



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:29 AM UTC

PDB ID : 6P60 / pdb_00006p60
Title : Vaccine-elicited NHP FP-targeting neutralizing antibody A12V163-a.02 in complex with HIV fusion peptide (residue 512-519)
Authors : Xu, K.; Liu, K.; Kwong, P.D.
Deposited on : 2019-05-31
Resolution : 2.50 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

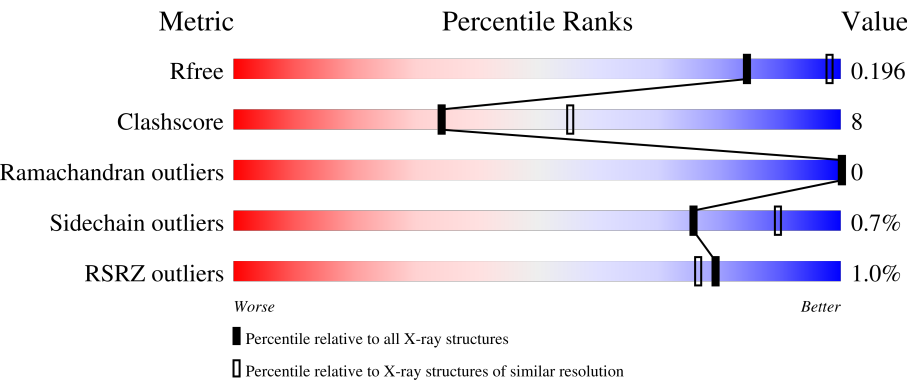
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	A	225	83%15%.
1	C	225	% 79%17%..
1	G	225	2% 78%18%.
1	J	225	2% 80%15%.
2	B	212	83%17%

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Mol	Chain	Length	Quality of chain
2	D	212	87% 13%
2	H	212	90% 10%
2	K	212	% 90% 10%
3	E	8	100%
3	F	8	12% 75% 12% 12%
3	I	8	12% 88% 12%
3	L	8	25% 75% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14008 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 Antibody A12V163-a.02 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1663	1050	280	329	4			
1	C	221	Total	C	N	O	S	0	0	0
			1663	1050	280	329	4			
1	G	215	Total	C	N	O	S	0	0	0
			1621	1028	271	318	4			
1	J	215	Total	C	N	O	S	0	0	0
			1621	1028	271	318	4			

- Molecule 2 is a protein called Antibody A12V163-a.02 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1572	982	262	323	5			
2	D	211	Total	C	N	O	S	0	0	0
			1572	982	262	323	5			
2	H	212	Total	C	N	O	S	0	0	0
			1581	987	264	325	5			
2	K	212	Total	C	N	O	S	0	0	0
			1581	987	264	325	5			

- Molecule 3 is a protein called HIV fusion peptide residue 512-519.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			51	35	8	8			
3	F	8	Total	C	N	O	0	0	0
			51	35	8	8			
3	I	8	Total	C	N	O	0	0	0
			51	35	8	8			
3	L	8	Total	C	N	O	0	0	0
			51	35	8	8			

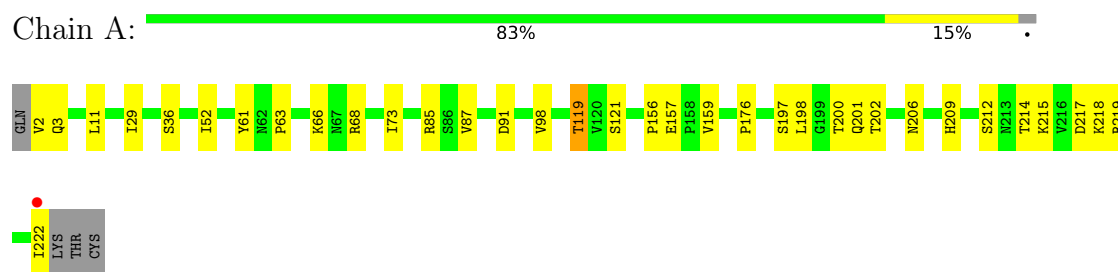
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total 137	O 137	0	0
4	B	104	Total 104	O 104	0	0
4	E	7	Total 7	O 7	0	0
4	C	133	Total 133	O 133	0	0
4	D	127	Total 127	O 127	0	0
4	F	5	Total 5	O 5	0	0
4	G	111	Total 111	O 111	0	0
4	H	92	Total 92	O 92	0	0
4	I	3	Total 3	O 3	0	0
4	J	127	Total 127	O 127	0	0
4	K	78	Total 78	O 78	0	0
4	L	6	Total 6	O 6	0	0

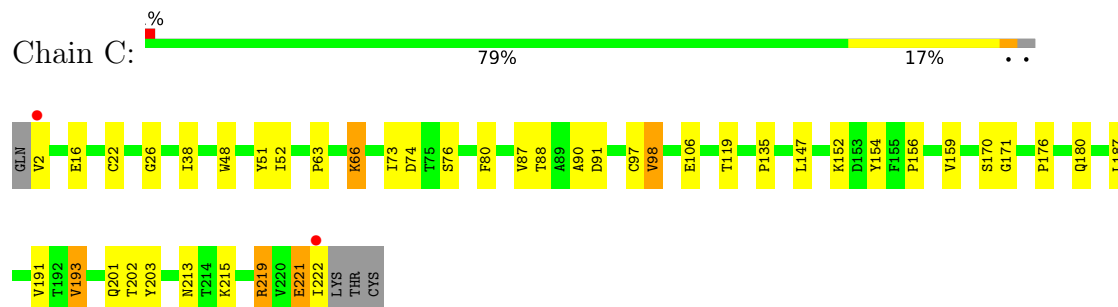
3 Residue-property plots [i](#)

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

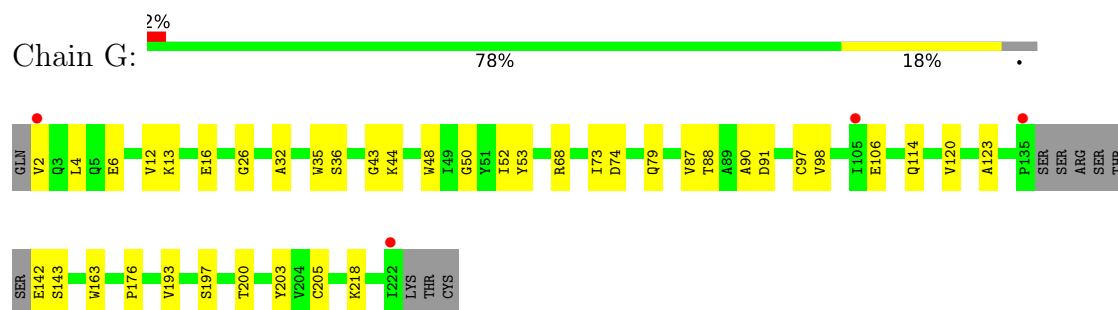
- Molecule 1: Antibody A12V163-a.02 heavy chain



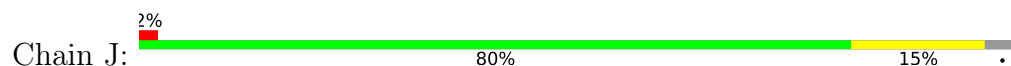
- Molecule 1: Antibody A12V163-a.02 heavy chain

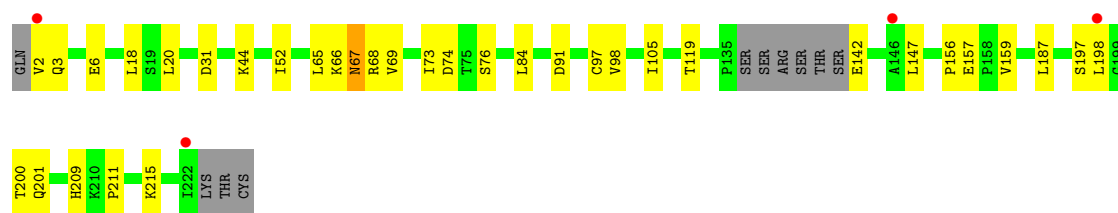


- Molecule 1: Antibody A12V163-a.02 heavy chain



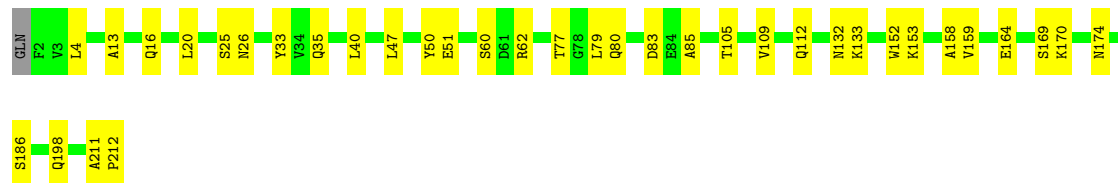
- Molecule 1: Antibody A12V163-a.02 heavy chain





- Molecule 2: Antibody A12V163-a.02 light chain

Chain B: 83% 17%



- Molecule 2: Antibody A12V163-a.02 light chain

Chain D: 87% 13%



- Molecule 2: Antibody A12V163-a.02 light chain

Chain H: 90% 10%



- Molecule 2: Antibody A12V163-a.02 light chain

Chain K: 90% 10%



- Molecule 3: HIV fusion peptide residue 512-519

Chain E: 100%

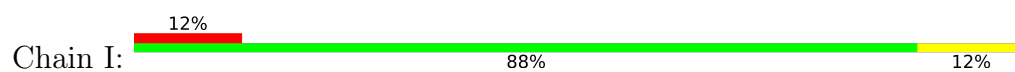
There are no outlier residues recorded for this chain.

- Molecule 3: HIV fusion peptide residue 512-519

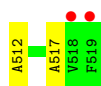
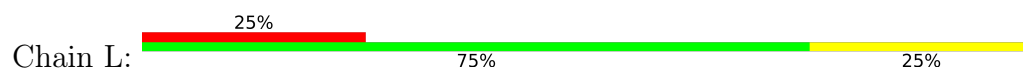
Chain F: 12% 75% 12% 12%



- Molecule 3: HIV fusion peptide residue 512-519



- Molecule 3: HIV fusion peptide residue 512-519



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.78Å 72.20Å 185.53Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	41.75 – 2.50 41.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (41.75-2.50) 97.9 (41.75-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.197 , 0.209 (Not available) , 0.196	Depositor DCC
R_{free} test set	3384 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14008	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0859e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	A	0.43	0/1703	0.73	0/2328
1	C	0.45	0/1703	0.90	8/2328 (0.3%)
1	G	0.42	0/1660	0.76	1/2269 (0.0%)
1	J	0.44	0/1660	0.78	2/2269 (0.1%)
2	B	0.38	0/1608	0.63	0/2194
2	D	0.39	0/1608	0.64	0/2194
2	H	0.37	0/1617	0.67	1/2206 (0.0%)
2	K	0.37	0/1617	0.67	1/2206 (0.0%)
3	E	0.32	0/51	0.52	0/68
3	F	0.45	0/51	0.84	0/68
3	I	0.32	0/51	0.53	0/68
3	L	0.33	0/51	0.77	0/68
All	All	0.41	0/13380	0.73	13/18266 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	GLU	CA-CB-CG	-10.17	93.76	114.10
1	C	221	GLU	CA-C-N	7.59	135.37	121.70
1	C	221	GLU	C-N-CA	7.59	135.37	121.70
1	G	106	GLU	CA-CB-CG	7.22	128.55	114.10
1	C	106	GLU	CA-CB-CG	7.04	128.17	114.10
1	C	219	ARG	CD-NE-CZ	-6.43	115.40	124.40
1	J	67	ASN	CB-CA-C	-6.31	97.13	110.31
2	K	149	GLU	CA-CB-CG	5.85	125.80	114.10
1	C	66	LYS	CG-CD-CE	5.71	124.44	111.30
2	H	149	GLU	N-CA-CB	5.65	120.66	110.83
1	J	142	GLU	CB-CA-C	-5.59	99.47	110.10
1	C	219	ARG	CB-CG-CD	-5.32	99.06	111.30
1	C	221	GLU	CG-CD-OE1	-5.32	106.17	118.40

There are no chirality outliers.

There are no planarity outliers.

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	A	1663	0	1641	26	0
1	C	1663	0	1641	40	1
1	G	1621	0	1600	26	0
1	J	1621	0	1600	29	0
2	B	1572	0	1512	25	0
2	D	1572	0	1512	21	1
2	H	1581	0	1523	15	0
2	K	1581	0	1523	13	0
3	E	51	0	53	0	0
3	F	51	0	53	3	0
3	I	51	0	53	1	0
3	L	51	0	53	3	0
4	A	137	0	0	6	0
4	B	104	0	0	9	2
4	C	133	0	0	14	1
4	D	127	0	0	9	2
4	E	7	0	0	0	0
4	F	5	0	0	0	0
4	G	111	0	0	3	2
4	H	92	0	0	5	0
4	I	3	0	0	0	0
4	J	127	0	0	8	2
4	K	78	0	0	1	1
4	L	6	0	0	1	0
All	All	14008	0	12764	195	6

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 8.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:ASN:OD1	1:J:68:ARG:HG3	1.12	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ARG:NH2	4:B:301:HOH:O	1.92	1.00
1:C:22:CYS:SG	4:C:323:HOH:O	2.19	1.00
1:J:67:ASN:OD1	1:J:68:ARG:CG	2.09	0.99
1:J:105:ILE:O	4:J:301:HOH:O	1.81	0.97
1:C:221:GLU:HG2	1:C:222:ILE:H	1.30	0.96
1:J:66:LYS:NZ	4:J:302:HOH:O	1.97	0.96
2:D:160:ASN:ND2	4:D:303:HOH:O	1.91	0.95
1:C:221:GLU:CG	1:C:222:ILE:H	1.78	0.94
2:D:61:ASP:O	4:D:301:HOH:O	1.86	0.90
1:A:218:LYS:NZ	4:A:301:HOH:O	2.03	0.89
2:D:88:TYR:OH	4:D:302:HOH:O	1.90	0.89
1:C:88:THR:HG22	1:C:90:ALA:H	1.38	0.86
2:D:79:LEU:O	4:D:304:HOH:O	1.92	0.86
1:A:2:VAL:HG12	1:A:3:GLN:HG3	1.59	0.83
1:C:180:GLN:NE2	4:C:302:HOH:O	2.11	0.83
1:J:2:VAL:HG12	1:J:3:GLN:HG3	1.63	0.81
2:B:198:GLN:NE2	4:B:305:HOH:O	2.14	0.81
1:G:88:THR:HG22	1:G:90:ALA:H	1.44	0.80
1:J:157:GLU:OE1	4:J:303:HOH:O	2.00	0.80
2:D:160:ASN:ND2	4:D:307:HOH:O	2.13	0.80
2:B:83:ASP:OD2	4:B:301:HOH:O	1.98	0.79
1:J:200:THR:HG23	1:J:201:GLN:HG2	1.68	0.75
2:H:47:LEU:O	4:H:301:HOH:O	2.05	0.75
1:J:31:ASP:OD1	4:J:304:HOH:O	2.04	0.74
1:C:16:GLU:OE1	4:C:301:HOH:O	2.05	0.73
2:H:55:ARG:NH2	2:H:59:VAL:O	2.21	0.73
1:A:63:PRO:HA	1:A:66:LYS:HG3	1.72	0.71
1:G:2:VAL:HG22	1:G:26:GLY:HA3	1.71	0.71
2:B:152:TRP:HB2	2:B:159:VAL:HG22	1.71	0.71
1:J:67:ASN:O	4:J:305:HOH:O	2.07	0.71
2:H:51:GLU:OE1	4:H:302:HOH:O	2.08	0.70
2:D:212:PRO:O	4:D:306:HOH:O	2.09	0.70
1:G:2:VAL:O	4:G:302:HOH:O	2.08	0.70
3:L:517:ALA:O	4:L:601:HOH:O	2.08	0.70
2:K:167:LYS:HG3	2:K:168:PRO:HD2	1.74	0.68
1:C:170:SER:O	4:C:303:HOH:O	2.12	0.67
1:C:2:VAL:HG22	1:C:26:GLY:HA3	1.77	0.67
1:C:221:GLU:HG2	1:C:222:ILE:N	2.08	0.66
1:G:142:GLU:N	4:G:303:HOH:O	2.27	0.66
2:D:62:ARG:NH1	2:D:83:ASP:OD2	2.30	0.65
1:C:135:PRO:HD3	1:C:147:LEU:HD23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LYS:NZ	4:B:311:HOH:O	2.30	0.64
2:B:79:LEU:HA	4:B:301:HOH:O	1.96	0.64
1:A:63:PRO:HA	1:A:66:LYS:HE3	1.80	0.64
1:G:13:LYS:NZ	1:G:123:ALA:O	2.31	0.64
2:D:37:TYR:CZ	2:D:47:LEU:HD13	2.34	0.63
2:K:33:TYR:HB3	2:K:51:GLU:HA	1.81	0.62
1:G:197:SER:HA	1:G:200:THR:HG22	1.82	0.61
1:J:44:LYS:NZ	4:J:308:HOH:O	2.33	0.61
1:C:63:PRO:HA	1:C:66:LYS:HG3	1.82	0.61
2:D:37:TYR:CE2	2:D:47:LEU:HD13	2.37	0.60
2:D:3:VAL:HG21	2:D:96:LEU:HD11	1.83	0.60
2:B:164:GLU:OE1	4:B:306:HOH:O	2.17	0.59
2:H:20:LEU:HB3	4:H:326:HOH:O	2.01	0.59
1:C:221:GLU:HG3	1:C:222:ILE:H	1.66	0.59
3:F:515:ILE:O	3:F:515:ILE:HG13	2.02	0.59
1:J:215:LYS:NZ	4:J:306:HOH:O	2.13	0.59
1:G:13:LYS:HB2	1:G:16:GLU:HG3	1.85	0.58
1:J:197:SER:O	1:J:200:THR:HG22	2.03	0.58
1:C:88:THR:HB	4:C:336:HOH:O	2.03	0.58
1:C:213:ASN:ND2	4:C:316:HOH:O	2.36	0.58
1:C:119:THR:HG21	1:C:156:PRO:HB2	1.84	0.58
1:J:52:ILE:HD13	1:J:73:ILE:HG13	1.85	0.58
1:C:152:LYS:NZ	4:C:317:HOH:O	2.37	0.58
1:C:87:VAL:HG23	1:C:91:ASP:HB2	1.85	0.57
1:C:201:GLN:NE2	1:C:202:THR:O	2.33	0.57
1:C:16:GLU:O	1:C:87:VAL:HG12	2.04	0.57
1:C:52:ILE:HD13	1:C:73:ILE:HG13	1.87	0.57
2:H:82:GLU:OE2	2:H:82:GLU:N	2.38	0.56
1:G:218:LYS:NZ	2:H:127:GLU:OE1	2.38	0.56
1:J:119:THR:HG21	1:J:156:PRO:HB2	1.88	0.56
1:A:206:ASN:ND2	1:A:217:ASP:OD2	2.37	0.56
1:A:36:SER:HB2	1:A:98:VAL:HG22	1.88	0.55
2:B:152:TRP:HB2	2:B:159:VAL:CG2	2.36	0.55
1:J:119:THR:HG21	1:J:156:PRO:CB	2.38	0.54
1:J:65:LEU:O	1:J:69:VAL:HG23	2.07	0.54
1:A:11:LEU:HD11	1:A:121:SER:HB3	1.90	0.54
1:C:38:ILE:HD12	1:C:98:VAL:HG11	1.90	0.54
2:K:82:GLU:N	2:K:82:GLU:OE1	2.40	0.53
1:C:154:TYR:CE1	1:C:159:VAL:HG13	2.44	0.53
2:B:33:TYR:HB3	2:B:51:GLU:HA	1.91	0.53
2:H:31:VAL:HG21	2:H:94:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:ARG:HH22	1:J:91:ASP:CG	2.16	0.53
2:B:169:SER:OG	4:B:303:HOH:O	2.11	0.53
2:B:20:LEU:HD12	2:B:105:THR:HG21	1.90	0.53
1:G:44:LYS:HD3	4:H:305:HOH:O	2.09	0.52
2:K:40:LEU:O	2:K:43:THR:HG22	2.09	0.52
1:C:2:VAL:N	4:C:322:HOH:O	2.42	0.52
1:A:68:ARG:O	1:A:85:ARG:HG2	2.09	0.52
2:H:33:TYR:HB3	2:H:51:GLU:HA	1.92	0.52
1:C:74:ASP:OD1	1:C:76:SER:OG	2.28	0.52
2:B:35:GLN:HG3	2:B:50:TYR:HA	1.92	0.52
2:K:208:LYS:NZ	4:K:312:HOH:O	2.43	0.52
1:J:159:VAL:HG12	1:J:187:LEU:HD21	1.91	0.51
2:H:208:LYS:NZ	4:H:304:HOH:O	2.26	0.51
1:A:52:ILE:HD13	1:A:73:ILE:HG13	1.92	0.51
1:A:159:VAL:HG12	1:A:209:HIS:CD2	2.45	0.51
2:D:55:ARG:NH2	4:D:305:HOH:O	2.06	0.51
2:K:3:VAL:HG21	2:K:96:LEU:HD11	1.92	0.51
1:G:193:VAL:HG21	1:G:203:TYR:OH	2.10	0.51
1:J:68:ARG:NH2	1:J:91:ASP:OD2	2.44	0.51
2:D:70:THR:HG22	2:D:70:THR:O	2.11	0.50
1:A:212:SER:OG	1:A:214:THR:HG22	2.11	0.50
2:K:51:GLU:OE2	3:L:512:ALA:N	2.44	0.50
1:G:32:ALA:HB1	1:G:53:TYR:OH	2.12	0.50
1:G:142:GLU:HG3	1:G:143:SER:H	1.77	0.49
1:J:200:THR:HG23	1:J:201:GLN:CG	2.39	0.49
2:B:47:LEU:O	4:B:307:HOH:O	2.20	0.49
1:C:159:VAL:HG22	1:C:187:LEU:HD21	1.94	0.48
2:H:55:ARG:HD3	2:H:63:PHE:O	2.12	0.48
2:B:40:LEU:HD23	2:B:85:ALA:HB2	1.95	0.48
1:A:36:SER:HB2	1:A:98:VAL:CG2	2.44	0.48
1:C:119:THR:HG21	1:C:156:PRO:CB	2.44	0.48
4:C:379:HOH:O	2:K:94:ILE:HD11	2.14	0.48
1:G:52:ILE:HD13	1:G:73:ILE:HG13	1.95	0.48
3:F:517:ALA:HB1	3:L:517:ALA:HB1	1.95	0.48
1:J:74:ASP:OD2	1:J:76:SER:OG	2.29	0.48
1:C:176:PRO:HG2	2:D:169:SER:OG	2.14	0.48
2:H:4:LEU:HD22	2:H:100:VAL:HG23	1.96	0.47
1:C:215:LYS:NZ	4:C:327:HOH:O	2.47	0.47
1:A:215:LYS:NZ	4:A:305:HOH:O	2.33	0.47
2:K:189:TRP:CE2	2:K:212:PRO:HG3	2.49	0.47
1:G:114:GLN:HG3	4:G:332:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:THR:HG22	4:J:323:HOH:O	2.14	0.47
1:G:36:SER:HB2	1:G:98:VAL:HG13	1.96	0.47
1:G:12:VAL:HG13	1:G:120:VAL:HG22	1.95	0.47
2:B:80:GLN:O	2:B:109:VAL:HG21	2.14	0.47
1:C:201:GLN:HG2	1:C:203:TYR:CZ	2.50	0.47
2:D:50:TYR:HD1	2:D:51:GLU:HG3	1.80	0.47
1:G:176:PRO:HG2	2:H:169:SER:OG	2.15	0.47
2:D:127:GLU:HA	2:D:130:GLN:HG3	1.96	0.46
2:H:36:TRP:HB2	2:H:49:ILE:HB	1.96	0.46
1:G:6:GLU:HG3	1:G:97:CYS:SG	2.56	0.46
2:D:199:VAL:O	2:D:205:THR:HA	2.15	0.46
1:C:171:GLY:O	1:C:191:VAL:HA	2.16	0.46
2:B:112:GLN:NE2	4:B:321:HOH:O	2.49	0.46
2:D:15:GLY:N	4:D:304:HOH:O	2.48	0.46
1:A:87:VAL:HG22	1:A:91:ASP:HB2	1.97	0.46
1:C:51:TYR:OH	4:C:304:HOH:O	2.21	0.46
1:G:4:LEU:HD21	1:G:35:TRP:HZ3	1.81	0.46
1:G:74:ASP:HB3	1:G:79:GLN:HG2	1.98	0.46
2:B:25:SER:OG	2:B:26:ASN:N	2.49	0.45
1:C:48:TRP:NE1	3:F:515:ILE:HD11	2.31	0.45
1:A:61:TYR:HB2	1:A:66:LYS:HG2	1.98	0.45
2:D:13:ALA:HB3	2:D:16:GLN:NE2	2.32	0.45
2:B:13:ALA:O	2:B:16:GLN:HB3	2.17	0.45
1:C:193:VAL:HG21	1:C:203:TYR:CE1	2.52	0.45
1:A:157:GLU:OE1	4:A:303:HOH:O	2.21	0.45
2:B:132:ASN:HA	2:B:186:SER:OG	2.17	0.44
1:C:80:PHE:CZ	1:C:97:CYS:HB2	2.52	0.44
2:B:62:ARG:HD2	2:B:77:THR:O	2.17	0.44
1:A:176:PRO:HG2	2:B:169:SER:OG	2.17	0.44
2:B:50:TYR:HD1	2:B:51:GLU:HG3	1.83	0.44
1:C:2:VAL:CG2	1:C:26:GLY:HA3	2.47	0.44
1:A:197:SER:HA	1:A:200:THR:HG22	1.99	0.43
2:D:55:ARG:HD2	4:D:305:HOH:O	2.17	0.43
2:H:62:ARG:HB3	2:H:77:THR:O	2.18	0.43
1:J:198:LEU:HD23	1:J:198:LEU:HA	1.84	0.43
1:J:69:VAL:HG22	1:J:84:LEU:CD1	2.48	0.43
2:D:3:VAL:HG21	2:D:96:LEU:CD1	2.49	0.43
1:C:63:PRO:HA	1:C:66:LYS:CG	2.49	0.43
1:C:202:THR:HG22	4:C:312:HOH:O	2.19	0.43
2:B:153:LYS:HD3	2:B:158:ALA:HA	2.00	0.43
2:K:84:GLU:HG3	2:K:109:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:VAL:CG2	1:G:26:GLY:HA3	2.44	0.43
1:A:198:LEU:HD13	1:A:198:LEU:HA	1.78	0.42
1:C:193:VAL:HG22	4:C:334:HOH:O	2.19	0.42
1:A:119:THR:HG21	1:A:156:PRO:HB2	2.01	0.42
1:G:43:GLY:O	1:G:44:LYS:HB2	2.17	0.42
2:K:112:GLN:HB2	2:K:144:TYR:CE1	2.55	0.42
1:J:6:GLU:HG3	1:J:97:CYS:SG	2.59	0.42
1:J:209:HIS:CD2	1:J:211:PRO:HD2	2.54	0.42
1:C:221:GLU:HG3	1:C:222:ILE:N	2.31	0.42
2:K:79:LEU:HD23	2:K:79:LEU:HA	1.92	0.42
2:B:211:ALA:HA	2:B:212:PRO:HD3	1.88	0.42
1:A:201:GLN:HG3	1:A:202:THR:N	2.35	0.41
2:B:170:LYS:HE3	2:B:174:ASN:HA	2.01	0.41
1:A:219:ARG:HG2	4:A:314:HOH:O	2.20	0.41
2:H:16:GLN:CG	2:H:17:ARG:N	2.84	0.41
1:A:68:ARG:NH2	1:A:91:ASP:OD2	2.53	0.41
3:I:519:PHE:CD1	3:I:519:PHE:C	2.98	0.41
1:J:18:LEU:HD21	1:J:20:LEU:HG	2.03	0.41
1:A:222:ILE:C	4:A:316:HOH:O	2.64	0.41
2:D:80:GLN:O	2:D:109:VAL:HG21	2.21	0.41
1:G:68:ARG:HH11	1:G:68:ARG:HD2	1.75	0.41
1:J:147:LEU:HD23	1:J:198:LEU:HD21	2.03	0.41
1:G:48:TRP:CZ2	1:G:50:GLY:HA2	2.56	0.41
1:A:29:ILE:HG13	1:A:29:ILE:O	2.21	0.40
1:C:213:ASN:OD1	4:C:305:HOH:O	2.22	0.40
1:A:219:ARG:NE	4:A:314:HOH:O	2.48	0.40
1:G:163:TRP:CH2	1:G:205:CYS:HB3	2.56	0.40
1:J:215:LYS:HE3	1:J:215:LYS:HB2	1.87	0.40
1:G:87:VAL:HG22	1:G:91:ASP:HB2	2.04	0.40
2:K:90:GLN:HG2	2:K:100:VAL:O	2.22	0.40

All (6) 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)
4:G:404:HOH:O	4:J:418:HOH:O[2_355]	1.86	0.34
4:B:385:HOH:O	4:G:381:HOH:O[1_545]	1.90	0.30
4:C:338:HOH:O	4:D:387:HOH:O[2_346]	1.98	0.22
4:J:401:HOH:O	4:K:354:HOH:O[2_255]	2.02	0.18
1:C:219:ARG:NH2	2:D:203:GLY:O[2_346]	2.16	0.04
4:B:319:HOH:O	4:D:307:HOH:O[2_446]	2.19	0.01

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	A	219/225 (97%)	214 (98%)	5 (2%)	0	100	100
1	C	219/225 (97%)	214 (98%)	5 (2%)	0	100	100
1	G	211/225 (94%)	207 (98%)	4 (2%)	0	100	100
1	J	211/225 (94%)	209 (99%)	2 (1%)	0	100	100
2	B	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
2	D	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
2	H	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
2	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
3	E	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
3	F	6/8 (75%)	3 (50%)	3 (50%)	0	100	100
3	I	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
3	L	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
All	All	1722/1780 (97%)	1676 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	191/195 (98%)	190 (100%)	1 (0%)	81	92
1	C	191/195 (98%)	189 (99%)	2 (1%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	185/195 (95%)	185 (100%)	0	100	100
1	J	121/195 (62%)	120 (99%)	1 (1%)	73	88
2	B	176/177 (99%)	174 (99%)	2 (1%)	65	84
2	D	176/177 (99%)	175 (99%)	1 (1%)	78	91
2	H	42/177 (24%)	41 (98%)	1 (2%)	43	70
2	K	177/177 (100%)	177 (100%)	0	100	100
3	E	4/4 (100%)	4 (100%)	0	100	100
3	F	4/4 (100%)	3 (75%)	1 (25%)	0	1
3	L	4/4 (100%)	4 (100%)	0	100	100
All	All	1271/1500 (85%)	1262 (99%)	9 (1%)	76	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	THR
2	B	4	LEU
2	B	60	SER
1	C	98	VAL
1	C	193	VAL
2	D	4	LEU
3	F	515	ILE
2	H	4	LEU
1	J	98	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	40	GLN
2	B	39	GLN
2	B	112	GLN
2	B	201	HIS
2	D	132	ASN
1	J	213	ASN
2	K	16	GLN
2	K	112	GLN
2	K	201	HIS

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	A	221/225 (98%)	-0.06	1 (0%) 87 85	27, 40, 59, 75	0
1	C	221/225 (98%)	-0.02	2 (0%) 81 78	26, 41, 60, 75	0
1	G	215/225 (95%)	-0.05	4 (1%) 66 62	29, 41, 61, 82	0
1	J	215/225 (95%)	-0.01	4 (1%) 66 62	30, 42, 62, 78	0
2	B	211/212 (99%)	-0.11	0 100 100	24, 43, 56, 65	0
2	D	211/212 (99%)	-0.16	0 100 100	25, 43, 57, 63	0
2	H	212/212 (100%)	-0.10	0 100 100	31, 45, 58, 65	0
2	K	212/212 (100%)	-0.04	2 (0%) 81 78	34, 46, 59, 70	0
3	E	8/8 (100%)	0.02	0 100 100	37, 38, 51, 52	0
3	F	8/8 (100%)	0.23	1 (12%) 8 6	36, 38, 49, 56	0
3	I	8/8 (100%)	0.43	1 (12%) 8 6	37, 43, 52, 53	0
3	L	8/8 (100%)	0.49	2 (25%) 2 1	37, 39, 57, 60	0
All	All	1750/1780 (98%)	-0.06	17 (0%) 79 76	24, 43, 59, 82	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	519	PHE	3.3
1	C	222	ILE	3.2
3	L	519	PHE	3.1
1	A	222	ILE	3.1
1	G	222	ILE	2.8
1	J	222	ILE	2.7
1	C	2	VAL	2.5
3	L	518	VAL	2.5
1	J	146	ALA	2.4
1	G	105	ILE	2.4
1	J	198	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	519	PHE	2.3
1	G	2	VAL	2.2
1	G	135	PRO	2.1
1	J	2	VAL	2.1
2	K	160	ASN	2.0
2	K	167	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 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.