



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2023 – 04:45 PM EDT

PDB ID : 3UC0
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 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 : 2.35
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) : 2.35

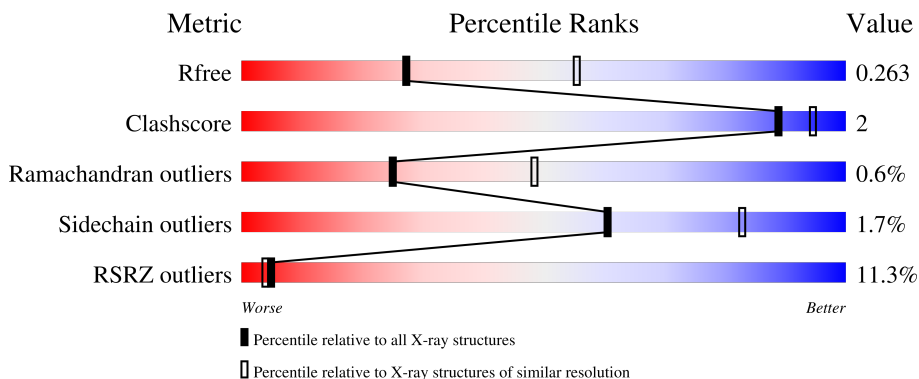
1 Overall quality at a glance

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.



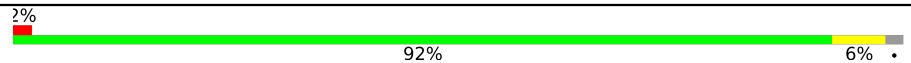
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 ≥ 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	 A horizontal bar chart representing the quality of chain. The bar is primarily green, indicating a high quality score of 92%. There is a small red segment at the beginning, labeled '2%', and a small yellow segment at the end, labeled '6%'. The total length of the bar is 100%.

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	M	216	-	-	-	X

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.

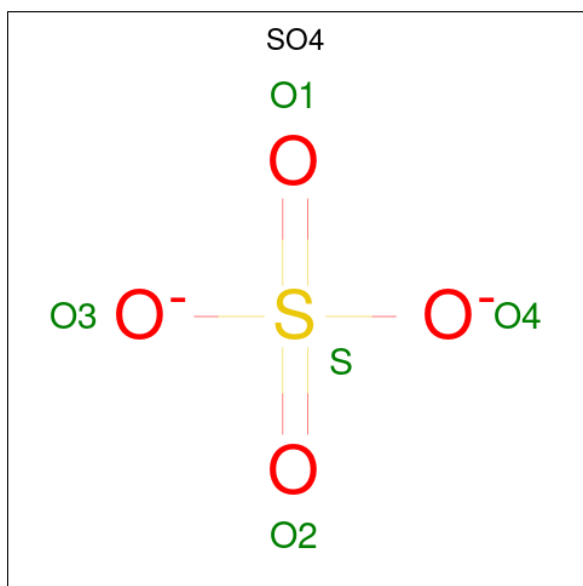
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	209	1607	1007	267	328	5	0	0	0
3	M	211	1626	1017	273	331	5	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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



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

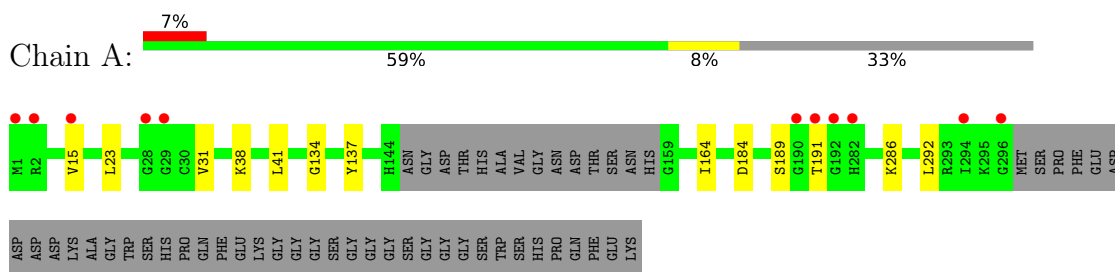
- Molecule 6 is water.

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

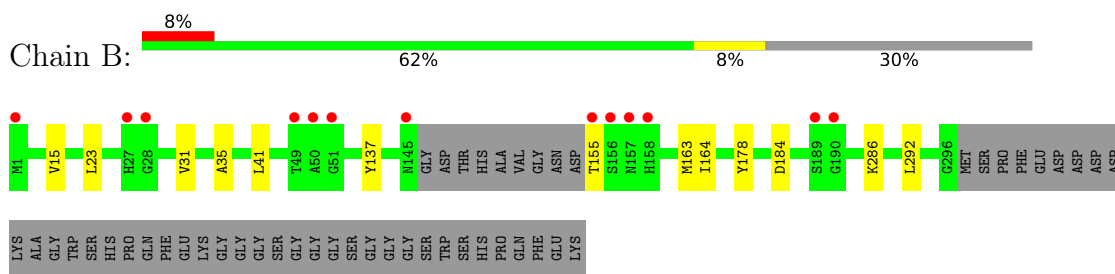
3 Residue-property plots [i](#)

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.

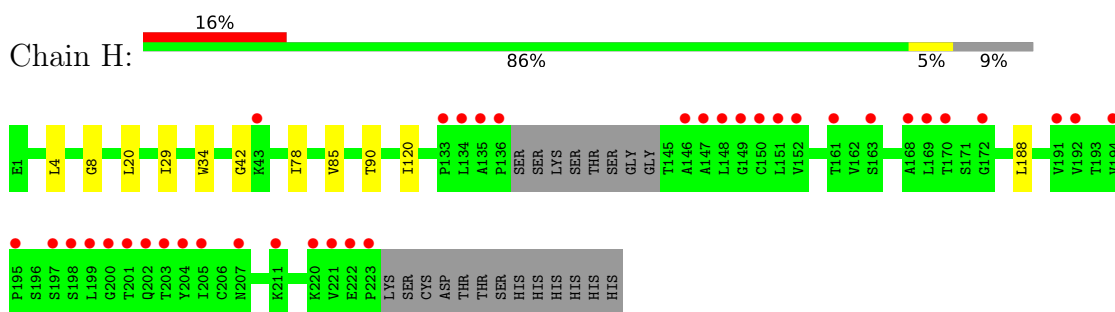
- Molecule 1: envelope protein



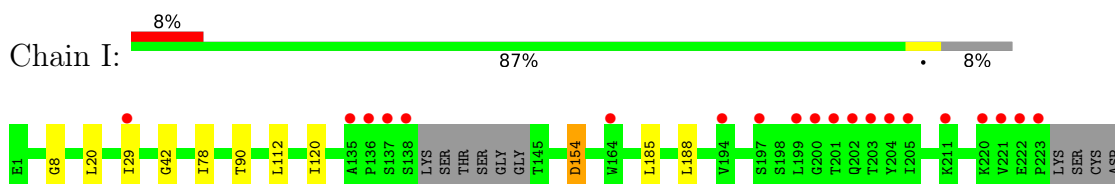
- Molecule 1: envelope protein



- Molecule 2: Heavy chain, monoclonal antibody 5H2

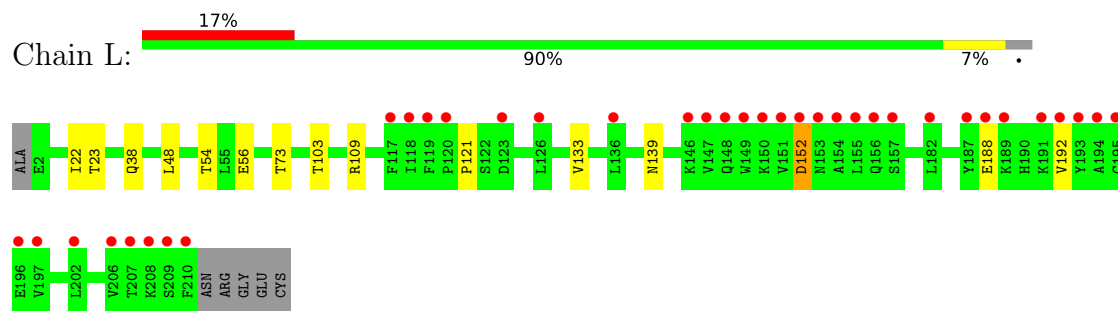


- Molecule 2: Heavy chain, monoclonal antibody 5H2

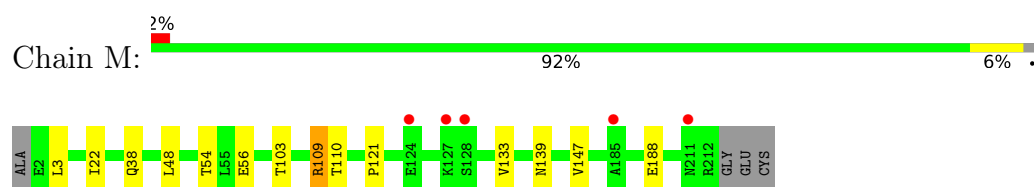


THR
THR
SER
HIS
HIS
HIS
HIS
HIS

- Molecule 3: Light chain, monoclonal antibody 5H2



- Molecule 3: Light chain, monoclonal antibody 5H2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.94Å 113.86Å 169.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 2.71 46.18 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.17-2.71) 97.6 (46.18-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	47.8	Xtrriage
Anisotropy	0.492	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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 [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	0.34	0/834	0.58	0/1127
1	B	0.35	0/856	0.58	0/1160
2	H	0.34	0/1641	0.59	0/2243
2	I	0.34	0/1657	0.58	0/2264
3	L	0.33	0/1641	0.57	0/2228
3	M	0.33	0/1660	0.57	0/2253
All	All	0.34	0/8289	0.58	0/11275

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	A	822	0	831	6	0
1	B	843	0	828	6	0
2	H	1603	0	1588	4	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:15:VAL:HG11	1:A:38:LYS:HG3	1.88	0.55
1:B:184:ASP:HB3	1:B:286:LYS:HB2	1.90	0.54
1:A:184:ASP:HB3	1:A:286:LYS:HB2	1.89	0.53
3:M:109:ARG:HG2	3:M:109:ARG:HH11	1.73	0.53
3:M:121:PRO:HD3	3:M:133:VAL:HG22	1.92	0.52
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.92	0.52
1:A:134:GLY:H	1:A:189:SER:HA	1.75	0.52
2:I:8:GLY:HA3	2:I:20:LEU:HD23	1.93	0.51
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.94	0.50
1:B:41:LEU:HD11	1:B:292:LEU:HD11	1.93	0.48
1:A:23:LEU:HD22	1:A:31:VAL:HG11	1.96	0.47
1:B:23:LEU:HD22	1:B:31:VAL:HG11	1.95	0.47
1:B:15:VAL:HG21	1:B:35:ALA:HB1	1.96	0.47
2:I:90:THR:HG23	2:I:120:ILE:HA	1.97	0.46
2:H:29:ILE:HD11	2:H:78:ILE:HG13	1.96	0.46
2:H:90:THR:HG23	2:H:120:ILE:HA	1.98	0.46
2:I:29:ILE:HD11	2:I:78:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HB2	1:A:164:ILE:HB	1.98	0.44
2:I:154:ASP:HB3	2:I:185:LEU:HD13	2.00	0.44
1:B:137:TYR:HB2	1:B:164:ILE:HB	2.00	0.43
2:H:4:LEU:HD21	2:H:34:TRP:CZ3	2.54	0.43
3:L:152:ASP:HA	3:L:192:VAL:HB	2.02	0.42
1:B:155:THR:HA	1:B:178:TYR:HE2	1.84	0.42
3:L:22:ILE:HD12	3:L:103:THR:HG21	2.00	0.42
3:L:23:THR:HG22	3:L:73:THR:HG22	2.02	0.41

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%)	29	53
2	I	213/236 (90%)	205 (96%)	6 (3%)	2 (1%)	17	38
3	L	207/215 (96%)	197 (95%)	8 (4%)	2 (1%)	15	35
3	M	209/215 (97%)	199 (95%)	9 (4%)	1 (0%)	29	53
All	All	1059/1232 (86%)	1012 (96%)	41 (4%)	6 (1%)	25	48

All (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

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Mol	Chain	Res	Type
3	L	152	ASP
2	I	154	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%)	73	89
1	B	91/132 (69%)	90 (99%)	1 (1%)	73	89
2	H	183/203 (90%)	181 (99%)	2 (1%)	73	89
2	I	186/203 (92%)	184 (99%)	2 (1%)	73	89
3	L	184/188 (98%)	180 (98%)	4 (2%)	52	78
3	M	186/188 (99%)	180 (97%)	6 (3%)	39	67
All	All	921/1046 (88%)	905 (98%)	16 (2%)	60	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	THR
1	B	163	MET
2	H	85	VAL
2	H	188	LEU
2	I	112	LEU
2	I	188	LEU
3	L	54	THR
3	L	56	GLU
3	L	109	ARG
3	L	188	GLU
3	M	3	LEU
3	M	54	THR
3	M	56	GLU
3	M	109	ARG
3	M	147	VAL
3	M	188	GLU

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

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 monosaccharides 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	M	219	-	4,4,4	0.17	0	6,6,6	0.06	0
5	SO4	M	217	-	4,4,4	0.13	0	6,6,6	0.12	0
5	SO4	I	237	-	4,4,4	0.16	0	6,6,6	0.05	0
4	GOL	A	337	-	5,5,5	0.36	0	5,5,5	0.48	0
5	SO4	M	220	-	4,4,4	0.19	0	6,6,6	0.07	0
5	SO4	H	238	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	M	216	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	B	338	-	4,4,4	0.16	0	6,6,6	0.05	0
5	SO4	M	221	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	B	337	-	4,4,4	0.18	0	6,6,6	0.04	0
5	SO4	H	237	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	M	218	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	338	-	4,4,4	0.16	0	6,6,6	0.04	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 [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, 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	111/165 (67%)	0.59	11 (9%) 7 6	31, 55, 80, 98	0
1	B	116/165 (70%)	0.66	13 (11%) 5 4	31, 51, 90, 102	0
2	H	215/236 (91%)	0.91	37 (17%) 1 1	29, 57, 104, 120	0
2	I	217/236 (91%)	0.72	20 (9%) 9 7	30, 55, 94, 124	0
3	L	209/215 (97%)	0.87	36 (17%) 1 1	33, 63, 108, 132	0
3	M	211/215 (98%)	0.24	5 (2%) 59 60	27, 43, 79, 113	0
All	All	1079/1232 (87%)	0.67	122 (11%) 5 4	27, 54, 100, 132	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	152	ASP	7.2
1	B	157	ASN	6.9
2	H	205	ILE	6.7
2	I	201	THR	6.0
2	H	220	LYS	5.6
3	L	153	ASN	5.5
2	H	200	GLY	5.4
2	H	223	PRO	5.4
2	H	135	ALA	5.1
2	H	221	VAL	5.1
2	I	223	PRO	4.8
3	L	210	PHE	4.8
2	H	204	TYR	4.6
1	B	50	ALA	4.6
3	L	119	PHE	4.6
3	L	192	VAL	4.6
2	H	197	SER	4.5
2	H	136	PRO	4.5
3	L	155	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	148	LEU	4.4
1	B	1	MET	4.4
2	H	168	ALA	4.3
3	L	123	ASP	4.2
2	H	149	GLY	4.2
2	I	199	LEU	4.2
2	I	200	GLY	4.2
3	L	197	VAL	4.1
2	H	201	THR	4.1
3	M	127	LYS	4.1
3	L	196	GLU	4.0
3	L	194	ALA	4.0
2	I	194	VAL	4.0
2	H	195	PRO	4.0
3	L	154	ALA	4.0
3	L	193	TYR	3.9
2	H	133	PRO	3.9
3	L	206	VAL	3.9
2	I	138	SER	3.9
3	L	151	VAL	3.9
1	A	1	MET	3.9
3	L	195	CYS	3.8
2	H	194	VAL	3.6
3	L	187	TYR	3.6
3	L	189	LYS	3.6
2	I	221	VAL	3.6
2	I	136	PRO	3.6
1	B	155	THR	3.5
3	L	182	LEU	3.5
2	H	222	GLU	3.5
2	H	146	ALA	3.4
2	I	220	LYS	3.4
1	B	156	SER	3.4
3	L	157	SER	3.3
3	L	202	LEU	3.3
3	M	185	ALA	3.3
3	L	191	LYS	3.2
2	H	199	LEU	3.2
3	L	149	TRP	3.2
3	L	148	GLN	3.2
2	H	202	GLN	3.1
3	L	147	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	L	209	SER	3.1
1	A	15	VAL	3.0
3	L	117	PHE	3.0
2	I	203	THR	3.0
1	A	28	GLY	2.9
2	H	134	LEU	2.9
1	B	158	HIS	2.9
2	I	135	ALA	2.9
3	L	120	PRO	2.9
1	B	27	HIS	2.8
3	L	208	LYS	2.8
2	H	192	VAL	2.8
2	I	222	GLU	2.8
1	A	296	GLY	2.8
3	L	136	LEU	2.7
1	A	2	ARG	2.7
2	H	163	SER	2.7
2	I	137	SER	2.7
2	H	147	ALA	2.6
1	B	28	GLY	2.6
2	I	164	TRP	2.5
3	M	211	ASN	2.5
2	H	203	THR	2.5
2	I	197	SER	2.5
2	I	204	TYR	2.5
1	A	192	GLY	2.4
1	B	189	SER	2.4
3	L	118	ILE	2.4
1	B	51	GLY	2.4
2	H	150	CYS	2.4
3	L	156	GLN	2.3
3	M	124	GLU	2.3
1	A	190	GLY	2.3
3	M	128	SER	2.3
1	A	294	ILE	2.3
2	H	151	LEU	2.3
1	A	191	THR	2.3
3	L	150	LYS	2.3
2	I	211	LYS	2.2
3	L	188	GLU	2.2
2	H	43	LYS	2.2
3	L	146	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	282	HIS	2.2
2	I	202	GLN	2.2
2	H	172	GLY	2.2
2	I	205	ILE	2.2
1	B	145	ASN	2.2
2	H	169	LEU	2.2
1	B	49	THR	2.2
2	H	198	SER	2.1
2	H	211	LYS	2.1
1	B	190	GLY	2.1
3	L	207	THR	2.1
1	A	29	GLY	2.1
2	H	170	THR	2.1
2	H	152	VAL	2.1
2	H	207	ASN	2.1
2	I	29	ILE	2.1
3	L	126	LEU	2.0
2	H	191	VAL	2.0
2	H	161	THR	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, 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(Å ²)	Q<0.9
5	SO4	M	216	5/5	0.69	0.46	142,147,147,148	0
5	SO4	B	338	5/5	0.72	0.32	121,125,126,127	0
5	SO4	H	238	5/5	0.75	0.26	118,123,123,124	0
5	SO4	I	237	5/5	0.83	0.26	141,145,146,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	M	219	5/5	0.86	0.26	96,100,101,101	0
5	SO4	A	338	5/5	0.90	0.20	146,150,151,152	0
4	GOL	A	337	6/6	0.91	0.20	76,77,77,78	0
5	SO4	M	218	5/5	0.92	0.18	87,91,92,93	0
5	SO4	M	221	5/5	0.92	0.16	123,128,128,129	0
5	SO4	B	337	5/5	0.93	0.22	68,72,73,74	0
5	SO4	H	237	5/5	0.93	0.23	81,86,86,87	0
5	SO4	M	220	5/5	0.94	0.21	94,98,99,100	0
5	SO4	M	217	5/5	0.97	0.17	88,92,93,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.