



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:33 PM UTC

PDB ID : 5FHC / pdb_00005fhc
Title : Crystal Structure of Protective Human Antibodies 100 and 114 in Complex with Ebola Virus Fusion Glycoprotein (GP)
Authors : Gilman, M.S.A.; McLellan, J.S.
Deposited on : 2015-12-21
Resolution : 6.70 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:

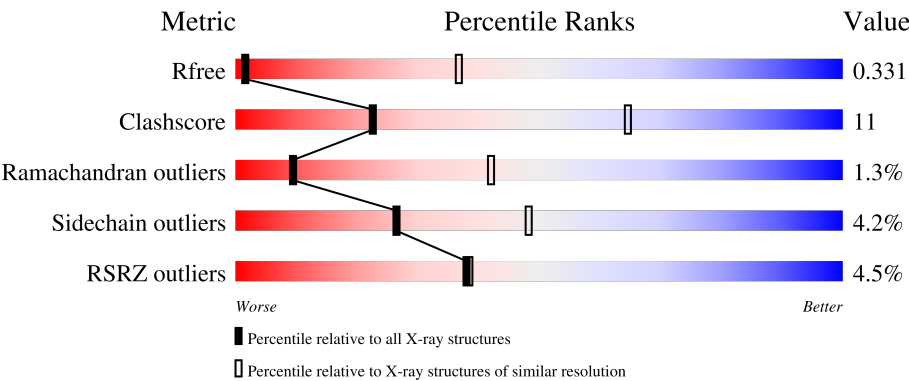
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.70 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	1162 (9.00-4.00)
Clashscore	190562	1001 (9.32-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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 $\leq 5\%$. 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	J	98	11% 66% 27% 5%
2	K	322	2% 45% 23% 29%
3	A	227	6% 72% 22%
4	B	207	2% 87% 12%
5	L	212	5% 80% 17%

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Mol	Chain	Length	Quality of chain
6	H	220	3% 80% 15% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8854 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	98	Total	C	N	O	S	0	0	0
			747	479	130	135	3			

- Molecule 2 is a protein called Envelope glycoprotein,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	230	Total	C	N	O	S	0	0	0
			1676	1065	287	320	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	309	SER	-	linker	UNP Q05320
K	310	ARG	-	linker	UNP Q05320

- Molecule 3 is a protein called Antibody 100 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	221	Total	C	N	O	S	0	0	0
			1667	1060	273	329	5			

- Molecule 4 is a protein called Antibody 100 Fab light chain.

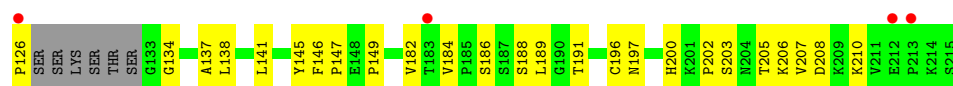
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	207	Total	C	N	O	S	0	0	0
			1564	980	258	320	6			

- Molecule 5 is a protein called Antibody 114 Fab light chain.

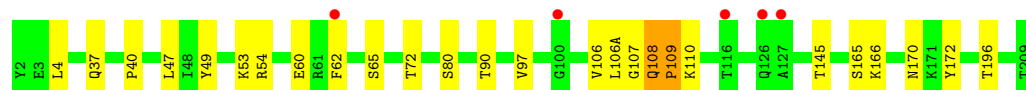
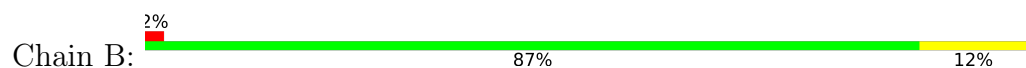
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	211	Total	C	N	O	S	0	0	0
			1605	1004	275	321	5			

- Molecule 6 is a protein called Antibody 114 Fab heavy chain.

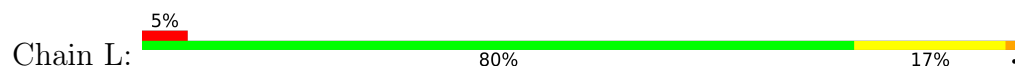
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	215	Total	C	N	O	S	0	0	0
			1595	1004	273	311	7			



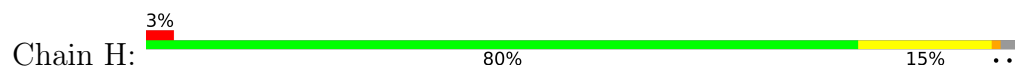
• Molecule 4: Antibody 100 Fab light chain



• Molecule 5: Antibody 114 Fab light chain



• Molecule 6: Antibody 114 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	169.67Å 169.67Å 376.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.85 – 6.70 47.85 – 6.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.85-6.70) 99.6 (47.85-6.70)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.260 , 0.343 0.275 , 0.331	Depositor DCC
R_{free} test set	202 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	277.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 378.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å ²)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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	J	0.48	0/763	1.03	6/1039 (0.6%)
2	K	0.43	0/1712	0.98	3/2336 (0.1%)
3	A	0.46	0/1713	0.96	5/2344 (0.2%)
4	B	0.37	0/1603	0.82	0/2191
5	L	0.51	1/1640 (0.1%)	0.95	10/2229 (0.4%)
6	H	0.46	1/1629 (0.1%)	0.94	7/2215 (0.3%)
All	All	0.45	2/9060 (0.0%)	0.94	31/12354 (0.3%)

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	J	0	1
2	K	0	1
5	L	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	110	VAL	CA-C	6.06	1.60	1.52
6	H	27	PHE	CA-C	5.73	1.60	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	149	PRO	N-CD-CG	-9.08	92.90	103.80
2	K	33	ILE	CA-C-N	8.43	128.36	119.85
2	K	33	ILE	C-N-CA	8.43	128.36	119.85
3	A	11	LEU	N-CA-C	8.08	123.53	109.96
3	A	112	SER	N-CA-C	7.91	121.26	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	149	PRO	CB-CG-CD	-7.85	87.34	105.40
6	H	115	SER	N-CA-C	7.84	121.56	110.50
6	H	149	PRO	CA-CB-CG	-7.78	89.22	104.00
6	H	149	PRO	N-CA-CB	-7.13	94.75	102.60
3	A	207	VAL	N-CA-C	7.07	118.30	108.12
5	L	153	ALA	CA-C-N	-7.04	113.19	123.05
5	L	153	ALA	C-N-CA	-7.04	113.19	123.05
1	J	525	ALA	N-CA-C	-6.95	104.37	112.92
5	L	106	ILE	CA-C-N	-6.65	113.32	122.30
5	L	106	ILE	C-N-CA	-6.65	113.32	122.30
3	A	113	SER	N-CA-C	6.39	121.08	113.28
1	J	512	ASN	CA-C-N	6.28	125.97	119.82
1	J	512	ASN	C-N-CA	6.28	125.97	119.82
5	L	110	VAL	N-CA-CB	-6.07	104.25	111.90
5	L	109	THR	CA-C-N	-5.85	115.30	123.13
5	L	109	THR	C-N-CA	-5.85	115.30	123.13
3	A	111	VAL	N-CA-C	5.79	116.77	107.73
6	H	149	PRO	CA-N-CD	-5.67	103.56	111.50
5	L	155	GLN	N-CA-C	5.58	118.42	110.10
2	K	223	THR	N-CA-C	5.50	118.42	109.24
6	H	115	SER	CB-CA-C	-5.30	99.78	109.54
1	J	522	ASP	N-CA-C	-5.25	103.38	110.68
1	J	572	PHE	N-CA-C	-5.18	105.54	111.14
1	J	564	GLU	N-CA-C	5.16	117.58	111.33
5	L	108	ARG	CA-C-N	5.12	129.83	121.74
5	L	108	ARG	C-N-CA	5.12	129.83	121.74

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	522	ASP	Peptide
2	K	54	ARG	Peptide
5	L	109	THR	Mainchain
5	L	110	VAL	Mainchain

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	J	747	0	727	33	1
2	K	1676	0	1530	75	0
3	A	1667	0	1628	37	3
4	B	1564	0	1505	17	0
5	L	1605	0	1565	31	2
6	H	1595	0	1577	35	0
All	All	8854	0	8532	183	3

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 11.

All (183) 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:A:11:LEU:HD13	3:A:147:PRO:HG3	1.40	1.01
5:L:108:ARG:HH12	5:L:111:ALA:HB2	1.36	0.87
3:A:11:LEU:CD1	3:A:147:PRO:HG3	2.04	0.86
5:L:108:ARG:NH1	5:L:111:ALA:HB2	1.97	0.80
5:L:155:GLN:OE1	5:L:158:ASN:ND2	2.14	0.80
3:A:10:GLY:HA2	3:A:202:PRO:HG3	1.67	0.77
2:K:223:THR:HG21	6:H:31:MET:O	1.85	0.76
4:B:40:PRO:HB3	4:B:166:LYS:HD2	1.68	0.76
3:A:200:HIS:HD1	3:A:203:SER:HG	1.34	0.75
2:K:114:LYS:HZ2	5:L:92:ASN:CG	1.95	0.74
6:H:29:LEU:O	6:H:71:ARG:NH2	2.21	0.73
3:A:108:LEU:HD23	3:A:149:PRO:HB3	1.69	0.73
3:A:11:LEU:HD12	3:A:110:THR:O	1.90	0.72
6:H:94:ARG:HB3	6:H:102:SER:HB2	1.73	0.71
2:K:114:LYS:NZ	5:L:92:ASN:HD21	1.88	0.71
3:A:112:SER:HG	3:A:146:PHE:HE2	1.40	0.70
6:H:210:LYS:NZ	6:H:212:GLU:OE2	2.16	0.70
2:K:221:GLN:HB3	6:H:97:ARG:HE	1.58	0.69
5:L:110:VAL:HG11	5:L:199:GLN:HB3	1.75	0.69
4:B:166:LYS:HG2	4:B:172:TYR:CE1	2.29	0.68
2:K:89:ARG:HG2	2:K:90:SER:N	2.08	0.68
6:H:97:ARG:NH1	6:H:97:ARG:HB3	2.10	0.67
3:A:115:SER:O	3:A:115:SER:OG	2.09	0.67
6:H:193:THR:HG23	6:H:210:LYS:HE2	1.78	0.66
1:J:562:ALA:HB1	2:K:180:VAL:HG23	1.78	0.65
1:J:527:ILE:HG22	3:A:96:SER:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:37:GLN:HB2	4:B:47:LEU:HD11	1.78	0.64
2:K:143:GLY:HA2	6:H:98:GLY:HA2	1.80	0.64
6:H:117:LYS:N	6:H:146:PHE:O	2.31	0.64
2:K:57:LEU:HD12	2:K:185:ILE:HD11	1.80	0.63
3:A:96:SER:OG	3:A:100(G):THR:OG1	2.12	0.63
5:L:19:ILE:HD11	5:L:75:ILE:HD12	1.80	0.63
5:L:40:PRO:HB2	5:L:165:GLU:HB3	1.80	0.63
1:J:523:GLU:HB3	4:B:53:LYS:NZ	2.14	0.62
1:J:526:ALA:HB1	3:A:98:SER:CB	2.30	0.62
3:A:25:SER:O	3:A:27:GLY:N	2.34	0.59
2:K:83:THR:HG21	2:K:232:TYR:OH	2.03	0.59
1:J:504:ILE:HG23	2:K:45:VAL:HG21	1.85	0.59
1:J:526:ALA:HB1	3:A:98:SER:HB3	1.83	0.59
2:K:223:THR:HG23	6:H:97:ARG:HG3	1.85	0.58
2:K:223:THR:CG2	6:H:97:ARG:HG3	2.34	0.58
2:K:114:LYS:NZ	5:L:92:ASN:ND2	2.51	0.57
1:J:580:ARG:NH2	2:K:127:ASP:O	2.33	0.57
1:J:579:LEU:H	1:J:579:LEU:HD12	1.69	0.57
2:K:114:LYS:HZ2	5:L:92:ASN:ND2	2.02	0.57
2:K:231:GLU:HB2	6:H:31:MET:SD	2.45	0.56
1:J:562:ALA:HA	2:K:182:ALA:HB2	1.87	0.56
5:L:108:ARG:HG3	5:L:140:TYR:CD2	2.40	0.56
1:J:522:ASP:O	1:J:524:GLY:N	2.39	0.55
3:A:110:THR:HG21	3:A:147:PRO:HB2	1.89	0.55
2:K:162:TYR:CE1	2:K:176:PHE:HB3	2.41	0.55
2:K:227:THR:CG2	6:H:54:SER:HB3	2.36	0.55
4:B:106(A):LEU:O	4:B:108:GLN:HG2	2.07	0.54
5:L:110:VAL:HG13	5:L:141:PRO:HD2	1.88	0.54
1:J:595:GLN:HG3	2:K:48:VAL:HG12	1.90	0.53
2:K:117:ASP:OD2	6:H:58:TYR:HB3	2.08	0.53
2:K:126:PRO:HG2	2:K:129:ILE:HD12	1.89	0.53
6:H:97:ARG:HB3	6:H:97:ARG:HH11	1.72	0.53
1:J:504:ILE:HD11	2:K:43:LEU:HD13	1.90	0.53
1:J:561:LEU:O	1:J:565:THR:HG23	2.07	0.53
3:A:50:TYR:HE1	3:A:58:ASN:HB3	1.73	0.53
3:A:197:ASN:ND2	3:A:208:ASP:OD1	2.30	0.53
1:J:573:LEU:HD21	2:K:97:VAL:HG22	1.91	0.53
2:K:90:SER:HB3	2:K:150:ASP:CG	2.34	0.52
1:J:516:HIS:HD1	2:K:104:TRP:CD1	2.27	0.52
4:B:166:LYS:HG2	4:B:172:TYR:HE1	1.74	0.51
2:K:152:ALA:HB3	2:K:170:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:100:TYR:HE2	3:A:100(G):THR:HG22	1.76	0.51
1:J:522:ASP:O	1:J:525:ALA:N	2.43	0.51
2:K:36:GLY:O	2:K:185:ILE:HG22	2.11	0.51
4:B:4:LEU:HD11	4:B:90:THR:HG22	1.93	0.51
3:A:114:ALA:HB3	3:A:146:PHE:CD2	2.46	0.50
6:H:56:ASP:OD1	6:H:56:ASP:N	2.41	0.50
2:K:224:GLY:O	2:K:230:THR:HG22	2.12	0.50
2:K:221:GLN:HG3	2:K:241:TYR:CE2	2.47	0.50
6:H:82:MET:HB3	6:H:82(C):LEU:HD21	1.93	0.49
2:K:227:THR:HG21	6:H:54:SER:HB3	1.94	0.49
3:A:112:SER:OG	3:A:146:PHE:HE2	1.94	0.49
1:J:506:ASN:HD22	1:J:556:CYS:C	2.19	0.49
2:K:232:TYR:HB3	2:K:244:LEU:HD12	1.92	0.49
5:L:18:ARG:HG2	5:L:76:SER:O	2.12	0.49
6:H:159:LEU:HD21	6:H:182:VAL:HG21	1.93	0.49
2:K:255:GLN:O	2:K:259:THR:HG23	2.13	0.49
6:H:149:PRO:HG2	6:H:149:PRO:O	2.04	0.49
4:B:65:SER:HG	4:B:72:THR:HG1	1.61	0.49
1:J:584:ILE:O	1:J:587:ARG:HB3	2.13	0.48
3:A:126:PRO:HG3	3:A:138:LEU:HB3	1.93	0.48
2:K:221:GLN:OE1	6:H:98:GLY:HA3	2.12	0.48
2:K:114:LYS:HZ1	5:L:92:ASN:HD21	1.58	0.48
5:L:13:ALA:C	5:L:107:LYS:H	2.21	0.48
3:A:50:TYR:CE1	3:A:58:ASN:HB3	2.48	0.48
1:J:592:PHE:HA	2:K:48:VAL:HG11	1.95	0.48
4:B:40:PRO:CB	4:B:166:LYS:HD2	2.43	0.48
6:H:11:LEU:HB2	6:H:147:PRO:HG3	1.96	0.48
2:K:94:PRO:HB3	2:K:169:VAL:HG21	1.94	0.48
2:K:245:GLU:H	2:K:248:PHE:HE2	1.62	0.48
2:K:259:THR:HA	2:K:262:THR:HG1	1.79	0.48
2:K:259:THR:HA	2:K:262:THR:OG1	2.14	0.48
1:J:518:TRP:CZ3	2:K:133:PRO:HG2	2.49	0.47
1:J:595:GLN:HG3	2:K:48:VAL:CG1	2.44	0.47
1:J:518:TRP:CH2	2:K:133:PRO:HG2	2.49	0.47
2:K:115:LYS:HA	2:K:145:GLY:O	2.14	0.47
5:L:110:VAL:HG22	5:L:141:PRO:HD3	1.96	0.47
3:A:184:VAL:HG21	3:A:189:LEU:HD23	1.95	0.47
2:K:79:VAL:HG21	2:K:220:TYR:CZ	2.49	0.47
3:A:116:THR:HB	3:A:203:SER:HB3	1.97	0.47
1:J:545:GLU:HG3	2:K:104:TRP:HE1	1.79	0.47
5:L:155:GLN:CD	5:L:158:ASN:HD21	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:11:LEU:HD22	6:H:147:PRO:HB3	1.97	0.46
2:K:97:VAL:HG12	2:K:98:ASN:N	2.30	0.46
2:K:120:GLU:HG2	2:K:172:ARG:HD3	1.97	0.46
3:A:100:TYR:CE2	3:A:100(G):THR:HG22	2.50	0.46
4:B:145:THR:HB	4:B:196:THR:OG1	2.16	0.46
1:J:595:GLN:HE21	1:J:595:GLN:HA	1.81	0.46
5:L:55:HIS:O	5:L:58:VAL:HG22	2.15	0.46
5:L:40:PRO:HB2	5:L:165:GLU:CB	2.45	0.46
2:K:33:ILE:HA	2:K:34:PRO:HD2	1.76	0.45
2:K:70:LEU:HB3	2:K:75:VAL:HG21	1.97	0.45
2:K:90:SER:HB3	2:K:150:ASP:H	1.81	0.45
1:J:526:ALA:HB1	3:A:98:SER:HB2	1.98	0.45
4:B:80:SER:HA	4:B:106:VAL:HG21	1.99	0.45
5:L:145:LYS:HB3	5:L:197:THR:HB	1.99	0.45
2:K:97:VAL:HG12	2:K:98:ASN:H	1.82	0.44
3:A:11:LEU:HD23	3:A:116:THR:HG22	1.99	0.44
2:K:85:ARG:HD2	2:K:178:GLU:OE2	2.16	0.44
2:K:123:PRO:HG3	2:K:151:PHE:CE1	2.53	0.44
2:K:141:VAL:HA	2:K:220:TYR:HB2	1.98	0.44
2:K:145:GLY:HA3	2:K:225:PHE:H	1.82	0.44
5:L:66:GLY:HA3	5:L:71:PHE:HA	1.99	0.44
1:J:586:ASN:O	1:J:590:ILE:HG13	2.18	0.44
2:K:231:GLU:CB	6:H:31:MET:SD	3.06	0.44
2:K:269:THR:O	5:L:56:ALA:HB1	2.17	0.44
3:A:12:VAL:HG11	3:A:18:LEU:HD13	1.99	0.44
5:L:14:SER:HB2	5:L:17:ASP:OD2	2.18	0.44
6:H:119:PRO:HB3	6:H:145:TYR:HB3	2.00	0.44
6:H:31:MET:HE3	6:H:31:MET:HB3	1.81	0.43
1:J:523:GLU:CB	4:B:53:LYS:NZ	2.81	0.43
4:B:106(A):LEU:O	4:B:107:GLY:C	2.61	0.43
5:L:13:ALA:O	5:L:107:LYS:N	2.44	0.43
6:H:168:ALA:HA	6:H:178:LEU:HB3	2.00	0.43
3:A:9:PRO:HB2	3:A:149:PRO:HG3	1.99	0.43
3:A:119:PRO:HB3	3:A:145:TYR:HB3	2.00	0.43
2:K:47:ASP:O	2:K:48:VAL:HB	2.18	0.43
2:K:227:THR:HG22	6:H:54:SER:HB3	2.00	0.43
1:J:520:THR:CG2	2:K:164:ARG:HD3	2.49	0.43
2:K:122:LEU:O	2:K:172:ARG:NH2	2.52	0.43
2:K:185:ILE:O	2:K:185:ILE:HG23	2.18	0.43
3:A:121:VAL:HA	3:A:141:LEU:O	2.19	0.43
1:J:527:ILE:HG22	3:A:96:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:126:PRO:HA	3:A:137:ALA:O	2.20	0.42
5:L:90:ASN:OD1	5:L:97:THR:HG22	2.19	0.42
3:A:24:VAL:HG13	3:A:76:ASN:ND2	2.35	0.42
4:B:109:PRO:HB2	4:B:110:LYS:H	1.67	0.42
6:H:52:GLY:O	6:H:71:ARG:HD3	2.19	0.42
3:A:134:GLY:O	3:A:186:SER:N	2.46	0.42
2:K:246:SER:O	2:K:248:PHE:N	2.53	0.42
6:H:143:LYS:NZ	6:H:171:GLN:OE1	2.52	0.42
1:J:529:LEU:HB3	1:J:532:ILE:HD12	2.02	0.42
1:J:573:LEU:HD21	2:K:97:VAL:CG2	2.49	0.42
4:B:54:ARG:HD3	4:B:62:PHE:O	2.19	0.42
2:K:241:TYR:CZ	6:H:97:ARG:NH2	2.87	0.42
5:L:123:GLU:O	5:L:126:LYS:HB2	2.20	0.42
6:H:22:CYS:HB3	6:H:78:LEU:HD23	2.02	0.42
2:K:117:ASP:OD2	6:H:58:TYR:CD2	2.73	0.41
2:K:138:VAL:HB	2:K:217:THR:HG22	2.03	0.41
5:L:110:VAL:HG13	5:L:141:PRO:CD	2.50	0.41
3:A:24:VAL:O	3:A:76:ASN:ND2	2.48	0.41
5:L:89:GLN:HB2	5:L:98:PHE:CD2	2.56	0.41
2:K:38:ILE:HD11	2:K:186:LEU:HD23	2.02	0.41
2:K:160:PHE:CD2	2:K:170:ILE:HG23	2.56	0.41
3:A:206:LYS:HE3	3:A:206:LYS:HB2	1.83	0.41
2:K:146:PRO:HB3	6:H:56:ASP:CG	2.45	0.41
3:A:188:SER:O	3:A:191:THR:OG1	2.37	0.41
5:L:37:GLN:HB2	5:L:47:LEU:HD11	2.02	0.41
6:H:12:ILE:HG13	6:H:13:GLN:N	2.35	0.41
1:J:518:TRP:CZ2	2:K:102:GLY:HA3	2.56	0.40
2:K:136:ARG:HG2	2:K:137:TYR:CE2	2.56	0.40
2:K:74:GLY:O	2:K:75:VAL:C	2.64	0.40
4:B:145:THR:HB	4:B:196:THR:HG1	1.87	0.40
1:J:524:GLY:HA3	4:B:49:TYR:OH	2.21	0.40
2:K:240:THR:HG21	2:K:266:ARG:HA	2.03	0.40
5:L:58:VAL:HA	5:L:59:PRO:HD3	1.93	0.40
5:L:141:PRO:HB2	5:L:143:GLU:OE1	2.20	0.40

All (3) 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)
3:A:16:ASP:OD2	5:L:126:LYS:NZ[5_565]	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:564:GLU:OE2	3:A:54:SER:OG[2_665]	2.07	0.13
3:A:210:LYS:NZ	5:L:15:VAL:O[6_555]	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	J	96/98 (98%)	83 (86%)	11 (12%)	2 (2%)	5	30
2	K	224/322 (70%)	183 (82%)	32 (14%)	9 (4%)	2	18
3	A	217/227 (96%)	206 (95%)	9 (4%)	2 (1%)	14	51
4	B	205/207 (99%)	196 (96%)	8 (4%)	1 (0%)	24	63
5	L	209/212 (99%)	199 (95%)	9 (4%)	1 (0%)	24	63
6	H	211/220 (96%)	205 (97%)	6 (3%)	0	100	100
All	All	1162/1286 (90%)	1072 (92%)	75 (6%)	15 (1%)	9	42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	521	GLN
2	K	48	VAL
2	K	119	SER
2	K	163	ASP
2	K	247	ARG
3	A	26	GLY
4	B	109	PRO
2	K	56	LYS
2	K	75	VAL
3	A	115	SER
5	L	26	SER
1	J	523	GLU
2	K	40	ASN

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Mol	Chain	Res	Type
2	K	127	ASP
2	K	116	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	73/78 (94%)	67 (92%)	6 (8%)	10	31
2	K	162/278 (58%)	153 (94%)	9 (6%)	19	40
3	A	191/197 (97%)	180 (94%)	11 (6%)	18	40
4	B	178/178 (100%)	173 (97%)	5 (3%)	38	60
5	L	181/182 (100%)	179 (99%)	2 (1%)	65	76
6	H	177/182 (97%)	170 (96%)	7 (4%)	28	49
All	All	962/1095 (88%)	922 (96%)	40 (4%)	26	48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	504	ILE
1	J	523	GLU
1	J	576	THR
1	J	579	LEU
1	J	591	ASP
1	J	595	GLN
2	K	43	LEU
2	K	69	ASN
2	K	81	SER
2	K	89	ARG
2	K	90	SER
2	K	98	ASN
2	K	113	ILE
2	K	120	GLU
2	K	170	ILE
3	A	7	SER

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Mol	Chain	Res	Type
3	A	11	LEU
3	A	24	VAL
3	A	28	SER
3	A	31	SER
3	A	50	TYR
3	A	71	VAL
3	A	121	VAL
3	A	182	VAL
3	A	196	CYS
3	A	205	THR
4	B	60	GLU
4	B	97	VAL
4	B	108	GLN
4	B	165	SER
4	B	170	ASN
5	L	106	ILE
5	L	154	LEU
6	H	29	LEU
6	H	40	THR
6	H	78	LEU
6	H	97	ARG
6	H	149	PRO
6	H	183	THR
6	H	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	512	ASN
1	J	595	GLN
3	A	1	GLN
3	A	39	GLN
4	B	38	GLN
4	B	50	GLN
4	B	126	GLN
5	L	3	GLN
5	L	38	GLN
6	H	39	GLN
6	H	82(A)	ASN
6	H	192	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 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

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, 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	J	98/98 (100%)	0.74	11 (11%) 10 18	230, 272, 373, 394	0
2	K	230/322 (71%)	0.29	7 (3%) 52 46	196, 279, 352, 446	0
3	A	221/227 (97%)	0.34	13 (5%) 28 32	227, 327, 418, 550	0
4	B	207/207 (100%)	0.13	5 (2%) 59 52	248, 306, 445, 566	0
5	L	211/212 (99%)	0.33	11 (5%) 33 35	231, 285, 351, 394	0
6	H	215/220 (97%)	0.25	6 (2%) 55 48	247, 280, 334, 396	0
All	All	1182/1286 (91%)	0.31	53 (4%) 38 38	196, 290, 388, 566	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	522	ASP	5.1
2	K	238	ASN	4.1
3	A	212	GLU	3.8
5	L	3	GLN	3.8
6	H	127	SER	3.5
1	J	589	ALA	3.5
3	A	28	SER	3.5
6	H	133	GLY	3.4
5	L	5	THR	3.4
5	L	24	ARG	3.3
6	H	48	VAL	3.3
5	L	95	PRO	3.2
1	J	511	CYS	3.2
1	J	579	LEU	3.1
2	K	111	LEU	3.1
1	J	543	TYR	3.1
5	L	2	ILE	3.1
1	J	558	LEU	3.0
2	K	170	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	48	ILE	2.9
1	J	502	GLU	2.7
6	H	51	VAL	2.7
6	H	45	LEU	2.7
3	A	27	GLY	2.7
3	A	26	GLY	2.6
3	A	25	SER	2.6
3	A	82(C)	VAL	2.6
4	B	126	GLN	2.6
1	J	586	ASN	2.5
3	A	56	SER	2.5
5	L	27	GLN	2.5
5	L	37	GLN	2.5
5	L	131	SER	2.5
2	K	156	GLU	2.4
1	J	526	ALA	2.4
4	B	62	PHE	2.4
5	L	209	PHE	2.4
3	A	213	PRO	2.4
3	A	31	SER	2.4
5	L	205	VAL	2.4
1	J	593	LEU	2.4
3	A	183	THR	2.3
1	J	521	GLN	2.3
6	H	174	GLY	2.3
4	B	100	GLY	2.2
4	B	127	ALA	2.2
4	B	116	THR	2.2
2	K	309	SER	2.2
5	L	82	ASP	2.1
2	K	77	THR	2.1
3	A	126	PRO	2.1
3	A	83	THR	2.1
2	K	266	ARG	2.0

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 [i](#)

There are no oligosaccharides 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.