	1:A:98:PHE:CE1	1.83	1.13
1:A:87:TYR:HB3	1:A:98:PHE:HE1	1.00	1.07
1:A:50:GLN:O	1:A:51:ASP:HB2	1.55	1.05
1:A:36:TYR:CE1	1:A:46:VAL:HG12	1.94	1.01
1:B:36:TYR:HE1	1:B:46:VAL:CG2	1.75	1.00
1:B:193:SER:HB3	1:B:208:THR:HG22	1.44	1.00
1:A:87:TYR:CB	1:A:98:PHE:HE1	1.76	0.97
1:B:132:LEU:HD12	1:B:179:LEU:HD23	1.45	0.97
1:B:123:GLU:HG3	2:B:370:HOH:O	1.63	0.97
1:B:193:SER:CB	1:B:208:THR:HG22	1.93	0.97
1:A:28:LEU:HD21	1:A:71:ALA:HB2	1.47	0.95
1:B:181:LEU:HD22	1:B:185:GLN:HB3	1.49	0.94
1:B:156:LYS:HZ3	1:B:157:ALA:HB3	1.34	0.93
1:B:67:SER:OG	1:B:68:GLY:N	2.01	0.92
1:A:31:ALA:HA	1:A:91:TRP:O	1.69	0.91
1:B:34:CYS:SG	1:B:49:TYR:HA	2.10	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:HG2	1:B:4:VAL:O	1.70	0.90
1:A:136:ILE:HG22	1:A:139:PHE:CE2	2.10	0.86
1:A:27:LYS:O	1:A:29:GLY:N	2.10	0.84
1:B:91:TRP:HZ3	1:B:95:ALA:C	1.82	0.83
1:A:49:TYR:C	1:A:51:ASP:H	1.78	0.82
1:B:156:LYS:NZ	1:B:157:ALA:HB3	1.92	0.82
1:B:54:ARG:HD3	1:B:58:ILE:HG22	1.62	0.82
1:B:139:PHE:CE2	1:B:144:VAL:HG13	2.16	0.80
1:B:162:THR:O	2:B:463:HOH:O	2.01	0.79
1:B:156:LYS:HG2	1:B:157:ALA:N	1.98	0.79
1:A:6:GLN:NE2	1:A:86:TYR:O	2.15	0.79
1:A:11:LEU:HD23	1:A:21:ILE:HG12	1.64	0.78
1:A:60:GLU:HB3	2:A:309:HOH:O	1.84	0.76
1:A:50:GLN:NE2	1:A:53:ARG:HG3	2.01	0.76
1:B:91:TRP:CH2	1:B:95:ALA:HA	2.21	0.76
1:A:190:ARG:NE	1:A:190:ARG:HA	2.00	0.75
1:B:47:VAL:HG12	1:B:58:ILE:CD1	2.17	0.75
1:B:32:TYR:CD1	1:B:50:GLN:HG2	2.22	0.75
1:B:4:VAL:HG21	1:B:90:VAL:HG21	1.69	0.74
1:B:90:VAL:O	1:B:96:VAL:HA	1.87	0.74
1:A:4:VAL:CG1	1:A:23:CYS:SG	2.76	0.73
1:A:28:LEU:CD2	1:A:71:ALA:HB2	2.19	0.73
1:A:173:TYR:N	1:A:173:TYR:CD1	2.56	0.73
1:A:167:GLN:HG3	1:A:170:ASN:OD1	1.88	0.73
1:A:22:THR:OG1	1:A:70:THR:HG23	1.89	0.73
1:B:52:ASN:OD1	2:B:427:HOH:O	2.06	0.72
1:B:156:LYS:HG2	1:B:157:ALA:H	1.53	0.72
1:B:91:TRP:CZ3	1:B:95:ALA:C	2.63	0.72
1:A:173:TYR:N	1:A:173:TYR:HD1	1.88	0.72
1:B:117:LEU:HD23	1:B:208:THR:HA	1.72	0.71
1:B:156:LYS:H	1:B:156:LYS:HD3	1.55	0.71
1:B:39:ARG:HD2	1:B:40:PRO:HD2	1.71	0.71
1:A:115:VAL:HG12	1:A:207:LYS:HG3	1.72	0.70
1:B:23:CYS:O	1:B:70:THR:HG23	1.91	0.70
1:A:9:SER:OG	1:A:141:PRO:HG2	1.90	0.70
1:A:65:SER:O	1:A:71:ALA:HA	1.92	0.69
1:B:11:LEU:O	1:B:104:LEU:HD12	1.93	0.69
1:A:20:ARG:HB2	1:A:20:ARG:HH11	1.57	0.69
1:A:7:PRO:O	1:A:101:GLY:O	2.10	0.69
1:A:49:TYR:C	1:A:51:ASP:N	2.46	0.68
1:A:149:LYS:HA	1:A:153:SER:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:O	1:A:48:ILE:CD1	2.33	0.68
1:B:119:PRO:HA	1:B:132:LEU:HD23	1.75	0.67
1:B:156:LYS:CG	1:B:157:ALA:H	2.07	0.67
1:A:166:LYS:HD3	2:A:377:HOH:O	1.95	0.67
1:A:31:ALA:HB1	1:A:90:VAL:HG13	1.76	0.67
1:A:50:GLN:O	1:A:51:ASP:CB	2.41	0.67
1:A:133:VAL:HG21	1:B:118:PHE:CE1	2.30	0.67
1:A:36:TYR:HE2	1:A:89:GLN:NE2	1.92	0.66
1:A:103:LYS:NZ	1:A:103:LYS:HB2	2.10	0.66
1:B:47:VAL:HG12	1:B:58:ILE:HD11	1.77	0.66
1:B:117:LEU:HD23	1:B:208:THR:CA	2.24	0.66
1:B:182:THR:C	1:B:184:GLU:H	1.97	0.65
1:A:20:ARG:CG	1:A:20:ARG:HH11	2.10	0.65
1:B:39:ARG:NH2	1:B:81:LEU:HD23	2.11	0.65
1:A:115:VAL:O	1:A:207:LYS:HG3	1.96	0.65
1:A:95:ALA:HA	2:A:320:HOH:O	1.96	0.65
1:A:54:ARG:HH21	1:A:60:GLU:HG2	1.60	0.65
1:B:136:ILE:HD13	1:B:136:ILE:N	2.11	0.65
1:A:58:ILE:CG2	1:A:59:PRO:HD2	2.27	0.65
1:A:11:LEU:CD2	1:A:21:ILE:HG12	2.26	0.65
1:B:193:SER:HB3	1:B:208:THR:CG2	2.26	0.64
1:A:49:TYR:O	1:A:51:ASP:N	2.31	0.64
1:A:54:ARG:NH2	1:A:60:GLU:HG2	2.12	0.63
1:A:14:SER:N	1:A:17:GLN:OE1	2.30	0.63
1:B:60:GLU:OE1	2:B:414:HOH:O	2.15	0.63
1:A:2:TYR:N	1:A:2:TYR:CD1	2.65	0.63
1:A:90:VAL:HG12	1:A:90:VAL:O	1.98	0.63
1:A:130:ALA:O	1:A:181:LEU:HD12	1.99	0.63
1:A:50:GLN:HE21	1:A:53:ARG:HB2	1.62	0.63
1:B:91:TRP:CZ3	1:B:95:ALA:HA	2.34	0.63
1:A:21:ILE:O	1:A:73:LEU:N	2.26	0.63
1:B:61:ARG:NH2	1:B:82:ASP:OD1	2.32	0.63
1:A:34:CYS:HA	1:A:48:ILE:O	1.99	0.62
1:A:3:GLU:HB2	1:A:26:GLU:OE2	1.98	0.62
1:B:181:LEU:HB3	1:B:185:GLN:HB2	1.81	0.62
1:B:41:GLY:O	1:B:42:GLN:NE2	2.31	0.62
1:A:8:PRO:HG2	1:A:198:HIS:O	1.99	0.62
1:B:12:SER:HB2	1:B:106(A):LEU:HD21	1.80	0.62
1:B:117:LEU:CD2	1:B:208:THR:HA	2.29	0.62
1:A:33:VAL:HA	1:A:89:GLN:O	1.99	0.62
1:A:50:GLN:HE22	1:A:53:ARG:HG3	1.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:NH1	1:A:63:SER:HA	2.15	0.61
1:B:13:VAL:CG1	1:B:14:SER:H	2.14	0.61
1:A:123:GLU:OE2	1:B:209:VAL:HG12	2.01	0.61
1:A:58:ILE:HG23	1:A:59:PRO:HD2	1.81	0.61
1:A:13:VAL:HG22	1:A:14:SER:N	2.16	0.61
1:A:181:LEU:HD12	1:A:181:LEU:O	2.00	0.61
1:B:13:VAL:HG12	1:B:14:SER:H	1.65	0.61
1:A:145:THR:O	1:A:196:VAL:HA	2.01	0.61
1:A:36:TYR:HE1	1:A:46:VAL:HG12	1.63	0.60
1:B:22:THR:HG22	1:B:72:THR:OG1	2.01	0.60
1:B:36:TYR:HE1	1:B:46:VAL:HG22	0.78	0.60
1:B:164:PRO:HA	1:B:174:ALA:O	2.01	0.60
1:A:3:GLU:CB	1:A:26:GLU:OE2	2.49	0.60
1:B:2:TYR:CD2	1:B:97:VAL:HG22	2.36	0.59
1:A:27:LYS:C	1:A:29:GLY:H	2.05	0.59
1:A:112:ALA:HB1	1:A:113:PRO:HD2	1.85	0.59
1:B:91:TRP:CD2	1:B:96:VAL:HG23	2.37	0.59
1:B:80:THR:C	1:B:82:ASP:H	2.06	0.59
1:B:91:TRP:CE3	1:B:96:VAL:HG23	2.37	0.59
1:B:181:LEU:HD23	1:B:185:GLN:OE1	2.03	0.59
1:B:37:GLN:HE21	1:B:86:TYR:HE1	1.49	0.59
1:B:156:LYS:HZ2	1:B:157:ALA:H	1.49	0.59
1:B:182:THR:HB	1:B:184:GLU:HB2	1.83	0.58
1:A:50:GLN:NE2	1:A:53:ARG:CG	2.66	0.58
1:B:210:ALA:O	1:B:212:THR:N	2.36	0.58
1:A:20:ARG:HH11	1:A:20:ARG:HG2	1.69	0.58
1:A:20:ARG:CB	1:A:20:ARG:HH11	2.16	0.58
1:B:148:TRP:HE1	1:B:177:SER:HB3	1.69	0.58
1:B:167:GLN:HB2	1:B:172:LYS:O	2.04	0.57
1:A:155:VAL:HG11	1:A:179:LEU:HD11	1.86	0.57
1:B:81:LEU:HD23	1:B:171:ASN:OD1	2.05	0.57
1:B:39:ARG:O	1:B:41:GLY:N	2.39	0.56
1:B:47:VAL:HG12	1:B:58:ILE:HD12	1.87	0.56
1:B:182:THR:HB	1:B:184:GLU:H	1.70	0.56
1:B:197:THR:HG23	1:B:204:THR:OG1	2.05	0.56
1:B:61:ARG:O	1:B:75:ILE:HA	2.05	0.56
1:A:136:ILE:HG22	1:A:139:PHE:HE2	1.63	0.56
1:B:140:TYR:CD1	1:B:140:TYR:C	2.79	0.56
1:A:136:ILE:HG22	1:A:139:PHE:CD2	2.40	0.56
1:B:142:GLY:HA3	1:B:173:TYR:CE2	2.41	0.56
1:A:11:LEU:HD23	1:A:21:ILE:CG1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:C	1:B:184:GLU:N	2.60	0.55
1:B:6:GLN:HG3	1:B:23:CYS:SG	2.46	0.55
1:B:3:GLU:HB3	2:B:428:HOH:O	2.05	0.55
1:B:155:VAL:HG11	1:B:179:LEU:HD11	1.88	0.55
1:B:68:GLY:O	1:B:70:THR:N	2.40	0.55
1:B:139:PHE:CD2	1:B:144:VAL:HG13	2.41	0.55
1:B:50:GLN:O	1:B:52:ASN:N	2.38	0.55
1:B:41:GLY:O	1:B:42:GLN:HB2	2.06	0.55
1:A:14:SER:O	1:A:16:GLY:N	2.40	0.55
1:A:4:VAL:HG13	1:A:23:CYS:SG	2.47	0.55
1:B:59:PRO:HD2	1:B:62:PHE:HE1	1.72	0.54
1:B:91:TRP:CZ3	1:B:95:ALA:CA	2.90	0.54
1:B:70:THR:HG22	1:B:71:ALA:O	2.07	0.54
1:A:120:PRO:HB2	1:A:125:LEU:CD1	2.37	0.54
1:A:60:GLU:O	1:A:60:GLU:OE1	2.25	0.54
1:B:165:SER:O	1:B:173:TYR:HA	2.08	0.54
1:B:35:TRP:HD1	1:B:48:ILE:HG22	1.73	0.53
1:A:163:THR:O	1:A:163:THR:HG22	2.08	0.53
1:A:36:TYR:CE2	1:A:89:GLN:NE2	2.75	0.53
1:B:150:ALA:HB2	1:B:155:VAL:CG2	2.39	0.53
1:A:136:ILE:CG2	1:A:139:PHE:CE2	2.89	0.53
1:B:2:TYR:CE2	1:B:97:VAL:HG22	2.44	0.53
1:B:156:LYS:N	1:B:156:LYS:HD3	2.23	0.53
1:B:3:GLU:CD	1:B:100:GLY:H	2.11	0.53
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.40	0.53
1:B:122:SER:O	1:B:125:LEU:N	2.42	0.53
1:B:162:THR:HB	1:B:175:ALA:HA	1.89	0.53
1:A:119:PRO:HB2	1:A:120:PRO:HD2	1.91	0.53
1:A:94:ASN:N	1:A:94:ASN:HD22	2.06	0.52
1:B:39:ARG:O	1:B:40:PRO:C	2.48	0.52
1:B:46:VAL:HG12	1:B:55:PRO:HG3	1.92	0.52
1:B:146:VAL:HG12	1:B:147:ALA:N	2.24	0.52
1:A:13:VAL:HG22	1:A:14:SER:O	2.10	0.52
1:B:34:CYS:SG	1:B:49:TYR:HB2	2.49	0.51
1:A:87:TYR:CB	1:A:98:PHE:CE1	2.64	0.51
1:A:60:GLU:CB	2:A:309:HOH:O	2.52	0.51
1:B:91:TRP:HH2	1:B:95:ALA:HA	1.75	0.51
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.45	0.51
1:A:208:THR:HG22	2:A:374:HOH:O	2.09	0.51
1:B:150:ALA:O	1:B:151:ASP:C	2.47	0.51
1:B:34:CYS:SG	1:B:49:TYR:CA	2.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:HA	1:B:176:SER:O	2.11	0.51
1:A:39:ARG:O	1:A:42:GLN:HB2	2.10	0.51
1:B:4:VAL:HA	2:B:412:HOH:O	2.10	0.50
1:B:156:LYS:HZ2	1:B:157:ALA:N	2.09	0.50
1:B:19:ALA:O	1:B:74:THR:HA	2.11	0.50
1:B:181:LEU:HB3	1:B:185:GLN:CB	2.41	0.50
1:B:41:GLY:O	2:B:410:HOH:O	2.20	0.50
1:B:146:VAL:HG13	1:B:196:VAL:HG22	1.94	0.50
1:A:50:GLN:HE21	1:A:53:ARG:CB	2.25	0.50
1:A:3:GLU:HB2	1:A:26:GLU:CD	2.31	0.50
1:B:3:GLU:CG	1:B:4:VAL:O	2.53	0.50
1:A:20:ARG:HB2	1:A:20:ARG:NH1	2.26	0.50
1:B:21:ILE:O	1:B:73:LEU:N	2.35	0.50
1:B:146:VAL:HG12	1:B:147:ALA:H	1.76	0.50
1:A:182:THR:OG1	1:A:185:GLN:HG3	2.12	0.50
1:B:34:CYS:O	1:B:88:CYS:HA	2.12	0.50
1:B:116:THR:O	1:B:134:CYS:HA	2.11	0.50
1:A:115:VAL:HG12	1:A:207:LYS:CG	2.39	0.49
1:A:34:CYS:HB2	1:A:89:GLN:HB3	1.94	0.49
1:A:195:GLN:HB2	1:A:206:GLU:OE1	2.12	0.49
1:B:24:SER:OG	1:B:70:THR:OG1	2.31	0.49
1:B:210:ALA:C	1:B:212:THR:H	2.16	0.49
1:B:79:GLN:O	1:B:106:VAL:HG21	2.13	0.49
1:B:27:LYS:O	1:B:29:GLY:N	2.45	0.49
1:A:3:GLU:HB2	1:A:26:GLU:CG	2.43	0.48
1:B:2:TYR:HD1	2:B:456:HOH:O	1.96	0.48
1:A:17:GLN:HB3	2:A:306:HOH:O	2.12	0.48
1:B:36:TYR:CE1	1:B:46:VAL:CG2	2.65	0.48
1:B:155:VAL:HG11	1:B:179:LEU:CD1	2.43	0.48
1:A:4:VAL:HG11	1:A:23:CYS:SG	2.54	0.48
1:B:183:PRO:O	1:B:187:LYS:HG2	2.13	0.48
1:B:22:THR:HG22	1:B:72:THR:HA	1.96	0.47
1:B:156:LYS:CE	1:B:157:ALA:HB3	2.43	0.47
1:B:162:THR:HG22	1:B:163:THR:O	2.15	0.47
1:A:147:ALA:HB3	1:A:195:GLN:HB3	1.96	0.47
1:B:49:TYR:HD2	1:B:55:PRO:HD3	1.78	0.47
1:B:114:SER:HB3	2:B:462:HOH:O	2.15	0.47
1:A:212:THR:HG22	1:B:215:SER:OXT	2.15	0.46
1:A:12:SER:HA	1:A:105:THR:O	2.15	0.46
1:A:123:GLU:O	1:A:124:GLU:C	2.53	0.46
1:B:67:SER:O	2:B:404:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLY:O	1:B:179:LEU:HA	2.15	0.46
1:B:20:ARG:HG3	1:B:72:THR:HG23	1.98	0.46
1:A:164:PRO:HA	1:A:174:ALA:O	2.15	0.46
1:A:92:ASP:O	1:A:94:ASN:ND2	2.49	0.46
1:B:54:ARG:HH11	1:B:54:ARG:HD2	1.48	0.46
1:B:70:THR:HG22	1:B:71:ALA:N	2.31	0.46
1:B:91:TRP:HZ3	1:B:95:ALA:CA	2.26	0.46
1:B:13:VAL:O	1:B:106(A):LEU:HB2	2.16	0.46
1:A:58:ILE:CG2	1:A:59:PRO:CD	2.95	0.45
1:A:3:GLU:HB3	1:A:26:GLU:OE2	2.15	0.45
1:B:160:GLU:O	1:B:177:SER:HA	2.16	0.45
1:B:42:GLN:HA	1:B:42:GLN:OE1	2.16	0.45
1:B:13:VAL:HG12	1:B:14:SER:N	2.29	0.45
1:B:47:VAL:HA	1:B:58:ILE:HG13	1.97	0.45
1:A:112:ALA:HB1	1:A:113:PRO:CD	2.46	0.45
1:A:127:ALA:O	1:A:128:ASN:CB	2.64	0.45
1:A:110:LYS:HE2	1:A:110:LYS:HB3	1.78	0.45
1:B:34:CYS:SG	1:B:49:TYR:CB	3.05	0.45
1:A:34:CYS:SG	2:A:331:HOH:O	2.61	0.45
1:B:22:THR:HG22	1:B:72:THR:CB	2.47	0.45
1:A:120:PRO:HB2	1:A:125:LEU:HD13	1.99	0.45
1:A:60:GLU:O	1:A:60:GLU:CD	2.54	0.45
1:A:58:ILE:HG22	1:A:59:PRO:HD2	1.99	0.45
1:B:17:GLN:HB3	1:B:18:THR:H	1.51	0.45
1:B:91:TRP:CZ3	1:B:95:ALA:O	2.69	0.45
1:A:64:GLY:HA2	1:A:72:THR:O	2.17	0.45
1:B:59:PRO:HD2	1:B:62:PHE:CE1	2.51	0.45
1:A:149:LYS:CA	1:A:153:SER:O	2.62	0.44
1:B:13:VAL:CG1	1:B:14:SER:N	2.79	0.44
1:A:14:SER:CB	1:A:17:GLN:OE1	2.65	0.44
1:B:66:SER:HA	1:B:70:THR:O	2.17	0.44
1:A:165:SER:O	1:A:173:TYR:HA	2.16	0.44
1:A:13:VAL:CG2	1:A:14:SER:N	2.81	0.44
1:B:24:SER:HG	1:B:70:THR:HG1	1.58	0.44
1:A:213:GLU:N	1:B:215:SER:OXT	2.50	0.44
2:A:476:HOH:O	1:B:163:THR:HG21	2.18	0.44
1:A:13:VAL:O	1:A:106:VAL:HA	2.18	0.44
1:B:193:SER:OG	1:B:208:THR:HG22	2.16	0.44
1:B:39:ARG:NH2	1:B:81:LEU:CD2	2.80	0.44
1:A:11:LEU:HD21	1:A:20:ARG:H	1.83	0.44
1:A:207:LYS:HB3	1:A:207:LYS:HE2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:O	1:A:163:THR:CG2	2.65	0.43
1:A:14:SER:HB2	1:A:17:GLN:OE1	2.18	0.43
1:A:80:THR:HG23	1:A:83:GLU:OE1	2.18	0.43
1:B:3:GLU:HG3	1:B:99:GLY:HA2	2.00	0.43
1:B:87:TYR:CE1	1:B:101:GLY:HA3	2.54	0.43
1:B:193:SER:CA	1:B:208:THR:HG22	2.48	0.43
1:A:167:GLN:N	1:A:172:LYS:O	2.50	0.43
1:B:91:TRP:CE3	1:B:95(A):SER:O	2.72	0.43
1:B:32:TYR:CE1	1:B:50:GLN:HG2	2.54	0.43
1:B:136:ILE:N	1:B:136:ILE:CD1	2.76	0.43
1:A:75:ILE:HD13	1:A:75:ILE:HG21	1.83	0.43
1:A:50:GLN:HE21	1:A:53:ARG:CG	2.32	0.42
1:A:114:SER:O	1:A:136:ILE:HA	2.19	0.42
1:B:39:ARG:HH21	1:B:81:LEU:CD2	2.31	0.42
1:B:114:SER:CB	2:B:462:HOH:O	2.67	0.42
1:B:94:ASN:O	1:B:95:ALA:HB3	2.20	0.42
1:B:11:LEU:O	1:B:104:LEU:HA	2.19	0.42
1:B:54:ARG:HA	1:B:55:PRO:HD2	1.67	0.42
1:B:89:GLN:HB3	1:B:89:GLN:HE21	1.41	0.42
1:B:6:GLN:HG2	1:B:7:PRO:HD2	2.02	0.42
1:A:91:TRP:CD2	1:A:96:VAL:HG12	2.55	0.42
1:B:96:VAL:HG12	1:B:96:VAL:O	2.19	0.42
1:B:97:VAL:CG1	1:B:98:PHE:N	2.83	0.42
1:A:21:ILE:HD11	1:A:104:LEU:HD12	2.02	0.42
1:A:35:TRP:CE2	1:A:73:LEU:HB2	2.55	0.42
1:A:166:LYS:HD2	1:A:171:ASN:OD1	2.20	0.42
1:A:162:THR:OG1	1:A:176:SER:N	2.47	0.42
1:A:159:VAL:HA	1:A:178:TYR:O	2.19	0.42
1:A:115:VAL:HG12	1:A:115:VAL:O	2.20	0.42
1:B:13:VAL:O	1:B:106(A):LEU:CD2	2.68	0.42
1:B:37:GLN:HA	1:B:85:ASP:O	2.20	0.42
1:B:11:LEU:HD22	1:B:21:ILE:HG12	2.02	0.42
1:B:2:TYR:N	1:B:2:TYR:CD1	2.87	0.42
1:A:36:TYR:CD1	1:A:46:VAL:HG12	2.50	0.41
1:A:103:LYS:HZ3	1:A:103:LYS:HB2	1.83	0.41
1:B:27:LYS:C	1:B:29:GLY:N	2.73	0.41
1:B:36:TYR:HE2	1:B:89:GLN:NE2	2.19	0.41
1:B:135:LEU:C	1:B:136:ILE:HD13	2.41	0.41
1:B:93:SER:OG	1:B:94:ASN:OD1	2.38	0.41
1:B:20:ARG:HA	1:B:73:LEU:O	2.20	0.41
1:B:156:LYS:NZ	1:B:157:ALA:CB	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:CD	1:B:157:ALA:H	2.34	0.41
1:B:182:THR:O	1:B:184:GLU:N	2.54	0.41
1:B:52:ASN:ND2	1:B:53:ARG:HG2	2.36	0.41
1:B:136:ILE:O	1:B:174:ALA:HA	2.20	0.41
1:B:83:GLU:OE1	1:B:105:THR:HG22	2.21	0.41
1:A:181:LEU:C	1:A:181:LEU:CD1	2.89	0.40
1:A:136:ILE:CG2	1:A:139:PHE:HE2	2.33	0.40
1:B:37:GLN:O	1:B:44:PRO:HA	2.20	0.40
1:B:122:SER:HA	1:B:125:LEU:HD12	2.03	0.40
1:A:39:ARG:HB3	2:A:312:HOH:O	2.21	0.40
1:A:20:ARG:HD3	1:A:20:ARG:HA	1.71	0.40
1:A:163:THR:O	1:A:164:PRO:C	2.58	0.40
1:A:150:ALA:HB1	1:A:189:HIS:CD2	2.57	0.40

All (2) 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:375:HOH:O	2:B:479:HOH:O[2_655]	2.12	0.08
1:B:215:SER:O	2:A:310:HOH:O[4_456]	2.16	0.04

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	210/212 (99%)	161 (77%)	33 (16%)	16 (8%)	1 1
1	B	210/212 (99%)	166 (79%)	27 (13%)	17 (8%)	1 1
All	All	420/424 (99%)	327 (78%)	60 (14%)	33 (8%)	1 1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	30	ASP
1	A	40	PRO
1	B	40	PRO
1	B	69	ASN
1	B	213	GLU
1	B	214	CYS
1	A	15	PRO
1	A	41	GLY
1	A	51	ASP
1	A	68	GLY
1	A	81	LEU
1	A	103	LYS
1	A	130	ALA
1	B	17	GLN
1	B	28	LEU
1	B	42	GLN
1	B	94	ASN
1	B	101	GLY
1	B	211	PRO
1	A	8	PRO
1	B	27	LYS
1	B	51	ASP
1	B	60	GLU
1	A	50	GLN
1	A	107	GLY
1	B	138	ASP
1	B	186	TRP
1	A	93	SER
1	B	198	HIS
1	A	198	HIS
1	A	7	PRO
1	B	13	VAL

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	181/181 (100%)	139 (77%)	42 (23%)	1 2
1	B	181/181 (100%)	139 (77%)	42 (23%)	1 2
All	All	362/362 (100%)	278 (77%)	84 (23%)	1 2

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	3	GLU
1	A	5	THR
1	A	17	GLN
1	A	20	ARG
1	A	27	LYS
1	A	28	LEU
1	A	37	GLN
1	A	42	GLN
1	A	50	GLN
1	A	51	ASP
1	A	54	ARG
1	A	56	SER
1	A	60	GLU
1	A	66	SER
1	A	73	LEU
1	A	74	THR
1	A	79	GLN
1	A	80	THR
1	A	81	LEU
1	A	91	TRP
1	A	94	ASN
1	A	98	PHE
1	A	103	LYS
1	A	105	THR
1	A	108	GLN
1	A	114	SER
1	A	116	THR
1	A	122	SER
1	A	138	ASP
1	A	144	VAL
1	A	149	LYS
1	A	152	SER
1	A	163	THR
1	A	179	LEU

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Mol	Chain	Res	Type
1	A	181	LEU
1	A	190	ARG
1	A	193	SER
1	A	207	LYS
1	A	208	THR
1	A	212	THR
1	A	214	CYS
1	B	5	THR
1	B	12	SER
1	B	24	SER
1	B	26	GLU
1	B	28	LEU
1	B	30	ASP
1	B	39	ARG
1	B	40	PRO
1	B	48	ILE
1	B	50	GLN
1	B	51	ASP
1	B	52	ASN
1	B	56	SER
1	B	69	ASN
1	B	73	LEU
1	B	75	ILE
1	B	80	THR
1	B	91	TRP
1	B	94	ASN
1	B	96	VAL
1	B	105	THR
1	B	106(A)	LEU
1	B	110	LYS
1	B	116	THR
1	B	134	CYS
1	B	135	LEU
1	B	136	ILE
1	B	149	LYS
1	B	151	ASP
1	B	152	SER
1	B	153	SER
1	B	156	LYS
1	B	165	SER
1	B	181	LEU
1	B	182	THR

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Mol	Chain	Res	Type
1	B	187	LYS
1	B	193	SER
1	B	197	THR
1	B	198	HIS
1	B	199	GLU
1	B	214	CYS
1	B	215	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	42	GLN
1	A	50	GLN
1	A	52	ASN
1	A	79	GLN
1	A	89	GLN
1	A	94	ASN
1	A	189	HIS
1	A	195	GLN
1	B	52	ASN
1	B	89	GLN
1	B	128	ASN
1	B	198	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	212/212 (100%)	-0.73	0	100	100	16, 16, 16, 16	0
1	B	212/212 (100%)	-0.73	0	100	100	16, 16, 16, 16	0
All	All	424/424 (100%)	-0.73	0	100	100	16, 16, 16, 16	0

There are no RSRZ outliers to report.

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.