



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:24 am GMT

PDB ID : 3QQ9  
Title : Crystal structure of FAB fragment of anti-human RSV (RESPIRATORY SYNCYTIAL VIRUS) F Protein MAB 101F  
Authors : Luo, J.; Tsui, P.; Spurlino, J.; Lewansowski, F.; Heavner, G.A.; Del Vecchio, F.  
Deposited on : 2011-02-15  
Resolution : 1.64 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

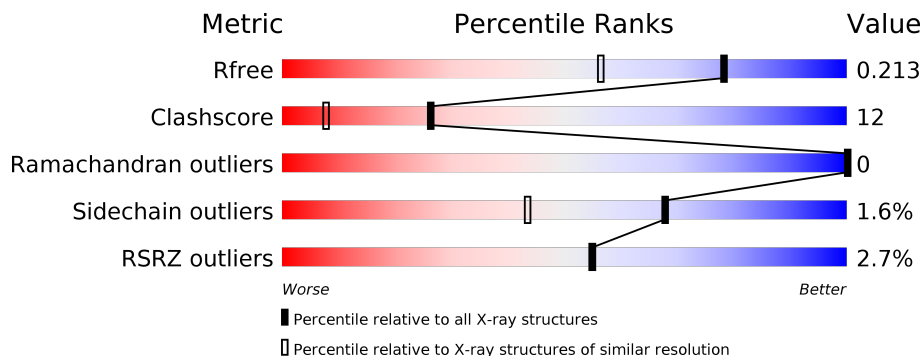
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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))
$R_{free}$	100719	2211 (1.66-1.62)
Clashscore	112137	2356 (1.66-1.62)
Ramachandran outliers	110173	2315 (1.66-1.62)
Sidechain outliers	110143	2315 (1.66-1.62)
RSRZ outliers	101464	2219 (1.66-1.62)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	C	218	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>79%</span> <span>21%</span> </div> </div>
1	L	218	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>85%</span> <span>14%</span> </div> </div>
2	D	227	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>78%</span> <span>15%</span> <span>6%</span> </div> </div>
2	H	227	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>88%</span> <span>7%</span> <span>5%</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	H	228	-	-	-	X
3	SO4	L	220	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14408 atoms, of which 6502 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.

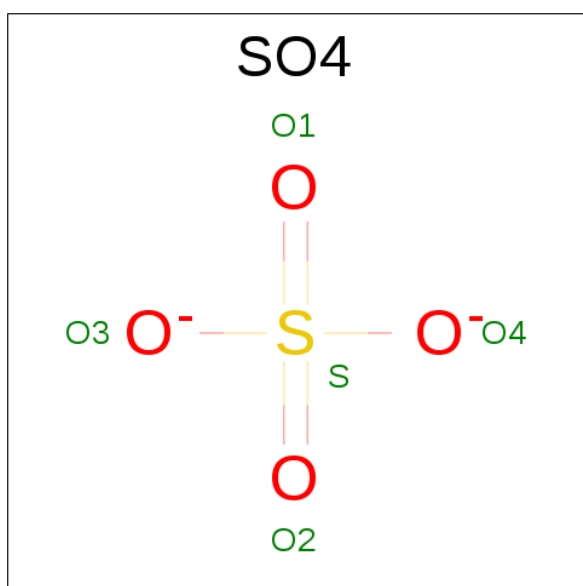
- Molecule 1 is a protein called 101F LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	217	Total	C	H	N	O	S	0	6	0
			3366	1075	1662	283	340	6			
1	C	217	Total	C	H	N	O	S	0	3	0
			3319	1062	1633	280	337	7			

- Molecule 2 is a protein called 101F HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	215	Total	C	H	N	O	S	0	4	0
			3248	1046	1613	266	317	6			
2	D	213	Total	C	H	N	O	S	0	3	0
			3214	1036	1594	263	316	5			

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

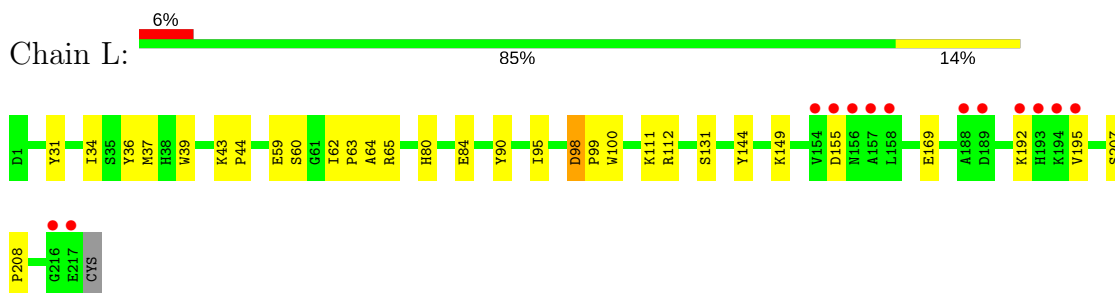
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	327	Total O 327 327	0	0
4	H	406	Total O 406 406	0	0
4	C	235	Total O 235 235	0	0
4	D	268	Total O 268 268	0	0

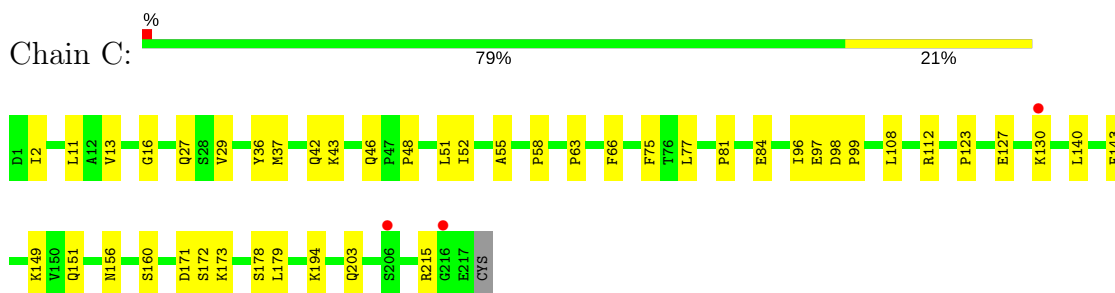
### 3 Residue-property plots [i](#)

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.

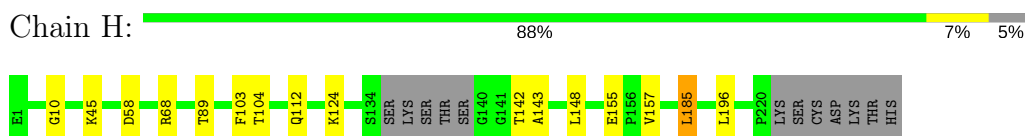
- Molecule 1: 101F LIGHT CHAIN



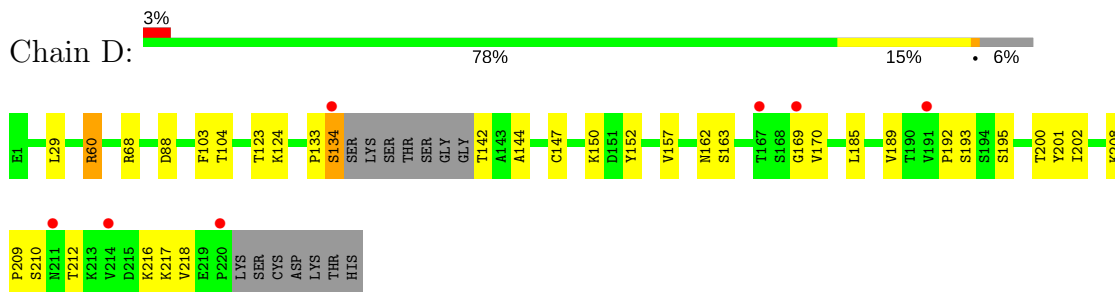
- Molecule 1: 101F LIGHT CHAIN



- Molecule 2: 101F HEAVY CHAIN



- Molecule 2: 101F HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.31Å 84.56Å 101.66Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	42.37 – 1.64 42.37 – 1.64	Depositor EDS
% Data completeness (in resolution range)	85.1 (42.37-1.64) 85.1 (42.37-1.64)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.47 (at 1.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.173 , 0.217 0.171 , 0.213	Depositor DCC
$R_{free}$ test set	4848 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.48 , 69.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PCA, 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	C	0.61	0/1735	0.65	0/2359
1	L	0.83	1/1762 (0.1%)	0.77	0/2395
2	D	0.69	0/1664	0.74	4/2273 (0.2%)
2	H	0.87	0/1682	0.86	3/2297 (0.1%)
All	All	0.76	1/6843 (0.0%)	0.76	7/9324 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	90	TYR	CD1-CE1	5.05	1.47	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	68	ARG	NE-CZ-NH2	-9.53	115.53	120.30
2	H	68	ARG	NE-CZ-NH1	7.33	123.97	120.30
2	D	68	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	D	60	ARG	NE-CZ-NH1	-6.60	117.00	120.30
2	D	60	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	D	68	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	H	185	LEU	CA-CB-CG	5.21	127.28	115.30

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	C	1686	1633	1633	50	0
1	L	1704	1662	1662	46	0
2	D	1620	1594	1600	42	0
2	H	1635	1613	1617	13	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	H	5	0	0	1	0
3	L	10	0	0	0	0
4	C	235	0	0	17	0
4	D	268	0	0	30	1
4	H	406	0	0	12	4
4	L	327	0	0	24	2
All	All	7906	6502	6512	153	4

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 12.

All (153) 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:D:189:VAL:HG23	4:D:497:HOH:O	1.47	1.13
1:C:48:PRO:HD3	4:C:462:HOH:O	1.49	1.10
1:C:97:GLU:OE2	4:C:376:HOH:O	1.81	0.99
1:C:140:LEU:O	4:C:479:HOH:O	1.80	0.98
1:C:143:PHE:HE2	4:C:479:HOH:O	1.48	0.95
2:H:155:GLU:OE2	4:H:459:HOH:O	1.83	0.94
2:D:134:SER:N	4:D:491:HOH:O	2.01	0.93
1:L:36:TYR:OH	4:L:341:HOH:O	1.87	0.93
2:D:170:VAL:CA	4:D:497:HOH:O	2.17	0.91
2:H:10:GLY:HA3	4:H:629:HOH:O	1.74	0.87
1:C:11:LEU:HD21	1:C:13:VAL:HG23	1.57	0.87
2:D:104:THR:OG1	4:D:461:HOH:O	1.91	0.86
1:C:143:PHE:CE2	4:C:479:HOH:O	2.26	0.84
2:D:170:VAL:N	4:D:497:HOH:O	2.12	0.83
1:C:171:ASP:OD2	1:C:173:LYS:HG2	1.79	0.82
2:D:147:CYS:HB2	4:D:482:HOH:O	1.78	0.81
2:D:201:TYR:HB2	4:D:490:HOH:O	1.82	0.80
1:L:36:TYR:CE2	4:L:445:HOH:O	2.34	0.80
2:D:170:VAL:HA	4:D:497:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:THR:HA	4:D:409:HOH:O	1.83	0.78
1:L:100:TRP:C	4:L:539:HOH:O	2.22	0.76
2:D:170:VAL:CG2	4:D:497:HOH:O	2.34	0.75
2:D:134:SER:CA	4:D:491:HOH:O	2.34	0.74
1:C:179:LEU:N	4:C:479:HOH:O	2.21	0.73
1:C:178:SER:HA	4:C:479:HOH:O	1.88	0.73
2:D:170:VAL:HG23	4:D:497:HOH:O	1.89	0.73
1:L:100:TRP:N	4:L:539:HOH:O	2.21	0.73
1:C:51:LEU:HB3	1:C:52:ILE:HD12	1.71	0.73
1:L:155:ASP:HA	1:L:195:VAL:HG22	1.73	0.71
1:C:37[B]:MET:HE1	1:C:55:ALA:HB2	1.72	0.71
1:C:37[B]:MET:HE1	1:C:75:PHE:CD2	2.26	0.70
1:L:144:TYR:CE1	4:L:550:HOH:O	2.44	0.70
1:C:127:GLU:HA	1:C:130:LYS:HE3	1.75	0.69
3:C:219:SO4:O4	4:C:481:HOH:O	2.10	0.68
1:C:43:LYS:NZ	4:C:427:HOH:O	2.23	0.67
1:L:64:ALA:C	4:L:276:HOH:O	2.33	0.67
2:H:58:ASP:OD2	4:H:561:HOH:O	2.12	0.67
1:L:155:ASP:HA	1:L:195:VAL:CG2	2.25	0.67
1:C:98:ASP:OD1	1:C:99:PRO:HA	1.95	0.67
1:C:42:GLN:NE2	4:C:462:HOH:O	2.28	0.66
1:L:36:TYR:CZ	4:L:445:HOH:O	2.44	0.66
1:C:37[B]:MET:CE	1:C:55:ALA:HB2	2.27	0.65
4:C:360:HOH:O	2:D:150:LYS:HE3	1.95	0.64
1:L:60:SER:O	4:L:391:HOH:O	2.14	0.64
1:C:11:LEU:HD22	1:C:108:LEU:HD13	1.78	0.64
1:L:207:SER:HB2	1:L:208:PRO:HD2	1.80	0.64
1:C:203:GLN:O	4:C:367:HOH:O	2.15	0.63
2:H:104:THR:OG1	4:H:539:HOH:O	2.16	0.62
2:D:202:ILE:HD12	2:D:217:LYS:HE3	1.81	0.62
1:L:207:SER:HA	4:L:486:HOH:O	2.00	0.62
3:H:228:SO4:O2	4:H:469:HOH:O	2.16	0.61
2:D:193:SER:CB	4:D:475:HOH:O	2.49	0.61
1:L:31:TYR:O	1:L:34[A]:ILE:HG22	2.00	0.61
1:L:64:ALA:HA	4:L:521:HOH:O	2.00	0.60
1:C:151:GLN:HG2	4:C:450:HOH:O	2.03	0.57
1:C:98:ASP:OD1	1:C:99:PRO:CA	2.53	0.56
1:L:207:SER:CA	4:L:486:HOH:O	2.52	0.56
1:L:44:PRO:CG	1:L:169:GLU:HG3	2.36	0.56
2:H:89:THR:HG22	4:H:631:HOH:O	2.05	0.56
1:C:37[B]:MET:HE1	1:C:75:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37[B]:MET:CE	1:C:75:PHE:CD2	2.89	0.56
1:C:37[B]:MET:HE1	1:C:55:ALA:CB	2.36	0.55
2:D:162:ASN:HA	4:D:454:HOH:O	2.06	0.55
1:L:37[B]:MET:HE1	1:L:39:TRP:NE1	2.21	0.55
1:L:34[A]:ILE:HD13	1:L:36:TYR:HE2	1.72	0.55
2:D:133:PRO:O	4:D:333:HOH:O	2.18	0.55
1:L:112:ARG:N	4:L:550:HOH:O	2.39	0.54
1:C:52:ILE:HD13	1:C:77:LEU:HD13	1.90	0.54
2:H:112:GLN:OE1	4:H:582:HOH:O	2.19	0.54
1:C:37[B]:MET:CE	1:C:75:PHE:CE2	2.91	0.53
2:D:202:ILE:CD1	2:D:217:LYS:HG3	2.38	0.53
1:L:111:LYS:HA	4:L:550:HOH:O	2.08	0.53
2:D:169:GLY:C	4:D:497:HOH:O	2.44	0.53
1:L:64:ALA:HA	4:L:488:HOH:O	2.08	0.53
2:D:147:CYS:CB	4:D:482:HOH:O	2.47	0.53
2:D:193:SER:HB2	4:D:475:HOH:O	2.08	0.53
2:H:148:LEU:HD12	4:H:615:HOH:O	2.10	0.52
1:L:111:LYS:CA	4:L:550:HOH:O	2.57	0.52
2:D:193:SER:HB3	4:D:475:HOH:O	2.09	0.52
1:C:46:GLN:HG2	4:D:444:HOH:O	2.10	0.51
1:L:84:GLU:HG2	4:L:340:HOH:O	2.11	0.51
4:L:445:HOH:O	2:D:103:PHE:HE2	1.94	0.51
1:L:95:ILE:HD11	2:H:103:PHE:O	2.09	0.51
1:L:34[A]:ILE:HG21	4:L:445:HOH:O	2.10	0.51
2:D:202:ILE:HD12	2:D:217:LYS:HG3	1.93	0.51
1:C:11:LEU:CD2	1:C:13:VAL:HG23	2.37	0.50
2:D:189:VAL:CG2	4:D:497:HOH:O	2.24	0.50
2:D:208:LYS:HB2	2:D:209:PRO:HD3	1.93	0.50
1:L:59:GLU:HB3	1:L:62:ILE:HG13	1.93	0.50
2:H:89:THR:CG2	4:H:631:HOH:O	2.60	0.49
1:C:16:GLY:HA2	1:C:81:PRO:HB2	1.95	0.49
1:C:11:LEU:C	1:C:11:LEU:HD23	2.33	0.48
1:C:112:ARG:HB2	4:C:387:HOH:O	2.13	0.48
2:D:124:LYS:NZ	4:D:467:HOH:O	2.45	0.48
1:C:11:LEU:HD21	1:C:13:VAL:CG2	2.37	0.48
1:L:195:VAL:HG23	1:L:195:VAL:O	2.13	0.48
1:L:131:SER:HB3	4:L:483:HOH:O	2.14	0.48
1:L:65[B]:ARG:HB2	1:L:80:HIS:O	2.13	0.48
2:D:192:PRO:HG2	2:D:195:SER:OG	2.13	0.47
1:L:111:LYS:HB3	4:L:550:HOH:O	2.15	0.47
1:L:37[B]:MET:CE	1:L:39:TRP:NE1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:LYS:HD2	1:C:215:ARG:HH11	1.80	0.47
1:L:37[B]:MET:CE	1:L:39:TRP:CE2	2.97	0.47
1:L:98:ASP:HA	1:L:99:PRO:C	2.35	0.47
1:C:84:GLU:OE1	1:C:172:SER:HA	2.14	0.46
1:C:130:LYS:HB2	1:C:130:LYS:NZ	2.30	0.46
2:D:200:THR:HG22	2:D:202:ILE:HD11	1.98	0.46
2:D:142:THR:N	4:D:475:HOH:O	2.49	0.46
1:L:63:PRO:CB	1:L:65[A]:ARG:NH1	2.79	0.46
1:C:27:GLN:HG3	4:C:469:HOH:O	2.16	0.46
2:H:124:LYS:HE2	4:H:417:HOH:O	2.15	0.46
1:C:29:VAL:HA	1:C:96:ILE:HG21	1.97	0.45
1:C:160:SER:HB2	4:C:477:HOH:O	2.16	0.45
1:C:2:ILE:CD1	1:C:96:ILE:HD11	2.46	0.45
1:L:65[B]:ARG:NH1	1:L:65[B]:ARG:HG3	2.31	0.45
1:C:149:LYS:HZ3	1:C:151:GLN:HG3	1.83	0.44
1:L:37[B]:MET:HE1	1:L:39:TRP:CE2	2.51	0.44
1:L:84:GLU:CD	1:L:84:GLU:H	2.20	0.44
1:C:58:PRO:HB3	4:C:442:HOH:O	2.18	0.44
2:D:193:SER:CB	4:D:458:HOH:O	2.65	0.44
2:D:200:THR:CG2	2:D:202:ILE:HD11	2.48	0.44
1:C:123:PRO:HD2	4:D:426:HOH:O	2.18	0.44
1:L:34[A]:ILE:HD13	1:L:36:TYR:CE2	2.53	0.44
1:C:37[B]:MET:HE2	1:C:37[B]:MET:HB3	1.67	0.43
1:C:63:PRO:HG2	1:C:66:PHE:CE2	2.53	0.43
2:D:163:SER:OG	4:D:455:HOH:O	2.19	0.43
2:D:208:LYS:N	2:D:209:PRO:CD	2.82	0.43
1:C:194:LYS:HD2	1:C:215:ARG:NH1	2.34	0.43
1:C:36:TYR:HB2	1:C:96:ILE:HG22	2.00	0.43
2:D:152:TYR:CE1	2:D:157:VAL:HG13	2.54	0.43
1:L:192:LYS:C	4:L:573:HOH:O	2.57	0.43
2:H:143:ALA:CB	2:H:196:LEU:HD11	2.48	0.43
1:L:43:LYS:NZ	4:L:425:HOH:O	2.51	0.43
1:C:2:ILE:HD11	1:C:96:ILE:HD11	2.01	0.42
2:H:148:LEU:CD1	4:H:615:HOH:O	2.67	0.42
2:D:202:ILE:HG23	2:D:217:LYS:HD2	2.00	0.42
1:L:64:ALA:HB3	4:L:276:HOH:O	2.19	0.42
2:D:163:SER:N	4:D:454:HOH:O	2.52	0.42
1:C:11:LEU:HD22	1:C:108:LEU:CD1	2.46	0.42
1:L:155:ASP:OD1	1:L:195:VAL:HG22	2.20	0.42
2:D:218:VAL:O	4:D:490:HOH:O	2.22	0.42
2:D:123:THR:HB	4:D:481:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:PRO:HA	2:D:144:ALA:O	2.19	0.41
2:H:45:LYS:HE2	4:H:408:HOH:O	2.19	0.41
1:L:44:PRO:CB	1:L:169:GLU:HG3	2.50	0.41
1:C:52:ILE:HD11	1:C:77:LEU:HD11	2.01	0.41
1:L:37[B]:MET:HE2	1:L:39:TRP:CE2	2.56	0.41
1:L:65[B]:ARG:HH11	1:L:65[B]:ARG:HG3	1.86	0.41
2:D:210:SER:OG	2:D:212:THR:HG23	2.21	0.41
2:D:193:SER:HB2	4:D:458:HOH:O	2.21	0.40
1:L:44:PRO:HG2	1:L:169:GLU:HG3	2.02	0.40

All (4) 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:H:571:HOH:O	4:D:442:HOH:O[2_556]	1.68	0.52
4:L:479:HOH:O	4:H:406:HOH:O[4_546]	1.99	0.21
4:L:449:HOH:O	4:H:570:HOH:O[4_546]	2.15	0.05
4:H:547:HOH:O	4:H:556:HOH:O[2_556]	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	C	218/218 (100%)	213 (98%)	5 (2%)	0	100	100
1	L	221/218 (101%)	214 (97%)	7 (3%)	0	100	100
2	D	212/227 (93%)	210 (99%)	2 (1%)	0	100	100
2	H	215/227 (95%)	212 (99%)	3 (1%)	0	100	100
All	All	866/890 (97%)	849 (98%)	17 (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	C	190/188 (101%)	189 (100%)	1 (0%)	91	83
1	L	193/188 (103%)	191 (99%)	2 (1%)	80	63
2	D	185/195 (95%)	179 (97%)	6 (3%)	44	14
2	H	186/195 (95%)	182 (98%)	4 (2%)	57	28
All	All	754/766 (98%)	741 (98%)	13 (2%)	68	40

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	98	ASP
1	L	149	LYS
2	H	142	THR
2	H	157[A]	VAL
2	H	157[B]	VAL
2	H	185	LEU
1	C	156	ASN
2	D	29	LEU
2	D	60	ARG
2	D	88	ASP
2	D	134	SER
2	D	185	LEU
2	D	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	PCA	D	1	2	8,8,9	1.65	1 (12%)	9,10,12	2.21	5 (55%)
2	PCA	H	1	2	8,8,9	1.97	2 (25%)	9,10,12	1.89	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CA-C	3.38	1.54	1.50
2	H	1	PCA	CD-N	4.15	1.46	1.34
2	D	1	PCA	CD-N	4.20	1.46	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	PCA	CA-N-CD	-3.52	101.53	113.58
2	D	1	PCA	OE-CD-CG	-3.09	121.18	126.86
2	H	1	PCA	CA-N-CD	-2.69	104.36	113.58
2	H	1	PCA	OE-CD-CG	-2.56	122.15	126.86
2	D	1	PCA	CB-CA-C	-2.37	109.44	112.70
2	H	1	PCA	O-C-CA	-2.30	119.79	125.15
2	H	1	PCA	CB-CA-C	-2.29	109.55	112.70
2	D	1	PCA	CG-CD-N	2.32	114.93	108.33
2	D	1	PCA	CB-CA-N	2.44	110.32	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
3	SO4	C	219	-	4,4,4	0.12	0	6,6,6	0.07	0
3	SO4	D	228	-	4,4,4	0.31	0	6,6,6	0.51	0
3	SO4	H	228	-	4,4,4	0.17	0	6,6,6	0.94	0
3	SO4	L	219	-	4,4,4	0.27	0	6,6,6	0.31	0
3	SO4	L	220	-	4,4,4	0.70	0	6,6,6	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	219	-	-	0/0/0/0	0/0/0/0
3	SO4	D	228	-	-	0/0/0/0	0/0/0/0
3	SO4	H	228	-	-	0/0/0/0	0/0/0/0
3	SO4	L	219	-	-	0/0/0/0	0/0/0/0
3	SO4	L	220	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	219	SO4	1	0
3	H	228	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	217/218 (99%)	0.09	3 (1%) 75 77	22, 39, 60, 77	0
1	L	217/218 (99%)	0.25	13 (5%) 23 19	16, 28, 50, 86	0
2	D	212/227 (93%)	0.16	7 (3%) 47 46	20, 32, 76, 96	0
2	H	214/227 (94%)	-0.09	0 100 100	16, 23, 36, 51	0
All	All	860/890 (96%)	0.10	23 (2%) 55 55	16, 30, 62, 96	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	216	GLY	5.3
1	L	157	ALA	4.0
1	L	158	LEU	3.7
2	D	211	ASN	3.6
1	L	154	VAL	3.4
2	D	167	THR	3.3
1	L	188	ALA	3.3
2	D	134	SER	3.0
2	D	220	PRO	2.9
2	D	191	VAL	2.7
2	D	169	GLY	2.7
1	L	193	HIS	2.6
1	L	155	ASP	2.6
1	L	192	LYS	2.5
1	C	130	LYS	2.5
1	C	216	GLY	2.5
1	L	156	ASN	2.4
1	L	194	LYS	2.3
2	D	214	VAL	2.2
1	L	189	ASP	2.2
1	C	206	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	195	VAL	2.2
1	L	217	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	PCA	H	1	8/9	0.97	0.12	-	22,24,27,29	0
2	PCA	D	1	8/9	0.98	0.07	-	25,37,45,53	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
3	SO4	H	228	5/5	0.94	0.15	2.89	43,51,58,61	0
3	SO4	L	220	5/5	0.95	0.12	2.65	34,36,42,43	0
3	SO4	C	219	5/5	0.98	0.08	-	59,60,63,63	0
3	SO4	D	228	5/5	0.98	0.06	-	33,33,38,39	0
3	SO4	L	219	5/5	0.98	0.09	-	42,50,60,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.