



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:24 PM UTC

PDB ID : 6NMR / pdb_00006nmr
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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

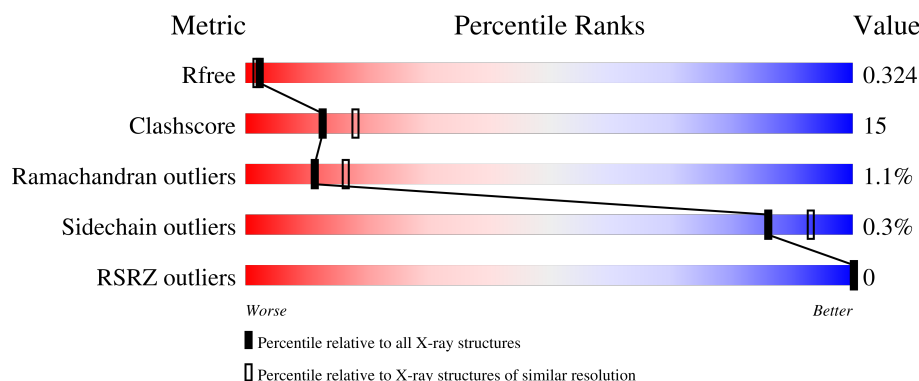
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

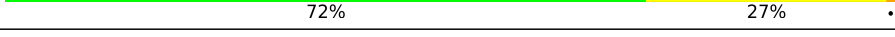
The reported resolution of this entry is 2.42 Å.

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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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.

Mol	Chain	Length	Quality of chain
1	B	215	 70% 28% ..
1	G	215	 77% 22%
1	K	215	 78% 21% .
1	L	215	 72% 27% .
2	A	229	 72% 23% 5%

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Mol	Chain	Length	Quality of chain
2	F	229	 67%24%••6%
2	H	229	 70%25%5%
2	J	229	 68%27%•5%
3	E	127	 57%31%•12%
3	I	127	 49%38%••12%
3	M	127	 58%30%12%
3	S	127	 62%21%••11%

2 Entry composition

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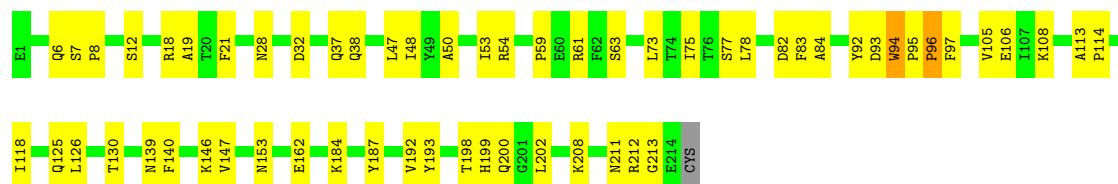
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	32	Total 32	O 32	0	0
4	S	19	Total 19	O 19	0	0
4	B	55	Total 55	O 55	0	0
4	A	28	Total 28	O 28	0	0
4	E	13	Total 13	O 13	0	0
4	G	42	Total 42	O 42	0	0
4	F	17	Total 17	O 17	0	0
4	I	6	Total 6	O 6	0	0
4	K	35	Total 35	O 35	0	0
4	J	28	Total 28	O 28	0	0
4	M	14	Total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

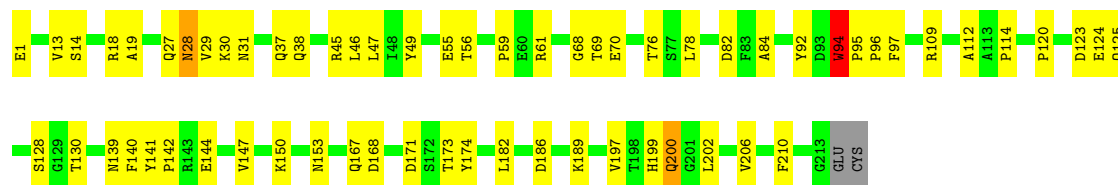
- Molecule 1: Fab 119 anti-SIRP-alpha antibody Variable Light Chain

Chain L: 



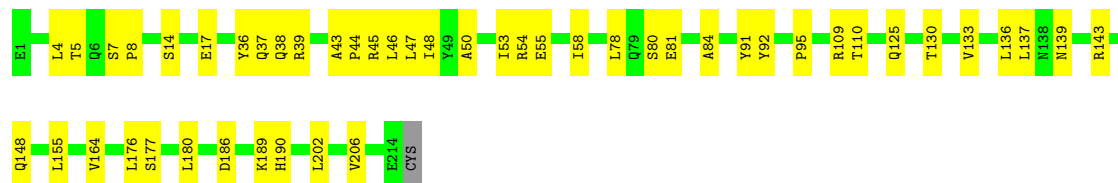
- Molecule 1: Fab 119 anti-SIRP-alpha antibody Variable Light Chain

Chain B: 



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

Chain G: 



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

Chain K: 





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

Chain H: 70% 25% 5%



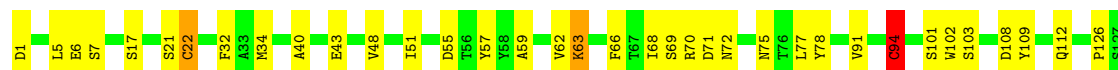
• Molecule 2: Fab 119 anti-SIRP-alpha antibody Variable Heavy Chain

Chain A: 72% 23% 5%



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

Chain F: 67% 24% 6% 3%



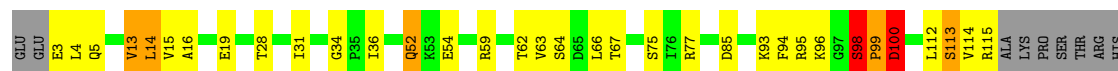
• Molecule 2: Fab 119 anti-SIRP-alpha antibody Variable Heavy Chain

Chain J: 68% 27% 5% 1%



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

Chain S: 62% 21% 11% 6%



HIS
HIS
HIS
HIS
HIS

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

Chain E:  57% 31% 12%

GLU E2 E3 L4 D10 A16 E19 T20 A21 T22 L23 R24 C25 S29 L30 I31 P32 V33 Q37 W38 F39 R40 G41 A42 Y50 N51 Q52 K53 F57 V60 V63 T67 K68 R69 N70 M71 M72 D73 F74 S75 I76 R77 P83 C91 R95 S98

P99 D100 D101 V102 S113 VAL ARG ALA LYS PRO SER THR ARG HIS HIS HIS HIS HIS HIS

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

Chain I:  49% 38% 12%

GLU GLU L4 P9 L14 V15 G18 E19 T20 A21 R24 C25 L30 G34 P35 I36 Q37 W38 F39 R40 G41 A42 P44 L48 T49 Y50 H51 Q52 K53 R59 T62 V63 S64 D65 L66 T67 K68 R69 N70 N71 F74 S75 I76 R77 I78 G79 A80 I81

T82 P83 A84 D85 A86 Y89 Y90 C91 F94 D101 F104 K105 S106 T110 E111 L112 S113 V114 ARG ALA LYS PRO SER THR ARG HIS HIS HIS HIS HIS HIS

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

Chain M:  58% 30% 12%

GLU GLU E3 L4 Q5 Q8 P9 D10 K11 V15 E19 T22 L23 R24 T28 P32 V33 G34 R40 I49 Y50 H56 F57 P58 R59 V60 V63 S64 K68 R69 N70 N71 D72 D73 F74 S75 I76 R77 P83 A84 D85 C91 F94 R95 K96

D100 G107 T110 V114 ARG ALA LYS PRO SER THR ARG HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.07Å 113.56Å 152.08Å 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 2.42Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.288 , 0.323 0.289 , 0.324	Depositor DCC
R_{free} test set	4000 reflections (4.89%)	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)	0.35 , 38.1	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	0.91	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

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	B	0.27	0/1663	0.69	5/2268 (0.2%)
1	G	0.16	0/1686	0.43	0/2293
1	K	0.18	0/1666	0.53	2/2267 (0.1%)
1	L	0.23	0/1684	0.47	0/2295
2	A	0.24	0/1640	0.52	0/2238
2	F	0.26	0/1617	0.56	1/2211 (0.0%)
2	H	0.17	0/1650	0.44	0/2251
2	J	0.27	0/1640	0.57	0/2239
3	E	0.23	0/824	0.63	2/1122 (0.2%)
3	I	0.48	0/845	0.81	5/1150 (0.4%)
3	M	0.20	0/849	0.55	0/1155
3	S	0.38	0/870	1.00	12/1182 (1.0%)
All	All	0.25	0/16634	0.59	27/22671 (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 (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	TRP	CA-C-N	-12.64	107.36	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	TRP	C-N-CA	-12.64	107.36	120.38
1	K	94	TRP	CA-C-N	-11.44	108.59	120.38
1	K	94	TRP	C-N-CA	-11.44	108.59	120.38
3	S	14	LEU	CB-CG-CD2	-9.76	81.44	110.70
3	S	100	ASP	N-CA-CB	9.36	126.31	110.49
1	B	200	GLN	CB-CA-C	-9.18	95.55	110.79
3	S	99	PRO	CA-C-N	8.54	137.86	121.54
3	S	99	PRO	C-N-CA	8.54	137.86	121.54
3	S	14	LEU	CB-CG-CD1	8.11	135.04	110.70
1	B	200	GLN	CA-CB-CG	6.97	128.03	114.10
3	S	100	ASP	CB-CA-C	-6.58	97.32	110.42
3	S	13	VAL	CA-C-N	-6.43	111.88	122.11
3	S	13	VAL	C-N-CA	-6.43	111.88	122.11
3	I	59	ARG	CG-CD-NE	-6.39	97.94	112.00
3	S	14	LEU	CD1-CG-CD2	-6.22	97.11	110.80
3	I	78	ILE	CA-C-N	5.86	132.90	121.41
3	I	78	ILE	C-N-CA	5.86	132.90	121.41
2	F	94	CYS	CB-CA-C	5.83	119.80	109.72
1	B	70	GLU	CA-CB-CG	-5.67	102.75	114.10
3	E	99	PRO	CA-C-N	5.55	132.14	121.54
3	E	99	PRO	C-N-CA	5.55	132.14	121.54
3	S	14	LEU	CA-CB-CG	5.51	135.59	116.30
3	I	79	GLY	N-CA-C	5.49	126.19	113.18
3	S	113	SER	CB-CA-C	5.47	121.31	110.42
3	I	59	ARG	NE-CZ-NH1	-5.36	116.14	121.50
3	S	99	PRO	N-CA-C	5.23	123.23	112.47

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 ⓘ

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	55	0
1	G	1649	0	1583	39	1
1	K	1627	0	1555	31	0
1	L	1645	0	1564	46	1
2	A	1601	0	1528	42	0
2	F	1578	0	1482	54	0
2	H	1611	0	1541	47	0
2	J	1601	0	1518	54	0
3	E	808	0	760	41	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	11	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	483	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 (483) 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:CG	3:M:69:ARG:HH22	1.62	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:108:ASP:OD1	3:M:69:ARG:NH2	1.90	1.05
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
3:I:20:THR:CG2	3:I:77:ARG:HG3	1.98	0.92
2:J:108:ASP:CG	3:M:69:ARG:NH2	2.27	0.92
2:H:127:SER:OG	4:H:301:HOH:O	1.87	0.91
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:102:TRP:NE1	3:M:64:SER:OG	2.16	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
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
3:S:64:SER:OG	4:S:201:HOH:O	1.89	0.71
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
3:S:98:SER:C	3:S:100:ASP:H	2.04	0.65
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:20:THR:OG1	3:I:79:GLY:O	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:55:GLU:CD	3:E:69:ARG:HH12	2.10	0.58
2:F:154:PRO:O	2:F:155:GLU:HB3	2.02	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
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
3:M:59:ARG:HH12	3:M:85:ASP:CG	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:LEU:CD2	1:G:55:GLU:HG3	2.37	0.54
2:J:81:MET:HE3	2:J:84:LEU:HD21	1.89	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:F:204:ASN:HD22	2:F:215:ASP:CG	2.20	0.49
3:I:42:ALA:HB2	3:I:90:TYR:CE2	2.48	0.49
2:H:102:TRP:HB2	3:S:52:GLN:CD	2.38	0.49
3:S:100:ASP:OD1	3:S:100:ASP:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:40:ALA:HB3	2:F:43:GLU:CD	2.38	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
3:E:30:LEU:HG	3:E:72:MET:HE2	1.96	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
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:211:ASN:C	1:L:213:GLY:H	2.21	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:M:50:TYR:CD2	3:M:76:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:98:SER:C	3:S:100:ASP:N	2.73	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:F:153:PHE:C	2:F:155:GLU:H	2.17	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
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:153:PHE:C	2:F:155:GLU:N	2.74	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
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
3:I:30:LEU:HD13	3:I:30:LEU:C	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:204:ASN:HD22	2:H:215:ASP:CG	2.26	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
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
3:S:62:THR:OG1	4:S:201:HOH:O	2.19	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
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:31:ILE:HA	3:E:32:PRO:C	2.42	0.44
3:E:50:TYR:HB2	3:E:60:VAL:HG11	1.99	0.44
2:J:97:ASP:HB3	2:J:105:ASP:CG	2.42	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:J:98:SER:HG	3:M:69:ARG:NH1	2.04	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:B:125:GLN:O	1:B:128:SER:OG	2.35	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
2:H:219:GLU:CD	4:H:304:HOH:O	2.56	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
2:H:3:GLN:CD	2:H:5:LEU:HD11	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:F:102:TRP:NE1	3:I:62:THR:OG1	2.52	0.42
3:E:22:THR:HA	3:E:76:ILE:O	2.19	0.42
3:E:75:SER:C	3:E:76:ILE:HD12	2.45	0.42
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
2:A:102:TRP:HB2	3:E:52:GLN:CD	2.45	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
2:J:100:VAL:O	2:J:101:SER:C	2.62	0.42
1:B:27:GLN:HG3	1:B:28:ASN:H	1.83	0.42
2:H:81:MET:HE1	2:H:116:VAL:HG21	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	211/215 (98%)	199 (94%)	9 (4%)	3 (1%)	9	12
1	G	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
1	K	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	14	20
1	L	212/215 (99%)	203 (96%)	7 (3%)	2 (1%)	14	20
2	A	213/229 (93%)	204 (96%)	8 (4%)	1 (0%)	24	35
2	F	211/229 (92%)	199 (94%)	8 (4%)	4 (2%)	6	7
2	H	214/229 (93%)	203 (95%)	10 (5%)	1 (0%)	24	35
2	J	214/229 (93%)	203 (95%)	8 (4%)	3 (1%)	9	12
3	E	110/127 (87%)	98 (89%)	11 (10%)	1 (1%)	14	20
3	I	110/127 (87%)	101 (92%)	7 (6%)	2 (2%)	6	8
3	M	110/127 (87%)	101 (92%)	8 (7%)	1 (1%)	14	20
3	S	111/127 (87%)	100 (90%)	8 (7%)	3 (3%)	4	3
All	All	2139/2284 (94%)	2017 (94%)	99 (5%)	23 (1%)	11	16

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	176 (100%)	0	100	100
1	G	182/187 (97%)	182 (100%)	0	100	100
1	K	175/187 (94%)	175 (100%)	0	100	100
1	L	180/187 (96%)	179 (99%)	1 (1%)	78	88
2	A	177/193 (92%)	176 (99%)	1 (1%)	78	88
2	F	170/193 (88%)	168 (99%)	2 (1%)	63	79
2	H	178/193 (92%)	178 (100%)	0	100	100
2	J	173/193 (90%)	173 (100%)	0	100	100
3	E	78/106 (74%)	78 (100%)	0	100	100
3	I	85/106 (80%)	85 (100%)	0	100	100
3	M	86/106 (81%)	86 (100%)	0	100	100
3	S	90/106 (85%)	89 (99%)	1 (1%)	65	81
All	All	1750/1944 (90%)	1745 (100%)	5 (0%)	86	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	77	SER
3	S	52	GLN
2	A	28	SER
2	F	22	CYS
2	F	94	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	79	GLN
2	H	39	GLN
2	H	72	ASN
2	H	171	HIS
3	S	37	GLN
1	B	37	GLN
1	B	125	GLN
1	B	138	ASN
1	B	190	HIS
1	B	200	GLN
2	A	39	GLN
2	A	72	ASN
2	A	80	GLN
2	A	171	HIS
3	E	70	ASN
1	G	79	GLN
1	G	190	HIS
2	F	39	GLN
2	F	80	GLN
2	F	112	GLN
3	I	52	GLN
3	I	70	ASN
1	K	38	GLN
2	J	39	GLN
2	J	82	ASN
3	M	71	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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%)	-1.01	0 100 100	30, 41, 50, 58	0
1	G	214/215 (99%)	-0.94	0 100 100	31, 45, 56, 72	0
1	K	213/215 (99%)	-1.00	0 100 100	27, 40, 51, 61	0
1	L	214/215 (99%)	-1.00	0 100 100	29, 42, 54, 60	0
2	A	217/229 (94%)	-0.91	0 100 100	30, 45, 61, 70	0
2	F	215/229 (93%)	-0.83	0 100 100	38, 54, 64, 73	0
2	H	218/229 (95%)	-0.94	0 100 100	31, 46, 57, 62	0
2	J	218/229 (95%)	-0.93	0 100 100	34, 49, 61, 68	0
3	E	112/127 (88%)	-0.70	0 100 100	45, 65, 79, 82	0
3	I	112/127 (88%)	-0.72	0 100 100	50, 66, 73, 78	0
3	M	112/127 (88%)	-0.83	0 100 100	45, 55, 64, 74	0
3	S	113/127 (88%)	-0.93	0 100 100	39, 48, 61, 65	0
All	All	2171/2284 (95%)	-0.91	0 100 100	27, 47, 67, 82	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.