Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:38 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

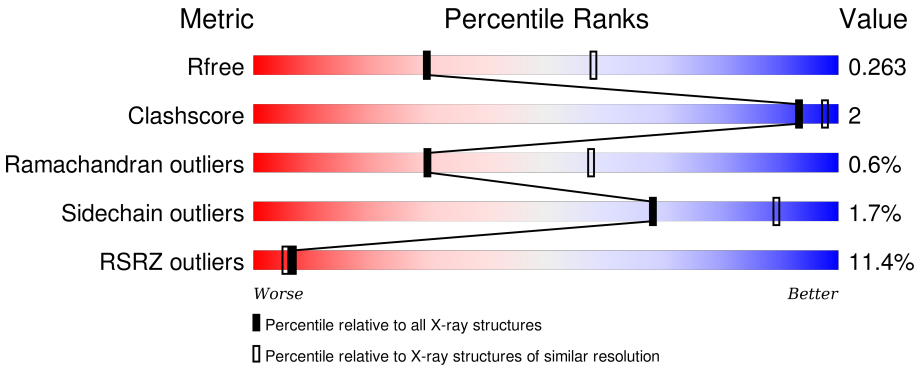
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.71 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}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7% 59% 8% 33%
1	B	165	8% 62% 8% 30%
2	H	236	16% 86% 5% 9%
2	I	236	8% 87% • 8%
3	L	215	17% 90% 7% •

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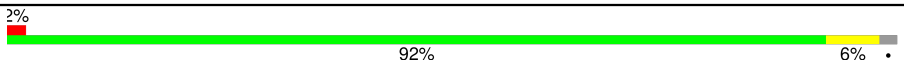
Mol	Chain	Length	Quality of chain
3	M	215	

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
1	A	111	Total	C	N	O	S	0	0	0
			822	515	142	157	8			
1	B	116	Total	C	N	O	S	0	0	0
			843	528	144	163	8			

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

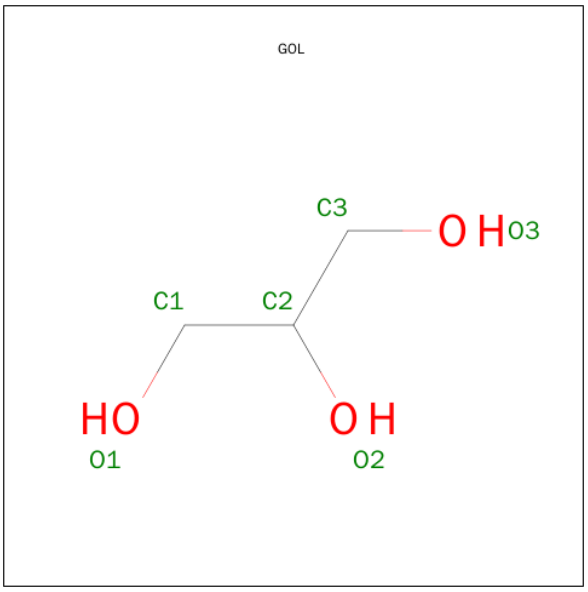
- Molecule 2 is a protein called Heavy chain, monoclonal antibody 5H2.

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

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

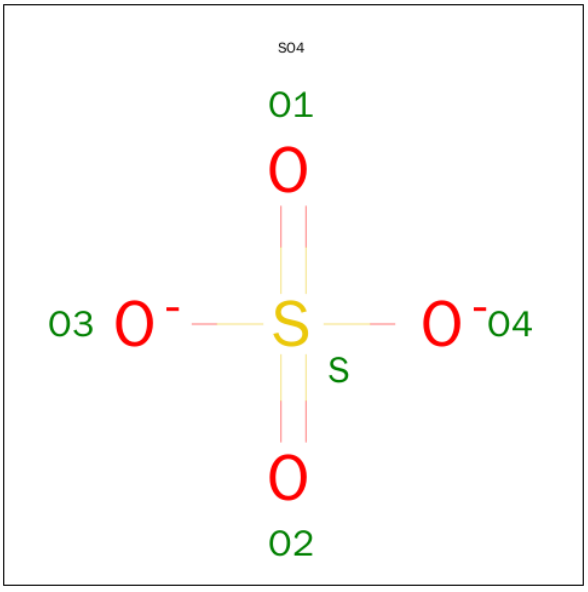
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1607	1007	267	328	5			
3	M	211	Total	C	N	O	S	0	0	0
			1626	1017	273	331	5			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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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.

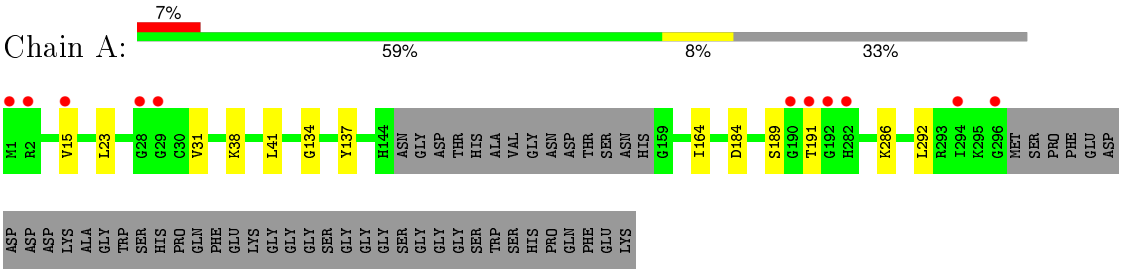
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	28	Total O 28 28	0	0
6	B	29	Total O 29 29	0	0
6	H	58	Total O 58 58	0	0
6	I	70	Total O 70 70	0	0
6	L	52	Total O 52 52	0	0
6	M	106	Total O 106 106	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

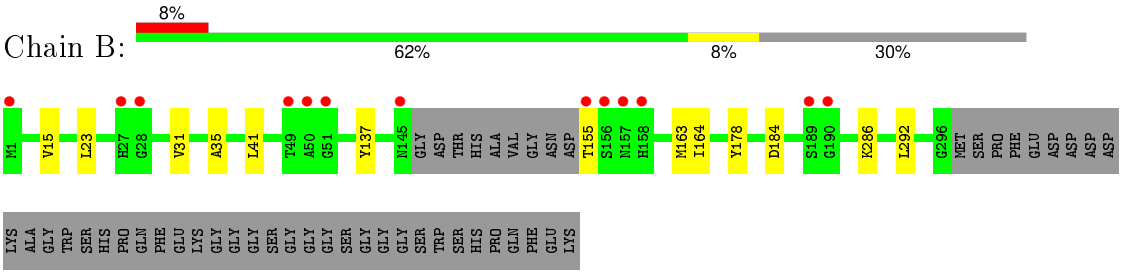
- Molecule 1: envelope protein

Chain A:



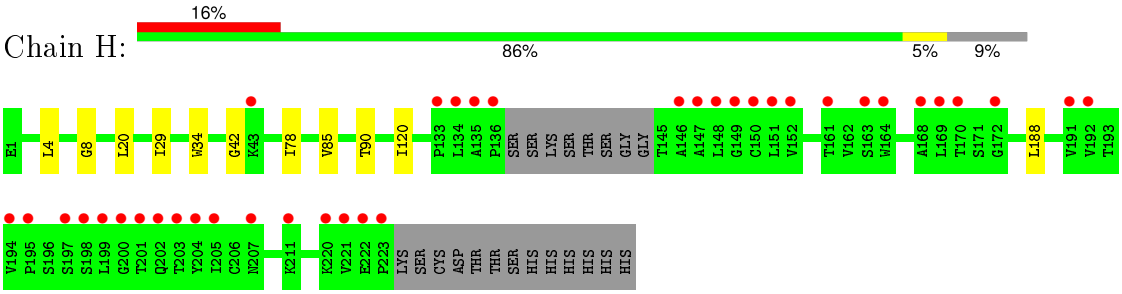
- Molecule 1: envelope protein

Chain B:



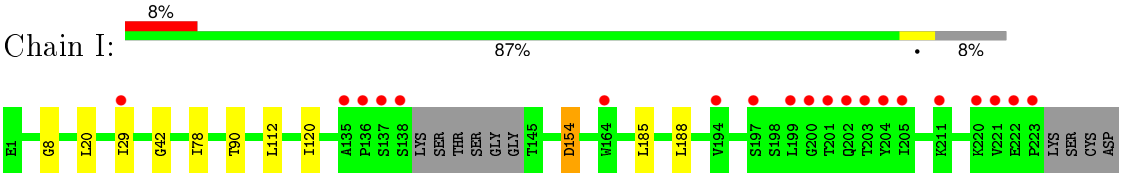
- Molecule 2: Heavy chain, monoclonal antibody 5H2

Chain H:

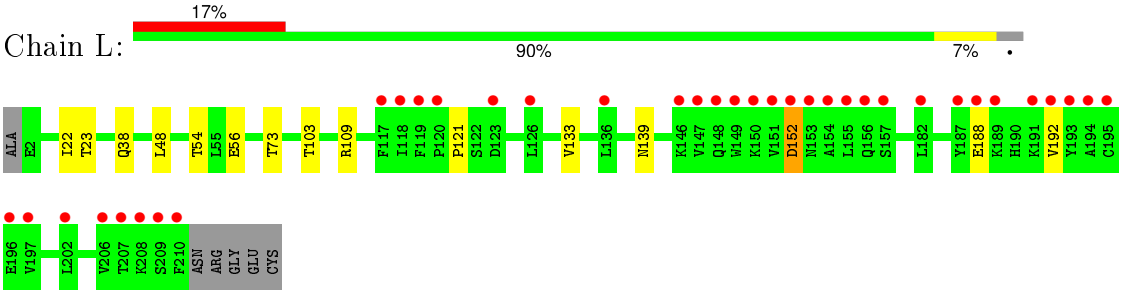


- Molecule 2: Heavy chain, monoclonal antibody 5H2

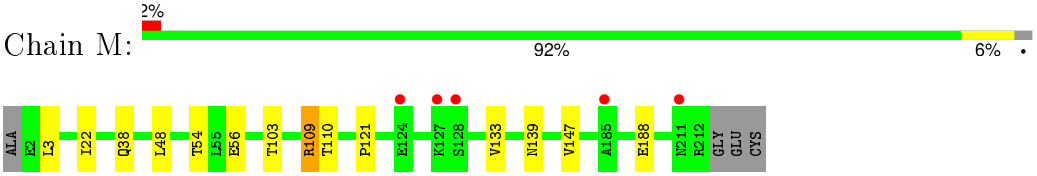
Chain I:



• 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
$< I/\sigma(I) >$ [1]	1.87 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.220 , 0.252 0.229 , 0.263	Depositor DCC
R_{free} test set	2088 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 41262 reflections	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.34	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

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
2:H:4:LEU:HD21	2:H:34:TRP:CZ3	2.54	0.43
1:B:137:TYR:HB2	1:B:164:ILE:HB	2.00	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%)	34	62
2	I	213/236 (90%)	205 (96%)	6 (3%)	2 (1%)	21	47
3	L	207/215 (96%)	197 (95%)	8 (4%)	2 (1%)	19	44
3	M	209/215 (97%)	199 (95%)	9 (4%)	1 (0%)	34	62
All	All	1059/1232 (86%)	1012 (96%)	41 (4%)	6 (1%)	30	58

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%)	80	94
1	B	91/132 (69%)	90 (99%)	1 (1%)	80	94
2	H	183/203 (90%)	181 (99%)	2 (1%)	80	94
2	I	186/203 (92%)	184 (99%)	2 (1%)	80	94
3	L	184/188 (98%)	180 (98%)	4 (2%)	60	86
3	M	186/188 (99%)	180 (97%)	6 (3%)	46	76
All	All	921/1046 (88%)	905 (98%)	16 (2%)	68	89

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

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

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 carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	GOL	A	337	-	5,5,5	0.31	0	5,5,5	0.50	0
5	SO4	A	338	-	4,4,4	0.11	0	6,6,6	0.07	0
5	SO4	B	337	-	4,4,4	0.07	0	6,6,6	0.08	0
5	SO4	B	338	-	4,4,4	0.09	0	6,6,6	0.08	0
5	SO4	H	237	-	4,4,4	0.05	0	6,6,6	0.11	0
5	SO4	H	238	-	4,4,4	0.06	0	6,6,6	0.09	0
5	SO4	I	237	-	4,4,4	0.09	0	6,6,6	0.08	0
5	SO4	M	216	-	4,4,4	0.10	0	6,6,6	0.09	0
5	SO4	M	217	-	4,4,4	0.19	0	6,6,6	0.15	0
5	SO4	M	218	-	4,4,4	0.08	0	6,6,6	0.08	0
5	SO4	M	219	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	M	220	-	4,4,4	0.12	0	6,6,6	0.08	0
5	SO4	M	221	-	4,4,4	0.12	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	-	-	0/4/4/4	0/0/0/0
5	SO4	A	338	-	-	0/0/0/0	0/0/0/0
5	SO4	B	337	-	-	0/0/0/0	0/0/0/0
5	SO4	B	338	-	-	0/0/0/0	0/0/0/0
5	SO4	H	237	-	-	0/0/0/0	0/0/0/0
5	SO4	H	238	-	-	0/0/0/0	0/0/0/0
5	SO4	I	237	-	-	0/0/0/0	0/0/0/0
5	SO4	M	216	-	-	0/0/0/0	0/0/0/0
5	SO4	M	217	-	-	0/0/0/0	0/0/0/0
5	SO4	M	218	-	-	0/0/0/0	0/0/0/0
5	SO4	M	219	-	-	0/0/0/0	0/0/0/0
5	SO4	M	220	-	-	0/0/0/0	0/0/0/0
5	SO4	M	221	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95^{th} 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%)	0.63	11 (9%) 9 7	31, 55, 80, 98	0
1	B	116/165 (70%)	0.71	13 (11%) 7 5	31, 51, 90, 102	0
2	H	215/236 (91%)	0.95	38 (17%) 2 1	29, 57, 104, 120	0
2	I	217/236 (91%)	0.76	20 (9%) 11 9	30, 55, 94, 124	0
3	L	209/215 (97%)	0.91	36 (17%) 2 1	33, 63, 108, 132	0
3	M	211/215 (98%)	0.28	5 (2%) 62 62	27, 43, 79, 113	0
All	All	1079/1232 (87%)	0.71	123 (11%) 7 5	27, 54, 100, 132	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	152	ASP	7.4
1	B	157	ASN	7.0
2	H	205	ILE	6.7
2	I	201	THR	6.1
2	H	220	LYS	5.8
3	L	153	ASN	5.6
2	H	200	GLY	5.5
2	H	223	PRO	5.5
2	H	135	ALA	5.2
2	H	221	VAL	5.2
2	I	223	PRO	4.9
3	L	210	PHE	4.9
2	H	204	TYR	4.7
1	B	50	ALA	4.7
3	L	119	PHE	4.6
3	L	192	VAL	4.6
2	H	197	SER	4.6
2	H	136	PRO	4.5
1	B	1	MET	4.5

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Mol	Chain	Res	Type	RSRZ
2	H	148	LEU	4.4
3	L	155	LEU	4.4
3	L	123	ASP	4.4
2	H	168	ALA	4.3
2	H	149	GLY	4.3
2	I	200	GLY	4.3
2	H	201	THR	4.2
3	L	197	VAL	4.2
2	I	199	LEU	4.2
3	M	127	LYS	4.2
3	L	196	GLU	4.1
3	L	194	ALA	4.1
2	I	194	VAL	4.1
1	A	1	MET	4.1
3	L	154	ALA	4.0
3	L	193	TYR	4.0
2	H	133	PRO	4.0
2	H	195	PRO	4.0
3	L	151	VAL	4.0
3	L	206	VAL	4.0
2	I	138	SER	4.0
3	L	195	CYS	3.9
3	L	187	TYR	3.7
2	H	194	VAL	3.7
3	L	189	LYS	3.7
2	I	221	VAL	3.6
1	B	155	THR	3.6
2	I	136	PRO	3.6
2	H	222	GLU	3.6
3	L	182	LEU	3.5
2	H	146	ALA	3.5
2	I	220	LYS	3.5
1	B	156	SER	3.4
3	L	157	SER	3.4
3	M	185	ALA	3.4
3	L	202	LEU	3.4
3	L	191	LYS	3.3
2	H	199	LEU	3.3
3	L	148	GLN	3.2
3	L	149	TRP	3.2
2	H	202	GLN	3.2
3	L	209	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	L	147	VAL	3.1
1	A	15	VAL	3.1
2	I	203	THR	3.1
3	L	117	PHE	3.1
1	A	28	GLY	3.0
1	B	158	HIS	2.9
2	H	134	LEU	2.9
2	I	135	ALA	2.9
3	L	120	PRO	2.9
3	L	208	LYS	2.9
2	I	222	GLU	2.9
1	B	27	HIS	2.8
2	H	192	VAL	2.8
1	A	296	GLY	2.8
1	A	2	ARG	2.8
3	L	136	LEU	2.8
2	H	163	SER	2.7
2	I	137	SER	2.7
2	H	147	ALA	2.7
1	B	28	GLY	2.7
2	I	164	TRP	2.6
3	M	211	ASN	2.6
2	H	203	THR	2.5
2	I	204	TYR	2.5
2	I	197	SER	2.5
1	A	192	GLY	2.5
1	B	51	GLY	2.4
1	B	189	SER	2.4
2	H	150	CYS	2.4
3	L	156	GLN	2.4
3	M	124	GLU	2.4
3	L	118	ILE	2.4
1	A	190	GLY	2.4
3	M	128	SER	2.4
1	A	294	ILE	2.3
3	L	150	LYS	2.3
1	A	191	THR	2.3
2	I	211	LYS	2.3
3	L	188	GLU	2.3
2	H	151	LEU	2.3
2	H	43	LYS	2.3
2	H	172	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	202	GLN	2.3
3	L	146	LYS	2.3
1	A	282	HIS	2.2
1	B	145	ASN	2.2
1	B	190	GLY	2.2
2	H	211	LYS	2.2
1	B	49	THR	2.2
2	I	205	ILE	2.2
3	L	207	THR	2.2
2	H	169	LEU	2.2
2	H	198	SER	2.2
1	A	29	GLY	2.2
2	H	170	THR	2.2
2	H	207	ASN	2.1
2	H	152	VAL	2.1
2	I	29	ILE	2.1
2	H	191	VAL	2.1
3	L	126	LEU	2.1
2	H	161	THR	2.1
2	H	164	TRP	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	M	216	5/5	0.69	0.46	15.29	142,147,147,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	H	238	5/5	0.75	0.26	1.86	118,123,123,124	0
5	SO4	M	219	5/5	0.86	0.26	1.66	96,100,101,101	0
5	SO4	M	220	5/5	0.94	0.21	1.17	94,98,99,100	0
5	SO4	I	237	5/5	0.83	0.25	0.68	141,145,146,147	0
5	SO4	B	337	5/5	0.93	0.22	0.09	68,72,73,74	0
4	GOL	A	337	6/6	0.91	0.20	0.05	76,77,77,78	0
5	SO4	M	218	5/5	0.92	0.18	0.02	87,91,92,93	0
5	SO4	M	221	5/5	0.92	0.16	-	123,128,128,129	0
5	SO4	A	338	5/5	0.90	0.19	-	146,150,151,152	0
5	SO4	H	237	5/5	0.93	0.23	-	81,86,86,87	0
5	SO4	M	217	5/5	0.97	0.17	-	88,92,93,94	0
5	SO4	B	338	5/5	0.72	0.32	-	121,125,126,127	0

6.5 Other polymers (i)

There are no such residues in this entry.