



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2017 – 01:47 PM EDT

PDB ID : 5MP6  
Title : Structure of the Unliganded Fab from HIV-1 Neutralizing Antibody CAP248-2B that Binds to the gp120 C-terminus - gp41 Interface, at two Angstrom resolution.  
Authors : Wibmer, C.K.; Gorman, J.; Kwong, P.D.  
Deposited on : 2016-12-15  
Resolution : 1.96 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 : rb-20029077  
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) : rb-20029077

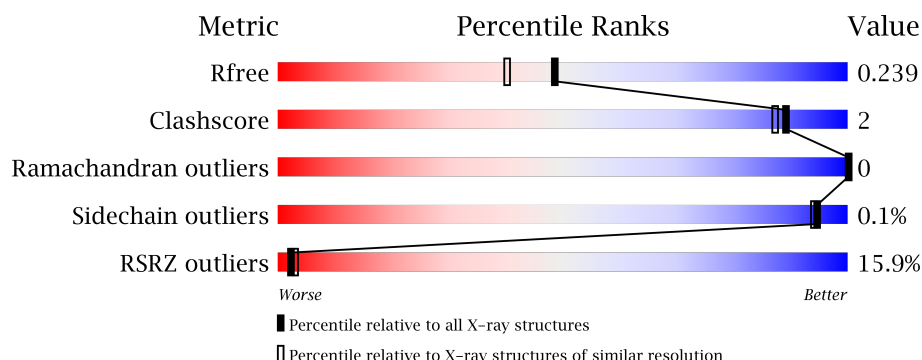
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	H	238	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>.</div> </div> </div>
1	P	238	<div> <div>18%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
2	L	225	<div> <div>4%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
2	Q	225	<div> <div>33%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </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	L	305	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13438 atoms, of which 6411 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.

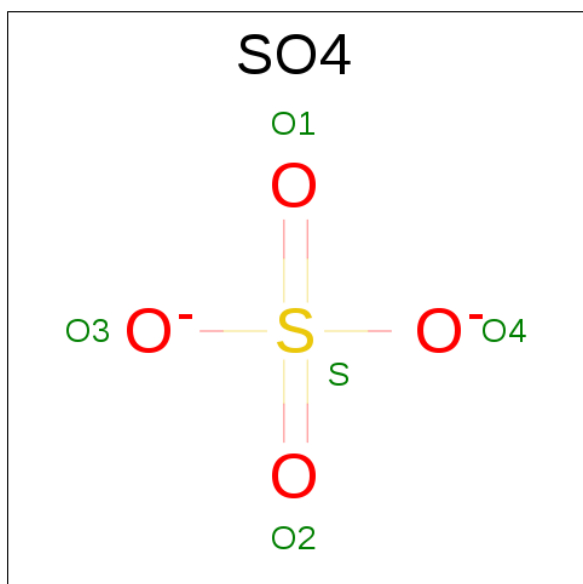
- Molecule 1 is a protein called CAP248-2B Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	P	211	Total	C	H	N	O	S	0	2	0
			3196	1026	1579	268	317	6			
1	H	230	Total	C	H	N	O	S	0	2	0
			3424	1095	1689	288	345	7			

- Molecule 2 is a protein called CAP248-2B Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	Q	208	Total	C	H	N	O	S	0	1	0
			3047	969	1500	256	318	4			
2	L	225	Total	C	H	N	O	S	0	5	0
			3331	1059	1643	278	346	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

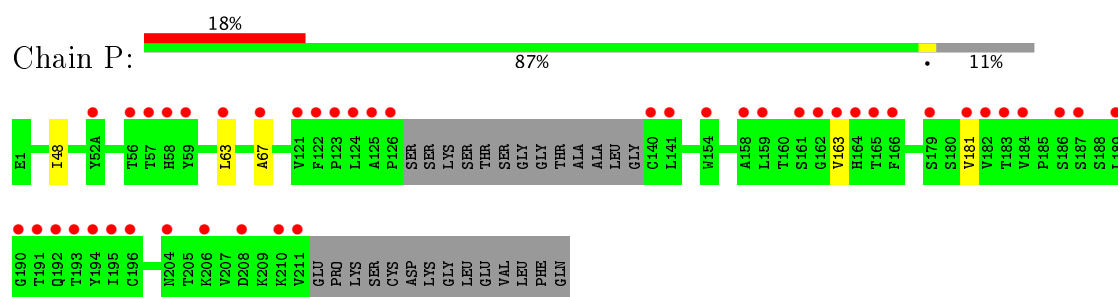
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	80	Total O 80 80	0	0
4	Q	53	Total O 53 53	0	0
4	H	113	Total O 113 113	0	0
4	L	124	Total O 124 124	0	0

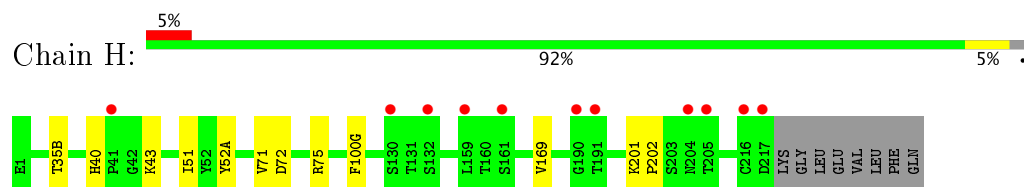
### 3 Residue-property plots [i](#)

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.

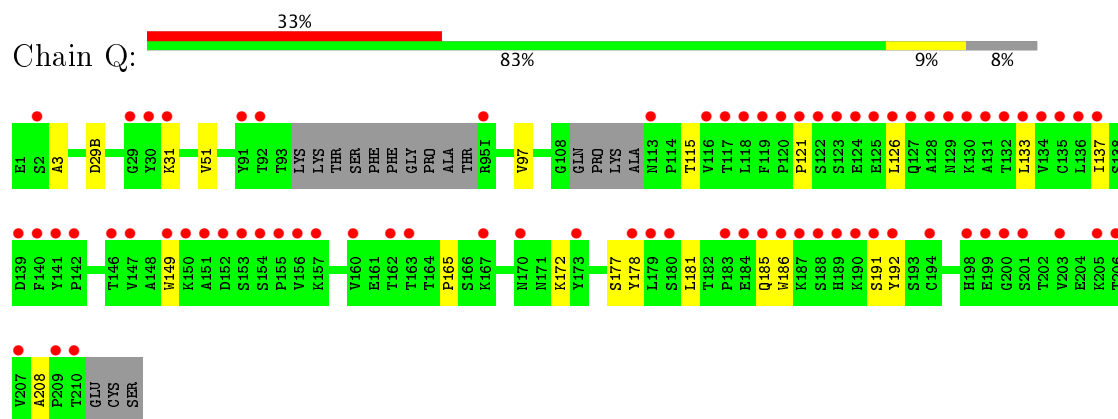
- Molecule 1: CAP248-2B Heavy Chain



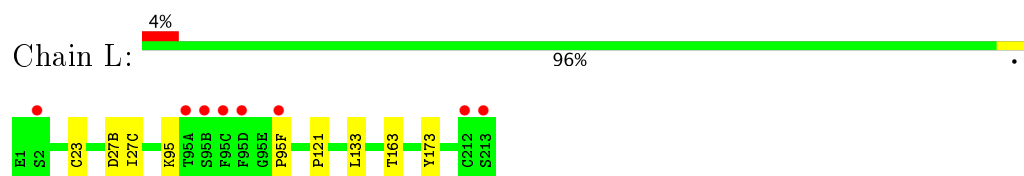
- Molecule 1: CAP248-2B Heavy Chain



- Molecule 2: CAP248-2B Light Chain



- Molecule 2: CAP248-2B Light Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.00 Å 85.90 Å 126.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.74 – 1.96 41.74 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.74-1.96) 99.5 (41.74-1.96)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.97 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.198 , 0.240 0.197 , 0.239	Depositor DCC
$R_{free}$ test set	2001 reflections (3.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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	H	0.30	0/1777	0.55	0/2430
1	P	0.30	0/1654	0.55	0/2262
2	L	0.32	0/1740	0.53	0/2373
2	Q	0.28	0/1581	0.51	0/2156
All	All	0.30	0/6752	0.54	0/9221

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	H	1735	1689	1694	8	0
1	P	1617	1579	1579	5	0
2	L	1688	1643	1644	7	0
2	Q	1547	1500	1495	11	0
3	H	30	0	0	0	0
3	L	25	0	0	1	0
3	P	10	0	0	0	0
3	Q	5	0	0	0	0
4	H	113	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	124	0	0	0	0
4	P	80	0	0	0	0
4	Q	53	0	0	0	0
All	All	7027	6411	6412	29	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 2.

All (29) 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:P:63:LEU:HD21	1:P:67:ALA:CB	2.41	0.51
2:L:27(B):ASP:OD1	2:L:27(C):ILE:N	2.39	0.50
2:L:173:TYR:OH	3:L:305:SO4:O3	2.27	0.47
1:P:48:ILE:HG23	1:P:63:LEU:HD22	1.96	0.47
1:P:48:ILE:HG23	1:P:63:LEU:CD2	2.43	0.47
2:L:95:LYS:HD2	2:L:95(F):PRO:HB3	1.98	0.46
2:Q:3:ALA:HA	2:Q:97:VAL:HG21	1.96	0.46
1:H:72:ASP:OD2	1:H:75:ARG:NH2	2.49	0.46
1:H:169:VAL:HG12	2:L:163:THR:HG22	1.98	0.45
1:P:163:VAL:HG23	1:P:181:VAL:O	2.17	0.45
2:Q:149:TRP:HE1	2:Q:177:SER:HG	1.65	0.44
2:Q:181:LEU:HD13	2:Q:185:GLN:HB2	2.00	0.44
2:L:121:PRO:HD3	2:L:133:LEU:CD2	2.49	0.43
1:H:40:HIS:O	1:H:43:LYS:N	2.51	0.43
2:Q:121:PRO:HD3	2:Q:133:LEU:HD23	2.01	0.42
2:Q:115:THR:O	2:Q:137:ILE:HA	2.19	0.42
1:P:63:LEU:HD21	1:P:67:ALA:HB2	2.02	0.42
1:H:35(B):THR:HG21	1:H:100(G):PHE:CE1	2.54	0.42
2:Q:133:LEU:O	2:Q:178:TYR:HA	2.19	0.42
1:H:169:VAL:HG12	2:L:163:THR:CG2	2.50	0.41
2:Q:191:SER:O	2:Q:208:ALA:HA	2.19	0.41
1:H:52(A):TYR:HD1	1:H:71[B]:VAL:HG11	1.85	0.41
2:Q:149:TRP:CZ3	2:Q:192:TYR:CE2	3.08	0.41
2:L:23:CYS:SG	2:L:27(C):ILE:HD11	2.61	0.41
1:H:51:ILE:HG21	1:H:71[A]:VAL:HG23	2.03	0.41
2:Q:165:PRO:HB3	2:Q:172:LYS:HA	2.02	0.41
2:Q:31:LYS:O	2:Q:51:VAL:HG23	2.20	0.41
1:H:201:LYS:N	1:H:202:PRO:CD	2.84	0.40
2:Q:126:LEU:HD22	2:Q:186:TRP:CZ2	2.57	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	H	230/238 (97%)	225 (98%)	5 (2%)	0	100	100
1	P	209/238 (88%)	202 (97%)	7 (3%)	0	100	100
2	L	228/225 (101%)	223 (98%)	5 (2%)	0	100	100
2	Q	203/225 (90%)	189 (93%)	14 (7%)	0	100	100
All	All	870/926 (94%)	839 (96%)	31 (4%)	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	H	198/203 (98%)	198 (100%)	0	100	100
1	P	184/203 (91%)	184 (100%)	0	100	100
2	L	193/188 (103%)	193 (100%)	0	100	100
2	Q	175/188 (93%)	174 (99%)	1 (1%)	89	88
All	All	750/782 (96%)	749 (100%)	1 (0%)	94	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	29(B)	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	58	HIS
2	L	39	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z  > 2$
1	PCA	H	1	1	8,8,9	1.88	2 (25%)	9,10,12	2.23	6 (66%)
2	PCA	L	1	2	8,8,9	2.13	2 (25%)	9,10,12	1.97	5 (55%)
1	PCA	P	1	1	8,8,9	1.97	2 (25%)	9,10,12	2.25	5 (55%)
2	PCA	Q	1	2	8,8,9	2.02	2 (25%)	9,10,12	2.17	6 (66%)

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
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
2	PCA	L	1	2	-	0/0/11/13	0/1/1/1
1	PCA	P	1	1	-	0/0/11/13	0/1/1/1
2	PCA	Q	1	2	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	PCA	CA-N	2.78	1.49	1.46
1	P	1	PCA	CA-N	3.25	1.50	1.46
2	Q	1	PCA	CA-N	3.28	1.50	1.46
2	L	1	PCA	CA-N	3.59	1.50	1.46
1	H	1	PCA	CD-N	4.16	1.46	1.34
1	P	1	PCA	CD-N	4.22	1.46	1.34
2	Q	1	PCA	CD-N	4.29	1.46	1.34
2	L	1	PCA	CD-N	4.31	1.47	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1	PCA	CB-CA-C	-3.56	107.80	112.70
1	H	1	PCA	CB-CA-C	-3.24	108.25	112.70
2	Q	1	PCA	OE-CD-CG	-3.03	121.28	126.86
1	H	1	PCA	OE-CD-CG	-3.02	121.29	126.86
2	L	1	PCA	CA-N-CD	-3.02	103.24	113.58
1	P	1	PCA	CA-N-CD	-3.00	103.32	113.58
1	P	1	PCA	OE-CD-CG	-2.96	121.42	126.86
2	Q	1	PCA	CA-N-CD	-2.94	103.51	113.58
1	H	1	PCA	CA-N-CD	-2.92	103.58	113.58
2	L	1	PCA	OE-CD-CG	-2.90	121.53	126.86
2	Q	1	PCA	CB-CA-C	-2.84	108.80	112.70
1	H	1	PCA	O-C-CA	-2.13	120.17	125.15
2	Q	1	PCA	O-C-CA	-2.11	120.23	125.15
2	L	1	PCA	CB-CA-C	-2.04	109.89	112.70
2	L	1	PCA	CG-CD-N	2.20	114.58	108.33
1	P	1	PCA	CG-CD-N	2.25	114.73	108.33
2	Q	1	PCA	CG-CD-N	2.27	114.77	108.33
1	H	1	PCA	CG-CD-N	2.28	114.81	108.33
2	L	1	PCA	CB-CA-N	2.34	110.03	103.30
1	P	1	PCA	CB-CA-N	2.47	110.38	103.30
2	Q	1	PCA	CB-CA-N	2.47	110.40	103.30
1	H	1	PCA	CB-CA-N	2.52	110.54	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](#)

14 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	H	301	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	H	302	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	H	303	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	H	304	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	H	305	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	H	306	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	L	302	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	L	303	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	L	304	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	L	305	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	P	301	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	P	302	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	Q	301	-	4,4,4	0.15	0	6,6,6	0.05	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	H	301	-	-	0/0/0/0	0/0/0/0
3	SO4	H	302	-	-	0/0/0/0	0/0/0/0
3	SO4	H	303	-	-	0/0/0/0	0/0/0/0
3	SO4	H	304	-	-	0/0/0/0	0/0/0/0
3	SO4	H	305	-	-	0/0/0/0	0/0/0/0
3	SO4	H	306	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	L	301	-	-	0/0/0/0	0/0/0/0
3	SO4	L	302	-	-	0/0/0/0	0/0/0/0
3	SO4	L	303	-	-	0/0/0/0	0/0/0/0
3	SO4	L	304	-	-	0/0/0/0	0/0/0/0
3	SO4	L	305	-	-	0/0/0/0	0/0/0/0
3	SO4	P	301	-	-	0/0/0/0	0/0/0/0
3	SO4	P	302	-	-	0/0/0/0	0/0/0/0
3	SO4	Q	301	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	305	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	H	229/238 (96%)	0.51	11 (4%) 31 42	21, 36, 76, 96	0
1	P	210/238 (88%)	1.26	44 (20%) 1 1	21, 44, 119, 141	0
2	L	224/225 (99%)	0.27	8 (3%) 43 54	19, 32, 65, 108	0
2	Q	207/225 (92%)	1.76	75 (36%) 0 0	22, 69, 107, 125	0
All	All	870/926 (93%)	0.93	138 (15%) 2 3	19, 39, 100, 141	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	126	LEU	11.0
2	Q	192	TYR	10.7
1	P	189	LEU	10.0
2	Q	186	TRP	9.2
1	P	161	SER	8.9
2	Q	191	SER	8.6
2	Q	119	PHE	8.2
2	Q	131	ALA	8.1
1	P	162	GLY	8.1
1	P	193	THR	8.1
2	Q	118	LEU	8.0
1	P	122	PHE	7.9
2	Q	190	LYS	7.3
2	L	95(A)	THR	6.7
1	P	181	VAL	6.7
1	P	158	ALA	6.0
2	Q	2	SER	5.9
1	P	125	ALA	5.9
1	P	67	ALA	5.7
2	Q	206	THR	5.7
1	P	123	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
2	Q	133	LEU	5.7
2	Q	134	VAL	5.6
2	Q	152	ASP	5.5
1	P	183	THR	5.5
1	P	182	VAL	5.3
1	P	190	GLY	5.3
1	P	140	CYS	5.2
1	P	191	THR	5.1
2	Q	149	TRP	5.0
2	Q	140	PHE	4.9
1	P	63	LEU	4.8
2	Q	180	SER	4.6
2	Q	135	CYS	4.6
2	Q	130	LYS	4.5
2	Q	210	THR	4.4
2	Q	147	VAL	4.3
1	P	187	SER	4.3
2	Q	136	LEU	4.3
1	P	124	LEU	4.3
1	P	184	VAL	4.3
1	P	194	TYR	4.2
2	Q	116	VAL	4.2
2	Q	207	VAL	4.2
2	Q	153	SER	4.1
1	P	159	LEU	4.0
2	L	95(B)	SER	4.0
1	P	57	THR	4.0
1	P	195	ILE	4.0
2	Q	122	SER	4.0
2	L	213	SER	4.0
2	Q	30	TYR	4.0
1	P	121	VAL	3.9
2	Q	123	SER	3.8
1	P	58	HIS	3.8
2	Q	201	SER	3.8
2	Q	121	PRO	3.7
2	Q	185	GLN	3.7
1	P	59	TYR	3.7
2	Q	156	VAL	3.7
2	Q	189	HIS	3.6
2	Q	157	LYS	3.6
1	P	196	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	P	166	PHE	3.6
1	P	210	LYS	3.5
2	L	212	CYS	3.5
1	H	130	SER	3.4
2	Q	205	LYS	3.4
1	P	126	PRO	3.3
2	L	95(C)	PHE	3.3
2	Q	139	ASP	3.3
1	P	192	GLN	3.3
2	Q	178	TYR	3.3
1	P	204	ASN	3.3
1	P	52(A)	TYR	3.3
1	H	216	CYS	3.3
1	P	164	HIS	3.2
1	H	159	LEU	3.2
2	Q	167	LYS	3.2
2	Q	117	THR	3.2
2	Q	128	ALA	3.2
2	Q	151	ALA	3.2
2	Q	132	THR	3.1
1	H	41	PRO	3.1
2	Q	187	LYS	3.1
1	P	211	VAL	3.0
2	Q	203	VAL	3.0
2	Q	209	PRO	3.0
2	L	2	SER	3.0
1	P	141	LEU	3.0
2	L	95(D)	PHE	2.9
1	H	190	GLY	2.9
2	Q	160	VAL	2.9
2	Q	188	SER	2.9
2	Q	179	LEU	2.9
2	Q	113	ASN	2.9
2	Q	155	PRO	2.8
2	Q	154	SER	2.8
2	Q	120	PRO	2.8
2	Q	129	ASN	2.8
2	Q	141	TYR	2.7
1	P	206	LYS	2.7
1	H	217	ASP	2.7
1	P	165	THR	2.7
2	Q	199	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	163	VAL	2.6
2	Q	95(I)	ARG	2.6
2	Q	91	TYR	2.6
2	Q	125	GLU	2.6
2	Q	150	LYS	2.6
2	Q	170	ASN	2.5
2	Q	173	TYR	2.5
2	Q	31	LYS	2.4
1	P	154	TRP	2.4
2	Q	137	ILE	2.4
2	Q	200	GLY	2.4
2	Q	127	GLN	2.4
2	Q	146	THR	2.3
1	P	179	SER	2.3
2	Q	142	PRO	2.3
2	Q	162	THR	2.3
1	H	132	SER	2.3
2	Q	163	THR	2.2
2	Q	194	CYS	2.2
2	Q	124	GLU	2.2
1	H	191	THR	2.2
1	H	204	ASN	2.2
1	P	208	ASP	2.2
2	L	95(F)	PRO	2.2
2	Q	92	THR	2.1
1	P	56	THR	2.1
1	H	205	THR	2.1
1	P	186	SER	2.1
2	Q	183	PRO	2.1
2	Q	184	GLU	2.1
2	Q	198	HIS	2.1
1	H	161	SER	2.0
2	Q	29	GLY	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
1	PCA	P	1	8/9	0.96	0.11	-	24,41,51,51	0
1	PCA	H	1	8/9	0.95	0.14	-	28,42,53,53	0
2	PCA	L	1	8/9	0.61	0.31	-	59,83,100,100	0
2	PCA	Q	1	8/9	0.72	0.39	-	75,87,104,104	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( $\text{\AA}^2$ )	Q<0.9
3	SO4	L	305	5/5	0.86	0.21	3.50	70,75,82,83	0
3	SO4	P	301	5/5	0.86	0.15	0.93	82,88,88,89	0
3	SO4	H	303	5/5	0.94	0.19	0.75	67,75,77,79	0
3	SO4	H	304	5/5	0.91	0.15	0.23	73,76,84,85	0
3	SO4	H	301	5/5	0.85	0.18	0.19	73,78,81,82	0
3	SO4	H	305	5/5	0.94	0.18	0.13	46,60,62,63	0
3	SO4	L	303	5/5	0.92	0.13	-0.49	78,79,80,84	0
3	SO4	H	306	5/5	0.80	0.19	-0.54	99,104,104,108	0
3	SO4	P	302	5/5	0.95	0.12	-0.70	78,78,83,86	0
3	SO4	L	302	5/5	0.95	0.10	-1.95	61,62,65,67	0
3	SO4	L	304	5/5	0.86	0.16	-	59,60,66,71	0
3	SO4	L	301	5/5	0.85	0.24	-	99,100,101,104	0
3	SO4	Q	301	5/5	0.95	0.14	-	87,88,90,92	0
3	SO4	H	302	5/5	0.94	0.16	-	87,90,91,92	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.