Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:39 PM BST

PDB ID	:	6P60
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 following versions of software and data (see references ⓘ) were used in the production of this report:

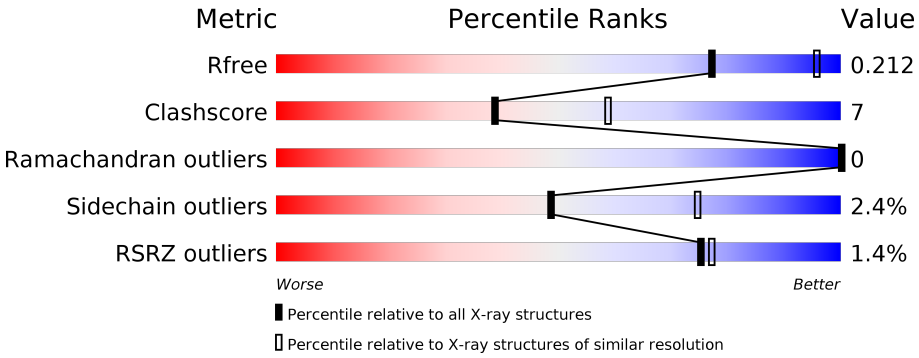
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	80% 17%
1	C	225	% 77% 19%
1	G	225	% 76% 19%
1	J	225	80% 14%
2	B	212	4% 81% 18%
2	D	212	2% 87% 13%

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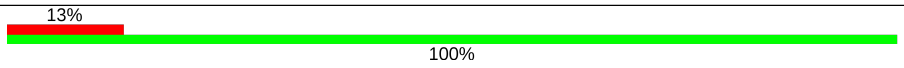
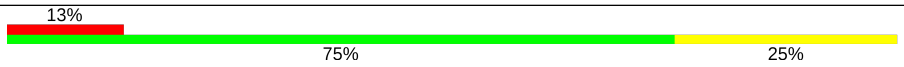
Mol	Chain	Length	Quality of chain
2	H	212	
2	K	212	
3	E	8	
3	F	8	
3	I	8	
3	L	8	

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.

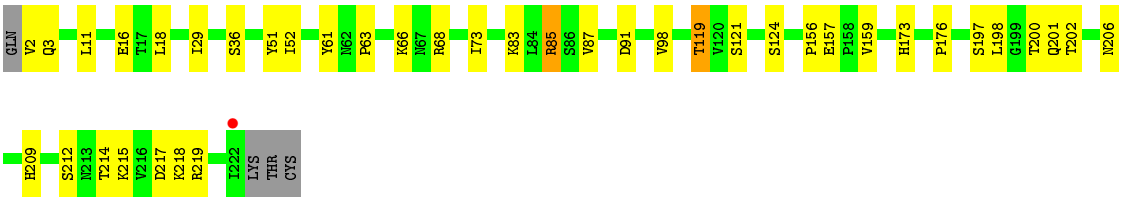
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	137	Total O 137 137	0	0
4	B	104	Total O 104 104	0	0
4	E	7	Total O 7 7	0	0
4	C	133	Total O 133 133	0	0
4	D	127	Total O 127 127	0	0
4	F	5	Total O 5 5	0	0
4	G	111	Total O 111 111	0	0
4	H	92	Total O 92 92	0	0
4	I	3	Total O 3 3	0	0
4	J	127	Total O 127 127	0	0
4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

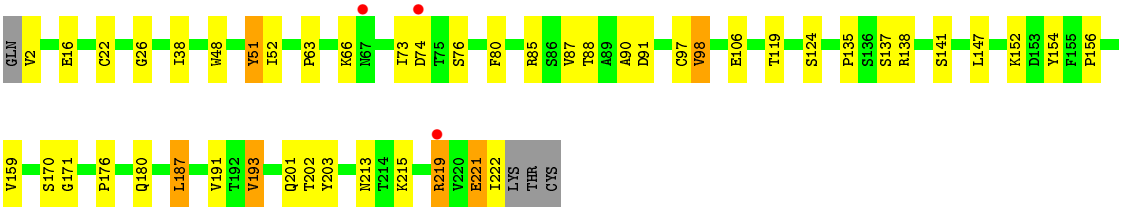
- Molecule 1: Antibody A12V163-a.02 heavy chain

Chain A:



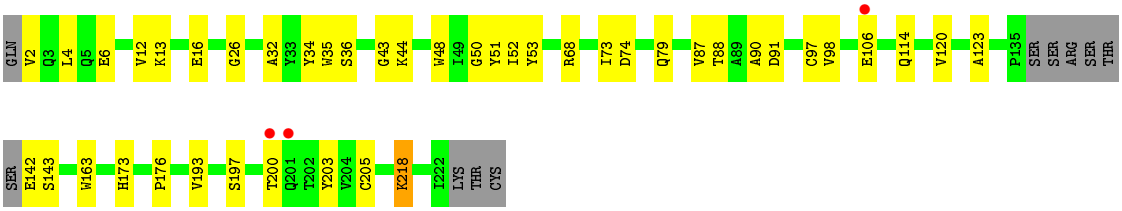
- Molecule 1: Antibody A12V163-a.02 heavy chain

Chain C:



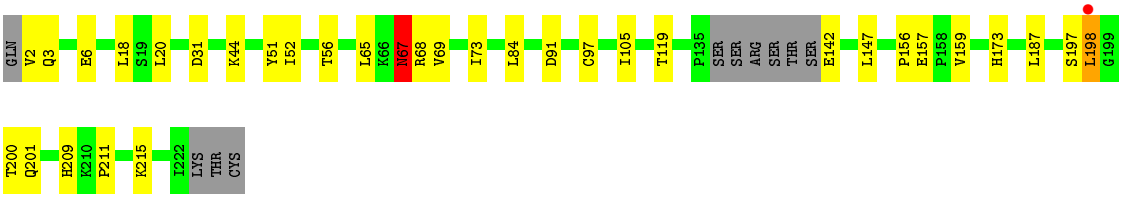
- Molecule 1: Antibody A12V163-a.02 heavy chain

Chain G:

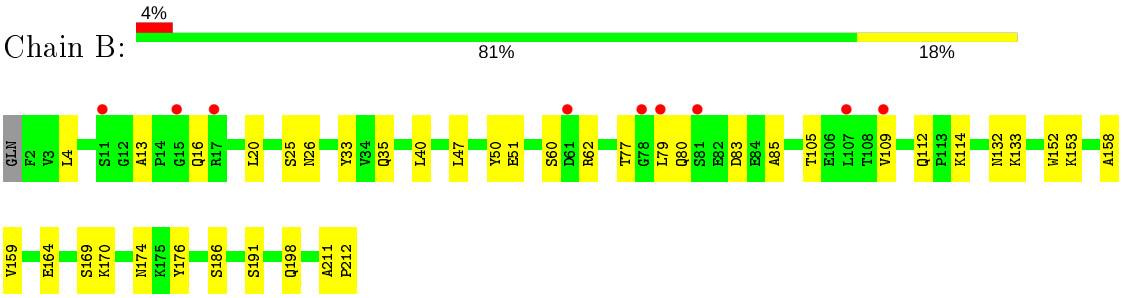


- Molecule 1: Antibody A12V163-a.02 heavy chain

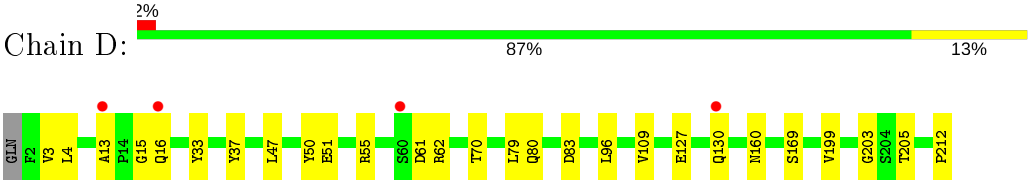
Chain J:



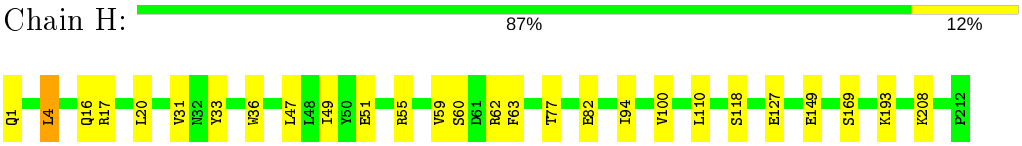
• Molecule 2: Antibody A12V163-a.02 light chain



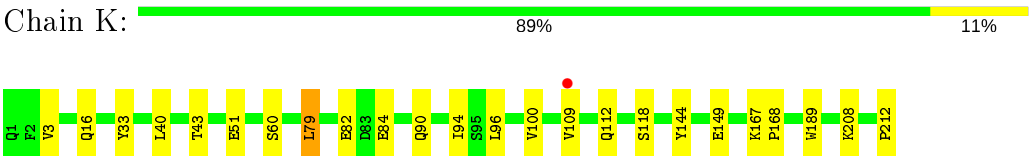
• Molecule 2: Antibody A12V163-a.02 light chain



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



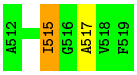
• Molecule 2: Antibody A12V163-a.02 light chain



• Molecule 3: HIV fusion peptide residue 512-519

There are no outlier residues recorded for this chain.

• Molecule 3: HIV fusion peptide residue 512-519



- Molecule 3: HIV fusion peptide residue 512-519

Chain I:

- Molecule 3: HIV fusion peptide residue 512-519

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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) 98.0 (41.75-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.197 , 0.209 0.198 , 0.212	Depositor DCC
R_{free} test set	3384 reflections (4.85%)	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 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.50	0/1703	0.74	2/2328 (0.1%)
1	C	0.52	0/1703	0.87	8/2328 (0.3%)
1	G	0.49	0/1660	0.72	1/2269 (0.0%)
1	J	0.51	0/1660	0.79	5/2269 (0.2%)
2	B	0.47	0/1608	0.65	0/2194
2	D	0.47	0/1608	0.65	0/2194
2	H	0.44	0/1617	0.67	1/2206 (0.0%)
2	K	0.45	0/1617	0.67	1/2206 (0.0%)
3	E	0.43	0/51	0.55	0/68
3	F	0.47	0/51	0.64	0/68
3	I	0.46	0/51	0.60	0/68
3	L	0.43	0/51	0.66	0/68
All	All	0.48	0/13380	0.72	18/18266 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	219	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	C	221	GLU	CA-CB-CG	-8.93	93.76	113.40
1	C	219	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	J	198	LEU	CA-CB-CG	-7.01	99.17	115.30
1	G	106	GLU	CA-CB-CG	6.88	128.55	113.40
1	C	106	GLU	CA-CB-CG	6.71	128.17	113.40
1	J	67	ASN	CB-CA-C	-6.63	97.13	110.40
1	C	221	GLU	CG-CD-OE1	-6.07	106.17	118.30
1	J	142	GLU	CA-C-N	-5.96	104.08	117.20
1	J	198	LEU	CB-CG-CD1	-5.94	100.90	111.00
1	C	219	ARG	CD-NE-CZ	-5.86	115.40	123.60
1	A	18	LEU	CA-CB-CG	5.80	128.64	115.30
2	K	149	GLU	CA-CB-CG	5.63	125.80	113.40
2	H	149	GLU	N-CA-CB	5.59	120.66	110.60
1	C	221	GLU	C-N-CA	5.47	135.37	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	142	GLU	CB-CA-C	-5.46	99.47	110.40
1	C	187	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	16	GLU	OE1-CD-OE2	5.01	129.32	123.30

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	25	0
1	C	1663	0	1641	41	1
1	G	1621	0	1600	27	0
1	J	1621	0	1600	27	0
2	B	1572	0	1512	26	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	0	0
3	L	51	0	53	3	0
4	A	137	0	0	5	0
4	B	104	0	0	10	2
4	C	133	0	0	14	1
4	D	127	0	0	8	2
4	E	7	0	0	0	0
4	F	5	0	0	0	0
4	G	111	0	0	4	2
4	H	92	0	0	5	0
4	I	3	0	0	0	0
4	J	127	0	0	6	2
4	K	78	0	0	1	1
4	L	6	0	0	1	0
All	All	14008	0	12764	193	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 7.

All (193) 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
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
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
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
1:G:34:TYR:OH	4:G:301:HOH:O	2.04	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:C:221:GLU:CG	1:C:222:ILE:N	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:176:TYR:OH	4:B:304:HOH:O	2.13	0.63
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: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: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:213:ASN:ND2	4:C:316:HOH:O	2.36	0.58
1:C:88:THR:HB	4:C:336:HOH:O	2.03	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
2:H:208:LYS:NZ	4:H:304:HOH:O	2.26	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:N	2:H:82:GLU:OE2	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:D:33:TYR:HH	1:J:56:THR:HG1	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:169:SER:OG	4:B:303:HOH:O	2.11	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
1:J:159:VAL:HG12	1:J:187:LEU:HD21	1.91	0.51
1:A:159:VAL:HG12	1:A:209:HIS:CD2	2.45	0.51
1:A:52:ILE:HD13	1:A:73:ILE:HG13	1.92	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:44:LYS:NZ	4:J:308:HOH:O	2.33	0.51
1:J:68:ARG:NH2	1:J:91:ASP:OD2	2.44	0.51
2:D:70:THR:O	2:D:70:THR:HG22	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
2:K:208:LYS:NZ	4:K:312:HOH:O	2.43	0.49
1:J:200:THR:HG23	1:J:201:GLN:CG	2.39	0.49
1:J:68:ARG:HH22	1:J:91:ASP:CG	2.16	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
1:G:52:ILE:HD13	1:G:73:ILE:HG13	1.95	0.48
4:C:379:HOH:O	2:K:94:ILE:HD11	2.14	0.48
3:F:517:ALA:HB1	3:L:517:ALA:HB1	1.95	0.48
1:C:176:PRO:HG2	2:D:169:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:A:215:LYS:NZ	4:A:305:HOH:O	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:VAL:HG21	2:D:96:LEU:CD1	2.49	0.43
1:C:202:THR:HG22	4:C:312:HOH:O	2.19	0.43
1:C:63:PRO:HA	1:C:66:LYS:CG	2.49	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
1:G:2:VAL:CG2	1:G:26:GLY:HA3	2.44	0.43
1:A:198:LEU:HA	1:A:198:LEU:HD13	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:209:HIS:CD2	1:J:211:PRO:HD2	2.54	0.42
1:J:6:GLU:HG3	1:J:97:CYS:SG	2.59	0.42
1:C:221:GLU:HG3	1:C:222:ILE:N	2.31	0.42
2:K:79:LEU:HA	2:K:79:LEU:HD23	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
1:J:18:LEU:HD21	1:J:20:LEU:HG	2.03	0.41
2:D:80:GLN:O	2:D:109:VAL:HG21	2.21	0.41
1:G:68:ARG:HD2	1:G:68:ARG:HH11	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:O	1:A:29:ILE:HG13	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:HB2	1:J:215:LYS:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	185 (97%)	6 (3%)	40 67
1	C	191/195 (98%)	183 (96%)	8 (4%)	30 54
1	G	185/195 (95%)	182 (98%)	3 (2%)	62 84
1	J	185/195 (95%)	182 (98%)	3 (2%)	62 84
2	B	176/177 (99%)	172 (98%)	4 (2%)	50 76
2	D	176/177 (99%)	175 (99%)	1 (1%)	86 95
2	H	177/177 (100%)	171 (97%)	6 (3%)	37 63
2	K	177/177 (100%)	173 (98%)	4 (2%)	50 76
3	E	4/4 (100%)	4 (100%)	0	100 100
3	F	4/4 (100%)	3 (75%)	1 (25%)	0 1
3	I	4/4 (100%)	4 (100%)	0	100 100
3	L	4/4 (100%)	4 (100%)	0	100 100
All	All	1474/1504 (98%)	1438 (98%)	36 (2%)	49 74

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	83	LYS
1	A	85	ARG
1	A	119	THR
1	A	124	SER
1	A	173	HIS
2	B	4	LEU
2	B	60	SER
2	B	114	LYS
2	B	191	SER
1	C	51	TYR
1	C	85	ARG
1	C	98	VAL
1	C	124	SER
1	C	137	SER
1	C	138	ARG
1	C	141	SER
1	C	193	VAL

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Mol	Chain	Res	Type
2	D	4	LEU
3	F	515	ILE
1	G	51	TYR
1	G	173	HIS
1	G	218	LYS
2	H	1	GLN
2	H	4	LEU
2	H	60	SER
2	H	110	LEU
2	H	118	SER
2	H	193	LYS
1	J	51	TYR
1	J	67	ASN
1	J	173	HIS
2	K	16	GLN
2	K	60	SER
2	K	79	LEU
2	K	118	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	213	ASN
2	K	16	GLN
2	K	38	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	221/225 (98%)	-0.09	1 (0%) 91 91	27, 40, 59, 75	0
1	C	221/225 (98%)	-0.02	3 (1%) 75 77	26, 41, 60, 75	0
1	G	215/225 (95%)	0.00	3 (1%) 75 77	29, 41, 61, 82	0
1	J	215/225 (95%)	-0.00	1 (0%) 91 91	30, 42, 62, 78	0
2	B	211/212 (99%)	0.11	9 (4%) 35 38	24, 43, 56, 65	0
2	D	211/212 (99%)	0.02	4 (1%) 66 69	25, 43, 57, 63	0
2	H	212/212 (100%)	-0.02	0 100 100	31, 45, 58, 65	0
2	K	212/212 (100%)	0.01	1 (0%) 91 91	34, 46, 59, 70	0
3	E	8/8 (100%)	0.46	0 100 100	37, 38, 51, 52	0
3	F	8/8 (100%)	0.58	0 100 100	36, 38, 49, 56	0
3	I	8/8 (100%)	0.59	1 (12%) 3 3	37, 43, 52, 53	0
3	L	8/8 (100%)	0.65	1 (12%) 3 3	37, 39, 57, 60	0
All	All	1750/1780 (98%)	0.01	24 (1%) 75 77	24, 43, 59, 82	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	519	PHE	2.8
1	C	67	ASN	2.8
1	J	198	LEU	2.8
2	B	79	LEU	2.7
3	I	519	PHE	2.7
1	G	200	THR	2.7
1	G	106	GLU	2.7
1	G	201	GLN	2.6
2	B	11	SER	2.6
2	D	16	GLN	2.5
2	B	17	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	61	ASP	2.4
1	A	222	ILE	2.4
1	C	74	ASP	2.4
2	B	109	VAL	2.4
2	D	13	ALA	2.4
1	C	219	ARG	2.3
2	B	78	GLY	2.3
2	B	81	SER	2.2
2	B	107	LEU	2.2
2	K	109	VAL	2.1
2	B	15	GLY	2.1
2	D	60	SER	2.0
2	D	130	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.