Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 12:03 PM EST

PDB ID	:	8SBL
Title	:	Structure of HLA-A*24:02 in complex with peptide, LYLPVRVLI
Authors	:	Mallik, L.; Young, M.C.; Sgourakis, N.G.
Deposited on	:	2023-04-03
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

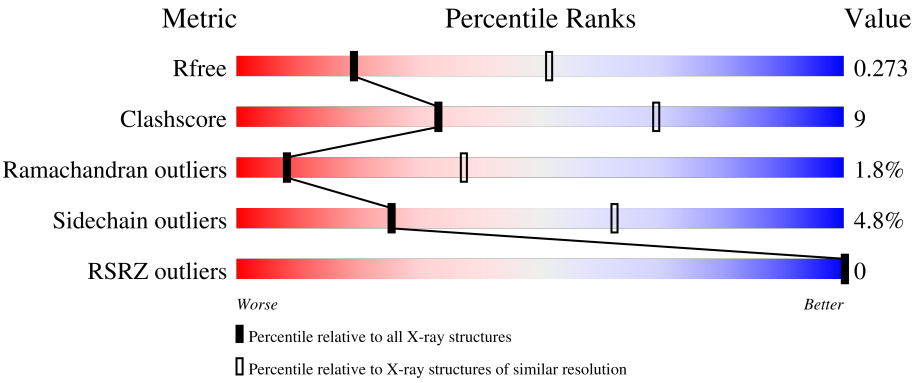
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	80% 16%
1	D	283	71% 23%
1	G	283	70% 25%
1	J	283	67% 29%
2	B	100	70% 27%

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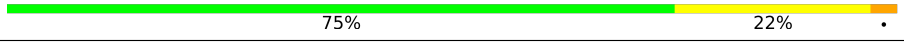
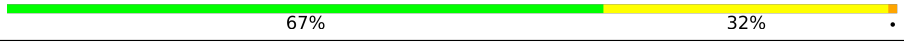
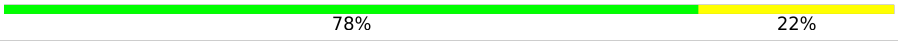
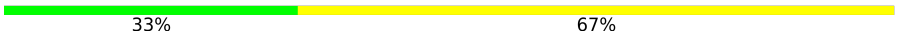
Mol	Chain	Length	Quality of chain
2	E	100	
2	H	100	
2	K	100	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12604 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2237	1392	405	430	10			
1	D	276	Total	C	N	O	S	0	0	0
			2237	1392	405	430	10			
1	G	276	Total	C	N	O	S	0	0	0
			2237	1392	405	430	10			
1	J	276	Total	C	N	O	S	0	0	0
			2237	1392	405	430	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A0A411J078
A	-1	ALA	-	expression tag	UNP A0A411J078
A	0	SER	-	expression tag	UNP A0A411J078
D	-2	MET	-	initiating methionine	UNP A0A411J078
D	-1	ALA	-	expression tag	UNP A0A411J078
D	0	SER	-	expression tag	UNP A0A411J078
G	-2	MET	-	initiating methionine	UNP A0A411J078
G	-1	ALA	-	expression tag	UNP A0A411J078
G	0	SER	-	expression tag	UNP A0A411J078
J	-2	MET	-	initiating methionine	UNP A0A411J078
J	-1	ALA	-	expression tag	UNP A0A411J078
J	0	SER	-	expression tag	UNP A0A411J078

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	K	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
E	1	MET	-	initiating methionine	UNP P61769
H	1	MET	-	initiating methionine	UNP P61769
K	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called LEU-TYR-LEU-PRO-VAL-ARG-VAL-LEU-ILE.

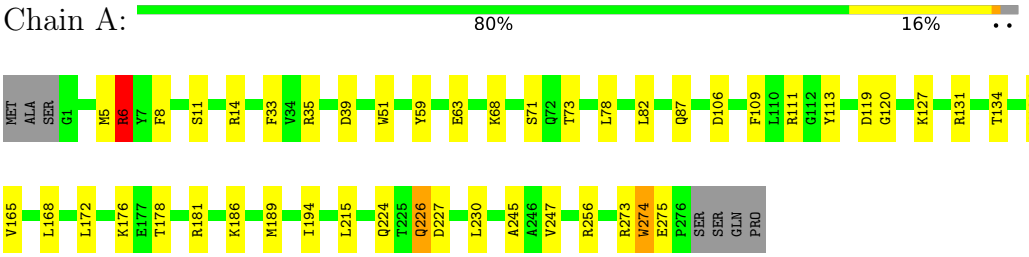
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			77	54	12	11			
3	F	9	Total	C	N	O	0	0	0
			77	54	12	11			
3	I	9	Total	C	N	O	0	0	0
			77	54	12	11			
3	L	9	Total	C	N	O	0	0	0
			77	54	12	11			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

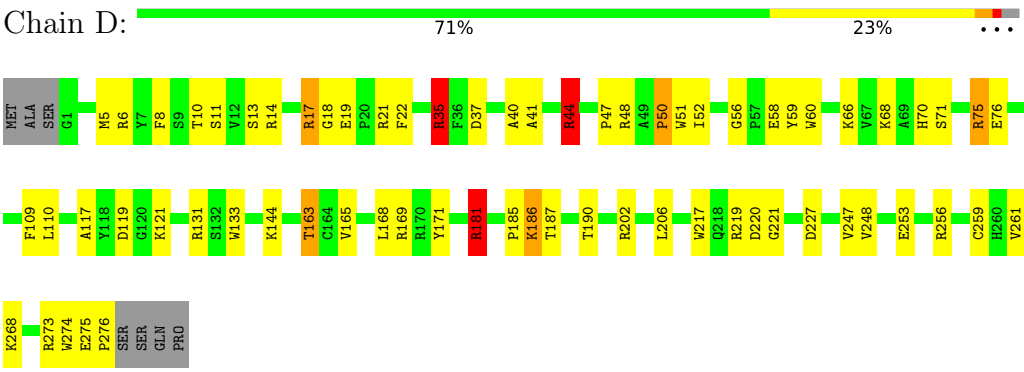
• Molecule 1: MHC class I antigen

Chain A:



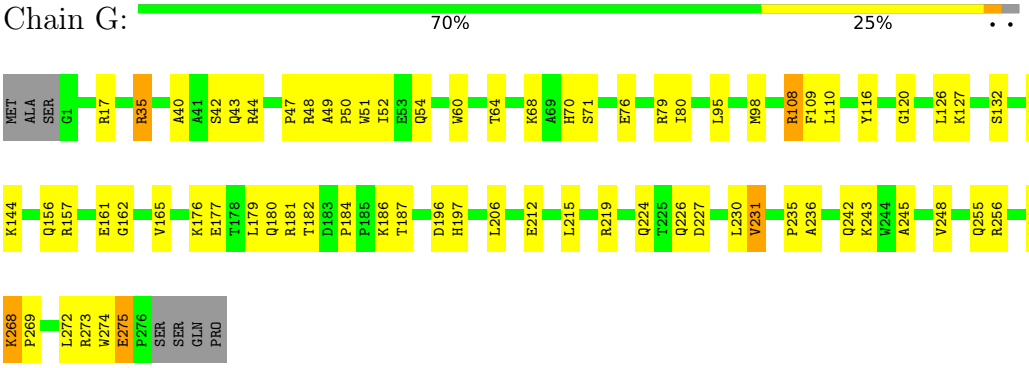
• Molecule 1: MHC class I antigen

Chain D:



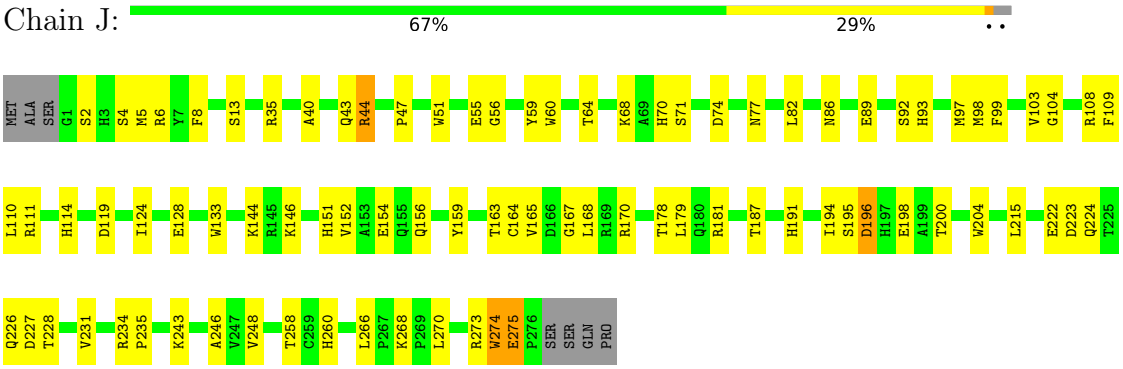
• Molecule 1: MHC class I antigen

Chain G:



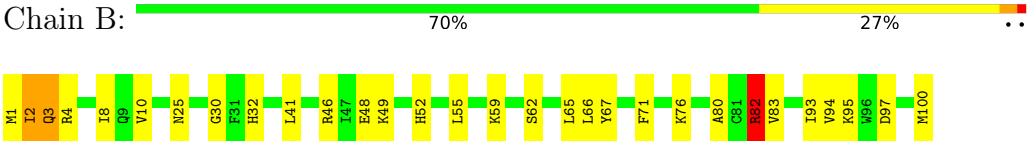
• Molecule 1: MHC class I antigen

Chain J:



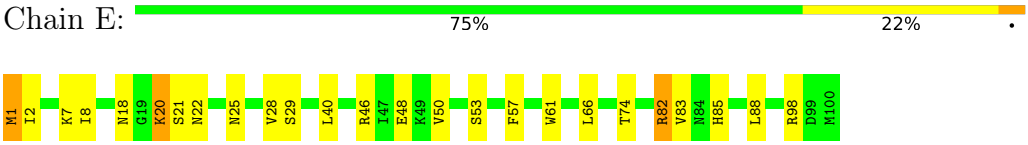
• Molecule 2: Beta-2-microglobulin

Chain B:



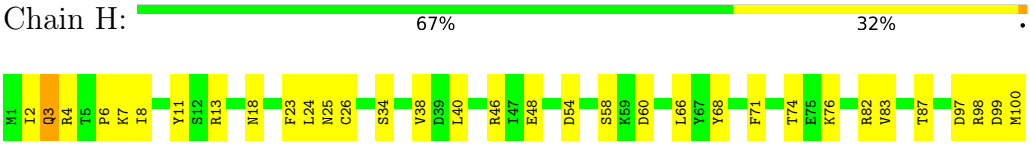
• Molecule 2: Beta-2-microglobulin

Chain E:



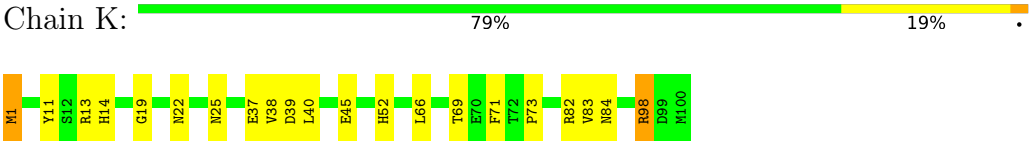
• Molecule 2: Beta-2-microglobulin

Chain H:



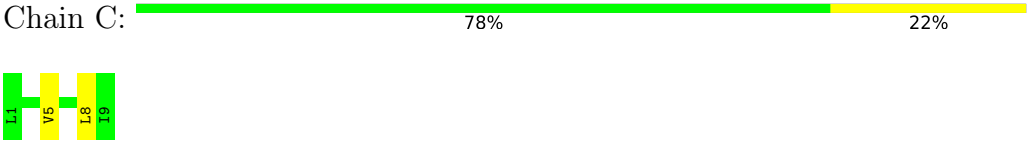
• Molecule 2: Beta-2-microglobulin

Chain K:



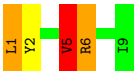
• Molecule 3: LEU-TYR-LEU-PRO-VAL-ARG-VAL-LEU-ILE

Chain C:



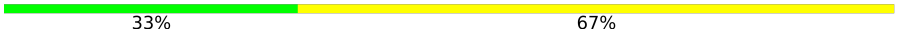
• Molecule 3: LEU-TYR-LEU-PRO-VAL-ARG-VAL-LEU-ILE

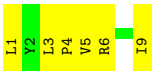
Chain F:



• Molecule 3: LEU-TYR-LEU-PRO-VAL-ARG-VAL-LEU-ILE

Chain I:





• Molecule 3: LEU-TYR-LEU-PRO-VAL-ARG-VAL-LEU-ILE

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.51Å 76.19Å 111.78Å 90.00° 109.76° 90.00°	Depositor
Resolution (Å)	105.19 – 3.00 105.20 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (105.19-3.00) 99.7 (105.20-3.00)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.193 , 0.270 0.210 , 0.273	Depositor DCC
R_{free} test set	2007 reflections (5.74%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12604	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	0/2298	0.71	0/3116
1	D	0.48	0/2298	0.73	0/3116
1	G	0.44	0/2298	0.73	0/3116
1	J	0.47	0/2298	0.72	0/3116
2	B	0.50	0/860	0.69	0/1162
2	E	0.49	0/860	0.71	0/1162
2	H	0.52	0/860	0.73	0/1162
2	K	0.49	0/860	0.69	0/1162
3	C	0.51	0/78	0.67	0/105
3	F	0.61	0/78	0.86	0/105
3	I	0.55	0/78	0.70	0/105
3	L	0.54	0/78	0.81	0/105
All	All	0.48	0/12944	0.72	0/17532

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	6
1	G	0	3
1	J	0	2
2	B	0	1
2	E	0	2
2	H	0	2
2	K	0	2
3	F	0	1
All	All	0	21

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	ARG	Sidechain
1	A	6	ARG	Sidechain
2	B	82	ARG	Sidechain
1	D	131	ARG	Sidechain
1	D	181	ARG	Sidechain
1	D	273	ARG	Sidechain
1	D	35	ARG	Sidechain
1	D	44	ARG	Sidechain
1	D	75	ARG	Sidechain
2	E	82	ARG	Sidechain
2	E	98	ARG	Sidechain
3	F	6	ARG	Sidechain
1	G	108	ARG	Sidechain
1	G	157	ARG	Sidechain
1	G	79	ARG	Sidechain
2	H	4	ARG	Sidechain
2	H	82	ARG	Sidechain
1	J	108	ARG	Sidechain
1	J	44	ARG	Sidechain
2	K	13	ARG	Sidechain
2	K	98	ARG	Sidechain

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	2237	0	2095	29	0
1	D	2237	0	2095	39	0
1	G	2237	0	2095	44	0
1	J	2237	0	2095	50	0
2	B	837	0	803	19	0
2	E	837	0	803	13	0
2	H	837	0	803	21	0
2	K	837	0	803	10	0
3	C	77	0	93	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	77	0	93	3	0
3	I	77	0	93	6	0
3	L	77	0	93	5	0
All	All	12604	0	11964	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (212) 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)
3:I:3:LEU:HD12	3:I:4:PRO:HD2	1.53	0.90
1:A:120:GLY:HA3	2:B:2:ILE:HG21	1.53	0.88
1:G:156:GLN:HE22	3:I:5:VAL:HG11	1.43	0.83
2:B:8:ILE:HG12	2:B:83:VAL:HG21	1.65	0.79
1:A:156:GLN:HE22	3:C:5:VAL:HG11	1.51	0.74
1:D:66:LYS:HE3	3:F:2:TYR:HB3	1.69	0.74
1:J:74:ASP:HA	1:J:77:ASN:HB2	1.70	0.73
2:B:25:ASN:HB3	2:B:66:LEU:HD11	1.70	0.73
2:H:18:ASN:OD1	2:H:98:ARG:NH2	2.21	0.72
1:G:70:HIS:HA	3:I:6:ARG:HD2	1.71	0.72
1:G:64:THR:HG22	1:G:68:LYS:HD2	1.72	0.71
1:G:35:ARG:NH1	2:H:54:ASP:OD1	2.22	0.71
2:K:25:ASN:HB3	2:K:66:LEU:HD11	1.71	0.70
3:I:5:VAL:O	3:I:6:ARG:NE	2.24	0.70
1:A:178:THR:HA	1:A:181:ARG:HH11	1.57	0.70
1:G:68:LYS:O	1:G:71:SER:HB3	1.91	0.70
1:A:131:ARG:HD2	1:A:157:ARG:NH1	2.07	0.69
1:J:70:HIS:HA	3:L:6:ARG:HD2	1.75	0.69
2:E:46:ARG:HH12	2:E:48:GLU:HG2	1.58	0.68
2:E:25:ASN:HB3	2:E:66:LEU:HD11	1.75	0.68
2:H:46:ARG:HH12	2:H:48:GLU:HG2	1.60	0.67
2:B:82:ARG:HG3	2:B:93:ILE:HG12	1.79	0.65
1:J:111:ARG:HD3	1:J:128:GLU:HG3	1.79	0.65
1:J:4:SER:HB2	1:J:6:ARG:HH12	1.61	0.64
1:D:253:GLU:OE1	1:D:256:ARG:NH1	2.32	0.63
1:J:68:LYS:O	1:J:71:SER:HB3	1.99	0.62
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.81	0.62
1:G:40:ALA:O	1:G:43:GLN:NE2	2.31	0.61
1:G:212:GLU:O	1:G:263:HIS:HD2	1.83	0.61
1:D:35:ARG:HG2	1:D:48:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:44:ARG:HD2	1:J:64:THR:HG21	1.83	0.60
1:J:156:GLN:HE22	3:L:5:VAL:HB	1.67	0.59
2:K:14:HIS:O	2:K:22:ASN:ND2	2.34	0.58
1:D:37:ASP:HB3	1:D:40:ALA:HB2	1.85	0.58
1:A:131:ARG:HD2	1:A:157:ARG:HH12	1.69	0.58
2:B:80:ALA:HB2	2:B:95:LYS:HD2	1.86	0.57
1:J:4:SER:HB2	1:J:6:ARG:NH1	2.19	0.57
1:J:235:PRO:HB2	2:K:66:LEU:HD22	1.85	0.57
1:D:121:LYS:HB2	2:E:2:ILE:HD13	1.85	0.57
2:H:46:ARG:NH1	2:H:48:GLU:HG2	2.18	0.57
2:B:46:ARG:HH12	2:B:48:GLU:HG2	1.69	0.56
1:J:8:PHE:CE1	1:J:98:MET:HG3	2.40	0.56
1:A:73:THR:HG23	3:C:8:LEU:HD12	1.87	0.56
1:A:6:ARG:HB3	1:A:8:PHE:CE1	2.40	0.56
1:G:196:ASP:OD1	1:G:197:HIS:NE2	2.39	0.56
1:D:68:LYS:O	1:D:71:SER:HB3	2.06	0.56
1:D:274:TRP:O	1:D:276:PRO:HD3	2.06	0.55
1:J:258:THR:HG22	1:J:273:ARG:HG3	1.87	0.55
2:K:38:VAL:HG22	2:K:83:VAL:HG22	1.89	0.55
1:A:178:THR:O	1:A:181:ARG:NH1	2.40	0.55
1:A:11:SER:HB3	1:A:78:LEU:HD11	1.88	0.55
1:G:227:ASP:HB3	1:G:248:VAL:HG22	1.88	0.55
1:G:231:VAL:O	1:G:243:LYS:NZ	2.41	0.54
1:D:70:HIS:HA	3:F:5:VAL:HG21	1.89	0.54
1:J:51:TRP:NE1	1:J:179:LEU:HD21	2.23	0.54
2:H:8:ILE:HG12	2:H:83:VAL:HG21	1.89	0.54
1:A:68:LYS:O	1:A:71:SER:HB3	2.07	0.53
1:D:8:PHE:HB3	2:E:57:PHE:CE2	2.43	0.53
1:G:64:THR:CG2	1:G:68:LYS:HD2	2.39	0.53
2:H:38:VAL:HG22	2:H:83:VAL:HG22	1.89	0.53
1:J:227:ASP:HB3	1:J:248:VAL:HG22	1.89	0.53
2:B:30:GLY:HA2	2:B:62:SER:OG	2.08	0.53
1:J:258:THR:HG1	1:J:260:HIS:HE2	1.57	0.53
2:B:97:ASP:HB3	2:B:100:MET:HB2	1.91	0.52
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.91	0.52
1:J:119:ASP:HB3	2:K:1:MET:HB2	1.91	0.52
1:J:40:ALA:O	1:J:43:GLN:NE2	2.42	0.52
1:J:8:PHE:HE1	1:J:98:MET:HG3	1.73	0.51
1:J:187:THR:HA	1:J:204:TRP:O	2.10	0.51
1:D:133:TRP:HB2	1:D:144:LYS:HG3	1.91	0.51
1:J:178:THR:O	1:J:181:ARG:NH1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:TYR:CD1	3:L:4:PRO:HD3	2.45	0.51
2:B:55:LEU:HA	2:B:65:LEU:HD21	1.93	0.51
1:D:41:ALA:HA	2:H:76:LYS:HD3	1.93	0.51
2:H:13:ARG:HB2	2:H:23:PHE:HB2	1.93	0.51
1:J:82:LEU:HD21	1:J:93:HIS:CD2	2.46	0.51
1:J:222:GLU:O	1:J:224:GLN:N	2.44	0.50
1:D:227:ASP:HB3	1:D:248:VAL:HG22	1.93	0.50
1:J:124:ILE:HD11	1:J:133:TRP:HB3	1.93	0.50
1:G:143:THR:HG23	3:I:9:ILE:HA	1.92	0.50
1:J:119:ASP:HB3	2:K:1:MET:CB	2.40	0.50
1:G:235:PRO:HG2	2:H:66:LEU:HD13	1.94	0.49
1:A:111:ARG:HG2	1:A:113:TYR:CZ	2.47	0.49
1:G:182:THR:O	1:G:184:PRO:HD3	2.13	0.49
1:D:117:ALA:HB2	2:E:61:TRP:CE2	2.48	0.49
2:E:20:LYS:HE3	2:E:20:LYS:HB2	1.54	0.49
1:G:230:LEU:HD13	1:G:245:ALA:HB2	1.94	0.49
2:H:26:CYS:HB2	2:H:40:LEU:HD21	1.95	0.49
1:J:164:CYS:O	1:J:167:GLY:N	2.46	0.49
1:G:35:ARG:HG3	1:G:48:ARG:HG3	1.95	0.48
2:E:40:LEU:HD12	2:E:50:VAL:HG22	1.95	0.48
1:J:231:VAL:O	1:J:243:LYS:NZ	2.46	0.48
2:E:46:ARG:NH1	2:E:48:GLU:HG2	2.27	0.48
1:G:177:GLU:O	1:G:181:ARG:HB3	2.13	0.48
1:D:163:THR:HG22	3:F:1:LEU:HD23	1.95	0.48
1:A:178:THR:HA	1:A:181:ARG:NH1	2.27	0.48
1:G:187:THR:HB	1:G:272:LEU:HD21	1.95	0.48
2:B:49:LYS:H	2:B:49:LYS:HD2	1.79	0.48
1:D:59:TYR:HH	1:D:171:TYR:HH	1.58	0.47
1:G:49:ALA:O	1:G:52:ILE:HG22	2.14	0.47
1:J:114:HIS:CD2	1:J:156:GLN:OE1	2.67	0.47
2:H:2:ILE:HG13	2:H:3:GLN:H	1.79	0.47
2:K:19:GLY:N	2:K:73:PRO:O	2.38	0.47
2:B:46:ARG:HH12	2:B:48:GLU:CG	2.27	0.47
1:D:14:ARG:HB2	1:D:17:ARG:HD2	1.97	0.47
1:D:76:GLU:HA	1:D:79:ARG:HG3	1.96	0.47
1:G:44:ARG:HD2	1:G:64:THR:HG21	1.97	0.47
1:D:50:PRO:O	1:D:52:ILE:N	2.47	0.47
2:E:53:SER:OG	2:E:66:LEU:N	2.42	0.46
1:G:95:LEU:HD11	1:G:116:TYR:HD1	1.80	0.46
1:D:35:ARG:O	1:D:35:ARG:HG3	2.16	0.46
1:J:104:GLY:N	1:J:110:LEU:HG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:40:LEU:HD13	2:K:69:THR:HG22	1.98	0.46
1:A:189:MET:HE2	1:A:274:TRP:HA	1.98	0.46
1:A:224:GLN:HG3	1:A:226:GLN:H	1.80	0.46
1:G:274:TRP:O	1:G:275:GLU:HG2	2.15	0.46
2:B:52:HIS:HB3	2:B:67:TYR:CD2	2.50	0.46
1:D:47:PRO:HB3	1:D:60:TRP:CH2	2.51	0.46
1:J:274:TRP:CG	1:J:275:GLU:N	2.84	0.46
2:E:18:ASN:HB3	2:E:74:THR:HA	1.98	0.46
2:B:41:LEU:HD23	2:B:46:ARG:HA	1.98	0.45
2:H:58:SER:HB2	2:H:60:ASP:OD1	2.17	0.45
1:J:5:MET:HB2	1:J:168:LEU:HD13	1.99	0.45
1:G:235:PRO:O	2:H:11:TYR:OH	2.17	0.45
1:G:236:ALA:O	2:H:13:ARG:HG3	2.17	0.45
1:J:51:TRP:CE2	1:J:179:LEU:HD21	2.51	0.45
2:B:10:VAL:HG21	2:B:94:VAL:O	2.17	0.45
1:D:186:LYS:HB2	1:D:186:LYS:HE2	1.41	0.45
1:G:206:LEU:HD23	1:G:242:GLN:NE2	2.31	0.45
1:D:185:PRO:HD3	1:D:263:HIS:CD2	2.51	0.45
1:J:144:LYS:HB3	1:J:144:LYS:HE2	1.80	0.45
1:J:156:GLN:HE22	3:L:5:VAL:CB	2.28	0.45
1:J:56:GLY:O	1:J:59:TYR:HB3	2.17	0.44
1:J:228:THR:HA	1:J:246:ALA:O	2.17	0.44
1:J:215:LEU:HD12	1:J:243:LYS:HD3	2.00	0.44
1:D:56:GLY:HA3	1:D:58:GLU:OE2	2.17	0.44
1:J:159:TYR:CD1	1:J:163:THR:HB	2.52	0.44
1:J:152:VAL:O	1:J:156:GLN:HG2	2.18	0.44
1:D:10:THR:O	1:D:22:PHE:HA	2.17	0.44
1:G:176:LYS:O	1:G:180:GLN:HB2	2.18	0.44
1:G:255:GLN:HB3	1:G:273:ARG:HD3	2.00	0.44
1:J:196:ASP:OD1	1:J:196:ASP:N	2.51	0.44
1:A:127:LYS:HG2	1:A:134:THR:OG1	2.18	0.44
2:E:8:ILE:HG12	2:E:83:VAL:HG21	1.99	0.44
2:H:99:ASP:O	2:H:100:MET:HG3	2.18	0.43
1:D:109:PHE:HB2	1:D:165:VAL:HG21	2.00	0.43
1:G:109:PHE:HB2	1:G:165:VAL:HG21	2.00	0.43
2:B:2:ILE:O	2:B:3:GLN:C	2.57	0.43
1:D:187:THR:HG21	1:D:261:VAL:HG21	2.00	0.43
2:H:74:THR:HB	1:J:195:SER:HA	2.00	0.43
1:J:235:PRO:HD2	2:K:11:TYR:OH	2.19	0.43
1:D:110:LEU:HD23	1:D:110:LEU:HA	1.82	0.43
3:L:6:ARG:HA	3:L:6:ARG:HD3	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD1	1:A:106:ASP:N	2.51	0.43
1:D:219:ARG:HD2	1:D:256:ARG:HH21	1.84	0.43
1:D:58:GLU:CD	1:D:58:GLU:H	2.21	0.43
1:D:44:ARG:HE	1:D:44:ARG:HB3	1.43	0.43
1:G:268:LYS:HB3	1:G:268:LYS:HE3	1.76	0.43
1:J:97:MET:HE1	1:J:99:PHE:CD2	2.53	0.43
1:G:219:ARG:HD2	1:G:256:ARG:NH2	2.33	0.43
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.93	0.42
1:D:119:ASP:HB3	2:E:1:MET:HA	2.01	0.42
1:J:55:GLU:OE1	1:J:170:ARG:NH1	2.53	0.42
1:J:151:HIS:HB2	1:J:154:GLU:CD	2.39	0.42
1:G:109:PHE:CD2	1:G:161:GLU:HA	2.54	0.42
1:J:2:SER:HB2	1:J:103:VAL:O	2.18	0.42
2:H:97:ASP:OD1	2:H:98:ARG:N	2.52	0.42
1:A:59:TYR:CZ	1:A:63:GLU:HG3	2.55	0.42
1:A:119:ASP:HB3	2:B:1:MET:HB2	2.02	0.42
1:G:35:ARG:HG3	1:G:48:ARG:CG	2.50	0.42
2:K:37:GLU:HB2	2:K:84:ASN:HB3	2.01	0.42
2:B:3:GLN:H	2:B:3:GLN:HG2	1.57	0.42
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.19	0.42
1:A:6:ARG:HA	1:A:6:ARG:HD3	1.81	0.42
1:A:33:PHE:HB3	1:A:51:TRP:CZ2	2.54	0.42
1:A:82:LEU:HD22	1:A:87:GLN:HB2	2.01	0.42
1:G:126:LEU:HD12	1:G:132:SER:O	2.20	0.42
1:A:109:PHE:HB2	1:A:165:VAL:HG21	2.01	0.42
2:E:85:HIS:HB3	2:E:88:LEU:HG	2.02	0.42
2:H:25:ASN:HB3	2:H:66:LEU:HD11	2.02	0.42
1:J:191:HIS:HA	1:J:200:THR:O	2.19	0.42
1:A:273:ARG:HB2	1:A:273:ARG:NH1	2.35	0.42
1:A:156:GLN:NE2	3:C:5:VAL:HG11	2.27	0.41
1:G:120:GLY:HA3	2:H:2:ILE:HG12	2.02	0.41
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.02	0.41
1:G:141:GLN:HA	1:G:144:LYS:HB3	2.02	0.41
1:D:181:ARG:HE	1:D:181:ARG:HB3	1.69	0.41
1:G:47:PRO:HB3	1:G:60:TRP:CH2	2.55	0.41
1:G:137:ASP:O	1:G:141:GLN:HG3	2.19	0.41
2:H:24:LEU:O	2:H:68:TYR:HA	2.20	0.41
1:G:51:TRP:CZ2	1:G:179:LEU:HD11	2.55	0.41
1:G:110:LEU:HD23	1:G:110:LEU:HA	1.83	0.41
1:G:42:SER:O	1:G:44:ARG:HG2	2.21	0.41
2:H:6:PRO:HD2	2:H:87:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:NH2	1:A:39:ASP:OD1	2.50	0.41
1:J:109:PHE:HB2	1:J:165:VAL:HG21	2.02	0.41
1:A:189:MET:CE	1:A:274:TRP:HA	2.51	0.41
2:B:4:ARG:HH21	2:B:62:SER:HB3	1.86	0.41
1:D:5:MET:O	1:D:6:ARG:HD3	2.21	0.41
1:G:127:LYS:HD3	1:G:132:SER:OG	2.21	0.41
1:G:215:LEU:CD2	1:G:261:VAL:HG22	2.50	0.41
1:J:194:ILE:HG13	1:J:198:GLU:HB3	2.03	0.41
1:D:266:LEU:HA	1:D:267:PRO:HD2	1.89	0.41
2:B:3:GLN:HA	2:B:32:HIS:O	2.21	0.40
1:D:13:SER:HG	1:D:93:HIS:H	1.63	0.40
1:D:35:ARG:HB3	1:D:48:ARG:HG3	2.03	0.40
1:G:196:ASP:OD1	1:G:197:HIS:CD2	2.74	0.40
3:I:1:LEU:HA	3:I:1:LEU:HD23	1.66	0.40
1:D:217:TRP:CD1	1:D:247:VAL:HG13	2.56	0.40
1:G:76:GLU:O	1:G:80:ILE:HG13	2.22	0.40
1:J:47:PRO:HB3	1:J:60:TRP:CH2	2.56	0.40
1:J:266:LEU:HD13	1:J:270:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	274/283 (97%)	249 (91%)	21 (8%)	4 (2%)	10 42
1	D	274/283 (97%)	247 (90%)	21 (8%)	6 (2%)	6 31
1	G	274/283 (97%)	246 (90%)	20 (7%)	8 (3%)	4 24
1	J	274/283 (97%)	240 (88%)	28 (10%)	6 (2%)	6 31
2	B	98/100 (98%)	94 (96%)	2 (2%)	2 (2%)	7 34
2	E	98/100 (98%)	94 (96%)	4 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	98/100 (98%)	92 (94%)	5 (5%)	1 (1%)	15 53
2	K	98/100 (98%)	92 (94%)	6 (6%)	0	100 100
3	C	7/9 (78%)	3 (43%)	4 (57%)	0	100 100
3	F	7/9 (78%)	4 (57%)	2 (29%)	1 (14%)	0 1
3	I	7/9 (78%)	4 (57%)	3 (43%)	0	100 100
3	L	7/9 (78%)	5 (71%)	2 (29%)	0	100 100
All	All	1516/1568 (97%)	1370 (90%)	118 (8%)	28 (2%)	8 37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ILE
1	G	226	GLN
1	J	223	ASP
1	J	226	GLN
1	J	274	TRP
1	A	226	GLN
1	A	274	TRP
2	B	2	ILE
2	B	3	GLN
1	D	17	ARG
1	D	51	TRP
3	F	5	VAL
1	G	17	ARG
2	H	3	GLN
1	J	86	ASN
1	D	220	ASP
1	G	54	GLN
1	G	162	GLY
1	G	267	PRO
1	D	50	PRO
1	G	275	GLU
1	A	275	GLU
1	J	89	GLU
1	J	275	GLU
1	G	269	PRO
1	D	221	GLY
1	G	50	PRO
1	D	18	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	232/238 (98%)	224 (97%)	8 (3%)	37 72
1	D	232/238 (98%)	217 (94%)	15 (6%)	17 50
1	G	232/238 (98%)	225 (97%)	7 (3%)	41 75
1	J	232/238 (98%)	225 (97%)	7 (3%)	41 75
2	B	95/95 (100%)	91 (96%)	4 (4%)	30 66
2	E	95/95 (100%)	87 (92%)	8 (8%)	11 38
2	H	95/95 (100%)	92 (97%)	3 (3%)	39 74
2	K	95/95 (100%)	88 (93%)	7 (7%)	13 44
3	C	9/9 (100%)	9 (100%)	0	100 100
3	F	9/9 (100%)	6 (67%)	3 (33%)	0 1
3	I	9/9 (100%)	9 (100%)	0	100 100
3	L	9/9 (100%)	7 (78%)	2 (22%)	1 4
All	All	1344/1368 (98%)	1280 (95%)	64 (5%)	25 62

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	35	ARG
1	A	138	MET
1	A	176	LYS
1	A	186	LYS
1	A	215	LEU
1	A	227	ASP
1	A	247	VAL
2	B	59	LYS
2	B	71	PHE
2	B	76	LYS
2	B	82	ARG
1	D	11	SER
1	D	19	GLU

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Mol	Chain	Res	Type
1	D	21	ARG
1	D	35	ARG
1	D	44	ARG
1	D	75	ARG
1	D	97	MET
1	D	163	THR
1	D	169	ARG
1	D	181	ARG
1	D	186	LYS
1	D	206	LEU
1	D	259	CYS
1	D	268	LYS
1	D	275	GLU
2	E	1	MET
2	E	7	LYS
2	E	20	LYS
2	E	21	SER
2	E	22	ASN
2	E	28	VAL
2	E	29	SER
2	E	82	ARG
3	F	1	LEU
3	F	5	VAL
3	F	6	ARG
1	G	35	ARG
1	G	98	MET
1	G	108	ARG
1	G	186	LYS
1	G	224	GLN
1	G	231	VAL
1	G	268	LYS
2	H	7	LYS
2	H	34	SER
2	H	71	PHE
1	J	13	SER
1	J	35	ARG
1	J	92	SER
1	J	146	LYS
1	J	196	ASP
1	J	234	ARG
1	J	268	LYS
2	K	1	MET

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Mol	Chain	Res	Type
2	K	39	ASP
2	K	45	GLU
2	K	52	HIS
2	K	71	PHE
2	K	82	ARG
2	K	98	ARG
3	L	1	LEU
3	L	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	D	156	GLN
1	D	192	HIS
1	G	156	GLN

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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	276/283 (97%)	-0.42	0	100	100	17, 32, 51, 62	0
1	D	276/283 (97%)	-0.50	0	100	100	15, 29, 47, 76	0
1	G	276/283 (97%)	-0.43	0	100	100	21, 32, 53, 76	0
1	J	276/283 (97%)	-0.39	0	100	100	22, 34, 50, 74	0
2	B	100/100 (100%)	-0.50	0	100	100	19, 30, 53, 59	0
2	E	100/100 (100%)	-0.43	0	100	100	19, 33, 51, 64	0
2	H	100/100 (100%)	-0.49	0	100	100	16, 29, 49, 62	0
2	K	100/100 (100%)	-0.48	0	100	100	21, 31, 49, 59	0
3	C	9/9 (100%)	-0.19	0	100	100	26, 30, 36, 37	0
3	F	9/9 (100%)	-0.20	0	100	100	20, 24, 34, 37	0
3	I	9/9 (100%)	-0.18	0	100	100	27, 33, 45, 54	0
3	L	9/9 (100%)	-0.23	0	100	100	30, 32, 43, 43	0
All	All	1540/1568 (98%)	-0.44	0	100	100	15, 32, 51, 76	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 monosaccharides 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.