



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:37 PM UTC

PDB ID : 3UC0 / pdb\_00003uc0  
Title : Crystal structure of domain I of the envelope glycoprotein ectodomain from dengue virus serotype 4 in complex with the fab fragment of the chimpanzee monoclonal antibody 5H2  
Authors : Cockburn, J.J.B.; Stura, E.A.; Navarro-Sanchez, M.E.; Rey, F.A.  
Deposited on : 2011-10-25  
Resolution : 2.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

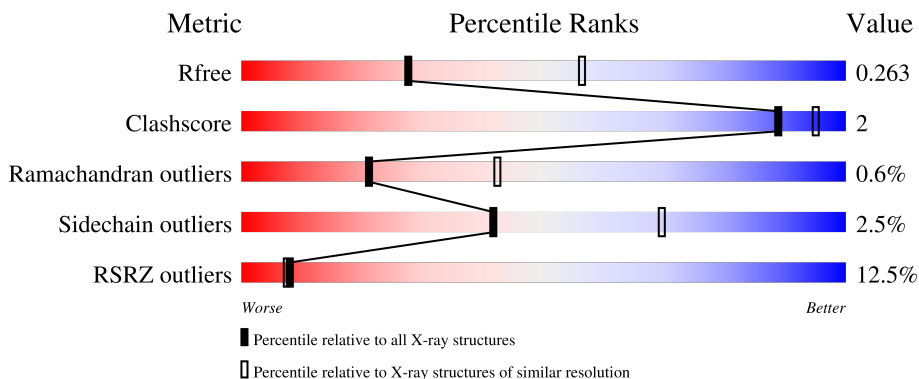
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



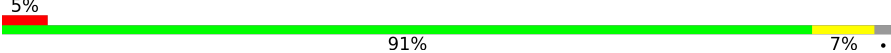
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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  $\geq 3$ , 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	165	
1	B	165	
2	H	236	
2	I	236	
3	L	215	

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Mol	Chain	Length	Quality of chain
3	M	215	 5% 91% 7%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8529 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 envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	111	822	515	142	157	8	0	0	0
1	B	116	843	528	144	163	8	0	0	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	linker	UNP Q91AI1
A	134	GLY	-	linker	UNP Q91AI1
A	191	THR	-	linker	UNP Q91AI1
A	299	PRO	-	expression tag	UNP Q91AI1
A	300	PHE	-	expression tag	UNP Q91AI1
A	301	GLU	-	expression tag	UNP Q91AI1
A	302	ASP	-	expression tag	UNP Q91AI1
A	303	ASP	-	expression tag	UNP Q91AI1
A	304	ASP	-	expression tag	UNP Q91AI1
A	305	ASP	-	expression tag	UNP Q91AI1
A	306	LYS	-	expression tag	UNP Q91AI1
A	307	ALA	-	expression tag	UNP Q91AI1
A	308	GLY	-	expression tag	UNP Q91AI1
A	309	TRP	-	expression tag	UNP Q91AI1
A	310	SER	-	expression tag	UNP Q91AI1
A	311	HIS	-	expression tag	UNP Q91AI1
A	312	PRO	-	expression tag	UNP Q91AI1
A	313	GLN	-	expression tag	UNP Q91AI1
A	314	PHE	-	expression tag	UNP Q91AI1
A	315	GLU	-	expression tag	UNP Q91AI1
A	316	LYS	-	expression tag	UNP Q91AI1
A	317	GLY	-	expression tag	UNP Q91AI1
A	318	GLY	-	expression tag	UNP Q91AI1
A	319	GLY	-	expression tag	UNP Q91AI1
A	320	SER	-	expression tag	UNP Q91AI1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	321	GLY	-	expression tag	UNP Q91AI1
A	322	GLY	-	expression tag	UNP Q91AI1
A	323	GLY	-	expression tag	UNP Q91AI1
A	324	SER	-	expression tag	UNP Q91AI1
A	325	GLY	-	expression tag	UNP Q91AI1
A	326	GLY	-	expression tag	UNP Q91AI1
A	327	GLY	-	expression tag	UNP Q91AI1
A	328	SER	-	expression tag	UNP Q91AI1
A	329	TRP	-	expression tag	UNP Q91AI1
A	330	SER	-	expression tag	UNP Q91AI1
A	331	HIS	-	expression tag	UNP Q91AI1
A	332	PRO	-	expression tag	UNP Q91AI1
A	333	GLN	-	expression tag	UNP Q91AI1
A	334	PHE	-	expression tag	UNP Q91AI1
A	335	GLU	-	expression tag	UNP Q91AI1
A	336	LYS	-	expression tag	UNP Q91AI1
B	51	GLY	-	linker	UNP Q91AI1
B	134	GLY	-	linker	UNP Q91AI1
B	191	THR	-	linker	UNP Q91AI1
B	299	PRO	-	expression tag	UNP Q91AI1
B	300	PHE	-	expression tag	UNP Q91AI1
B	301	GLU	-	expression tag	UNP Q91AI1
B	302	ASP	-	expression tag	UNP Q91AI1
B	303	ASP	-	expression tag	UNP Q91AI1
B	304	ASP	-	expression tag	UNP Q91AI1
B	305	ASP	-	expression tag	UNP Q91AI1
B	306	LYS	-	expression tag	UNP Q91AI1
B	307	ALA	-	expression tag	UNP Q91AI1
B	308	GLY	-	expression tag	UNP Q91AI1
B	309	TRP	-	expression tag	UNP Q91AI1
B	310	SER	-	expression tag	UNP Q91AI1
B	311	HIS	-	expression tag	UNP Q91AI1
B	312	PRO	-	expression tag	UNP Q91AI1
B	313	GLN	-	expression tag	UNP Q91AI1
B	314	PHE	-	expression tag	UNP Q91AI1
B	315	GLU	-	expression tag	UNP Q91AI1
B	316	LYS	-	expression tag	UNP Q91AI1
B	317	GLY	-	expression tag	UNP Q91AI1
B	318	GLY	-	expression tag	UNP Q91AI1
B	319	GLY	-	expression tag	UNP Q91AI1
B	320	SER	-	expression tag	UNP Q91AI1
B	321	GLY	-	expression tag	UNP Q91AI1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	322	GLY	-	expression tag	UNP Q91AI1
B	323	GLY	-	expression tag	UNP Q91AI1
B	324	SER	-	expression tag	UNP Q91AI1
B	325	GLY	-	expression tag	UNP Q91AI1
B	326	GLY	-	expression tag	UNP Q91AI1
B	327	GLY	-	expression tag	UNP Q91AI1
B	328	SER	-	expression tag	UNP Q91AI1
B	329	TRP	-	expression tag	UNP Q91AI1
B	330	SER	-	expression tag	UNP Q91AI1
B	331	HIS	-	expression tag	UNP Q91AI1
B	332	PRO	-	expression tag	UNP Q91AI1
B	333	GLN	-	expression tag	UNP Q91AI1
B	334	PHE	-	expression tag	UNP Q91AI1
B	335	GLU	-	expression tag	UNP Q91AI1
B	336	LYS	-	expression tag	UNP Q91AI1

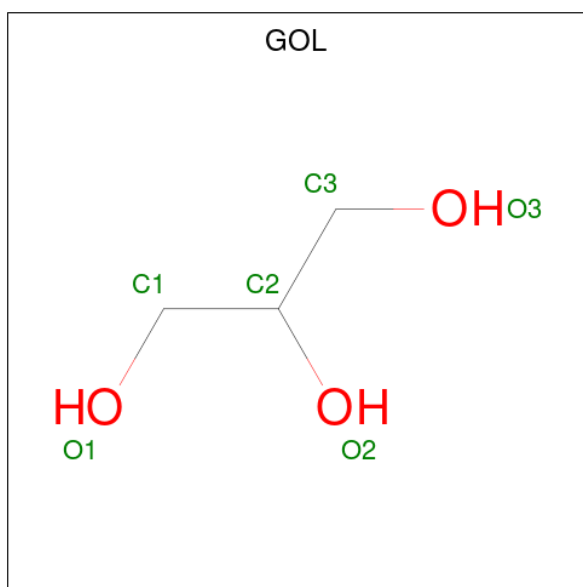
- Molecule 2 is a protein called Heavy chain, monoclonal antibody 5H2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	215	1603	1018	264	317	4	0	0	0
2	I	217	1619	1026	266	323	4	0	0	0

- Molecule 3 is a protein called Light chain, monoclonal antibody 5H2.

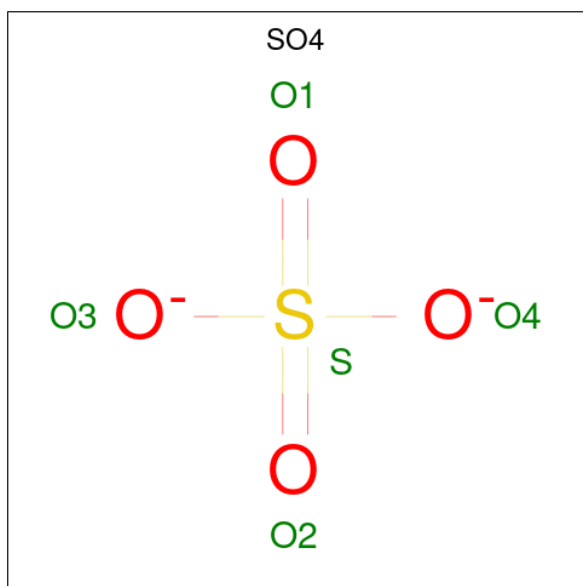
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	209	1607	1007	267	328	5	0	0	0
3	M	211	1626	1017	273	331	5	0	0	0

- Molecule 4 is GLYCEROL (CCD ID: 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	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

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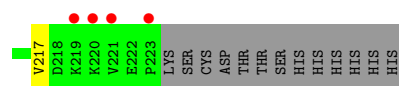
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		

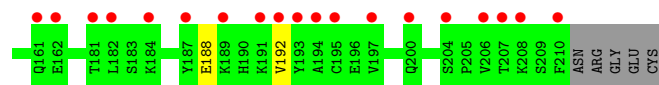
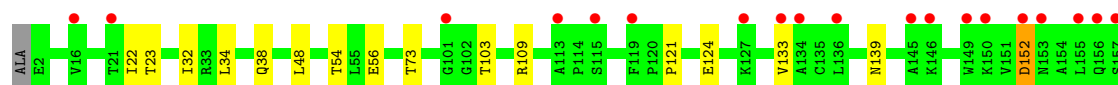
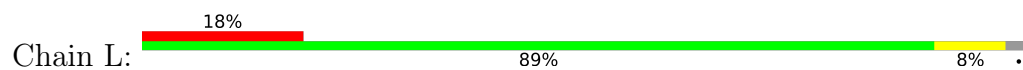
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	29	Total	O	0	0
			29	29		
6	H	58	Total	O	0	0
			58	58		
6	I	70	Total	O	0	0
			70	70		
6	L	52	Total	O	0	0
			52	52		
6	M	106	Total	O	0	0
			106	106		

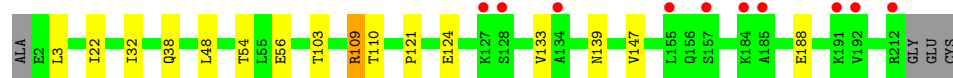
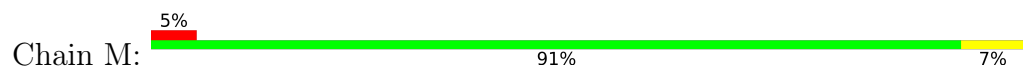




- Molecule 3: Light chain, monoclonal antibody 5H2



- Molecule 3: Light chain, monoclonal antibody 5H2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.94Å 113.86Å 169.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 2.71 46.17 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.17-2.71) 97.6 (46.17-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.73Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.9.3, BUSTER 2.9.3	Depositor
R, $R_{free}$	0.220 , 0.252 0.229 , 0.263	Depositor DCC
$R_{free}$ test set	2088 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtrriage
Anisotropy	0.492	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.18 % 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 9.2016e-03. 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: SO4, GOL

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	0.70	0/834	1.06	0/1127
1	B	0.71	0/856	1.07	0/1160
2	H	0.67	0/1641	1.10	1/2243 (0.0%)
2	I	0.67	0/1657	1.10	1/2264 (0.0%)
3	L	0.66	0/1641	1.05	0/2228
3	M	0.66	0/1660	1.04	0/2253
All	All	0.67	0/8289	1.07	2/11275 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	H	67	VAL	N-CA-C	5.88	117.47	108.71
2	I	67	VAL	N-CA-C	5.61	117.67	108.97

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	822	0	831	6	0
1	B	843	0	828	6	0
2	H	1603	0	1588	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1619	0	1602	4	0
3	L	1607	0	1561	5	0
3	M	1626	0	1580	5	0
4	A	6	0	8	0	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	H	10	0	0	0	0
5	I	5	0	0	0	0
5	M	30	0	0	0	0
6	A	28	0	0	0	0
6	B	29	0	0	0	0
6	H	58	0	0	0	0
6	I	70	0	0	0	0
6	L	52	0	0	0	0
6	M	106	0	0	0	0
All	All	8529	0	7998	30	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.

The worst 5 of 30 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:A:41:LEU:HD11	1:A:292:LEU:HD11	1.75	0.69
3:M:38:GLN:HB2	3:M:48:LEU:HD11	1.85	0.59
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.85	0.58
3:M:109:ARG:HG2	3:M:110:THR:N	2.17	0.58
3:M:22:ILE:HD12	3:M:103:THR:HG21	1.89	0.55

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/165 (65%)	102 (95%)	5 (5%)	0	100	100
1	B	112/165 (68%)	106 (95%)	6 (5%)	0	100	100
2	H	211/236 (89%)	203 (96%)	7 (3%)	1 (0%)	24	46
2	I	213/236 (90%)	205 (96%)	6 (3%)	2 (1%)	14	33
3	L	207/215 (96%)	197 (95%)	8 (4%)	2 (1%)	12	30
3	M	209/215 (97%)	199 (95%)	9 (4%)	1 (0%)	24	46
All	All	1059/1232 (86%)	1012 (96%)	41 (4%)	6 (1%)	21	42

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	42	GLY
2	I	42	GLY
3	L	139	ASN
3	M	139	ASN
3	L	152	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/132 (69%)	90 (99%)	1 (1%)	65	84
1	B	91/132 (69%)	91 (100%)	0	100	100
2	H	183/203 (90%)	180 (98%)	3 (2%)	55	78
2	I	186/203 (92%)	182 (98%)	4 (2%)	45	72
3	L	184/188 (98%)	177 (96%)	7 (4%)	29	56
3	M	186/188 (99%)	178 (96%)	8 (4%)	26	52
All	All	921/1046 (88%)	898 (98%)	23 (2%)	42	69

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	188	GLU

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Mol	Chain	Res	Type
3	M	54	THR
3	M	32	ILE
3	M	56	GLU
2	I	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	138	ASN
3	M	200	GLN
3	M	211	ASN
2	H	76	ASN
2	I	76	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 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
5	SO4	B	338	-	4,4,4	0.28	0	6,6,6	0.07	0
4	GOL	A	337	-	5,5,5	0.37	0	5,5,5	0.50	0
5	SO4	H	237	-	4,4,4	0.26	0	6,6,6	0.10	0
5	SO4	M	217	-	4,4,4	0.23	0	6,6,6	0.15	0
5	SO4	M	221	-	4,4,4	0.26	0	6,6,6	0.07	0
5	SO4	M	216	-	4,4,4	0.26	0	6,6,6	0.08	0
5	SO4	M	220	-	4,4,4	0.30	0	6,6,6	0.09	0
5	SO4	A	338	-	4,4,4	0.27	0	6,6,6	0.06	0
5	SO4	I	237	-	4,4,4	0.27	0	6,6,6	0.07	0
5	SO4	M	219	-	4,4,4	0.28	0	6,6,6	0.09	0
5	SO4	M	218	-	4,4,4	0.26	0	6,6,6	0.07	0
5	SO4	B	337	-	4,4,4	0.30	0	6,6,6	0.07	0
5	SO4	H	238	-	4,4,4	0.26	0	6,6,6	0.08	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	337	-	-	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	337	GOL	O1-C1-C2-C3
4	A	337	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	111/165 (67%)	0.93	15 (13%) 7 6	31, 55, 80, 98	0
1	B	116/165 (70%)	0.94	13 (11%) 10 9	31, 51, 90, 102	0
2	H	215/236 (91%)	0.96	35 (16%) 4 4	29, 57, 104, 120	0
2	I	217/236 (91%)	0.87	24 (11%) 10 9	30, 55, 94, 124	0
3	L	209/215 (97%)	1.08	38 (18%) 3 3	33, 63, 108, 132	0
3	M	211/215 (98%)	0.43	10 (4%) 36 33	27, 43, 79, 113	0
All	All	1079/1232 (87%)	0.86	135 (12%) 8 7	27, 54, 100, 132	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	THR	6.7
1	B	157	ASN	5.9
3	L	210	PHE	5.3
2	I	223	PRO	5.1
2	H	223	PRO	4.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	SO4	A	338	5/5	0.65	0.19	146,150,151,152	0
5	SO4	B	338	5/5	0.66	0.19	121,125,126,127	0
5	SO4	H	238	5/5	0.68	0.23	118,123,123,124	0
5	SO4	I	237	5/5	0.73	0.17	141,145,146,147	0
5	SO4	M	216	5/5	0.77	0.19	142,147,147,148	0
5	SO4	M	219	5/5	0.81	0.21	96,100,101,101	0
5	SO4	M	220	5/5	0.81	0.17	94,98,99,100	0
5	SO4	M	221	5/5	0.82	0.15	123,128,128,129	0
5	SO4	M	218	5/5	0.88	0.20	87,91,92,93	0
5	SO4	H	237	5/5	0.88	0.13	81,86,86,87	0
4	GOL	A	337	6/6	0.89	0.19	76,77,77,78	0
5	SO4	B	337	5/5	0.91	0.21	68,72,73,74	0
5	SO4	M	217	5/5	0.93	0.09	88,92,93,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.