



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:35 AM UTC

PDB ID : 5TKJ / pdb_00005tkj
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 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

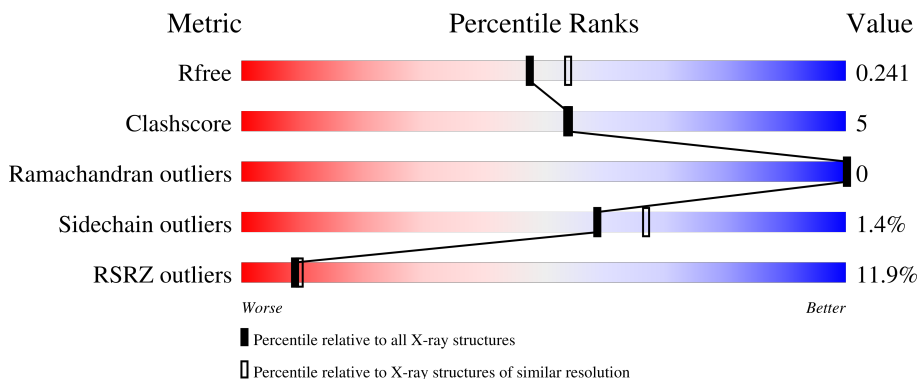
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 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	221	 2% 91% 5%
1	D	221	 % 90% 6% 5%
1	G	221	 10% 88% 6% 6%
1	J	221	 26% 81% 14% 5%
2	B	219	 94% 5%

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Mol	Chain	Length	Quality of chain
2	E	219	<p>%</p> <p>90% 9% .</p>
2	H	219	<p>21%</p> <p>85% 11% ..</p>
2	K	219	<p>29%</p> <p>81% 16% ..</p>
3	C	8	<p>25%</p> <p>75% 25%</p>
3	F	8	<p>12%</p> <p>100%</p>
3	I	8	<p>25%</p> <p>100%</p>
3	L	8	<p>25%</p> <p>100%</p>

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
			Total	C	N	O	S			
1	A	211	Total 1620	C 1037	N 266	O 312	S 5	0	0	0
1	D	211	Total 1620	C 1037	N 266	O 312	S 5	0	0	0
1	G	208	Total 1604	C 1028	N 263	O 308	S 5	0	0	0
1	J	211	Total 1620	C 1037	N 266	O 312	S 5	0	0	0

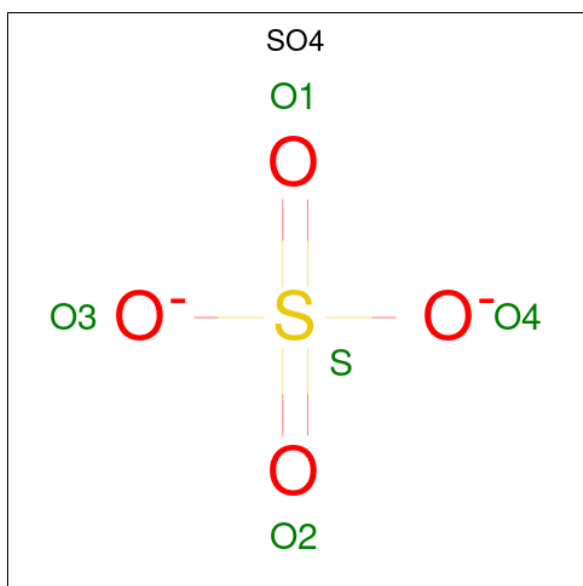
- Molecule 2 is a protein called vFP1.01 chimeric mouse antibody light chain.

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

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

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

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

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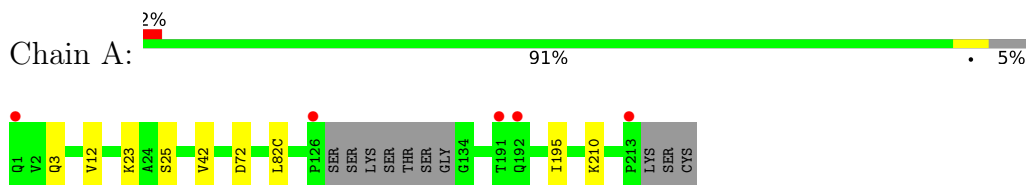
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	180	Total 180	O 180	0	0
5	F	2	Total 2	O 2	0	0
5	G	98	Total 98	O 98	0	0
5	H	70	Total 70	O 70	0	0
5	I	3	Total 3	O 3	0	0
5	J	87	Total 87	O 87	0	0
5	K	64	Total 64	O 64	0	0
5	L	3	Total 3	O 3	0	0

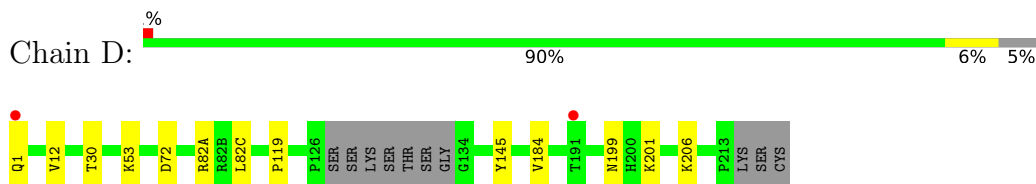
3 Residue-property plots i

These plots are drawn for all protein, RNA, 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.

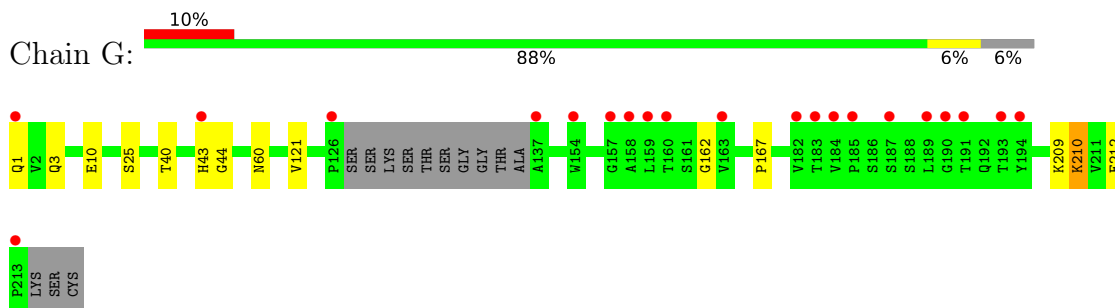
- Molecule 1: vFP1.01 chimeric mouse antibody heavy chain



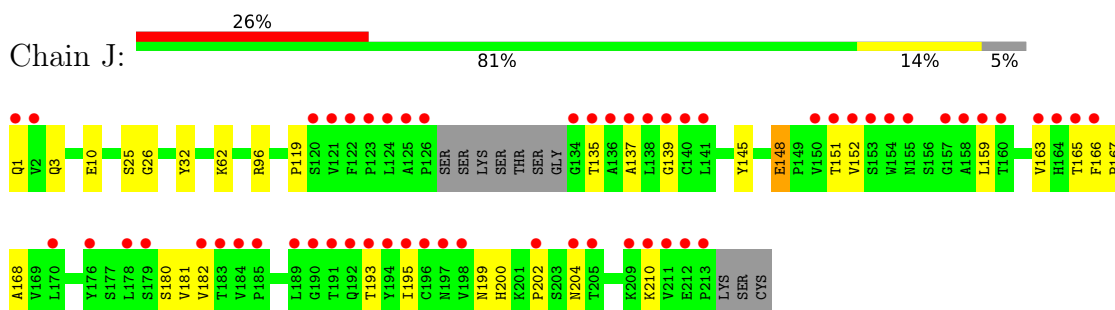
- Molecule 1: vFP1.01 chimeric mouse antibody heavy chain



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



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

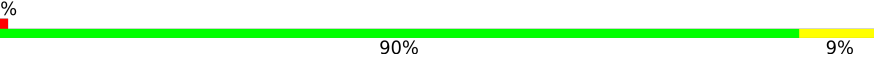


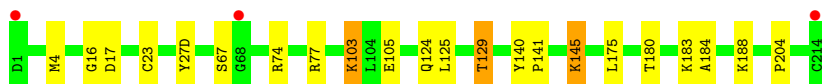
- Molecule 2: vFP1.01 chimeric mouse antibody light chain

Chain B:  94% 5%




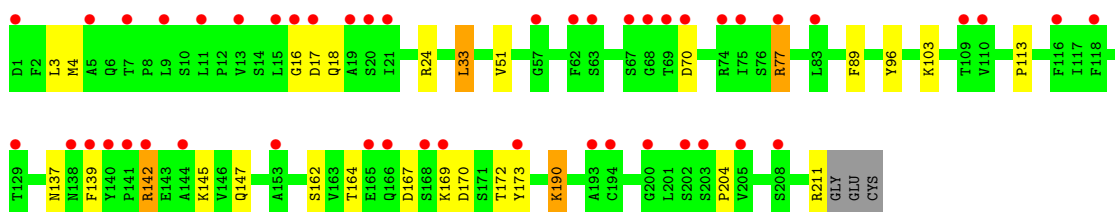
- Molecule 2: vFP1.01 chimeric mouse antibody light chain

Chain E:  90% 9%




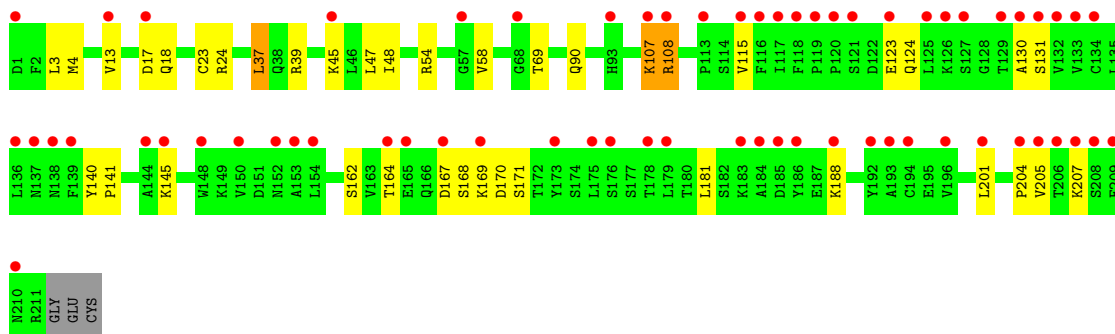
- Molecule 2: vFP1.01 chimeric mouse antibody light chain

Chain H:  21% 85% 11%




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

Chain K:  29% 81% 16%



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

Chain C:  25% 75% 25%



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

Chain F:  12% 100%



- 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 43.54 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.54-2.12) 99.7 (43.54-2.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.198 , 0.241 0.199 , 0.241	Depositor DCC
R_{free} test set	5932 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/1665	0.59	0/2279
1	D	0.41	0/1665	0.59	0/2279
1	G	0.32	0/1649	0.53	0/2257
1	J	0.32	0/1665	0.54	0/2279
2	B	0.42	0/1729	0.63	0/2344
2	E	0.39	0/1735	0.64	0/2352
2	H	0.33	0/1716	0.59	0/2327
2	K	0.30	0/1716	0.57	0/2327
3	C	0.37	0/51	0.65	0/68
3	F	0.35	0/51	0.72	0/68
3	I	0.26	0/51	0.50	0/68
3	L	0.34	0/51	0.53	0/68
All	All	0.36	0/13744	0.59	0/18716

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	1620	0	1589	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1620	0	1589	9	0
1	G	1604	0	1574	12	0
1	J	1620	0	1589	21	0
2	B	1691	0	1641	12	0
2	E	1697	0	1646	15	0
2	H	1678	0	1632	33	0
2	K	1678	0	1632	39	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	2	0
5	E	180	0	0	5	0
5	F	2	0	0	0	0
5	G	98	0	0	6	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	130	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 (130) 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

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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:J:62:LYS:NZ	5:J:402:HOH:O	2.12	0.73
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: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: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:145:LYS:HE2	2:K:145:LYS:HZ2	1.62	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:D:201:LYS:NZ	5:D:402:HOH:O	2.34	0.57
2:K:4:MET:HE3	2:K:23:CYS:SG	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:ARG:HD2	2:H:173:TYR:CE2	2.43	0.53
2:K:37:LEU:HD11	2:K:39:ARG:HG3	1.91	0.53
2:K:168:SER:HB3	2:K:169:LYS:HZ2	1.74	0.53
2:H:16:GLY:O	2:H:77:ARG:HG2	2.10	0.51
2:H:147:GLN:CD	2:K:145:LYS:HZ3	2.17	0.51
2:B:4:MET:HE3	2:B:23:CYS:SG	2.49	0.51
2:H:3:LEU:C	2:H:4:MET:HE2	2.36	0.51
1:J:151:THR:OG1	1:J:199:ASN:HB3	2.11	0.50
2:E:4:MET:HE3	2:E:23:CYS:SG	2.52	0.50
2:K:124:GLN:OE1	2:K:131:SER:N	2.40	0.50
2:B:127:SER:OG	5:B:302:HOH:O	2.11	0.49
2:E:67:SER:O	5:E:302:HOH:O	2.20	0.49
2:H:137:ASN:C	5:H:306:HOH:O	2.54	0.49
1:D:1:GLN:OE1	1:D:1:GLN:N	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
2:K:188:LYS:O	2:K:188:LYS:NZ	2.26	0.49
2:H:3:LEU:O	2:H:4:MET:HE2	2.12	0.48
1:J:165:THR:HA	1:J:180:SER:HA	1.96	0.48
1:D:72:ASP:OD2	1:G:10:GLU:OE2	2.30	0.48
2:E:17:ASP:OD2	5:E:301:HOH:O	2.19	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:E:27(D):TYR:OH	5:E:303:HOH:O	2.20	0.47
2:B:145:LYS:HE2	5:B:430:HOH:O	2.12	0.47
2:H:147:GLN:HB2	2:K:145:LYS:HZ2	1.79	0.47
2:K:140:TYR:CG	2:K:141:PRO:HA	2.50	0.47
2:H:147:GLN:CB	2:K:145:LYS:NZ	2.77	0.47
1:J:32:TYR:CE2	1:J:96:ARG:HB2	2.49	0.47
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: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:HD3	2:H:142:ARG:HA	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:OE2	2:K:123:GLU:N	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:K:168:SER:HB3	2:K:169:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:40:THR:C	5:G:401:HOH:O	2.59	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
2:E:175:LEU:C	2:E:175:LEU:HD23	2.43	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
2:K:108:ARG:HE	2:K:108:ARG:HB2	1.46	0.43
2:B:169:LYS:HE3	2:B:169:LYS:HB2	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:HB3	2:K:145:LYS:HE2	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:NH1	2:B:24:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4:MET:SD	2:K:90:GLN:HB2	2.62	0.40

There are no symmetry-related clashes.

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	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 [i](#)

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%)	65	74
1	D	182/191 (95%)	181 (100%)	1 (0%)	81	87
1	G	181/191 (95%)	180 (99%)	1 (1%)	78	85
1	J	182/191 (95%)	180 (99%)	2 (1%)	65	74
2	B	192/193 (100%)	191 (100%)	1 (0%)	81	87
2	E	193/193 (100%)	190 (98%)	3 (2%)	55	63
2	H	191/193 (99%)	186 (97%)	5 (3%)	40	45
2	K	191/193 (99%)	185 (97%)	6 (3%)	35	38
3	C	4/4 (100%)	4 (100%)	0	100	100
3	F	4/4 (100%)	4 (100%)	0	100	100
3	I	4/4 (100%)	4 (100%)	0	100	100
3	L	4/4 (100%)	4 (100%)	0	100	100
All	All	1510/1552 (97%)	1489 (99%)	21 (1%)	59	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	42	VAL
2	B	145	LYS
1	D	184	VAL
2	E	103	LYS
2	E	129	THR
2	E	145	LYS
1	G	210	LYS
2	H	33	LEU
2	H	77	ARG
2	H	142	ARG
2	H	172	THR
2	H	190	LYS
1	J	135	THR
1	J	148	GLU
2	K	3	LEU
2	K	13	VAL
2	K	37	LEU

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Mol	Chain	Res	Type
2	K	45	LYS
2	K	107	LYS
2	K	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	171	GLN
2	B	160	GLN
1	D	39	GLN
1	D	97	ASN
2	E	53	ASN
1	G	5	GLN
1	G	97	ASN
2	H	160	GLN
1	J	5	GLN
1	J	97	ASN
1	J	164	HIS
2	K	199	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](#)

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	G	302	-	4,4,4	0.20	0	6,6,6	0.28	0
4	SO4	A	301	-	4,4,4	0.25	0	6,6,6	0.17	0
4	SO4	A	302	-	4,4,4	0.27	0	6,6,6	0.45	0
4	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.33	0
4	SO4	G	301	-	4,4,4	0.18	0	6,6,6	0.35	0
4	SO4	J	301	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	D	302	-	4,4,4	0.24	0	6,6,6	0.15	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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/221 (95%)	-0.19	5 (2%) 59 62	17, 28, 52, 74	0
1	D	211/221 (95%)	-0.20	2 (0%) 81 83	19, 30, 51, 70	0
1	G	208/221 (94%)	0.57	21 (10%) 12 13	24, 47, 88, 114	0
1	J	211/221 (95%)	1.03	57 (27%) 1 1	22, 48, 110, 136	0
2	B	218/219 (99%)	-0.22	1 (0%) 87 89	19, 29, 52, 93	0
2	E	219/219 (100%)	-0.10	3 (1%) 73 76	23, 32, 55, 100	0
2	H	216/219 (98%)	1.34	47 (21%) 2 2	41, 63, 90, 113	0
2	K	216/219 (98%)	1.40	64 (29%) 1 1	31, 72, 96, 109	0
3	C	8/8 (100%)	0.98	2 (25%) 2 2	25, 27, 63, 118	0
3	F	8/8 (100%)	0.28	1 (12%) 8 9	24, 30, 61, 76	0
3	I	8/8 (100%)	1.52	2 (25%) 2 2	32, 38, 97, 127	0
3	L	8/8 (100%)	1.41	2 (25%) 2 2	26, 33, 101, 119	0
All	All	1742/1792 (97%)	0.46	207 (11%) 9 9	17, 39, 91, 136	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	519	PHE	7.5
1	J	182	VAL	6.0
3	L	519	PHE	5.9
1	J	138	LEU	5.5
3	C	519	PHE	5.3
3	L	518	VAL	5.3
2	H	173	TYR	5.1
1	J	184	VAL	5.0
1	J	211	VAL	4.7
3	I	518	VAL	4.6
1	G	189	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	J	194	TYR	4.5
1	A	126	PRO	4.5
2	K	153	ALA	4.5
2	E	214	CYS	4.3
2	H	142	ARG	4.2
1	J	183	THR	4.2
2	K	134	CYS	4.1
1	J	154	TRP	4.0
2	K	1	ASP	4.0
2	K	152	ASN	3.9
1	J	1	GLN	3.9
1	J	195	ILE	3.9
1	J	189	LEU	3.8
1	J	140	CYS	3.7
1	J	135	THR	3.7
1	J	126	PRO	3.6
1	J	196	CYS	3.6
1	G	194	TYR	3.6
2	K	129	THR	3.5
1	G	158	ALA	3.5
2	K	113	PRO	3.5
1	J	134	GLY	3.5
1	J	191	THR	3.5
2	H	68	GLY	3.5
2	K	194	CYS	3.5
1	J	121	VAL	3.5
1	A	1	GLN	3.5
1	G	191	THR	3.5
2	K	68	GLY	3.4
1	J	210	LYS	3.4
1	J	158	ALA	3.3
1	J	124	LEU	3.3
2	K	125	LEU	3.3
1	J	213	PRO	3.2
2	H	75	ILE	3.2
2	K	205	VAL	3.2
1	A	192	GLN	3.2
2	K	209	PHE	3.2
2	K	208	SER	3.2
1	J	193	THR	3.2
2	H	194	CYS	3.2
1	D	1	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	K	115	VAL	3.1
3	F	519	PHE	3.1
2	K	130	ALA	3.1
2	H	77	ARG	3.1
1	G	1	GLN	3.1
1	J	152	VAL	3.1
2	K	132	VAL	3.1
1	J	185	PRO	3.1
1	J	150	VAL	3.1
2	K	116	PHE	3.0
2	K	120	PRO	3.0
1	J	125	ALA	3.0
2	K	139	PHE	3.0
1	J	136	ALA	3.0
2	K	108	ARG	3.0
2	K	145	LYS	3.0
1	G	182	VAL	3.0
1	J	159	LEU	3.0
2	E	1	ASP	3.0
2	H	17	ASP	3.0
2	K	188	LYS	3.0
1	G	163	VAL	2.9
1	G	126	PRO	2.9
2	H	19	ALA	2.9
3	C	518	VAL	2.9
2	H	1	ASP	2.9
1	J	209	LYS	2.9
2	K	118	PHE	2.9
2	K	192	TYR	2.9
2	K	144	ALA	2.9
2	H	200	GLY	2.9
2	K	13	VAL	2.8
1	G	193	THR	2.8
1	G	190	GLY	2.8
2	H	205	VAL	2.8
2	E	68	GLY	2.8
2	H	57	GLY	2.8
2	H	7	THR	2.8
1	J	190	GLY	2.7
2	H	5	ALA	2.7
2	K	148	TRP	2.7
1	J	160	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	K	175	LEU	2.7
1	J	202	PRO	2.7
2	H	15	LEU	2.7
2	K	136	LEU	2.7
2	K	119	PRO	2.7
1	J	179	SER	2.7
2	K	133	VAL	2.7
1	J	137	ALA	2.6
2	H	109	THR	2.6
2	H	169	LYS	2.6
1	A	191	THR	2.6
1	G	159	LEU	2.6
1	J	141	LEU	2.6
1	J	120	SER	2.6
1	G	160	THR	2.6
2	H	63	SER	2.6
2	K	127	SER	2.6
1	J	197	ASN	2.6
1	G	183	THR	2.6
2	H	144	ALA	2.6
2	K	206	THR	2.6
1	J	123	PRO	2.6
2	H	67	SER	2.6
1	G	184	VAL	2.5
1	J	122	PHE	2.5
2	H	139	PHE	2.5
2	K	196	VAL	2.5
2	H	140	TYR	2.5
1	J	178	LEU	2.5
2	K	154	LEU	2.5
2	H	62	PHE	2.5
1	J	164	HIS	2.5
2	H	110	VAL	2.5
1	J	205	THR	2.5
2	K	164	THR	2.5
2	H	193	ALA	2.5
2	H	118	PHE	2.5
1	J	155	ASN	2.5
2	H	168	SER	2.4
2	K	176	SER	2.4
1	G	137	ALA	2.4
2	K	193	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	208	SER	2.4
1	J	151	THR	2.4
1	J	163	VAL	2.4
2	H	141	PRO	2.4
1	J	192	GLN	2.4
1	J	166	PHE	2.4
1	J	198	VAL	2.4
2	K	117	ILE	2.4
2	H	74	ARG	2.4
2	K	150	VAL	2.4
1	G	187	SER	2.4
1	J	165	THR	2.4
2	H	129	THR	2.4
2	K	178	THR	2.4
2	K	165	GLU	2.3
2	H	9	LEU	2.3
2	K	138	ASN	2.3
2	K	210	ASN	2.3
1	G	157	GLY	2.3
2	K	126	LYS	2.3
2	K	183	LYS	2.3
2	K	121	SER	2.3
2	H	153	ALA	2.3
2	K	173	TYR	2.3
2	K	137	ASN	2.3
2	H	11	LEU	2.3
2	H	16	GLY	2.3
2	K	201	LEU	2.3
2	K	107	LYS	2.3
2	K	57	GLY	2.3
2	H	203	SER	2.3
2	K	167	ASP	2.3
2	K	184	ALA	2.3
2	K	179	LEU	2.3
2	H	166	GLN	2.2
2	K	169	LYS	2.2
2	K	123	GLU	2.2
1	G	154	TRP	2.2
1	A	213	PRO	2.2
2	K	131	SER	2.2
1	J	204	ASN	2.2
2	H	21	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	116	PHE	2.2
1	D	191	THR	2.2
1	G	185	PRO	2.1
2	K	204	PRO	2.1
1	J	170	LEU	2.1
1	J	176	TYR	2.1
2	H	70	ASP	2.1
2	H	83	LEU	2.1
1	G	43	HIS	2.1
2	K	93	HIS	2.1
1	J	2	VAL	2.1
2	K	45	LYS	2.1
2	K	207	LYS	2.1
1	J	212	GLU	2.1
2	H	138	ASN	2.1
2	K	186	TYR	2.1
1	J	139	GLY	2.1
2	H	165	GLU	2.0
2	H	13	VAL	2.0
1	J	153	SER	2.0
2	H	20	SER	2.0
2	H	202	SER	2.0
2	B	1	ASP	2.0
2	K	17	ASP	2.0
2	K	185	ASP	2.0
1	G	213	PRO	2.0
2	H	69	THR	2.0
1	J	157	GLY	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](#)

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	0.72	0.28	101,108,110,113	0
4	SO4	D	301	5/5	0.90	0.12	50,50,57,61	0
4	SO4	G	301	5/5	0.96	0.09	45,49,54,56	0
4	SO4	A	302	5/5	0.96	0.12	46,46,59,67	0
4	SO4	G	302	5/5	0.97	0.07	42,42,47,50	0
4	SO4	D	302	5/5	0.98	0.06	33,34,38,40	0
4	SO4	A	301	5/5	0.98	0.05	33,35,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.