



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:25 pm BST

PDB ID : 5TKJ
Title : Structure of vaccine-elicited diverse HIV-1 neutralizing antibody vFP1.01 in complex with HIV-1 fusion peptide residue 512-519
Authors : Xu, K.; Liu, K.; Kwong, P.D.
Deposited on : 2016-10-06
Resolution : 2.12 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

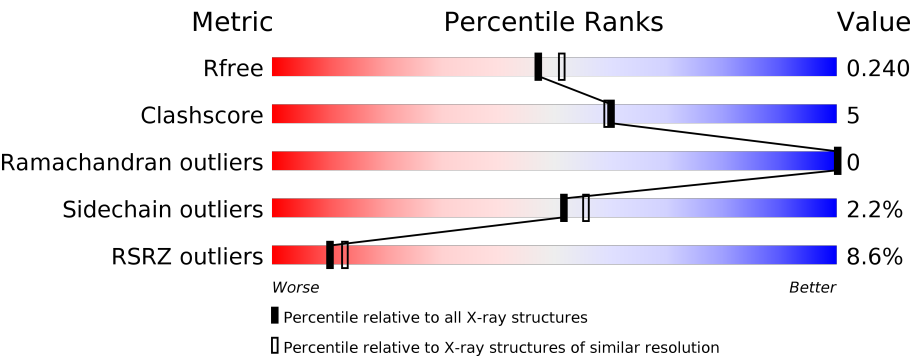
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 $\leq 5\%$. 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	221	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>91% . 5%</div></div>
1	D	221	<div><div></div><div></div><div></div><div></div><div></div></div> <div>89% 6% 5%</div>
1	G	221	<div><div>10%</div><div></div><div></div><div></div><div></div></div> <div>86% 8% 6%</div>
1	J	221	<div><div>25%</div><div></div><div></div><div></div><div></div></div> <div>80% 15% 5%</div>
2	B	219	<div><div></div><div></div><div></div><div></div><div></div></div> <div>94% 5%</div>
2	E	219	<div><div>%</div><div></div><div></div><div></div><div></div></div> <div>91% 8% .</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	219	
2	K	219	
3	C	8	
3	F	8	
3	I	8	
3	L	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	302	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14526 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 vFP1.01 chimeric mouse antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1620	1037	266	312	5			
1	D	211	Total	C	N	O	S	0	0	0
			1620	1037	266	312	5			
1	G	208	Total	C	N	O	S	0	0	0
			1604	1028	263	308	5			
1	J	211	Total	C	N	O	S	0	0	0
			1620	1037	266	312	5			

- Molecule 2 is a protein called vFP1.01 chimeric mouse antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1691	1064	284	338	5			
2	E	219	Total	C	N	O	S	0	0	0
			1697	1067	285	339	6			
2	H	216	Total	C	N	O	S	0	0	0
			1678	1057	282	334	5			
2	K	216	Total	C	N	O	S	0	0	0
			1678	1057	282	334	5			

- Molecule 3 is a protein called HIV-1 fusion peptide residue 512-519.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	196	Total	O	0	0
			196	196		
5	B	186	Total	O	0	0
			186	186		
5	C	3	Total	O	0	0
			3	3		
5	D	187	Total	O	0	0
			187	187		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	180	Total 180	O 180	0	0
5	F	2	Total 2	O 2	0	0
5	G	98	Total 98	O 98	0	0
5	H	70	Total 70	O 70	0	0
5	I	3	Total 3	O 3	0	0
5	J	87	Total 87	O 87	0	0
5	K	64	Total 64	O 64	0	0
5	L	3	Total 3	O 3	0	0

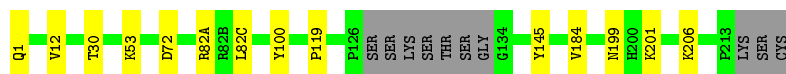
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

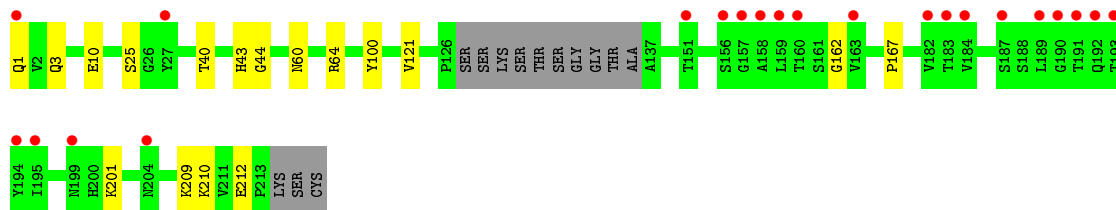
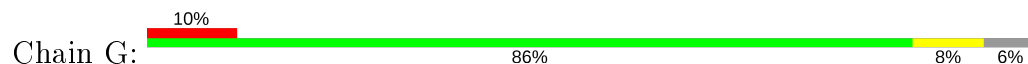
- Molecule 1: vFP1.01 chimeric mouse antibody heavy chain

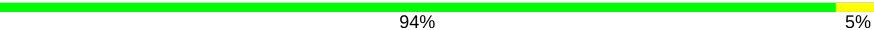


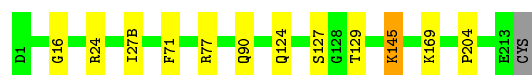
- Molecule 1: vFP1.01 chimeric mouse antibody heavy chain



- Molecule 1: vFP1.01 chimeric mouse antibody heavy chain

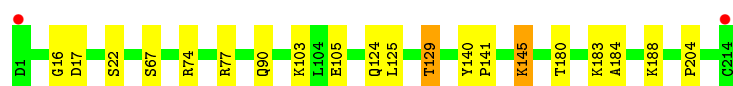


Chain B:  94% 5%




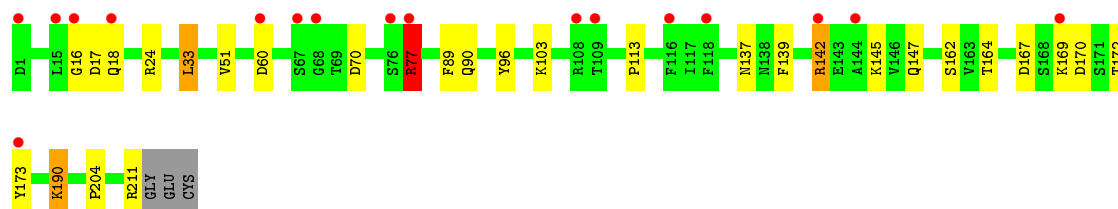
- Molecule 2: vFP1.01 chimeric mouse antibody light chain

Chain E:  91% 8%




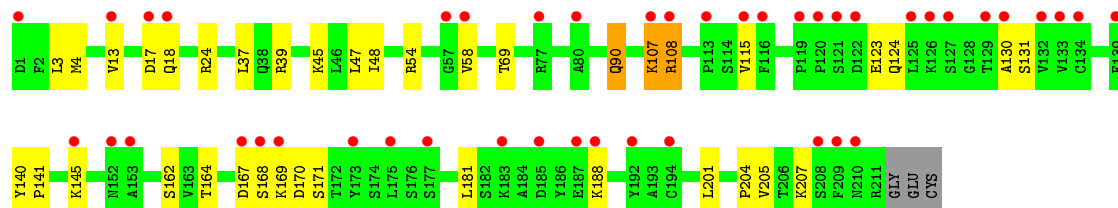
- Molecule 2: vFP1.01 chimeric mouse antibody light chain

Chain H:  85% 11% 8%




- Molecule 2: vFP1.01 chimeric mouse antibody light chain

Chain K:  81% 16% 20%



- Molecule 3: HIV-1 fusion peptide residue 512-519

Chain C:  75% 13% 13% 13%

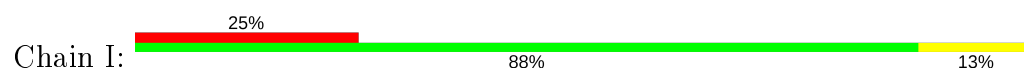


- Molecule 3: HIV-1 fusion peptide residue 512-519

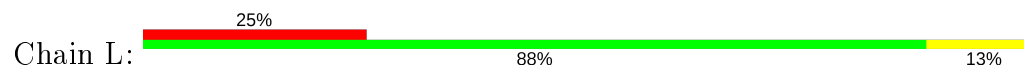
Chain F:  100% 13%



- Molecule 3: HIV-1 fusion peptide residue 512-519



- Molecule 3: HIV-1 fusion peptide residue 512-519



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.16Å 120.18Å 226.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.54 – 2.12 47.17 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.54-2.12) 99.7 (47.17-2.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.10 _2155	Depositor
R, R_{free}	0.198 , 0.241 0.199 , 0.240	Depositor DCC
R_{free} test set	5932 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14526	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 50.68 % 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 6.2457e-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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.47	0/1665	0.62	0/2279
1	D	0.48	0/1665	0.63	0/2279
1	G	0.39	0/1649	0.57	0/2257
1	J	0.39	0/1665	0.57	0/2279
2	B	0.50	0/1729	0.63	0/2344
2	E	0.48	0/1735	0.63	0/2352
2	H	0.40	0/1716	0.62	1/2327 (0.0%)
2	K	0.36	0/1716	0.60	0/2327
3	C	0.44	0/51	0.59	0/68
3	F	0.47	0/51	0.60	0/68
3	I	0.33	0/51	0.56	0/68
3	L	0.41	0/51	0.58	0/68
All	All	0.44	0/13744	0.61	1/18716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	77	ARG	NE-CZ-NH1	-5.97	117.31	120.30

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	1620	0	1589	4	0
1	D	1620	0	1589	8	0
1	G	1604	0	1574	11	0
1	J	1620	0	1589	21	0
2	B	1691	0	1641	11	0
2	E	1697	0	1646	12	0
2	H	1678	0	1632	31	0
2	K	1678	0	1632	38	0
3	C	51	0	53	1	0
3	F	51	0	53	0	0
3	I	51	0	53	0	0
3	L	51	0	53	0	0
4	A	10	0	0	2	0
4	D	10	0	0	0	0
4	G	10	0	0	0	0
4	J	5	0	0	0	0
5	A	196	0	0	2	0
5	B	186	0	0	4	0
5	C	3	0	0	0	0
5	D	187	0	0	1	0
5	E	180	0	0	4	0
5	F	2	0	0	0	0
5	G	98	0	0	5	0
5	H	70	0	0	4	0
5	I	3	0	0	0	0
5	J	87	0	0	4	0
5	K	64	0	0	3	0
5	L	3	0	0	0	0
All	All	14526	0	13104	121	0

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 5.

All (121) 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)
2:K:108:ARG:NH1	2:K:170:ASP:O	1.83	1.09
2:B:169:LYS:NZ	5:B:301:HOH:O	2.00	0.94
2:E:103:LYS:NZ	2:E:105:GLU:OE2	2.06	0.88
4:A:302:SO4:S	5:A:401:HOH:O	2.33	0.86
2:H:145:LYS:NZ	2:K:145:LYS:HD2	1.91	0.86
4:A:302:SO4:O3	5:A:401:HOH:O	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:VAL:O	5:J:401:HOH:O	1.98	0.81
2:K:108:ARG:CZ	2:K:171:SER:HB2	2.10	0.80
2:H:103:LYS:NZ	2:H:173:TYR:OH	2.15	0.80
1:G:43:HIS:N	5:G:401:HOH:O	2.16	0.78
1:G:44:GLY:N	5:G:401:HOH:O	2.07	0.78
1:G:40:THR:O	5:G:401:HOH:O	2.06	0.73
2:H:147:GLN:HB2	2:K:145:LYS:NZ	2.05	0.70
2:H:142:ARG:HD2	2:H:173:TYR:CD2	2.27	0.69
2:B:16:GLY:HA2	2:B:77:ARG:HG3	1.75	0.69
2:B:127:SER:OG	5:B:302:HOH:O	2.11	0.69
1:J:62:LYS:NZ	5:J:402:HOH:O	2.12	0.67
2:E:184:ALA:O	2:E:188:LYS:HG2	1.94	0.67
2:H:204:PRO:HG2	2:K:204:PRO:HG2	1.78	0.66
2:H:145:LYS:HE2	2:K:145:LYS:HZ2	1.60	0.66
2:K:181:LEU:O	5:K:301:HOH:O	2.14	0.65
1:J:167:PRO:HG2	2:K:162:SER:HB2	1.78	0.64
2:H:145:LYS:HZ1	2:K:145:LYS:HD2	1.63	0.64
2:H:145:LYS:CE	2:K:145:LYS:HZ2	2.10	0.64
2:H:167:ASP:HB3	2:H:170:ASP:OD2	1.96	0.64
2:H:167:ASP:OD2	2:H:169:LYS:HE2	1.97	0.63
1:G:162:GLY:O	5:G:402:HOH:O	2.16	0.61
1:J:193:THR:HG23	1:J:210:LYS:HE3	1.83	0.60
1:J:137:ALA:HA	5:J:401:HOH:O	2.02	0.60
2:H:24:ARG:HD3	2:H:70:ASP:OD2	2.02	0.59
2:H:145:LYS:HZ2	2:K:145:LYS:HD2	1.67	0.59
2:E:16:GLY:HA2	2:E:77:ARG:HG3	1.84	0.58
2:H:142:ARG:NH1	2:H:173:TYR:CD1	2.71	0.58
1:G:167:PRO:HG2	2:H:162:SER:HB2	1.85	0.58
1:D:12:VAL:HG21	1:D:82(C):LEU:HD13	1.86	0.58
2:K:130:ALA:N	5:K:301:HOH:O	2.37	0.57
1:G:3:GLN:HG2	1:G:25:SER:HB3	1.87	0.56
2:H:113:PRO:HA	5:H:306:HOH:O	2.05	0.56
1:A:12:VAL:HG21	1:A:82(C):LEU:HD13	1.88	0.56
1:D:199:ASN:OD1	1:D:201:LYS:HE2	2.05	0.56
2:K:115:VAL:O	2:K:207:LYS:HE3	2.06	0.56
2:B:204:PRO:HG2	2:E:204:PRO:HG2	1.89	0.55
1:G:1:GLN:OE1	1:G:1:GLN:N	2.32	0.55
2:K:17:ASP:OD1	2:K:18:GLN:N	2.38	0.55
2:E:74:ARG:NH1	5:E:307:HOH:O	2.36	0.53
1:J:1:GLN:O	1:J:26:GLY:HA3	2.08	0.53
2:H:142:ARG:HD2	2:H:173:TYR:CE2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:168:SER:HB3	2:K:169:LYS:HZ2	1.74	0.53
2:K:37:LEU:HD11	2:K:39:ARG:HG3	1.91	0.53
2:H:16:GLY:O	2:H:77:ARG:HG2	2.10	0.51
1:J:151:THR:OG1	1:J:199:ASN:HB3	2.11	0.50
2:K:124:GLN:OE1	2:K:131:SER:N	2.40	0.50
2:E:67:SER:O	5:E:302:HOH:O	2.20	0.49
1:D:1:GLN:N	1:D:1:GLN:OE1	2.35	0.49
1:G:121:VAL:O	1:G:209:LYS:HE3	2.13	0.49
2:H:190:LYS:HE3	2:H:211:ARG:NH2	2.28	0.49
1:J:165:THR:HA	1:J:180:SER:HA	1.96	0.48
2:E:17:ASP:OD2	5:E:301:HOH:O	2.19	0.48
1:D:72:ASP:OD2	1:G:10:GLU:OE2	2.30	0.48
1:J:119:PRO:HB3	1:J:145:TYR:HB3	1.96	0.48
2:H:17:ASP:OD1	2:H:18:GLN:N	2.45	0.48
2:B:145:LYS:HE2	5:B:430:HOH:O	2.12	0.47
2:K:140:TYR:CG	2:K:141:PRO:HA	2.50	0.47
2:H:147:GLN:HB2	2:K:145:LYS:HZ2	1.80	0.47
1:J:32:TYR:CE2	1:J:96:ARG:HB2	2.49	0.47
2:H:147:GLN:CB	2:K:145:LYS:NZ	2.77	0.47
2:K:188:LYS:NZ	2:K:188:LYS:O	2.26	0.46
1:A:195:ILE:HG12	1:A:210:LYS:HG3	1.96	0.46
2:K:108:ARG:NE	2:K:171:SER:HB2	2.30	0.46
2:E:180:THR:HB	5:E:426:HOH:O	2.15	0.46
2:H:137:ASN:C	5:H:306:HOH:O	2.54	0.46
2:K:47:LEU:HA	2:K:58:VAL:HG21	1.98	0.46
1:A:3:GLN:HG2	1:A:25:SER:HB3	1.97	0.46
2:H:142:ARG:HA	2:H:142:ARG:HD3	1.49	0.46
1:J:148:GLU:OE2	1:J:168:ALA:HB3	2.16	0.46
1:J:200:HIS:CD2	1:J:202:PRO:HD2	2.51	0.46
2:K:123:GLU:N	2:K:123:GLU:OE2	2.38	0.45
2:H:33:LEU:HB3	2:H:51:VAL:HG22	1.98	0.45
2:B:27(B):ILE:HD11	2:B:71:PHE:CE1	2.52	0.45
2:H:147:GLN:CD	2:K:145:LYS:HZ3	2.19	0.45
2:K:168:SER:HB3	2:K:169:LYS:NZ	2.32	0.45
1:J:163:VAL:HG12	1:J:182:VAL:HB	1.99	0.45
1:J:166:PHE:CE1	2:K:164:THR:HG23	2.53	0.44
2:B:145:LYS:HE3	5:B:333:HOH:O	2.17	0.44
2:B:145:LYS:HD2	2:E:145:LYS:NZ	2.32	0.44
2:K:69:THR:N	5:K:303:HOH:O	2.28	0.44
1:A:72:ASP:OD2	1:J:10:GLU:OE2	2.34	0.44
2:H:89:PHE:CZ	2:H:96:TYR:HB3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:108:ARG:HB2	2:K:108:ARG:HE	1.46	0.43
2:B:169:LYS:HB2	2:B:169:LYS:HE3	1.78	0.43
2:E:124:GLN:HG2	2:E:129:THR:O	2.18	0.43
2:H:24:ARG:O	5:H:301:HOH:O	2.21	0.43
1:G:60:ASN:ND2	5:G:412:HOH:O	2.51	0.43
1:D:199:ASN:ND2	1:D:206:LYS:HG2	2.33	0.43
1:D:30:THR:O	1:D:53:LYS:HE3	2.18	0.43
2:H:204:PRO:HG2	2:K:204:PRO:CG	2.45	0.43
2:E:125:LEU:O	2:E:183:LYS:HD2	2.19	0.43
2:K:201:LEU:HD13	2:K:205:VAL:HG23	2.01	0.42
3:C:518:VAL:O	3:C:519:PHE:HB2	2.20	0.42
2:B:124:GLN:HG2	2:B:129:THR:O	2.19	0.42
2:K:24:ARG:HA	2:K:69:THR:O	2.19	0.42
1:J:159:LEU:HD21	1:J:182:VAL:HG21	2.01	0.42
2:K:48:ILE:HD13	2:K:54:ARG:HA	2.01	0.42
1:J:152:VAL:N	5:J:404:HOH:O	2.47	0.42
1:J:139:GLY:HA3	1:J:181:VAL:HG12	2.02	0.42
1:J:204:ASN:O	1:J:204:ASN:ND2	2.53	0.41
2:H:164:THR:O	2:H:173:TYR:CD2	2.73	0.41
1:D:82(A):ARG:NH2	5:D:414:HOH:O	2.53	0.41
1:G:210:LYS:HE3	1:G:212:GLU:OE2	2.20	0.41
2:K:145:LYS:HE2	2:K:145:LYS:HB3	1.54	0.41
2:K:107:LYS:HB3	2:K:107:LYS:HE2	1.76	0.41
2:K:167:ASP:HB3	2:K:170:ASP:OD1	2.20	0.41
2:B:24:ARG:HB3	2:B:24:ARG:NH1	2.35	0.41
2:H:139:PHE:HD1	5:H:306:HOH:O	2.04	0.41
1:J:195:ILE:HD13	1:J:210:LYS:HA	2.02	0.41
1:J:3:GLN:HG2	1:J:25:SER:HB3	2.01	0.41
1:D:119:PRO:HB3	1:D:145:TYR:HB3	2.04	0.40
2:H:16:GLY:HA2	2:H:77:ARG:HE	1.85	0.40
2:E:140:TYR:CG	2:E:141:PRO:HA	2.56	0.40
2:K:167:ASP:O	2:K:171:SER:HA	2.21	0.40
2:K:4:MET:SD	2:K:90:GLN:HB2	2.62	0.40

There are no symmetry-related clashes.

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	207/221 (94%)	203 (98%)	4 (2%)	0	100	100
1	D	207/221 (94%)	203 (98%)	4 (2%)	0	100	100
1	G	204/221 (92%)	200 (98%)	4 (2%)	0	100	100
1	J	207/221 (94%)	203 (98%)	4 (2%)	0	100	100
2	B	216/219 (99%)	213 (99%)	3 (1%)	0	100	100
2	E	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
2	H	214/219 (98%)	210 (98%)	4 (2%)	0	100	100
2	K	214/219 (98%)	211 (99%)	3 (1%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
3	I	6/8 (75%)	6 (100%)	0	0	100	100
3	L	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1710/1792 (95%)	1679 (98%)	31 (2%)	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	182/191 (95%)	180 (99%)	2 (1%)	73	79
1	D	182/191 (95%)	180 (99%)	2 (1%)	73	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	181/191 (95%)	178 (98%)	3 (2%)	60	66
1	J	182/191 (95%)	178 (98%)	4 (2%)	52	55
2	B	192/193 (100%)	190 (99%)	2 (1%)	76	81
2	E	193/193 (100%)	189 (98%)	4 (2%)	53	57
2	H	191/193 (99%)	184 (96%)	7 (4%)	34	34
2	K	191/193 (99%)	185 (97%)	6 (3%)	40	42
3	C	4/4 (100%)	3 (75%)	1 (25%)	0	0
3	F	4/4 (100%)	4 (100%)	0	100	100
3	I	4/4 (100%)	3 (75%)	1 (25%)	0	0
3	L	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	1510/1552 (97%)	1477 (98%)	33 (2%)	52	55

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	100	TYR
2	B	90	GLN
2	B	145	LYS
3	C	519	PHE
1	D	100	TYR
1	D	184	VAL
2	E	22	SER
2	E	90	GLN
2	E	129	THR
2	E	145	LYS
1	G	64	ARG
1	G	100	TYR
1	G	201	LYS
2	H	33	LEU
2	H	60	ASP
2	H	77	ARG
2	H	90	GLN
2	H	142	ARG
2	H	172	THR
2	H	190	LYS
3	I	519	PHE
1	J	64	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	100	TYR
1	J	135	THR
1	J	148	GLU
2	K	3	LEU
2	K	13	VAL
2	K	45	LYS
2	K	90	GLN
2	K	107	LYS
2	K	108	ARG
3	L	519	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	138	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.45	0
4	SO4	G	302	-	4,4,4	0.13	0	6,6,6	0.31	0
4	SO4	G	301	-	4,4,4	0.13	0	6,6,6	0.33	0
4	SO4	D	301	-	4,4,4	0.16	0	6,6,6	0.37	0
4	SO4	A	301	-	4,4,4	0.19	0	6,6,6	0.19	0
4	SO4	J	301	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	D	302	-	4,4,4	0.20	0	6,6,6	0.19	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	SO4	2	0

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	211/221 (95%)	-0.08	3 (1%) 75 78	17, 28, 52, 74	0
1	D	211/221 (95%)	-0.08	0 100 100	19, 30, 51, 70	0
1	G	208/221 (94%)	0.46	22 (10%) 6 7	24, 47, 88, 114	0
1	J	211/221 (95%)	1.16	55 (26%) 0 0	22, 48, 110, 136	0
2	B	218/219 (99%)	-0.36	0 100 100	19, 29, 52, 93	0
2	E	219/219 (100%)	-0.25	2 (0%) 84 86	23, 32, 55, 100	0
2	H	216/219 (98%)	0.64	17 (7%) 12 16	41, 63, 90, 113	0
2	K	216/219 (98%)	0.88	44 (20%) 1 1	31, 72, 96, 109	0
3	C	8/8 (100%)	0.94	1 (12%) 3 5	25, 27, 63, 118	0
3	F	8/8 (100%)	0.08	1 (12%) 3 5	24, 30, 61, 76	0
3	I	8/8 (100%)	1.60	2 (25%) 0 0	32, 38, 97, 127	0
3	L	8/8 (100%)	1.75	2 (25%) 0 0	26, 33, 101, 119	0
All	All	1742/1792 (97%)	0.31	149 (8%) 10 13	17, 39, 91, 136	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	519	PHE	10.1
1	J	182	VAL	10.1
3	L	519	PHE	9.2
1	J	195	ILE	8.8
1	J	138	LEU	8.4
1	J	134	GLY	8.3
1	J	190	GLY	8.1
1	J	184	VAL	7.8
2	E	214	CYS	7.7
3	L	518	VAL	6.3
3	C	519	PHE	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	158	ALA	5.9
1	J	157	GLY	5.8
1	J	210	LYS	5.6
1	J	192	GLN	5.3
1	J	193	THR	5.3
1	J	125	ALA	5.3
1	J	153	SER	5.1
1	J	183	THR	5.1
2	H	173	TYR	4.9
2	K	152	ASN	4.9
1	J	211	VAL	4.8
1	G	193	THR	4.5
1	J	152	VAL	4.5
1	J	160	THR	4.5
1	J	154	TRP	4.4
1	J	151	THR	4.4
1	J	194	TYR	4.4
1	G	182	VAL	4.3
1	J	197	ASN	4.3
1	J	199	ASN	4.3
1	J	204	ASN	4.3
2	H	77	ARG	4.3
1	G	1	GLN	4.2
1	J	139	GLY	4.1
1	G	187	SER	4.1
1	J	189	LEU	4.0
2	K	125	LEU	4.0
2	K	139	PHE	3.8
2	K	108	ARG	3.8
1	J	163	VAL	3.8
3	F	519	PHE	3.8
1	J	120	SER	3.7
1	J	202	PRO	3.7
1	J	1	GLN	3.7
1	G	158	ALA	3.6
1	J	150	VAL	3.6
1	J	196	CYS	3.5
1	J	135	THR	3.5
2	H	169	LYS	3.5
1	J	140	CYS	3.5
1	J	205	THR	3.5
1	G	156	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	159	LEU	3.4
1	J	191	THR	3.4
2	K	126	LYS	3.4
1	J	124	LEU	3.3
1	G	184	VAL	3.3
2	K	173	TYR	3.3
1	G	194	TYR	3.2
2	K	210	ASN	3.2
1	G	160	THR	3.2
2	H	68	GLY	3.1
3	I	518	VAL	3.1
1	G	163	VAL	3.1
2	K	115	VAL	3.1
1	G	204	ASN	3.0
2	K	153	ALA	3.0
2	H	142	ARG	3.0
2	K	129	THR	3.0
2	K	192	TYR	3.0
2	K	168	SER	3.0
2	K	169	LYS	2.9
1	J	207	VAL	2.9
1	J	209	LYS	2.9
1	J	137	ALA	2.8
2	K	57	GLY	2.8
1	G	199	ASN	2.8
2	H	16	GLY	2.8
1	G	191	THR	2.8
2	K	113	PRO	2.8
1	G	190	GLY	2.8
1	J	185	PRO	2.8
2	K	122	ASP	2.8
2	H	67	SER	2.8
2	K	187	GLU	2.7
2	H	15	LEU	2.7
2	H	108	ARG	2.7
2	H	118	PHE	2.7
2	H	116	PHE	2.7
2	K	175	LEU	2.7
2	K	208	SER	2.7
2	K	209	PHE	2.7
1	J	164	HIS	2.6
2	K	119	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	195	ILE	2.6
2	K	121	SER	2.6
1	J	187	SER	2.6
1	J	188	SER	2.6
1	J	206	LYS	2.6
2	K	80	ALA	2.6
1	G	151	THR	2.5
2	H	18	GLN	2.5
2	K	58	VAL	2.5
2	H	76	SER	2.5
2	K	116	PHE	2.5
2	H	1	ASP	2.5
1	G	157	GLY	2.5
1	J	122	PHE	2.5
2	K	18	GLN	2.4
2	K	77	ARG	2.4
1	J	212	GLU	2.4
1	G	159	LEU	2.4
2	H	109	THR	2.3
1	J	208	ASP	2.3
1	A	192	GLN	2.3
1	J	198	VAL	2.3
1	J	156	SER	2.3
2	K	177	SER	2.3
2	K	188	LYS	2.3
2	K	134	CYS	2.3
2	K	185	ASP	2.3
1	A	1	GLN	2.3
1	A	68	ILE	2.3
2	K	130	ALA	2.2
2	K	132	VAL	2.2
2	K	133	VAL	2.2
1	G	192	GLN	2.2
1	J	162	GLY	2.2
1	G	189	LEU	2.2
1	J	176	TYR	2.2
2	K	145	LYS	2.2
1	G	27	TYR	2.1
2	K	120	PRO	2.1
2	K	13	VAL	2.1
2	H	144	ALA	2.1
2	K	1	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	166	PHE	2.1
2	K	194	CYS	2.1
2	H	60	ASP	2.1
2	K	183	LYS	2.1
1	J	141	LEU	2.0
2	E	1	ASP	2.0
2	K	167	ASP	2.0
2	K	107	LYS	2.0
2	K	17	ASP	2.0
2	K	127	SER	2.0
1	J	200	HIS	2.0
1	G	183	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	J	301	5/5	0.58	0.36	101,108,110,113	0
4	SO4	G	301	5/5	0.98	0.18	45,49,54,56	0
4	SO4	D	301	5/5	0.98	0.19	50,50,57,61	0
4	SO4	A	302	5/5	0.98	0.18	46,46,59,67	0
4	SO4	A	301	5/5	0.99	0.16	33,35,39,40	0
4	SO4	G	302	5/5	0.99	0.17	42,42,47,50	0
4	SO4	D	302	5/5	0.99	0.16	33,34,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.