



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:12 PM BST

PDB ID : 5YD3  
Title : Crystal structure of the scFv antibody 4B08 with epitope peptide  
Authors : Caaveiro, J.M.M.; Miyanabe, K.; Tsumoto, K.  
Deposited on : 2017-09-11  
Resolution : 1.35 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

<https://www.wwpdb.org/validation/2017/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:

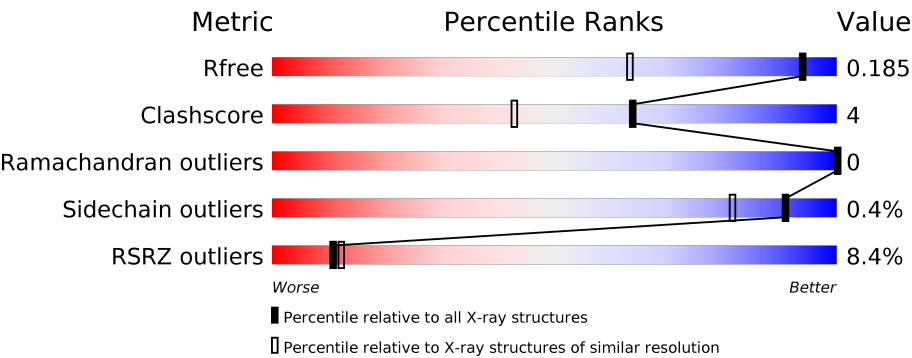
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

# 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 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 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	251	<div><div>2%</div><div><div></div><div>88%</div><div></div><div>8%</div></div><div></div></div>
1	C	251	<div><div>2%</div><div><div></div><div>84%</div><div>7%</div><div>9%</div></div><div></div></div>
1	E	251	<div><div>2%</div><div><div></div><div>88%</div><div></div><div>8%</div></div><div></div></div>
1	G	251	<div><div>23%</div><div><div></div><div>75%</div><div>13%</div><div>10%</div></div><div></div></div>
2	B	9	<div><div></div><div><div></div><div>89%</div><div></div><div>11%</div></div><div></div></div>
2	D	9	<div><div>11%</div><div><div></div><div>89%</div><div></div><div>11%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	9	<div><div></div><div>33%</div><div></div><div>100%</div></div>
2	H	9	<div><div></div><div>44%</div><div></div><div>44%</div><div></div><div>33%</div><div></div><div>22%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8826 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 scFv 4B08.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	12	0
			1854	1172	312	360	10			
1	C	229	Total	C	N	O	S	0	10	0
			1842	1168	309	356	9			
1	E	230	Total	C	N	O	S	0	9	0
			1833	1164	306	354	9			
1	G	226	Total	C	N	O	S	0	35	0
			2025	1294	332	387	12			

- Molecule 2 is a protein called Epitope peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			70	45	9	16			
2	D	8	Total	C	N	O	0	0	0
			70	45	9	16			
2	F	9	Total	C	N	O	0	0	0
			78	49	10	19			
2	H	7	Total	C	N	O	0	5	0
			104	65	13	26			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	1
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is water.

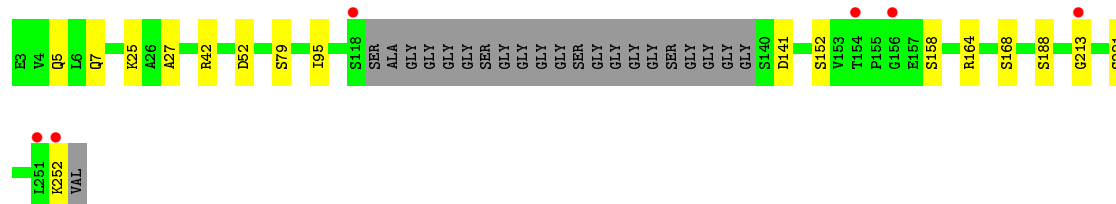
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total	O	0	7
			231	231		
5	B	13	Total	O	0	0
			13	13		
5	C	223	Total	O	0	8
			229	229		
5	D	11	Total	O	0	0
			11	11		
5	E	236	Total	O	0	7
			241	241		
5	F	19	Total	O	0	1
			20	20		
5	G	139	Total	O	0	6
			143	143		

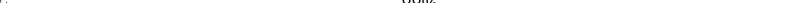


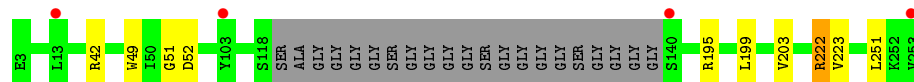
- Molecule 1: scFv 4B08



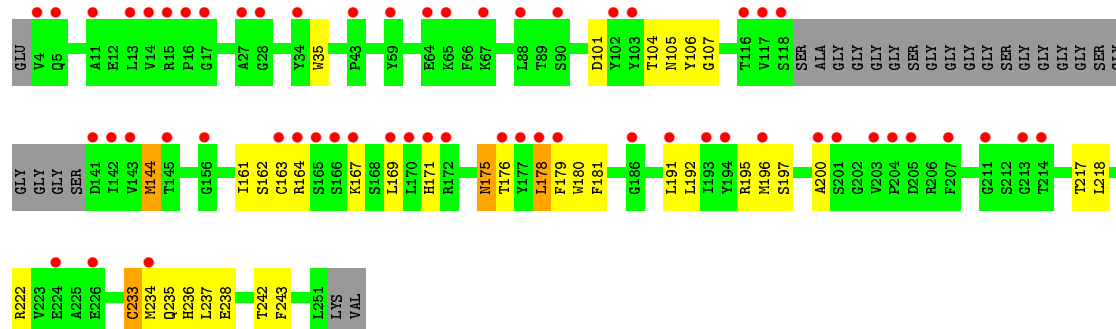
- Chain C:  2% 84% 7% 9%




- Chain E:  2% 88% 8%




- Chain G:  23% 75% 13% 10%



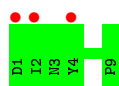
## ● Molecule 2: Epitope peptide

Chain B:  89% 11%


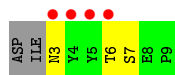
## ● Molecule 2: Epitope peptide

Chain D:  11% 89% 11%

## ● Molecule 2: Epitope peptide

Chain F:  33% 100%

## ● Molecule 2: Epitope peptide

Chain H:  44% 44% 33% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.48Å 72.97Å 86.99Å 90.00° 114.30° 90.00°	Depositor
Resolution (Å)	33.10 – 1.35 33.14 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.3 (33.10-1.35) 96.3 (33.14-1.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.136 , 0.184 0.136 , 0.185	Depositor DCC
$R_{free}$ test set	1868 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.10 % 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 4.5130e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, 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	0.75	1/1932 (0.1%)	0.89	3/2614 (0.1%)
1	C	0.78	2/1915 (0.1%)	0.90	3/2594 (0.1%)
1	E	0.71	0/1902	0.87	4/2577 (0.2%)
1	G	0.77	1/2100 (0.0%)	0.94	4/2852 (0.1%)
2	B	0.78	0/72	0.69	0/97
2	D	0.79	0/72	0.70	0/97
2	F	0.70	0/80	0.79	0/108
2	H	0.74	0/107	0.61	0/143
All	All	0.75	4/8180 (0.0%)	0.90	14/11082 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	233	CYS	CB-SG	-7.58	1.69	1.82
1	A	238	GLU	CD-OE2	-5.83	1.19	1.25
1	C	188[A]	SER	CB-OG	5.04	1.48	1.42
1	C	188[B]	SER	CB-OG	5.04	1.48	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	144	MET	CG-SD-CE	11.05	117.88	100.20
1	A	52	ASP	CB-CG-OD2	-9.14	110.08	118.30
1	E	52	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	E	222	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	52	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	52	ASP	CB-CG-OD1	5.68	123.42	118.30
1	A	141	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	52	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	E	222	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	195	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	G	233	CYS	O-C-N	5.26	131.12	122.70
1	G	106[A]	TYR	N-CA-C	-5.24	96.85	111.00
1	G	106[B]	TYR	N-CA-C	-5.24	96.85	111.00
1	C	141	ASP	CB-CG-OD2	-5.15	113.67	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1854	0	1803	5	0
1	C	1842	0	1789	11	0
1	E	1833	0	1789	6	0
1	G	2025	0	1930	45	0
2	B	70	0	59	0	0
2	D	70	0	59	0	0
2	F	78	0	66	0	0
2	H	104	0	82	3	0
3	A	20	0	0	0	0
3	C	5	0	0	0	0
3	E	20	0	0	0	0
3	G	5	0	0	0	0
4	A	12	0	16	1	0
5	A	231	0	0	0	0
5	B	13	0	0	0	0
5	C	229	0	0	3	0
5	D	11	0	0	0	0
5	E	241	0	0	2	0
5	F	20	0	0	0	0
5	G	143	0	0	2	0
All	All	8826	0	7593	65	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 4.

All (65) 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:G:171:HIS:HB2	1:G:237[A]:LEU:HD11	1.30	1.12
1:G:144:MET:HE1	1:G:169:LEU:HD11	1.12	1.11
1:G:180[A]:TRP:CE2	1:G:218:LEU:HB2	2.13	0.84
1:G:144:MET:HE1	1:G:169:LEU:CD1	2.06	0.76
1:G:144:MET:CE	1:G:169:LEU:HD11	2.07	0.75
1:G:171:HIS:CB	1:G:237[A]:LEU:HD11	2.16	0.71
2:H:3:ASN:HD22	2:H:6[A]:THR:HG22	1.56	0.70
1:G:234[A]:MET:HA	1:G:242[A]:THR:O	1.92	0.69
1:G:233:CYS:O	1:G:243[A]:PHE:HA	1.94	0.68
1:G:235[B]:GLN:HE22	1:G:238[B]:GLU:H	1.43	0.66
1:G:162[B]:SER:HA	1:G:217:THR:HA	1.80	0.64
1:G:178[A]:LEU:HB3	1:G:196[A]:MET:HA	1.80	0.63
1:G:180[A]:TRP:O	1:G:192:LEU:N	2.33	0.61
1:G:169:LEU:HD13	1:G:235[A]:GLN:HB3	1.81	0.61
1:G:171:HIS:HB2	1:G:237[A]:LEU:CD1	2.20	0.60
1:G:167:LYS:HE2	1:G:238[B]:GLU:OE2	2.03	0.59
1:G:178[A]:LEU:HD22	1:G:235[A]:GLN:HA	1.84	0.59
1:G:235[B]:GLN:NE2	1:G:237[B]:LEU:H	2.01	0.58
1:E:42:ARG:HD2	5:E:437:HOH:O	2.03	0.58
1:G:161[B]:ILE:O	1:G:218:LEU:N	2.35	0.57
1:G:180[A]:TRP:CD2	1:G:218:LEU:HB2	2.40	0.57
1:C:252:LYS:HE2	5:C:418:HOH:O	2.03	0.57
2:H:3:ASN:ND2	2:H:6[A]:THR:HG22	2.18	0.57
1:G:235[B]:GLN:HE21	1:G:237[B]:LEU:H	1.53	0.57
1:G:101[A]:ASP:OD2	1:G:104[A]:THR:N	2.34	0.56
1:G:105[A]:ASN:O	1:G:107[A]:GLY:N	2.40	0.55
1:G:169:LEU:O	1:G:237[A]:LEU:HD22	2.06	0.55
1:G:234[A]:MET:SD	1:G:235[A]:GLN:O	2.65	0.54
1:G:164:ARG:NH1	5:G:401:HOH:O	2.40	0.54
1:C:95:ILE:HD11	1:E:222:ARG:NH1	2.23	0.54
1:G:178[A]:LEU:HD21	1:G:235[A]:GLN:HB3	1.90	0.53
1:G:163[B]:CYS:HB3	1:G:180[B]:TRP:CZ2	2.45	0.51
1:G:175:ASN:ND2	5:G:404:HOH:O	2.44	0.50
1:A:62:TYR:CE2	4:A:305[B]:GOL:H12	2.48	0.49
1:G:175:ASN:OD1	1:G:195[B]:ARG:NE	2.45	0.49
1:G:35:TRP:CG	2:H:7[A]:SER:HB3	2.48	0.49
1:C:25:LYS:NZ	1:C:79[B]:SER:OG	2.46	0.48
1:E:223:VAL:HG12	1:E:251:LEU:HD21	1.95	0.48
1:G:236[A]:HIS:ND1	1:G:236[A]:HIS:O	2.46	0.47
1:A:93[A]:SER:HB3	1:G:222:ARG:HH22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234[A]:MET:HG3	1:G:243[A]:PHE:CE2	2.48	0.47
1:A:7:GLN:NE2	1:C:213:GLY:HA3	2.29	0.46
1:G:178[A]:LEU:HD22	1:G:178[A]:LEU:HA	1.47	0.46
1:G:163[B]:CYS:HB3	1:G:180[B]:TRP:CH2	2.49	0.46
1:C:152:SER:OG	1:C:252:LYS:HG3	2.16	0.45
1:G:196[B]:MET:SD	1:G:197:SER:HB3	2.57	0.45
1:C:164:ARG:NH1	5:C:405:HOH:O	2.46	0.44
1:G:180[A]:TRP:CG	1:G:218:LEU:HD13	2.52	0.44
1:C:5[B]:GLN:HE21	1:C:7:GLN:HE21	1.65	0.44
1:C:42[B]:ARG:HD2	5:C:447:HOH:O	2.16	0.44
1:E:42:ARG:NH1	5:E:405:HOH:O	2.51	0.44
1:A:219[B]:ARG:NH1	1:A:221[B]:SER:OG	2.51	0.44
1:G:176[A]:THR:O	1:G:178[A]:LEU:HB2	2.18	0.43
1:G:178[A]:LEU:CB	1:G:196[A]:MET:HA	2.48	0.43
1:A:7:GLN:NE2	1:C:168:SER:OG	2.52	0.43
1:G:105[A]:ASN:C	1:G:107[A]:GLY:N	2.72	0.43
1:G:181:PHE:HE1	1:G:234[A]:MET:HB3	1.83	0.42
1:G:191[A]:LEU:HG	1:G:200:ALA:CB	2.49	0.42
1:G:179[A]:PHE:HB2	1:G:234[A]:MET:HE3	2.01	0.42
1:G:163[B]:CYS:CB	1:G:180[B]:TRP:CH2	3.03	0.42
1:E:49:TRP:CH2	1:E:51:GLY:HA2	2.55	0.42
1:G:180[A]:TRP:CE3	1:G:218:LEU:HD22	2.54	0.41
1:E:199:LEU:HD11	1:E:203:VAL:HG12	2.03	0.41
1:C:158:SER:HB3	1:C:221:SER:O	2.21	0.41
1:C:5[A]:GLN:HB2	1:C:27:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/251 (95%)	237 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	235/251 (94%)	233 (99%)	2 (1%)	0	100	100
1	E	235/251 (94%)	232 (99%)	3 (1%)	0	100	100
1	G	253/251 (101%)	241 (95%)	12 (5%)	0	100	100
2	B	6/9 (67%)	6 (100%)	0	0	100	100
2	D	6/9 (67%)	6 (100%)	0	0	100	100
2	F	7/9 (78%)	7 (100%)	0	0	100	100
2	H	9/9 (100%)	9 (100%)	0	0	100	100
All	All	990/1040 (95%)	971 (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	206/199 (104%)	205 (100%)	1 (0%)	88	74
1	C	204/199 (102%)	204 (100%)	0	100	100
1	E	204/199 (102%)	204 (100%)	0	100	100
1	G	222/199 (112%)	219 (99%)	3 (1%)	67	36
2	B	8/9 (89%)	8 (100%)	0	100	100
2	D	8/9 (89%)	8 (100%)	0	100	100
2	F	9/9 (100%)	9 (100%)	0	100	100
2	H	12/9 (133%)	12 (100%)	0	100	100
All	All	873/832 (105%)	869 (100%)	4 (0%)	91	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	GLU
1	G	175	ASN

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Mol	Chain	Res	Type
1	G	178[A]	LEU
1	G	178[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	GLN
1	C	198	ASN
1	G	5	GLN
1	G	7	GLN
1	G	198	ASN
2	H	3	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 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	E	304	-	4,4,4	0.39	0	6,6,6	0.66	0
3	SO4	E	303	-	4,4,4	0.49	0	6,6,6	0.55	0
3	SO4	C	301	-	4,4,4	0.38	0	6,6,6	0.94	0
3	SO4	E	301	-	4,4,4	0.61	0	6,6,6	0.69	0
4	GOL	A	305[B]	-	5,5,5	0.32	0	5,5,5	0.80	0
4	GOL	A	305[A]	-	5,5,5	0.38	0	5,5,5	0.49	0
3	SO4	A	301	-	4,4,4	0.43	0	6,6,6	0.49	0
3	SO4	E	302	-	4,4,4	0.45	0	6,6,6	0.49	0
3	SO4	G	301	-	4,4,4	0.52	0	6,6,6	0.46	0
3	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.52	0
3	SO4	A	302[B]	-	4,4,4	0.26	0	6,6,6	0.31	0
3	SO4	A	304	-	4,4,4	0.94	0	6,6,6	0.41	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
4	GOL	A	305[B]	-	-	0/4/4/4	-
4	GOL	A	305[A]	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305[A]	GOL	C1-C2-C3-O3
4	A	305[A]	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305[B]	GOL	1	0



## 5.7 Other polymers

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, 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	A	231/251 (92%)	0.14	4 (1%) 70 74	6, 9, 23, 41	0
1	C	229/251 (91%)	0.24	6 (2%) 56 62	5, 9, 24, 42	0
1	E	230/251 (91%)	0.22	4 (1%) 70 74	8, 13, 26, 44	0
1	G	226/251 (90%)	1.29	58 (25%) 0 0	10, 21, 36, 46	3 (1%)
2	B	8/9 (88%)	0.38	0 100 100	8, 11, 24, 30	0
2	D	8/9 (88%)	0.85	1 (12%) 3 4	7, 10, 21, 39	0
2	F	9/9 (100%)	2.09	3 (33%) 0 0	11, 13, 27, 50	0
2	H	7/9 (77%)	3.95	4 (57%) 0 0	14, 17, 47, 51	0
All	All	948/1040 (91%)	0.52	80 (8%) 11 12	5, 13, 30, 51	3 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	5[A]	TYR	11.1
2	H	4	TYR	7.9
1	G	193[B]	ILE	7.7
2	F	2	ILE	7.4
1	G	14	VAL	6.7
1	G	117	VAL	6.3
1	G	194[B]	TYR	6.1
1	G	203	VAL	6.1
1	G	213	GLY	5.7
1	G	13	LEU	5.7
2	F	1	ASP	5.6
1	G	27	ALA	5.2
1	C	251	LEU	5.1
1	G	205	ASP	5.0
1	G	143	VAL	4.9
1	G	171	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	253	VAL	4.4
2	D	2	ILE	4.3
1	G	59	TYR	4.2
1	G	166	SER	4.1
1	G	169	LEU	4.0
1	G	172	ARG	3.9
1	G	214	THR	3.8
1	G	43	PRO	3.7
1	G	178[A]	LEU	3.7
1	G	118	SER	3.7
1	G	176[A]	THR	3.5
1	G	177[A]	TYR	3.5
1	G	141[A]	ASP	3.5
1	G	163[A]	CYS	3.2
1	G	142	ILE	3.2
1	E	140	SER	3.1
1	G	170	LEU	3.1
2	F	4	TYR	3.1
1	G	64	GLU	3.0
1	G	28	GLY	2.8
1	G	156	GLY	2.8
1	G	4	VAL	2.8
1	E	103	TYR	2.7
1	G	65	LYS	2.7
1	A	139	GLY	2.7
1	C	252	LYS	2.7
1	C	156	GLY	2.6
1	G	201	SER	2.6
1	G	17	GLY	2.6
1	G	103[A]	TYR	2.6
1	G	226	GLU	2.6
1	G	90	SER	2.6
1	G	186	GLY	2.5
1	G	164	ARG	2.5
1	C	154	THR	2.5
1	G	67	LYS	2.5
1	G	179[A]	PHE	2.5
1	G	200	ALA	2.5
2	H	6[A]	THR	2.4
2	H	3	ASN	2.4
1	G	11	ALA	2.4
1	G	167	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	13	LEU	2.4
1	G	204	PRO	2.3
1	G	88	LEU	2.3
1	G	191[A]	LEU	2.3
1	C	213	GLY	2.3
1	G	16	PRO	2.3
1	G	116	THR	2.3
1	G	34	TYR	2.3
1	G	207	PHE	2.3
1	G	5	GLN	2.2
1	C	118	SER	2.2
1	G	165	SER	2.2
1	G	145	THR	2.1
1	A	138	GLY	2.1
1	G	211	GLY	2.1
1	A	178	LEU	2.1
1	A	118	SER	2.1
1	G	196[A]	MET	2.1
1	G	234[A]	MET	2.1
1	G	102[A]	TYR	2.1
1	G	224	GLU	2.1
1	G	15	ARG	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 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	302[B]	5/5	0.86	0.13	25,30,32,35	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	304	5/5	0.88	0.23	29,30,32,36	0
4	GOL	A	305[B]	6/6	0.90	0.28	15,22,26,28	6
4	GOL	A	305[A]	6/6	0.90	0.28	14,29,32,33	6
3	SO4	E	301	5/5	0.93	0.16	15,16,19,23	5
3	SO4	E	304	5/5	0.94	0.13	27,31,36,38	5
3	SO4	G	301	5/5	0.94	0.23	35,36,47,60	0
3	SO4	E	303	5/5	0.97	0.22	24,29,34,36	0
3	SO4	A	301	5/5	0.97	0.27	34,37,50,59	0
3	SO4	E	302	5/5	0.97	0.13	26,28,30,33	0
3	SO4	C	301	5/5	0.98	0.11	19,23,29,35	0
3	SO4	A	303	5/5	0.98	0.13	19,25,36,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.