



Full wwPDB X-ray Structure Validation Report

(i)

Jun 24, 2024 – 06:30 PM EDT

PDB ID : 6NMR
Title : Blocking Fab 119 anti-SIRP-alpha antibody in complex with SIRP-alpha Variant 1
Authors : Wibowo, A.S.; Carter, J.J.; Sim, J.
Deposited on : 2019-01-11
Resolution : 2.42 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

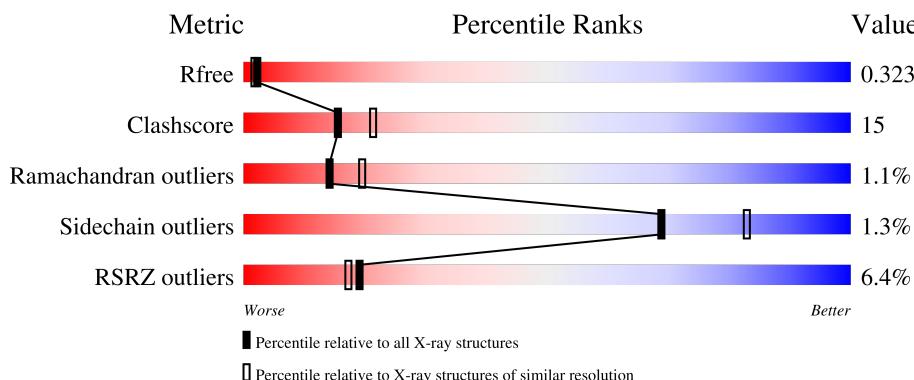
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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.



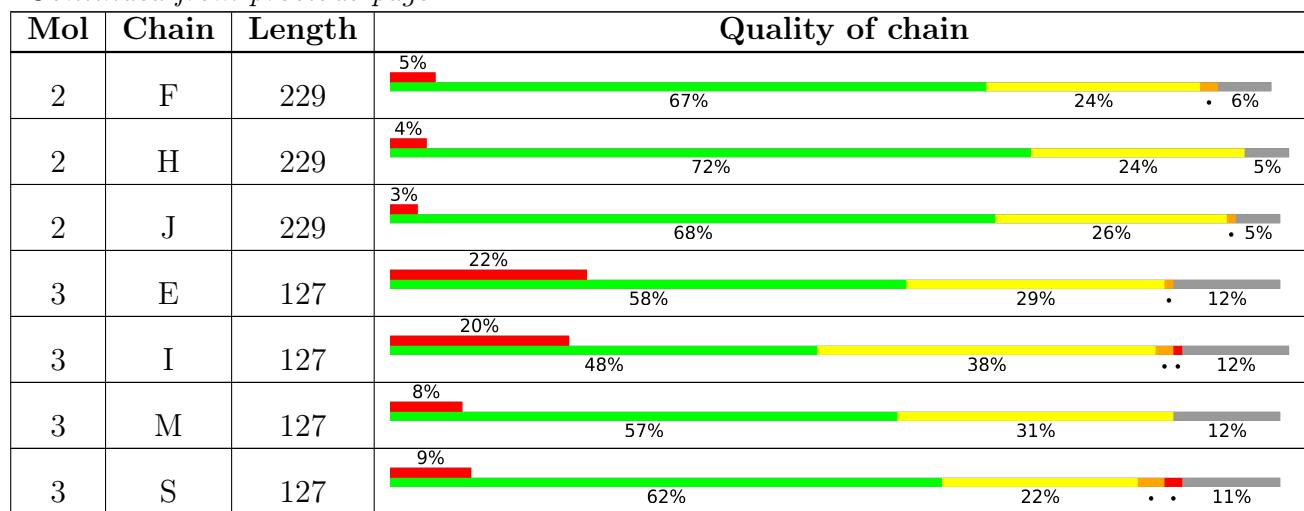
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 $\leq 5\%$. 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.



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16599 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 Fab 119 anti-SIRP-alpha antibody Variable Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
		1645	1035	277	329	4				
1	B	213	Total	C	N	O	S	0	0	0
		1624	1023	272	325	4				
1	G	214	Total	C	N	O	S	0	0	0
		1649	1037	276	332	4				
1	K	213	Total	C	N	O	S	0	0	0
		1627	1029	274	320	4				

- Molecule 2 is a protein called Fab 119 anti-SIRP-alpha antibody Variable Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
		1611	1019	264	322	6				
2	A	217	Total	C	N	O	S	0	0	0
		1601	1013	262	320	6				
2	F	215	Total	C	N	O	S	0	0	0
		1578	999	258	315	6				
2	J	218	Total	C	N	O	S	0	0	0
		1601	1013	265	317	6				

- Molecule 3 is a protein called Tyrosine-protein phosphatase non-receptor type substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	113	Total	C	N	O	S	0	0	0
		853	537	151	162	3				
3	E	112	Total	C	N	O	S	0	0	0
		808	508	144	153	3				
3	I	112	Total	C	N	O	S	0	0	0
		828	524	147	154	3				
3	M	112	Total	C	N	O	S	0	0	0
		832	525	147	158	2				

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	80	ALA	ASN	conflict	UNP P78324
S	120	THR	-	expression tag	UNP P78324
S	121	ARG	-	expression tag	UNP P78324
S	122	HIS	-	expression tag	UNP P78324
S	123	HIS	-	expression tag	UNP P78324
S	124	HIS	-	expression tag	UNP P78324
S	125	HIS	-	expression tag	UNP P78324
S	126	HIS	-	expression tag	UNP P78324
S	127	HIS	-	expression tag	UNP P78324
E	80	ALA	ASN	conflict	UNP P78324
E	120	THR	-	expression tag	UNP P78324
E	121	ARG	-	expression tag	UNP P78324
E	122	HIS	-	expression tag	UNP P78324
E	123	HIS	-	expression tag	UNP P78324
E	124	HIS	-	expression tag	UNP P78324
E	125	HIS	-	expression tag	UNP P78324
E	126	HIS	-	expression tag	UNP P78324
E	127	HIS	-	expression tag	UNP P78324
I	80	ALA	ASN	conflict	UNP P78324
I	120	THR	-	expression tag	UNP P78324
I	121	ARG	-	expression tag	UNP P78324
I	122	HIS	-	expression tag	UNP P78324
I	123	HIS	-	expression tag	UNP P78324
I	124	HIS	-	expression tag	UNP P78324
I	125	HIS	-	expression tag	UNP P78324
I	126	HIS	-	expression tag	UNP P78324
I	127	HIS	-	expression tag	UNP P78324
M	80	ALA	ASN	conflict	UNP P78324
M	120	THR	-	expression tag	UNP P78324
M	121	ARG	-	expression tag	UNP P78324
M	122	HIS	-	expression tag	UNP P78324
M	123	HIS	-	expression tag	UNP P78324
M	124	HIS	-	expression tag	UNP P78324
M	125	HIS	-	expression tag	UNP P78324
M	126	HIS	-	expression tag	UNP P78324
M	127	HIS	-	expression tag	UNP P78324

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	53	Total O 53 53	0	0

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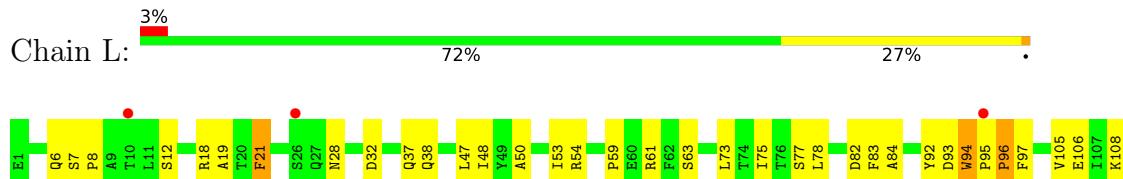
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	32	Total O 32 32	0	0
4	S	19	Total O 19 19	0	0
4	B	55	Total O 55 55	0	0
4	A	28	Total O 28 28	0	0
4	E	13	Total O 13 13	0	0
4	G	42	Total O 42 42	0	0
4	F	17	Total O 17 17	0	0
4	I	6	Total O 6 6	0	0
4	K	35	Total O 35 35	0	0
4	J	28	Total O 28 28	0	0
4	M	14	Total O 14 14	0	0

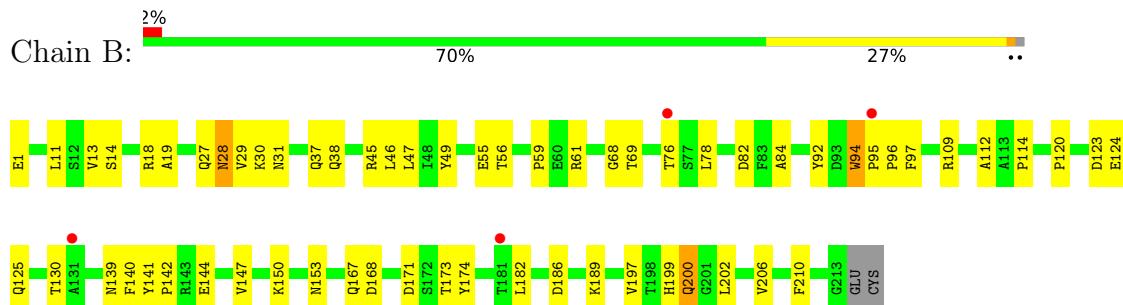
3 Residue-property plots

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.

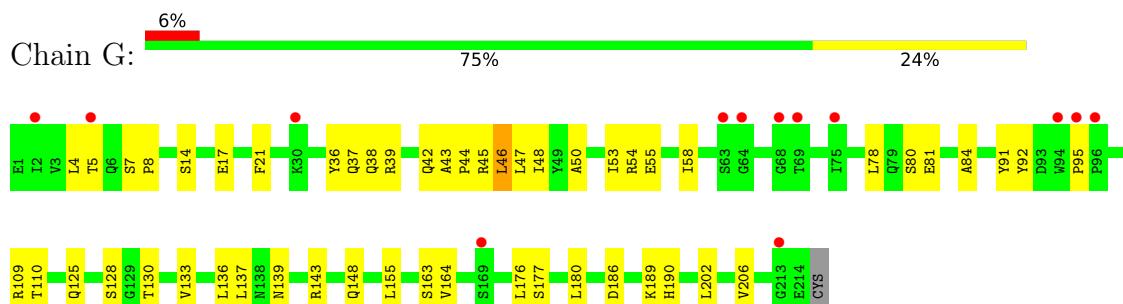
- Molecule 1: Fab 119 anti-SIRP-alpha antibody Variable Light Chain



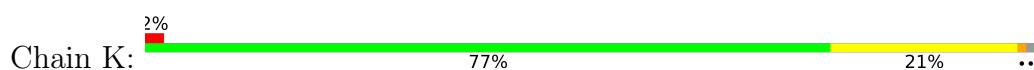
- Molecule 1: Fab 119 anti-SIRP-alpha antibody Variable Light Chain

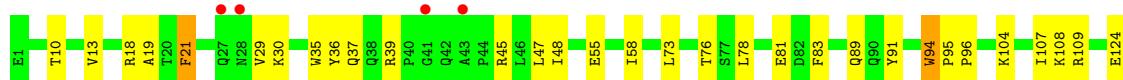


- Molecule 1: Fab 119 anti-SIRP-alpha antibody Variable Light Chain



- Molecule 1: Fab 119 anti-SIRP-alpha antibody Variable Light Chain





- Molecule 2: Fab 119 anti-SIRP-alpha antibody Variable Heavy Chain



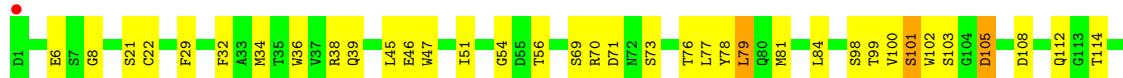
- Molecule 2: Fab 119 anti-SIRP-alpha antibody Variable Heavy Chain

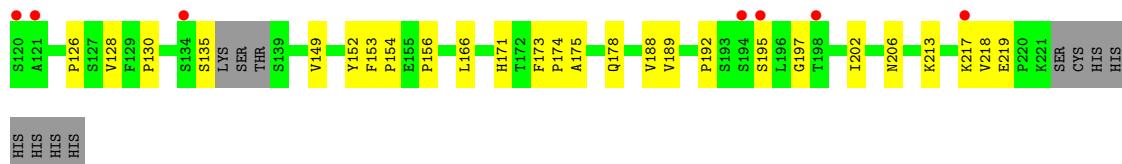


- Molecule 2: Fab 119 anti-SIRP-alpha antibody Variable Heavy Chain

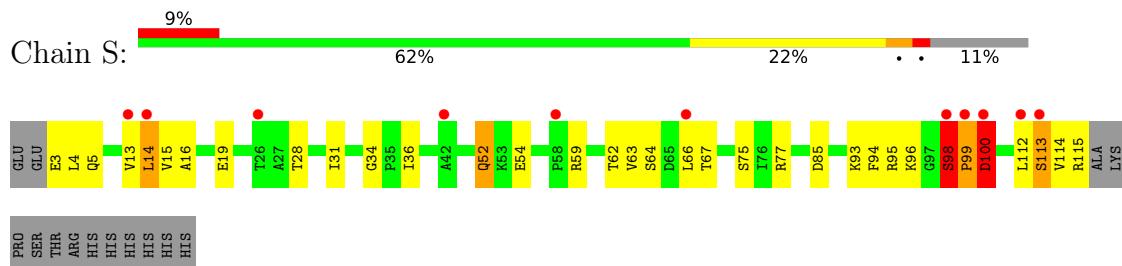


- Molecule 2: Fab 119 anti-SIRP-alpha antibody Variable Heavy Chain

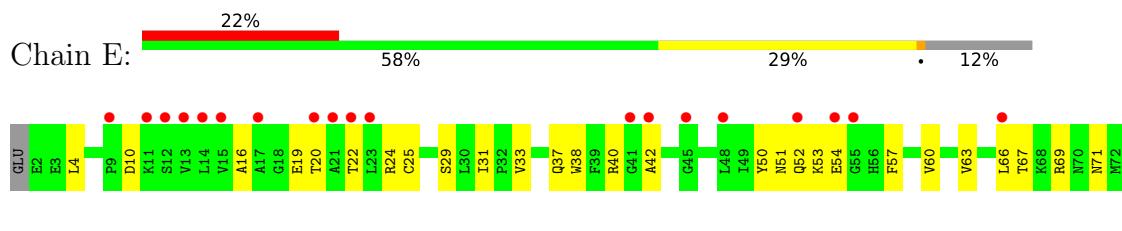




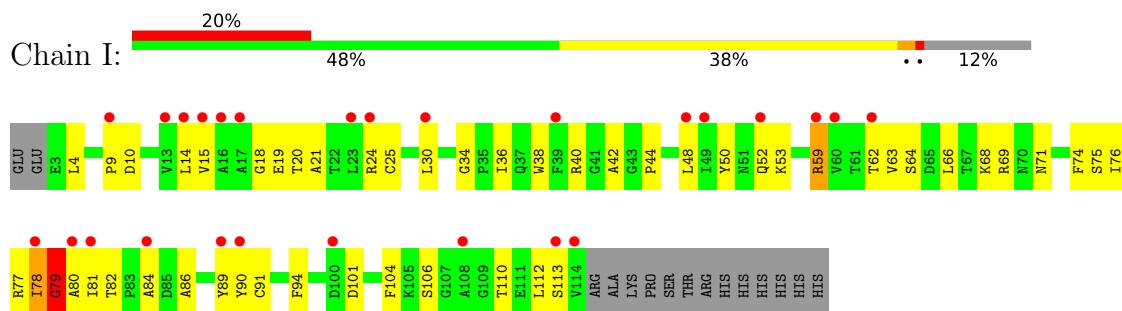
- Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1



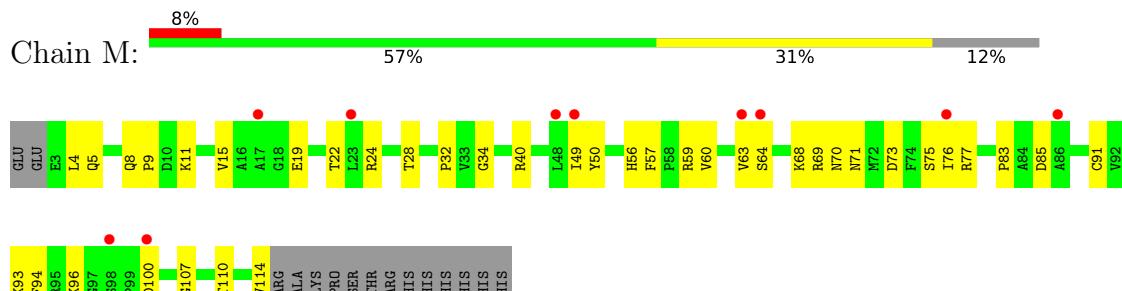
- Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1



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- Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.07 Å 113.56 Å 152.08 Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	38.01 – 2.42 38.01 – 2.42	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.01-2.42) 90.9 (38.01-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle^1$	1.46 (at 2.42 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R , R_{free}	0.288 , 0.323 0.288 , 0.323	Depositor DCC
R_{free} test set	4000 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.207 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16599	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

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	B	0.34	0/1663	0.60	2/2268 (0.1%)
1	G	0.28	0/1686	0.53	0/2293
1	K	0.28	0/1666	0.51	0/2267
1	L	0.33	0/1684	0.55	0/2295
2	A	0.32	0/1640	0.57	0/2238
2	F	0.32	0/1617	0.60	0/2211
2	H	0.28	0/1650	0.52	0/2251
2	J	0.34	0/1640	0.58	0/2239
3	E	0.31	0/824	0.63	1/1122 (0.1%)
3	I	0.49	0/845	0.82	6/1150 (0.5%)
3	M	0.30	0/849	0.59	0/1155
3	S	0.39	0/870	1.08	8/1182 (0.7%)
All	All	0.33	0/16634	0.62	17/22671 (0.1%)

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	B	0	2
1	K	0	1
1	L	0	2
2	F	0	1
3	E	0	1
3	S	0	1
All	All	0	8

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	S	14	LEU	CB-CG-CD2	-17.39	81.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	14	LEU	CB-CG-CD1	14.14	135.04	111.00
3	S	14	LEU	CA-CB-CG	8.82	135.59	115.30
3	S	100	ASP	N-CA-CB	8.73	126.31	110.60
3	I	59	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	B	200	GLN	CB-CA-C	-7.42	95.55	110.40
3	I	10	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	200	GLN	CA-CB-CG	6.65	128.03	113.40
3	I	59	ARG	CG-CD-NE	-6.60	97.94	111.80
3	S	100	ASP	CB-CA-C	-6.54	97.32	110.40
3	S	99	PRO	C-N-CA	6.46	137.86	121.70
3	I	10	ASP	CB-CG-OD1	6.06	123.75	118.30
3	S	113	SER	CB-CA-C	5.90	121.31	110.10
3	I	79	GLY	N-CA-C	5.24	126.19	113.10
3	S	100	ASP	CB-CG-OD1	-5.14	113.67	118.30
3	I	78	ILE	C-N-CA	5.05	132.90	122.30
3	E	66	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	30	LYS	Peptide
1	B	94	TRP	Peptide
3	E	98	SER	Peptide
2	F	153	PHE	Peptide
1	K	94	TRP	Peptide
1	L	7	SER	Peptide
1	L	94	TRP	Peptide
3	S	98	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1624	0	1534	54	0
1	G	1649	0	1583	39	1
1	K	1627	0	1555	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1645	0	1564	46	1
2	A	1601	0	1528	41	0
2	F	1578	0	1482	54	0
2	H	1611	0	1541	43	0
2	J	1601	0	1518	52	0
3	E	808	0	760	37	0
3	I	828	0	810	55	0
3	M	832	0	812	35	0
3	S	853	0	840	36	0
4	A	28	0	0	11	0
4	B	55	0	0	13	0
4	E	13	0	0	3	0
4	F	17	0	0	9	0
4	G	42	0	0	9	0
4	H	32	0	0	10	0
4	I	6	0	0	3	0
4	J	28	0	0	9	0
4	K	35	0	0	5	0
4	L	53	0	0	16	0
4	M	14	0	0	0	0
4	S	19	0	0	5	0
All	All	16599	0	15527	471	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (471) 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:S:14:LEU:HD23	3:S:113:SER:HB3	1.27	1.17
2:J:98:SER:OG	3:M:69:ARG:NH1	1.82	1.11
2:J:108:ASP:OD1	3:M:69:ARG:NH2	1.90	1.05
2:J:108:ASP:CG	3:M:69:ARG:HH22	1.62	1.03
1:L:54:ARG:NH1	4:L:302:HOH:O	1.90	1.01
3:S:14:LEU:CD2	3:S:113:SER:HB3	1.96	0.95
2:A:68:ILE:O	4:A:301:HOH:O	1.84	0.95
2:F:173:PHE:O	4:F:301:HOH:O	1.84	0.95
1:K:76:THR:O	4:K:301:HOH:O	1.87	0.93
2:J:102:TRP:HE1	3:M:64:SER:HG	1.08	0.93
3:I:20:THR:CG2	3:I:77:ARG:HG3	1.98	0.92
2:H:127:SER:OG	4:H:301:HOH:O	1.87	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:64:SER:OG	4:S:201:HOH:O	1.89	0.90
1:B:139:ASN:HA	1:B:173:THR:HG21	1.51	0.90
3:E:101:ASP:OD1	4:E:201:HOH:O	1.90	0.90
1:L:199:HIS:O	4:L:301:HOH:O	1.89	0.89
2:J:69:SER:HB2	2:J:78:TYR:HB2	1.54	0.89
3:I:63:VAL:O	4:I:201:HOH:O	1.90	0.89
3:E:10:ASP:OD1	4:E:202:HOH:O	1.91	0.89
1:L:200:GLN:NE2	4:L:304:HOH:O	1.98	0.88
2:J:108:ASP:CG	3:M:69:ARG:NH2	2.27	0.87
2:J:76:THR:O	4:J:301:HOH:O	1.93	0.86
2:J:197:GLY:O	4:J:302:HOH:O	1.94	0.86
2:A:6:GLU:O	4:A:302:HOH:O	1.94	0.84
3:I:63:VAL:HG11	3:I:75:SER:HB2	1.58	0.84
3:I:19:GLU:HG3	3:I:20:THR:N	1.93	0.84
1:B:139:ASN:O	4:B:301:HOH:O	1.98	0.82
1:B:139:ASN:HA	1:B:173:THR:CG2	2.10	0.82
1:G:55:GLU:OE2	3:I:69:ARG:NH1	2.12	0.81
1:L:75:ILE:O	4:L:303:HOH:O	1.97	0.81
2:A:39:GLN:NE2	4:A:304:HOH:O	2.13	0.81
2:A:151:ASP:OD1	4:A:303:HOH:O	2.00	0.79
2:F:17:SER:OG	4:F:302:HOH:O	2.01	0.79
2:H:218:VAL:O	4:H:302:HOH:O	2.00	0.78
1:B:1:GLU:OE1	4:B:302:HOH:O	2.00	0.78
2:F:71:ASP:O	4:F:303:HOH:O	2.01	0.78
2:J:73:SER:OG	4:J:303:HOH:O	2.00	0.77
3:I:30:LEU:HD13	3:I:30:LEU:O	1.83	0.77
2:H:155:GLU:O	4:H:303:HOH:O	2.02	0.76
2:H:96:LYS:NZ	4:H:308:HOH:O	2.17	0.76
2:A:128:VAL:HG22	2:A:149:VAL:HG22	1.68	0.76
1:B:124:GLU:OE1	4:B:304:HOH:O	2.04	0.76
2:A:70:ARG:HE	2:A:72:ASN:HD21	1.33	0.76
2:A:29:PHE:O	2:A:70:ARG:NH1	2.20	0.75
1:B:45:ARG:NH2	4:B:306:HOH:O	2.09	0.75
3:I:20:THR:HG22	3:I:77:ARG:HG3	1.69	0.75
2:H:219:GLU:OE2	4:H:304:HOH:O	2.05	0.74
1:B:168:ASP:OD1	4:B:303:HOH:O	2.03	0.74
2:F:153:PHE:O	2:F:155:GLU:N	2.16	0.74
2:F:102:TRP:HB3	3:I:52:GLN:HG3	1.69	0.74
3:S:59:ARG:NH2	3:S:85:ASP:OD2	2.22	0.72
1:G:46:LEU:HD23	1:G:55:GLU:HG3	1.70	0.72
2:H:112:GLN:O	4:H:305:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:19:GLU:HG3	3:I:20:THR:H	1.52	0.72
1:G:36:TYR:CZ	1:G:46:LEU:HD12	2.24	0.72
2:F:133:PRO:HD2	2:F:220:PRO:HG3	1.70	0.72
2:F:150:LYS:NZ	4:F:306:HOH:O	2.22	0.72
1:K:37:GLN:HB2	1:K:47:LEU:HD11	1.72	0.71
1:B:199:HIS:O	4:B:305:HOH:O	2.09	0.70
1:K:83:PHE:CZ	1:K:107:ILE:HG13	2.27	0.70
3:M:5:GLN:H	3:M:28:THR:HB	1.56	0.69
1:G:190:HIS:ND1	4:G:305:HOH:O	2.24	0.69
1:L:139:ASN:O	4:L:305:HOH:O	2.10	0.69
2:F:72:ASN:HA	4:F:303:HOH:O	1.92	0.69
2:F:126:PRO:HB3	2:F:152:TYR:HB3	1.73	0.68
1:L:113:ALA:O	4:L:305:HOH:O	2.12	0.68
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.75	0.68
3:I:15:VAL:HG23	3:I:19:GLU:HG2	1.76	0.67
1:K:37:GLN:OE1	1:K:45:ARG:NH2	2.27	0.67
1:G:17:GLU:O	1:G:78:LEU:HD23	1.94	0.67
2:F:128:VAL:HG11	2:F:205:VAL:HG11	1.77	0.67
3:I:19:GLU:O	3:I:80:ALA:HA	1.95	0.67
2:A:89:THR:HA	4:A:305:HOH:O	1.94	0.66
1:B:123:ASP:N	4:B:304:HOH:O	2.29	0.66
1:B:125:GLN:OE1	4:B:307:HOH:O	2.14	0.66
3:I:86:ALA:HA	3:I:112:LEU:HD22	1.76	0.66
1:K:10:THR:HG22	1:K:104:LYS:HD3	1.78	0.66
1:K:30:LYS:O	4:K:302:HOH:O	2.13	0.66
3:M:22:THR:HG23	3:M:63:VAL:HG21	1.76	0.66
2:J:135:SER:O	4:J:304:HOH:O	2.14	0.66
1:L:6:GLN:O	4:L:306:HOH:O	2.15	0.65
3:E:25:CYS:HB2	3:E:38:TRP:HZ2	1.61	0.65
2:F:102:TRP:HE1	3:I:62:THR:HG1	1.45	0.65
3:I:20:THR:HG21	3:I:77:ARG:HG3	1.77	0.65
1:B:144:GLU:O	4:B:308:HOH:O	2.15	0.65
3:I:14:LEU:HA	3:I:113:SER:HB2	1.79	0.64
3:E:83:PRO:HG2	3:I:24:ARG:HH12	1.62	0.64
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.44	0.64
2:H:217:LYS:HE2	2:H:219:GLU:HG3	1.79	0.64
2:H:93:TYR:OH	4:H:307:HOH:O	2.15	0.64
2:A:118:VAL:HG23	4:A:305:HOH:O	1.97	0.64
3:S:75:SER:OG	4:S:202:HOH:O	2.15	0.63
1:K:163:SER:OG	4:K:303:HOH:O	2.14	0.63
2:F:6:GLU:HG3	2:F:22:CYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:63:VAL:HB	3:M:75:SER:HB2	1.79	0.63
2:F:91:VAL:HG11	4:F:308:HOH:O	1.97	0.63
2:A:130:PRO:HB3	2:A:218:VAL:HG12	1.81	0.63
3:E:20:THR:CG2	3:E:77:ARG:HG2	2.29	0.63
3:I:63:VAL:CG1	3:I:75:SER:HB2	2.28	0.62
2:A:12:VAL:HG11	2:A:18:LEU:HG	1.81	0.62
2:F:6:GLU:OE1	2:F:94:CYS:N	2.30	0.62
1:L:18:ARG:HG2	4:L:303:HOH:O	1.99	0.62
3:S:15:VAL:HG22	3:S:19:GLU:HB2	1.81	0.62
3:E:83:PRO:CG	3:I:24:ARG:HH12	2.11	0.62
2:A:135:SER:O	2:A:136:LYS:HG3	2.00	0.61
1:G:36:TYR:CE2	1:G:46:LEU:HD12	2.35	0.61
3:I:66:LEU:HD12	3:I:66:LEU:H	1.66	0.61
2:J:29:PHE:O	2:J:70:ARG:NH2	2.32	0.61
2:J:70:ARG:HA	4:J:301:HOH:O	2.00	0.61
3:I:101:ASP:OD1	3:I:101:ASP:N	2.32	0.61
2:J:130:PRO:HB2	2:J:218:VAL:HG13	1.83	0.61
3:S:98:SER:C	3:S:100:ASP:H	2.04	0.61
2:F:69:SER:HB2	2:F:78:TYR:HB2	1.82	0.60
2:J:108:ASP:OD2	3:M:69:ARG:NH2	2.33	0.60
4:G:323:HOH:O	2:F:134:SER:HB3	2.01	0.60
1:K:109:ARG:NH1	1:K:171:ASP:O	2.32	0.60
2:J:32:PHE:O	2:J:70:ARG:NH2	2.32	0.60
2:A:166:LEU:HD21	2:A:189:VAL:HG21	1.84	0.60
1:B:13:VAL:HG21	1:B:78:LEU:HD13	1.83	0.59
3:E:20:THR:HG22	3:E:77:ARG:HG2	1.82	0.59
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.83	0.59
1:L:61:ARG:NH1	1:L:82:ASP:OD1	2.35	0.59
2:A:101:SER:HB2	3:E:67:THR:HA	1.83	0.59
2:J:175:ALA:N	4:J:306:HOH:O	2.28	0.59
1:L:108:LYS:HE3	4:L:349:HOH:O	2.01	0.59
1:B:46:LEU:HD22	2:A:108:ASP:HA	1.84	0.59
3:M:56:HIS:O	3:M:56:HIS:ND1	2.35	0.59
3:M:4:LEU:HD23	3:M:32:PRO:HD2	1.85	0.59
2:F:154:PRO:O	2:F:155:GLU:HB3	2.02	0.58
2:J:102:TRP:NE1	3:M:64:SER:OG	2.16	0.58
1:B:202:LEU:HB2	4:B:305:HOH:O	2.02	0.58
3:I:82:THR:HG23	3:I:84:ALA:H	1.67	0.58
1:L:202:LEU:O	4:L:301:HOH:O	2.17	0.58
2:H:4:LEU:HB3	2:H:94:CYS:SG	2.43	0.58
3:I:15:VAL:CG2	3:I:19:GLU:HG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:ALA:N	2:H:191:VAL:O	2.22	0.58
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.86	0.58
3:M:40:ARG:HB2	3:M:49:ILE:HD11	1.86	0.58
2:H:149:VAL:CG1	2:H:185:LEU:HB3	2.34	0.57
1:B:27:GLN:O	1:B:69:THR:HG22	2.04	0.57
1:G:39:ARG:NH1	1:G:81:GLU:HB2	2.19	0.57
1:B:38:GLN:NE2	4:A:304:HOH:O	2.33	0.57
1:B:61:ARG:NH1	1:B:82:ASP:OD2	2.37	0.57
3:M:69:ARG:HG2	3:M:69:ARG:HH11	1.70	0.57
2:J:192:PRO:HG2	2:J:195:SER:OG	2.04	0.57
3:I:18:GLY:N	4:I:204:HOH:O	2.35	0.57
1:K:78:LEU:HD11	1:K:83:PHE:CZ	2.40	0.57
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.88	0.56
3:E:71:ASN:ND2	3:E:73:ASP:O	2.34	0.56
2:F:32:PHE:O	2:F:70:ARG:NH1	2.29	0.56
2:H:55:ASP:HB3	3:S:95:ARG:NH1	2.21	0.56
2:A:4:LEU:HB3	2:A:22:CYS:SG	2.46	0.56
1:L:50:ALA:HB3	1:L:53:ILE:HD12	1.87	0.56
1:L:32:ASP:HB2	1:L:92:TYR:HB2	1.88	0.56
1:G:109:ARG:NH2	4:G:310:HOH:O	2.37	0.56
2:A:102:TRP:CH2	3:E:76:ILE:HD11	2.41	0.55
1:B:49:TYR:CE1	2:A:100:VAL:HG11	2.42	0.55
3:S:113:SER:O	3:S:114:VAL:HG23	2.05	0.55
2:A:91:VAL:HG22	2:A:115:LEU:HB2	1.89	0.55
2:A:176:VAL:HG23	4:A:310:HOH:O	2.07	0.55
2:H:96:LYS:HE2	2:H:97:ASP:O	2.07	0.55
1:L:12:SER:OG	1:L:106:GLU:OE2	2.22	0.54
1:G:137:LEU:HB2	1:G:176:LEU:HB3	1.89	0.54
2:F:202:ILE:CG2	2:F:215:ASP:HB3	2.37	0.54
3:S:14:LEU:HD11	3:S:115:ARG:HB2	1.88	0.54
3:E:37:GLN:HG2	3:E:51:ASN:HD22	1.71	0.54
1:G:46:LEU:CD2	1:G:55:GLU:HG3	2.37	0.54
4:A:320:HOH:O	3:E:95:ARG:HG3	2.06	0.54
1:G:8:PRO:HA	4:G:304:HOH:O	2.08	0.54
1:K:55:GLU:HB3	1:K:58:ILE:HD13	1.88	0.54
2:J:99:THR:HG22	2:J:100:VAL:O	2.08	0.54
1:B:59:PRO:HB2	1:B:61:ARG:HG2	1.89	0.54
1:B:55:GLU:CD	3:E:69:ARG:HH12	2.10	0.54
2:A:100:VAL:HG22	2:A:106:PHE:HE2	1.73	0.54
1:G:14:SER:HB2	1:G:17:GLU:HG3	1.89	0.54
1:G:139:ASN:ND2	4:G:314:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:83:PRO:HA	3:M:114:VAL:HG21	1.89	0.53
2:F:75:ASN:HA	4:F:303:HOH:O	2.08	0.53
3:S:62:THR:OG1	4:S:201:HOH:O	2.19	0.53
2:A:27:PHE:CD2	2:A:96:LYS:HE3	2.44	0.53
2:A:19:ARG:NH2	4:A:306:HOH:O	2.34	0.53
3:M:91:CYS:O	3:M:107:GLY:N	2.40	0.53
1:K:143:ARG:CZ	1:K:164:VAL:HG11	2.39	0.53
1:L:63:SER:HB3	4:L:314:HOH:O	2.08	0.53
2:F:191:VAL:HG11	2:F:201:TYR:CE2	2.43	0.53
1:K:91:TYR:HE2	2:J:103:SER:HB2	1.73	0.53
2:F:155:GLU:O	4:F:305:HOH:O	2.18	0.52
1:L:19:ALA:HB2	1:L:78:LEU:HD11	1.92	0.52
1:K:21:PHE:HE2	1:K:73:LEU:HD23	1.75	0.52
1:B:109:ARG:HH21	1:B:112:ALA:HB2	1.75	0.52
3:S:4:LEU:HA	3:S:28:THR:HB	1.92	0.52
3:S:14:LEU:CD1	3:S:115:ARG:HB2	2.40	0.52
1:B:150:LYS:HD2	1:B:153:ASN:HA	1.90	0.52
2:F:48:VAL:HG13	2:F:62:VAL:HG21	1.90	0.52
2:F:128:VAL:HG11	2:F:205:VAL:HG21	1.91	0.52
3:E:25:CYS:HB2	3:E:38:TRP:CZ2	2.42	0.52
3:I:15:VAL:HG13	3:I:81:ILE:HG21	1.92	0.52
1:K:163:SER:OG	2:J:173:PHE:HB3	2.10	0.52
3:S:98:SER:O	3:S:100:ASP:N	2.43	0.52
1:L:53:ILE:CD1	3:S:67:THR:HG22	2.40	0.52
1:B:141:TYR:CD1	1:B:142:PRO:HA	2.45	0.52
2:A:102:TRP:CZ2	3:E:76:ILE:HD11	2.45	0.52
3:S:85:ASP:O	3:S:112:LEU:HD12	2.10	0.51
1:K:163:SER:HB3	1:K:177:SER:OG	2.10	0.51
2:J:22:CYS:HB3	2:J:77:LEU:HB3	1.92	0.51
3:M:34:GLY:HA3	3:M:94:PHE:O	2.09	0.51
3:S:63:VAL:HG13	3:S:77:ARG:HH21	1.75	0.51
3:E:38:TRP:CZ2	3:E:91:CYS:HB2	2.45	0.51
2:H:126:PRO:HB3	2:H:152:TYR:HB3	1.91	0.51
3:M:5:GLN:HB2	3:M:28:THR:OG1	2.11	0.51
1:G:202:LEU:HD13	1:G:206:VAL:HG23	1.92	0.51
2:J:6:GLU:N	2:J:112:GLN:OE1	2.41	0.51
1:G:45:ARG:HA	4:G:317:HOH:O	2.10	0.51
2:F:178:GLN:OE1	2:F:184:SER:HB2	2.11	0.51
1:K:185:ALA:O	4:K:304:HOH:O	2.19	0.51
2:J:8:GLY:HA3	2:J:114:THR:HG21	1.92	0.51
3:I:15:VAL:HG21	3:I:21:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:OD1	1:B:173:THR:OG1	2.24	0.50
1:G:143:ARG:NH1	1:G:164:VAL:HG21	2.26	0.50
1:L:146:LYS:HB3	1:L:198:THR:HB	1.92	0.50
2:H:170:VAL:HG22	2:H:189:VAL:HG22	1.94	0.50
3:E:83:PRO:HG2	3:I:24:ARG:NH1	2.24	0.50
1:L:53:ILE:HD13	3:S:67:THR:HG22	1.94	0.50
3:I:18:GLY:HA2	3:I:80:ALA:HB1	1.93	0.50
1:L:192:VAL:HG22	1:L:211:ASN:OD1	2.12	0.50
2:H:29:PHE:O	2:H:70:ARG:NH1	2.45	0.50
2:J:81:MET:HB3	2:J:84:LEU:HD21	1.92	0.50
2:J:126:PRO:HB3	2:J:152:TYR:HB3	1.92	0.50
3:M:15:VAL:HG22	3:M:19:GLU:HB2	1.92	0.50
3:E:95:ARG:N	3:E:102:VAL:O	2.36	0.50
1:K:36:TYR:HE1	1:K:89:GLN:HB3	1.76	0.50
3:M:59:ARG:HH12	3:M:85:ASP:CG	2.15	0.50
1:L:18:ARG:NH2	4:L:307:HOH:O	2.16	0.49
3:E:24:ARG:NH1	3:E:75:SER:OG	2.45	0.49
1:B:186:ASP:HA	1:B:189:LYS:HE2	1.95	0.49
3:I:21:ALA:O	3:I:77:ARG:HA	2.13	0.49
2:F:195:SER:O	2:F:199:GLN:HB2	2.12	0.49
3:M:57:PHE:HB2	3:M:60:VAL:HG12	1.93	0.49
3:I:68:LYS:O	3:I:71:ASN:HB2	2.12	0.49
1:L:38:GLN:NE2	2:H:39:GLN:HE22	2.08	0.49
3:I:42:ALA:HB2	3:I:90:TYR:CE2	2.48	0.49
1:B:94:TRP:HZ2	3:E:33:VAL:HG21	1.77	0.49
3:I:24:ARG:HA	3:I:75:SER:OG	2.12	0.49
3:S:100:ASP:OD1	3:S:100:ASP:O	2.30	0.49
2:A:157:VAL:HG12	4:A:312:HOH:O	2.13	0.49
1:L:38:GLN:HE22	2:H:39:GLN:NE2	2.09	0.48
1:L:93:ASP:HA	4:L:324:HOH:O	2.13	0.48
3:E:63:VAL:HB	3:E:75:SER:HB2	1.95	0.48
1:G:80:SER:OG	4:G:303:HOH:O	2.19	0.48
3:I:25:CYS:HB2	3:I:38:TRP:CZ2	2.47	0.48
2:H:96:LYS:NZ	2:H:108:ASP:OD2	2.33	0.48
3:S:4:LEU:HD23	3:S:31:ILE:O	2.12	0.48
1:B:112:ALA:HB3	1:B:141:TYR:H	1.78	0.48
2:J:153:PHE:HB3	4:J:311:HOH:O	2.12	0.48
3:M:68:LYS:O	3:M:71:ASN:HB2	2.13	0.48
3:S:5:GLN:H	3:S:28:THR:HB	1.78	0.48
3:I:4:LEU:HD21	3:I:104:PHE:CE2	2.48	0.48
2:F:59:ALA:O	2:F:63:LYS:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:SER:HB3	2:J:173:PHE:CZ	2.49	0.48
1:B:112:ALA:HB3	1:B:141:TYR:N	2.29	0.48
3:I:50:TYR:HD2	3:I:76:ILE:HD12	1.79	0.48
1:L:18:ARG:HD2	4:L:307:HOH:O	2.14	0.47
1:B:182:LEU:HD22	1:B:186:ASP:OD2	2.14	0.47
3:E:42:ALA:O	4:E:203:HOH:O	2.19	0.47
3:I:34:GLY:HA3	3:I:94:PHE:O	2.14	0.47
2:H:154:PRO:HB2	2:H:156:PRO:HD2	1.95	0.47
1:G:95:PRO:HB3	2:F:57:TYR:HB3	1.96	0.47
3:I:9:PRO:HD2	3:I:24:ARG:HB2	1.95	0.47
2:J:202:ILE:HG12	2:J:217:LYS:HA	1.95	0.47
1:B:14:SER:N	4:B:311:HOH:O	2.33	0.47
2:A:70:ARG:NE	2:A:72:ASN:HD21	2.09	0.47
1:G:50:ALA:HB3	1:G:53:ILE:HD12	1.96	0.47
2:F:62:VAL:HG13	2:F:66:PHE:HB2	1.96	0.47
2:F:108:ASP:HB3	3:I:69:ARG:HH11	1.79	0.47
1:K:96:PRO:HA	2:J:47:TRP:CZ3	2.49	0.47
1:L:114:PRO:HB3	1:L:140:PHE:HB3	1.96	0.47
3:S:34:GLY:HA3	3:S:94:PHE:O	2.15	0.47
1:B:29:VAL:O	1:B:68:GLY:HA2	2.14	0.47
1:B:55:GLU:OE2	3:E:69:ARG:NH1	2.47	0.47
2:F:51:ILE:HD12	2:F:68:ILE:HG23	1.95	0.47
3:I:25:CYS:HB2	3:I:38:TRP:HZ2	1.78	0.47
1:K:35:TRP:HB2	1:K:48:ILE:HB	1.95	0.47
2:J:39:GLN:HB2	2:J:45:LEU:HD23	1.97	0.47
3:M:8:GLN:NE2	3:M:110:THR:OG1	2.48	0.47
3:I:20:THR:OG1	3:I:79:GLY:O	2.10	0.47
3:M:50:TYR:CD2	3:M:76:ILE:HD11	2.49	0.47
2:F:62:VAL:CG1	2:F:66:PHE:HB2	2.44	0.47
1:L:83:PHE:CD1	1:L:105:VAL:HG12	2.50	0.46
3:S:66:LEU:HB3	4:S:211:HOH:O	2.14	0.46
1:B:38:GLN:O	1:B:84:ALA:HB1	2.15	0.46
2:F:101:SER:OG	2:F:102:TRP:N	2.48	0.46
3:M:63:VAL:CG2	3:M:77:ARG:HB2	2.45	0.46
1:L:200:GLN:HG2	4:L:310:HOH:O	2.15	0.46
1:B:19:ALA:HB2	1:B:78:LEU:HD11	1.96	0.46
2:F:134:SER:OG	2:F:135:SER:N	2.47	0.46
2:J:128:VAL:HG22	2:J:149:VAL:HG22	1.97	0.46
2:J:98:SER:O	2:J:105:ASP:HA	2.16	0.46
2:A:91:VAL:HA	2:A:115:LEU:HA	1.98	0.46
3:I:24:ARG:HA	3:I:75:SER:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ASN:ND2	4:H:314:HOH:O	2.49	0.46
1:B:200:GLN:HG2	4:B:347:HOH:O	2.16	0.46
2:F:34:MET:HB3	2:F:77:LEU:HD22	1.98	0.46
3:I:20:THR:HG21	3:I:77:ARG:CG	2.45	0.46
1:L:95:PRO:HB2	1:L:96:PRO:HD3	1.96	0.46
1:B:167:GLN:HA	1:B:173:THR:O	2.16	0.46
1:B:125:GLN:HG2	1:B:130:THR:O	2.16	0.46
2:J:174:PRO:HA	4:J:306:HOH:O	2.15	0.46
2:F:204:ASN:HD22	2:F:215:ASP:CG	2.20	0.46
3:I:106:SER:O	4:I:202:HOH:O	2.20	0.46
3:M:63:VAL:HG22	3:M:77:ARG:HB2	1.99	0.45
2:J:81:MET:HE3	2:J:84:LEU:HD21	1.98	0.45
3:M:69:ARG:HH11	3:M:69:ARG:CG	2.27	0.45
1:G:136:LEU:HD12	1:G:176:LEU:O	2.16	0.45
3:M:9:PRO:HD2	3:M:24:ARG:HB2	1.98	0.45
3:M:71:ASN:HD21	3:M:73:ASP:HB3	1.82	0.45
2:H:133:PRO:HG3	2:H:145:LEU:HB3	1.98	0.45
2:A:98:SER:OG	3:E:69:ARG:HD2	2.17	0.45
1:G:186:ASP:HA	1:G:189:LYS:HD3	1.99	0.45
2:F:158:THR:HB	2:F:206:ASN:HB3	1.99	0.45
1:K:124:GLU:O	1:K:127:LYS:HG2	2.17	0.45
2:J:102:TRP:HB2	4:J:315:HOH:O	2.16	0.45
2:H:149:VAL:HG12	2:H:185:LEU:HB3	1.97	0.45
3:S:63:VAL:HG22	3:S:77:ARG:HG3	1.98	0.45
3:S:100:ASP:OD1	3:S:100:ASP:C	2.55	0.45
2:A:169:GLY:O	2:A:189:VAL:HA	2.17	0.45
1:L:126:LEU:O	1:L:184:LYS:HD2	2.17	0.45
1:L:92:TYR:OH	3:S:54:GLU:HG3	2.17	0.45
2:F:5:LEU:O	2:F:22:CYS:HA	2.16	0.45
2:A:4:LEU:HB3	2:A:94:CYS:SG	2.57	0.44
2:J:29:PHE:CE1	2:J:34:MET:HG3	2.52	0.44
1:L:125:GLN:HG2	1:L:130:THR:O	2.16	0.44
1:B:109:ARG:NH2	1:B:112:ALA:HB2	2.32	0.44
1:B:168:ASP:HB3	1:B:173:THR:H	1.81	0.44
1:G:38:GLN:HB2	1:G:44:PRO:HB3	1.98	0.44
2:F:160:SER:OG	2:F:204:ASN:HB2	2.17	0.44
3:I:4:LEU:HD21	3:I:104:PHE:HE2	1.81	0.44
2:H:161:TRP:CZ3	2:H:203:CYS:HB3	2.53	0.44
2:F:204:ASN:HA	2:F:215:ASP:OD1	2.18	0.44
3:M:11:LYS:HB3	3:M:11:LYS:HE3	1.77	0.44
3:M:60:VAL:CG2	3:M:76:ILE:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:TRP:CE2	3:S:96:LYS:HE3	2.52	0.44
2:H:68:ILE:HD11	2:H:77:LEU:HD11	1.98	0.44
2:J:100:VAL:HG12	2:J:101:SER:H	1.83	0.44
2:J:166:LEU:HD13	2:J:189:VAL:HG21	1.98	0.44
2:H:102:TRP:HB2	3:S:52:GLN:CD	2.38	0.44
1:G:91:TYR:HE2	2:F:103:SER:HB3	1.81	0.44
2:J:70:ARG:HG2	2:J:71:ASP:N	2.32	0.44
3:E:50:TYR:HB2	3:E:60:VAL:HG11	1.99	0.44
2:H:2:VAL:HG22	2:H:27:PHE:CD1	2.53	0.44
1:B:114:PRO:HB3	1:B:140:PHE:HB3	1.98	0.44
1:G:109:ARG:HG2	1:G:110:THR:H	1.82	0.44
2:F:40:ALA:HB3	2:F:43:GLU:CD	2.38	0.44
2:F:154:PRO:HG2	2:F:209:PRO:CB	2.48	0.44
1:L:97:PHE:HB2	2:H:47:TRP:CG	2.53	0.43
2:H:65:ARG:NH1	2:H:88:ASP:OD2	2.51	0.43
1:G:7:SER:OG	4:G:304:HOH:O	2.21	0.43
1:L:38:GLN:O	1:L:84:ALA:HB1	2.18	0.43
1:L:21:PHE:HE1	1:L:73:LEU:HD23	1.82	0.43
1:K:94:TRP:O	3:M:96:LYS:NZ	2.52	0.43
1:B:92:TYR:CE1	3:E:53:LYS:HG3	2.53	0.43
2:A:18:LEU:HD23	2:A:18:LEU:HA	1.71	0.43
1:K:13:VAL:HG21	1:K:19:ALA:HB2	2.00	0.43
1:G:48:ILE:HD13	1:G:54:ARG:HA	1.99	0.43
3:I:63:VAL:HG13	3:I:64:SER:N	2.33	0.43
1:K:202:LEU:HD13	1:K:206:VAL:HG23	2.00	0.43
1:L:147:VAL:HB	1:L:162:GLU:OE1	2.18	0.43
3:S:36:ILE:HD13	3:S:93:LYS:HA	2.00	0.43
3:M:63:VAL:HG22	3:M:77:ARG:HD3	2.01	0.43
1:L:211:ASN:C	1:L:213:GLY:H	2.21	0.43
1:B:202:LEU:HD13	1:B:206:VAL:HG23	2.01	0.43
2:A:34:MET:HB3	2:A:77:LEU:HD22	2.00	0.43
3:E:4:LEU:HB3	3:E:29:SER:OG	2.19	0.43
1:G:5:THR:HG23	4:G:322:HOH:O	2.19	0.43
2:H:198:THR:HA	4:H:324:HOH:O	2.19	0.43
3:E:50:TYR:HD1	3:E:57:PHE:CD1	2.36	0.43
2:H:126:PRO:HB2	2:H:149:VAL:HG22	2.01	0.43
1:B:96:PRO:HA	2:A:47:TRP:CZ3	2.53	0.43
2:H:199:GLN:O	4:H:309:HOH:O	2.21	0.42
1:K:39:ARG:NH2	1:K:81:GLU:O	2.49	0.42
2:F:77:LEU:HB3	4:F:307:HOH:O	2.18	0.42
3:E:22:THR:HA	3:E:76:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG11	2:H:109:TYR:CG	2.55	0.42
1:B:94:TRP:CZ2	3:E:33:VAL:HG21	2.53	0.42
2:A:161:TRP:CZ3	2:A:203:CYS:HB3	2.53	0.42
3:E:38:TRP:NE1	3:E:76:ILE:HD13	2.34	0.42
3:M:40:ARG:O	3:M:40:ARG:HG2	2.20	0.42
3:S:14:LEU:HD21	3:S:115:ARG:HG3	2.00	0.42
1:G:148:GLN:HG2	1:G:155:LEU:HD11	2.02	0.42
1:K:186:ASP:HA	1:K:189:LYS:HG2	1.99	0.42
2:H:166:LEU:HD21	2:H:189:VAL:HG11	2.01	0.42
1:G:177:SER:HB3	2:F:173:PHE:CZ	2.55	0.42
1:K:18:ARG:NH1	4:K:312:HOH:O	2.53	0.42
1:B:27:GLN:HG3	1:B:28:ASN:H	1.83	0.42
2:F:1:ASP:OD1	2:F:1:ASP:N	2.53	0.42
2:F:71:ASP:HB2	2:F:78:TYR:HE1	1.85	0.42
2:A:149:VAL:O	2:A:185:LEU:N	2.51	0.42
2:A:198:THR:HG23	2:A:199:GLN:HG3	2.02	0.42
2:J:38:ARG:NE	2:J:46:GLU:OE2	2.36	0.42
1:L:48:ILE:HD13	1:L:73:LEU:HD13	2.02	0.41
1:L:118:ILE:HB	1:L:208:LYS:HB3	2.02	0.41
2:H:160:SER:OG	2:H:204:ASN:HB2	2.20	0.41
1:B:120:PRO:HB3	1:B:210:PHE:CE1	2.55	0.41
3:E:40:ARG:HE	3:E:40:ARG:HB3	1.55	0.41
1:G:39:ARG:HG3	1:G:84:ALA:HB2	2.02	0.41
1:B:141:TYR:CG	1:B:142:PRO:HA	2.55	0.41
1:G:109:ARG:HG2	1:G:110:THR:N	2.35	0.41
2:J:36:TRP:NE1	2:J:79:LEU:HB2	2.35	0.41
2:H:200:THR:HG23	2:H:217:LYS:HG3	2.02	0.41
1:B:61:ARG:CB	1:B:76:THR:HG22	2.51	0.41
2:F:102:TRP:NE1	3:I:62:THR:OG1	2.52	0.41
2:J:217:LYS:HG2	2:J:219:GLU:OE2	2.19	0.41
1:L:59:PRO:HB2	1:L:61:ARG:HG2	2.02	0.41
2:A:99:THR:O	3:E:69:ARG:HG3	2.19	0.41
1:K:146:LYS:HB3	1:K:198:THR:HB	2.02	0.41
1:L:187:TYR:HA	1:L:193:TYR:OH	2.20	0.41
3:S:3:GLU:OE2	3:S:3:GLU:HA	2.20	0.41
3:S:98:SER:C	3:S:100:ASP:N	2.73	0.41
1:G:92:TYR:CE1	3:I:53:LYS:HG2	2.55	0.41
2:F:205:VAL:HG22	2:F:214:VAL:O	2.20	0.41
2:J:154:PRO:HB2	2:J:156:PRO:HD2	2.02	0.41
2:H:153:PHE:CD1	2:H:154:PRO:HA	2.55	0.41
3:S:13:VAL:HG13	3:S:112:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:SER:N	2:F:21:SER:O	2.52	0.41
2:J:99:THR:HB	3:M:70:ASN:HA	2.03	0.41
2:J:130:PRO:HB3	2:J:218:VAL:HG22	2.02	0.41
1:B:147:VAL:HG23	1:B:197:VAL:HG22	2.02	0.41
2:A:81:MET:HB3	2:A:84:LEU:HD21	2.02	0.41
3:I:19:GLU:CG	3:I:20:THR:N	2.72	0.41
2:J:206:ASN:HB2	2:J:213:LYS:HE3	2.03	0.41
2:H:12:VAL:HG11	2:H:18:LEU:HD13	2.02	0.41
1:B:97:PHE:HB2	2:A:47:TRP:CG	2.56	0.41
1:G:43:ALA:HB2	2:F:112:GLN:HA	2.01	0.41
2:F:153:PHE:C	2:F:155:GLU:N	2.74	0.41
2:J:6:GLU:HA	2:J:21:SER:O	2.21	0.41
2:J:166:LEU:HD23	2:J:166:LEU:HA	1.77	0.41
2:H:96:LYS:HG2	2:H:97:ASP:N	2.35	0.41
2:A:202:ILE:HG12	2:A:217:LYS:HB2	2.02	0.41
3:E:83:PRO:HG3	3:I:24:ARG:HH12	1.84	0.41
1:G:38:GLN:NE2	1:G:44:PRO:HD3	2.35	0.41
1:G:186:ASP:O	1:G:189:LYS:HG2	2.20	0.41
1:K:21:PHE:CE2	1:K:73:LEU:HD23	2.56	0.41
1:K:141:TYR:CG	1:K:142:PRO:HA	2.56	0.41
1:B:18:ARG:NH2	4:B:315:HOH:O	2.45	0.41
1:B:55:GLU:HG3	1:B:56:THR:N	2.36	0.41
2:A:18:LEU:HD12	2:A:116:VAL:HG13	2.03	0.41
3:E:98:SER:OG	1:K:108:LYS:NZ	2.39	0.41
1:G:125:GLN:HG2	1:G:130:THR:O	2.20	0.41
2:F:108:ASP:OD1	2:F:109:TYR:N	2.54	0.41
3:I:40:ARG:HG2	3:I:40:ARG:O	2.20	0.41
2:J:171:HIS:HB2	2:J:188:VAL:HG23	2.02	0.41
3:S:14:LEU:HD23	3:S:113:SER:CB	2.20	0.40
3:E:4:LEU:HD23	3:E:31:ILE:O	2.21	0.40
1:G:47:LEU:HD23	1:G:58:ILE:HD12	2.02	0.40
3:I:63:VAL:HG12	3:I:75:SER:O	2.20	0.40
3:I:89:TYR:HB2	3:I:110:THR:HG22	2.04	0.40
2:J:51:ILE:HD13	2:J:56:THR:HG22	2.03	0.40
3:S:3:GLU:HB3	4:S:204:HOH:O	2.20	0.40
1:B:173:THR:HG22	1:B:174:TYR:N	2.36	0.40
1:G:133:VAL:HB	1:G:180:LEU:HB3	2.04	0.40
3:I:38:TRP:O	3:I:48:LEU:HD12	2.21	0.40
1:L:28:ASN:OD1	4:L:308:HOH:O	2.22	0.40
3:E:16:ALA:O	3:E:19:GLU:HB3	2.21	0.40
3:I:36:ILE:HG13	3:I:74:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:38:TRP:CZ2	3:I:91:CYS:HB2	2.56	0.40
1:L:212:ARG:O	1:L:212:ARG:HG2	2.21	0.40
2:H:153:PHE:O	2:H:207:HIS:HE1	2.04	0.40
3:I:20:THR:HA	3:I:78:ILE:O	2.22	0.40
2:H:132:ALA:HA	2:H:133:PRO:HD3	1.93	0.40
3:S:16:ALA:HB3	3:S:19:GLU:OE2	2.22	0.40
2:F:55:ASP:OD1	2:F:55:ASP:N	2.50	0.40
2:J:178:GLN:HE21	2:J:178:GLN:HB2	1.76	0.40

All (1) 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:L:153:ASN:ND2	1:G:4:LEU:O[2_755]	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	B	211/215 (98%)	199 (94%)	9 (4%)	3 (1%)	11 14
1	G	212/215 (99%)	205 (97%)	7 (3%)	0	100 100
1	K	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17 24
1	L	212/215 (99%)	203 (96%)	7 (3%)	2 (1%)	17 24
2	A	213/229 (93%)	204 (96%)	8 (4%)	1 (0%)	29 40
2	F	211/229 (92%)	199 (94%)	8 (4%)	4 (2%)	8 9
2	H	214/229 (93%)	203 (95%)	10 (5%)	1 (0%)	29 40
2	J	214/229 (93%)	203 (95%)	8 (4%)	3 (1%)	11 14
3	E	110/127 (87%)	98 (89%)	11 (10%)	1 (1%)	17 24
3	I	110/127 (87%)	101 (92%)	7 (6%)	2 (2%)	8 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	M	110/127 (87%)	101 (92%)	8 (7%)	1 (1%)	17 24
3	S	111/127 (87%)	100 (90%)	8 (7%)	3 (3%)	5 4
All	All	2139/2284 (94%)	2017 (94%)	99 (5%)	23 (1%)	14 19

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	8	PRO
3	S	98	SER
3	S	99	PRO
3	S	100	ASP
3	E	100	ASP
2	F	153	PHE
2	F	154	PRO
2	F	155	GLU
2	J	101	SER
2	J	105	ASP
2	H	105	ASP
1	B	31	ASN
3	I	44	PRO
3	I	79	GLY
1	L	96	PRO
2	F	63	LYS
2	A	133	PRO
3	M	100	ASP
1	B	28	ASN
2	J	54	GLY
1	K	95	PRO
1	B	95	PRO
1	K	29	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	B	176/187 (94%)	175 (99%)	1 (1%)	86 93
1	G	182/187 (97%)	177 (97%)	5 (3%)	44 63
1	K	175/187 (94%)	173 (99%)	2 (1%)	73 86
1	L	180/187 (96%)	177 (98%)	3 (2%)	60 77
2	A	177/193 (92%)	174 (98%)	3 (2%)	60 77
2	F	170/193 (88%)	168 (99%)	2 (1%)	71 84
2	H	178/193 (92%)	177 (99%)	1 (1%)	86 93
2	J	173/193 (90%)	172 (99%)	1 (1%)	86 93
3	E	78/106 (74%)	76 (97%)	2 (3%)	46 64
3	I	85/106 (80%)	84 (99%)	1 (1%)	71 84
3	M	86/106 (81%)	85 (99%)	1 (1%)	71 84
3	S	90/106 (85%)	89 (99%)	1 (1%)	73 86
All	All	1750/1944 (90%)	1727 (99%)	23 (1%)	69 83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	PHE
1	L	77	SER
1	L	186	ASP
2	H	61	SER
3	S	52	GLN
1	B	11	LEU
2	A	13	GLN
2	A	28	SER
2	A	119	SER
3	E	52	GLN
3	E	54	GLU
1	G	21	PHE
1	G	42	GLN
1	G	46	LEU
1	G	128	SER
1	G	163	SER
2	F	22	CYS
2	F	94	CYS
3	I	59	ARG
1	K	21	PHE
1	K	166	GLU
2	J	79	LEU

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Mol	Chain	Res	Type
3	M	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	B	200	GLN
2	A	39	GLN
2	A	72	ASN
3	E	52	GLN
1	G	79	GLN
1	G	138	ASN
3	M	8	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data 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	B	213/215 (99%)	0.26	4 (1%) 66 64	30, 41, 50, 58	0
1	G	214/215 (99%)	0.47	13 (6%) 21 19	31, 45, 56, 72	0
1	K	213/215 (99%)	0.26	5 (2%) 60 57	27, 40, 51, 61	0
1	L	214/215 (99%)	0.36	6 (2%) 53 50	29, 42, 54, 60	0
2	A	217/229 (94%)	0.49	7 (3%) 47 45	30, 45, 61, 70	0
2	F	215/229 (93%)	0.68	12 (5%) 24 22	38, 54, 64, 73	0
2	H	218/229 (95%)	0.46	10 (4%) 32 30	31, 46, 57, 62	0
2	J	218/229 (95%)	0.54	8 (3%) 41 40	34, 49, 61, 68	0
3	E	112/127 (88%)	1.36	28 (25%) 0 0	45, 65, 79, 82	0
3	I	112/127 (88%)	1.22	26 (23%) 0 0	50, 66, 73, 78	0
3	M	112/127 (88%)	0.83	10 (8%) 9 8	45, 55, 64, 74	0
3	S	113/127 (88%)	0.58	11 (9%) 7 6	39, 48, 61, 65	0
All	All	2171/2284 (95%)	0.55	140 (6%) 19 17	27, 47, 67, 82	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	13	VAL	6.0
3	I	60	VAL	5.4
2	J	198	THR	5.3
3	M	98	SER	5.0
3	S	99	PRO	5.0
3	I	23	LEU	4.9
1	L	95	PRO	4.7
3	E	15	VAL	4.6
3	E	55	GLY	4.2
3	M	63	VAL	4.0
3	I	9	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	211	ASN	3.9
3	E	14	LEU	3.9
1	G	94	TRP	3.8
3	E	21	ALA	3.8
3	I	80	ALA	3.7
3	S	113	SER	3.7
3	E	9	PRO	3.7
3	S	14	LEU	3.6
3	I	30	LEU	3.6
3	I	108	ALA	3.6
3	E	84	ALA	3.5
2	J	134	SER	3.5
2	J	1	ASP	3.4
3	E	45	GLY	3.3
3	M	100	ASP	3.3
1	G	64	GLY	3.3
1	L	26	SER	3.3
1	G	75	ILE	3.3
3	E	17	ALA	3.2
2	F	22	CYS	3.2
3	I	49	ILE	3.2
1	G	213	GLY	3.2
3	E	20	THR	3.2
2	J	121	ALA	3.1
3	I	59	ARG	3.1
3	M	23	LEU	3.1
2	J	194	SER	3.1
1	L	130	THR	3.0
3	I	114	VAL	3.0
1	B	181	THR	3.0
3	E	23	LEU	2.9
2	F	133	PRO	2.9
1	B	95	PRO	2.8
2	A	214	VAL	2.8
2	F	220	PRO	2.8
2	H	60	ASP	2.8
1	G	169	SER	2.8
3	I	90	TYR	2.7
2	F	144	ALA	2.7
3	E	12	SER	2.7
1	G	69	THR	2.7
2	H	157	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	I	14	LEU	2.7
1	K	43	ALA	2.7
3	I	48	LEU	2.7
3	S	98	SER	2.6
3	E	66	LEU	2.6
3	M	49	ILE	2.6
3	I	113	SER	2.6
3	E	41	GLY	2.6
1	K	213	GLY	2.6
3	E	54	GLU	2.6
2	H	109	TYR	2.6
3	E	42	ALA	2.5
2	H	137	SER	2.5
3	M	76	ILE	2.5
1	K	41	GLY	2.5
1	G	5	THR	2.5
3	S	58	PRO	2.5
3	E	86	ALA	2.5
3	I	16	ALA	2.5
2	F	103	SER	2.5
3	E	109	GLY	2.5
2	H	135	SER	2.4
2	A	222	SER	2.4
3	I	78	ILE	2.4
3	S	100	ASP	2.4
3	E	22	THR	2.4
2	F	196	LEU	2.4
2	H	134	SER	2.4
2	A	198	THR	2.4
3	E	106	SER	2.4
1	G	2	ILE	2.4
3	E	111	GLU	2.4
1	G	63	SER	2.4
3	S	112	LEU	2.4
1	K	28	ASN	2.3
1	B	131	ALA	2.3
1	L	10	THR	2.3
3	E	48	LEU	2.3
3	I	39	PHE	2.3
3	E	97	GLY	2.3
2	F	215	ASP	2.3
3	I	89	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	15	VAL	2.3
2	A	68	ILE	2.3
1	G	30	LYS	2.3
3	S	42	ALA	2.3
1	K	27	GLN	2.3
2	J	120	SER	2.3
3	E	78	ILE	2.3
2	A	166	LEU	2.3
1	G	95	PRO	2.2
2	A	108	ASP	2.2
3	I	84	ALA	2.2
3	I	17	ALA	2.2
3	S	66	LEU	2.2
3	M	64	SER	2.2
3	M	86	ALA	2.2
3	M	17	ALA	2.2
1	G	96	PRO	2.2
3	S	13	VAL	2.1
1	L	129	GLY	2.1
3	S	26	THR	2.1
3	I	62	THR	2.1
3	M	48	LEU	2.1
3	I	100	ASP	2.1
1	G	68	GLY	2.1
2	F	94	CYS	2.1
2	A	220	PRO	2.1
2	F	154	PRO	2.1
3	E	52	GLN	2.1
3	I	52	GLN	2.1
2	H	196	LEU	2.1
1	B	76	THR	2.1
3	E	11	LYS	2.1
3	I	24	ARG	2.1
3	I	13	VAL	2.1
2	J	195	SER	2.1
2	H	161	TRP	2.1
3	E	112	LEU	2.0
2	H	156	PRO	2.0
2	F	165	ALA	2.0
2	F	62	VAL	2.0
1	L	182	LEU	2.0
3	E	99	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	84	LEU	2.0
3	I	81	ILE	2.0
2	J	217	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.