



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2022 – 04:22 PM EDT

PDB ID : 7TCQ
Title : Crystal structure of SARS-CoV-2 neutralizing antibody WS6 in complex with spike S2 peptide
Authors : Zhou, T.; Kwong, P.D.
Deposited on : 2021-12-28
Resolution : 2.02 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:

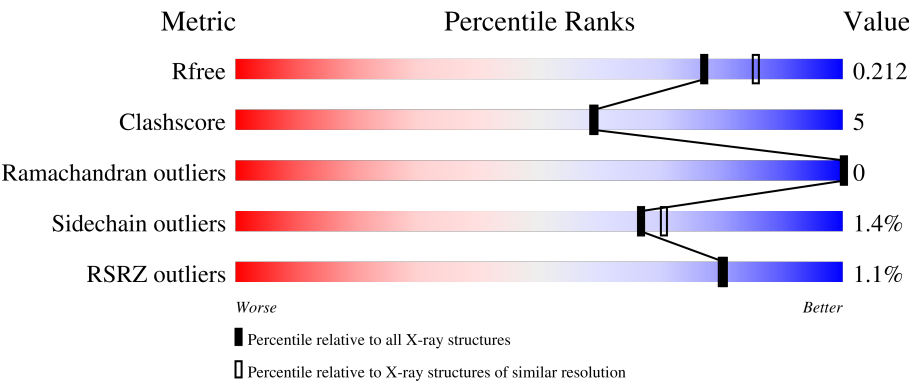
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	216	<div><div></div><div>87%12%</div></div>
1	H	216	<div><div></div><div>92%8%</div></div>
2	L	212	<div><div></div><div>%93%7%</div></div>
3	C	12	<div><div></div><div>75%25%</div></div>
3	D	12	<div><div></div><div>67%33%</div></div>

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Mol	Chain	Length	Quality of chain
4	B	212	<div><div></div><div>3%</div><div>84%</div><div>16%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7607 atoms, of which 20 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 Anti-SARS-CoV-2 antibody WS6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	2	0
			1639	1035	268	329	7			
1	A	213	Total	C	N	O	S	0	1	0
			1612	1020	263	322	7			

- Molecule 2 is a protein called Anti-SARS-CoV-2 antibody WS6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1638	1023	271	337	7			

- Molecule 3 is a protein called Pegylated spike S2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	0	0	0
			105	71	14	20			
3	D	12	Total	C	N	O	0	0	0
			105	71	14	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1147	ACE	-	acetylation	UNP P0DTC2
C	1158	I2J	-	insertion	UNP P0DTC2
D	1147	ACE	-	acetylation	UNP P0DTC2
D	1158	I2J	-	insertion	UNP P0DTC2

- Molecule 4 is a protein called Anti-SARS-CoV-2 antibody WS6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	212	Total	C	N	O	S	0	0	0
			1639	1023	272	337	7			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	H	O	0	0
			17	4	10	3		
6	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	228	Total 228	O 228	0	0
7	L	195	Total 195	O 195	0	0
7	C	14	Total 14	O 14	0	0
7	A	169	Total 169	O 169	0	0
7	B	117	Total 117	O 117	0	0
7	D	12	Total 12	O 12	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.

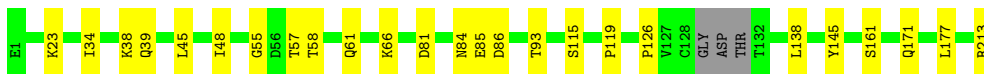
- Molecule 1: Anti-SARS-CoV-2 antibody WS6 Fab heavy chain

Chain H: 



- Molecule 1: Anti-SARS-CoV-2 antibody WS6 Fab heavy chain

Chain A: 



- Molecule 2: Anti-SARS-CoV-2 antibody WS6 Fab light chain

Chain L: 



- Molecule 3: Pegylated spike S2 peptide

Chain C: 

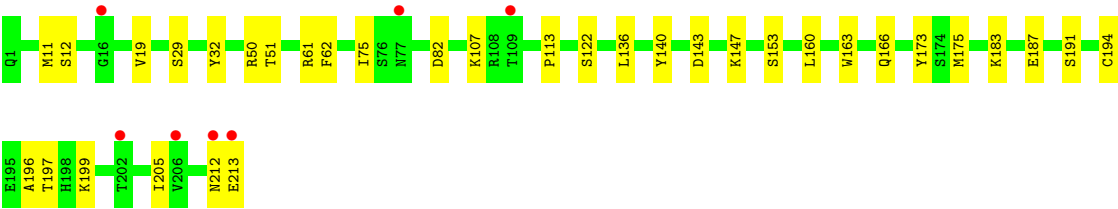
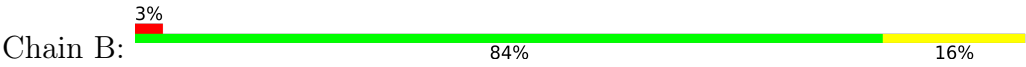


- Molecule 3: Pegylated spike S2 peptide

Chain D: 



- Molecule 4: Anti-SARS-CoV-2 antibody WS6 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.06Å 64.52Å 137.96Å 90.00° 117.34° 90.00°	Depositor
Resolution (Å)	40.23 – 2.02 40.23 – 2.02	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.23-2.02) 94.6 (40.23-2.02)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.172 , 0.213 0.170 , 0.212	Depositor DCC
R_{free} test set	1989 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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, ACE, PCA, I2J, PEG

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	0.39	0/1658	0.59	1/2268 (0.0%)
1	H	0.43	0/1689	0.62	0/2312
2	L	0.47	0/1672	0.62	0/2279
3	C	0.78	0/98	0.65	0/128
3	D	0.67	0/98	0.57	0/128
4	B	0.35	0/1680	0.56	0/2288
All	All	0.42	0/6895	0.60	1/9403 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	177	LEU	CA-CB-CG	6.30	129.78	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1157	LYS	Mainchain

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	1612	0	1561	14	0
1	H	1639	0	1587	10	0
2	L	1638	0	1560	12	0
3	C	105	0	96	4	0
3	D	105	0	96	4	1
4	B	1639	0	1564	19	1
5	A	35	0	0	0	0
5	B	10	0	0	1	0
5	C	5	0	0	0	0
5	H	35	0	0	1	0
5	L	15	0	0	0	0
6	C	7	10	10	0	0
6	L	7	10	10	1	0
7	A	169	0	0	4	1
7	B	117	0	0	2	0
7	C	14	0	0	1	0
7	D	12	0	0	0	0
7	H	228	0	0	3	2
7	L	195	0	0	3	1
All	All	7587	20	6484	62	3

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 (62) 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)
3:C:1147:ACE:H2	3:C:1151:GLU:H	1.23	1.02
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.47	0.96
1:H:61:GLN:NE2	7:H:401:HOH:O	2.03	0.91
3:C:1147:ACE:H3	7:C:1310:HOH:O	1.70	0.90
4:B:107:LYS:NZ	7:B:402:HOH:O	2.17	0.77
1:A:171:GLN:NE2	4:B:160:LEU:HD21	2.03	0.73
3:C:1147:ACE:CH3	3:C:1151:GLU:H	2.01	0.73
1:A:115:SER:OG	7:A:401:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40[B]:ARG:NH2	7:H:403:HOH:O	2.22	0.72
1:H:56[B]:ASP:OD2	3:C:1157:LYS:HG3	1.91	0.70
2:L:109:THR:HG22	7:L:524:HOH:O	1.92	0.69
3:D:1147:ACE:H2	3:D:1151:GLU:H	1.58	0.68
1:A:61:GLN:OE1	7:A:402:HOH:O	2.13	0.67
1:A:171:GLN:NE2	7:A:403:HOH:O	2.22	0.66
5:B:301:SO4:O2	7:B:401:HOH:O	2.13	0.65
2:L:155:ARG:NH2	7:L:402:HOH:O	2.31	0.64
2:L:9:ALA:O	2:L:10:ILE:HD13	1.98	0.62
3:D:1147:ACE:H1	3:D:1151:GLU:HG3	1.81	0.62
2:L:184:ASP:OD1	7:L:401:HOH:O	2.17	0.59
4:B:136:LEU:CD2	4:B:196:ALA:HB2	2.33	0.59
1:A:55:GLY:O	1:A:57:THR:HG23	2.03	0.58
5:H:301:SO4:O4	7:H:402:HOH:O	2.16	0.57
2:L:91:TYR:O	6:L:304:PEG:H21	2.06	0.56
4:B:183:LYS:O	4:B:187:GLU:HG2	2.06	0.56
1:A:66:LYS:HE2	1:A:86:ASP:OD1	2.08	0.53
1:A:213:ARG:HD3	7:A:407:HOH:O	2.08	0.53
4:B:61:ARG:NH2	4:B:82:ASP:OD1	2.42	0.53
1:A:34:ILE:HD12	1:A:93:THR:O	2.10	0.52
4:B:107:LYS:HE2	4:B:140:TYR:OH	2.12	0.49
2:L:1:PCA:HB2	2:L:97:THR:HG21	1.95	0.48
1:H:184:THR:O	1:H:187:THR:HB	2.13	0.48
4:B:113:PRO:HG2	4:B:205:ILE:HD12	1.96	0.48
1:H:145:TYR:CE2	1:H:150:VAL:HG13	2.49	0.47
4:B:62:PHE:CE1	4:B:75:ILE:HG12	2.49	0.47
1:H:73:THR:OG1	1:H:74:PRO:HD3	2.15	0.47
4:B:163:TRP:CD1	4:B:175:MET:HG3	2.51	0.46
4:B:11:MET:CE	4:B:19:VAL:HG13	2.45	0.46
4:B:61:ARG:HH21	4:B:82:ASP:CG	2.19	0.46
4:B:166:GLN:HG3	4:B:173:TYR:CZ	2.51	0.46
4:B:32:TYR:HB3	4:B:50:ARG:HA	1.99	0.45
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.99	0.44
1:H:154:TRP:CZ3	1:H:195:CYS:HB3	2.52	0.44
4:B:147:LYS:NZ	4:B:197:THR:HG23	2.33	0.44
2:L:73:LEU:C	2:L:73:LEU:HD23	2.39	0.43
1:H:95:THR:HA	1:H:98:TYR:O	2.19	0.43
2:L:193:THR:CG2	2:L:206:VAL:HG13	2.49	0.43
4:B:136:LEU:HD23	4:B:196:ALA:HB2	1.99	0.43
1:H:188:TRP:CG	1:H:189:PRO:HA	2.53	0.43
2:L:142:LYS:HB3	2:L:173:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HB2	1:A:48:ILE:HD11	2.01	0.42
1:A:126:PRO:HD3	1:A:138:LEU:HD23	2.01	0.42
1:A:84[B]:ASN:OD1	1:A:85:GLU:OE2	2.37	0.42
1:A:58:THR:HG21	3:D:1156:PHE:O	2.20	0.42
4:B:147:LYS:HZ3	4:B:147:LYS:HG3	1.62	0.41
2:L:193:THR:HG23	2:L:206:VAL:HG13	2.02	0.41
4:B:136:LEU:HD21	4:B:196:ALA:HB2	2.01	0.41
1:H:35:HIS:O	1:H:92:CYS:HA	2.21	0.41
4:B:212:ASN:O	4:B:213:GLU:C	2.59	0.41
2:L:184:ASP:O	2:L:188:ARG:HG3	2.20	0.41
1:A:39:GLN:HB2	1:A:45:LEU:HD23	2.03	0.41
3:D:1147:ACE:CH3	3:D:1151:GLU:H	2.30	0.40
4:B:50:ARG:O	4:B:51:THR:HB	2.21	0.40

All (3) 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:B:32:TYR:OH	3:D:1151:GLU:OE2[2_556]	2.00	0.20
7:H:593:HOH:O	7:A:543:HOH:O[3_545]	2.12	0.08
7:H:574:HOH:O	7:L:571:HOH:O[4_555]	2.18	0.02

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	210/216 (97%)	207 (99%)	3 (1%)	0	100	100
1	H	216/216 (100%)	211 (98%)	5 (2%)	0	100	100
2	L	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
3	C	10/12 (83%)	10 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	10/12 (83%)	10 (100%)	0	0	100	100
4	B	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
All	All	866/880 (98%)	847 (98%)	19 (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	183/184 (100%)	180 (98%)	3 (2%)	62	66
1	H	186/184 (101%)	186 (100%)	0	100	100
2	L	187/187 (100%)	187 (100%)	0	100	100
3	C	10/10 (100%)	10 (100%)	0	100	100
3	D	10/10 (100%)	10 (100%)	0	100	100
4	B	188/188 (100%)	180 (96%)	8 (4%)	29	25
All	All	764/763 (100%)	753 (99%)	11 (1%)	67	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	81	ASP
1	A	161	SER
4	B	12	SER
4	B	29	SER
4	B	122	SER
4	B	143	ASP
4	B	153	SER
4	B	191	SER
4	B	194	CYS
4	B	199	LYS

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

Mol	Chain	Res	Type
1	H	61	GLN
2	L	190	ASN
1	A	171	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	L	1	2	7,8,9	1.72	1 (14%)	9,10,12	1.85	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	L	1	2	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	PCA	CD-N	4.39	1.46	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	PCA	CA-N-CD	-2.62	104.60	113.58
2	L	1	PCA	CG-CD-N	2.53	114.94	108.39
2	L	1	PCA	CB-CA-N	2.52	110.54	103.30
2	L	1	PCA	OE-CD-CG	-2.24	122.85	126.76

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
2	L	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	$\# Z > 2$
6	PEG	L	304	-	6,6,6	0.24	0	5,5,5	0.16	0
5	SO4	A	302	-	4,4,4	0.17	0	6,6,6	0.24	0
5	SO4	H	301	-	4,4,4	0.15	0	6,6,6	0.18	0
5	SO4	H	304	-	4,4,4	0.19	0	6,6,6	0.09	0
5	SO4	B	301	-	4,4,4	0.16	0	6,6,6	0.23	0
5	SO4	H	307	-	4,4,4	0.28	0	6,6,6	0.35	0
5	SO4	L	303	-	4,4,4	0.28	0	6,6,6	0.40	0
5	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.26	0
5	SO4	L	302	-	4,4,4	0.17	0	6,6,6	0.32	0
5	SO4	H	305	-	4,4,4	0.17	0	6,6,6	0.38	0
5	SO4	H	302	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	305	-	4,4,4	0.18	0	6,6,6	0.16	0
5	SO4	A	306	-	4,4,4	0.20	0	6,6,6	0.17	0
5	SO4	A	307	-	4,4,4	0.20	0	6,6,6	0.08	0
5	SO4	L	301	-	4,4,4	0.22	0	6,6,6	0.16	0
5	SO4	H	306	-	4,4,4	0.13	0	6,6,6	0.26	0
6	PEG	C	1202	-	6,6,6	0.18	0	5,5,5	0.05	0
5	SO4	A	303	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	B	302	-	4,4,4	0.19	0	6,6,6	0.15	0
5	SO4	H	303	-	4,4,4	0.17	0	6,6,6	0.16	0
5	SO4	C	1201	-	4,4,4	0.23	0	6,6,6	0.18	0
5	SO4	A	301	-	4,4,4	0.21	0	6,6,6	0.27	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
6	PEG	C	1202	-	-	0/4/4/4	-
6	PEG	L	304	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	304	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	304	PEG	1	0
5	H	301	SO4	1	0
5	B	301	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	213/216 (98%)	-0.31	0 100 100	22, 30, 48, 75	0
1	H	216/216 (100%)	-0.42	1 (0%) 91 91	16, 25, 41, 76	0
2	L	211/212 (99%)	-0.29	2 (0%) 84 83	16, 25, 41, 81	0
3	C	10/12 (83%)	-0.26	0 100 100	21, 31, 40, 42	0
3	D	10/12 (83%)	-0.25	0 100 100	26, 34, 40, 44	0
4	B	212/212 (100%)	-0.12	7 (3%) 46 46	26, 39, 59, 88	0
All	All	872/880 (99%)	-0.29	10 (1%) 80 80	16, 30, 52, 88	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	212	ASN	4.8
2	L	212	ASN	4.0
4	B	202	THR	3.3
1	H	1	GLU	3.1
4	B	109	THR	2.9
4	B	77	ASN	2.8
4	B	206	VAL	2.6
4	B	16	GLY	2.2
2	L	109	THR	2.1
4	B	213	GLU	2.1

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. 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(\AA^2)	Q<0.9
2	PCA	L	1	8/9	0.97	0.09	21,26,35,39	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
5	SO4	H	307	5/5	0.74	0.38	47,56,73,82	0
6	PEG	L	304	7/7	0.81	0.26	39,47,53,55	0
6	PEG	C	1202	7/7	0.81	0.24	45,54,66,66	0
5	SO4	L	303	5/5	0.83	0.36	38,48,53,67	0
5	SO4	H	305	5/5	0.84	0.26	54,58,67,69	0
5	SO4	A	303	5/5	0.86	0.27	60,64,75,78	0
5	SO4	A	304	5/5	0.88	0.21	40,57,64,68	0
5	SO4	A	305	5/5	0.92	0.37	56,62,70,77	0
5	SO4	A	306	5/5	0.92	0.38	62,63,67,82	0
5	SO4	H	306	5/5	0.93	0.30	38,52,60,60	0
5	SO4	A	307	5/5	0.93	0.35	55,61,70,71	0
5	SO4	C	1201	5/5	0.95	0.21	46,50,57,60	0
5	SO4	H	304	5/5	0.95	0.13	39,53,64,69	0
5	SO4	L	301	5/5	0.96	0.19	50,55,59,62	0
5	SO4	B	302	5/5	0.97	0.24	54,58,62,63	0
5	SO4	A	302	5/5	0.97	0.16	39,48,59,60	0
5	SO4	B	301	5/5	0.97	0.13	50,55,61,65	0
5	SO4	H	301	5/5	0.98	0.20	44,45,51,55	0
5	SO4	A	301	5/5	0.98	0.13	33,41,49,56	0
5	SO4	L	302	5/5	0.98	0.09	28,30,36,39	0
5	SO4	H	302	5/5	0.98	0.18	50,59,61,61	0
5	SO4	H	303	5/5	0.99	0.12	34,42,47,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.