



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:14 pm GMT

PDB ID : 5T6L
Title : Crystal structure of 10E8 Fab in complex with the MPER epitope scaffold T117v2
Authors : Irimia, A.; Wilson, I.A.
Deposited on : 2016-09-01
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

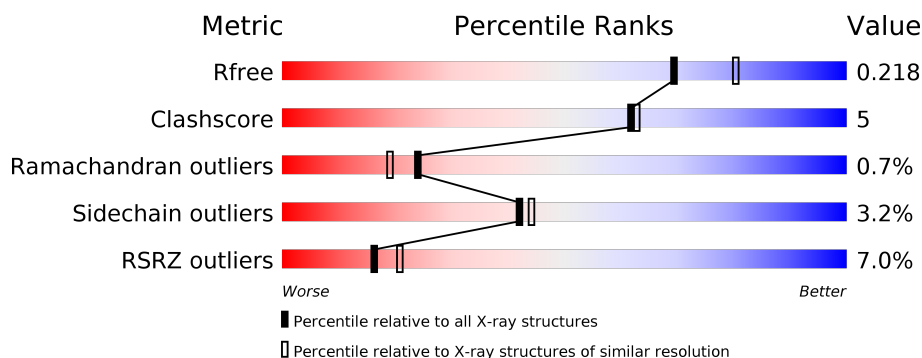
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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 $\leq 5\%$. 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	236	<div> <div>8%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	H	236	<div> <div>14%</div> <div>75%</div> <div>17%</div> <div>5%</div> </div>
2	B	215	<div> <div>2%</div> <div>95%</div> <div>•</div> </div>
2	L	215	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
3	G	163	<div> <div>4%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
3	I	163	<div> <div>4%</div> <div>75%</div> <div>17%</div> <div>7%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9545 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 Antibody 10E8 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	224	Total	C	N	O	S	0	4	0
			1744	1112	290	334	8			
1	A	223	Total	C	N	O	S	0	4	0
			1678	1069	280	321	8			

- Molecule 2 is a protein called Antibody 10E8 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	7	0
			1624	1008	279	331	6			
2	B	212	Total	C	N	O	S	0	0	0
			1563	973	265	321	4			

- Molecule 3 is a protein called 10E8 EPITOPE SCAFFOLD T117V2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	153	Total	C	N	O	S	0	0	0
			1209	778	206	220	5			
3	I	152	Total	C	N	O	S	0	4	0
			1205	780	201	220	4			

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



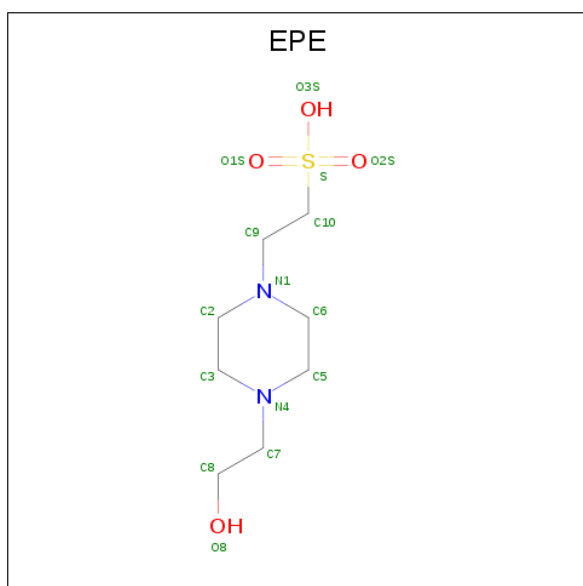
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total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

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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	110	Total	O	0	0
			110	110		
6	L	89	Total	O	0	0
			89	89		
6	A	87	Total	O	0	0
			87	87		
6	B	65	Total	O	0	0
			65	65		
6	G	35	Total	O	0	0
			35	35		

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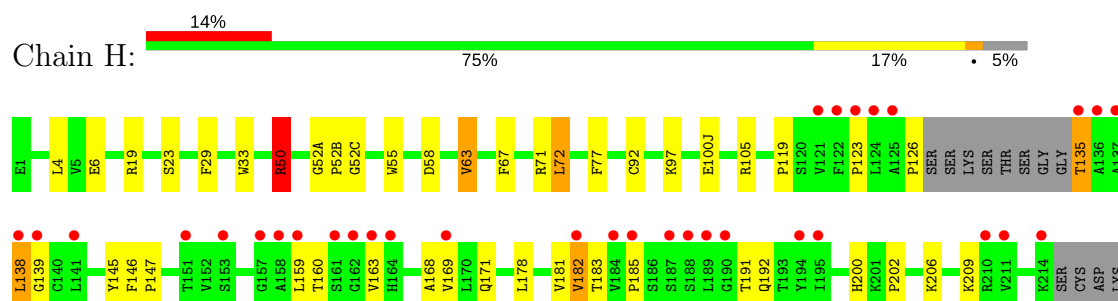
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	19	Total	O	0	0
			19	19		

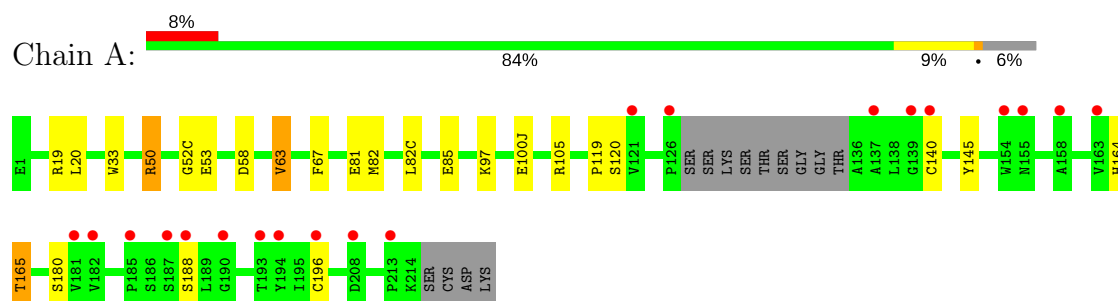
3 Residue-property plots [i](#)

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

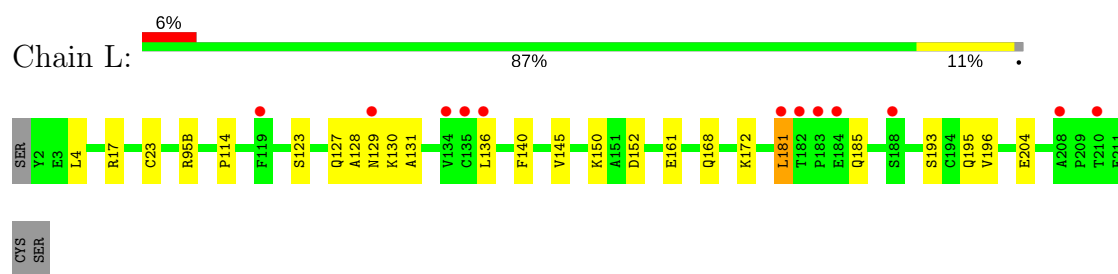
• Molecule 1: Antibody 10E8 FAB HEAVY CHAIN



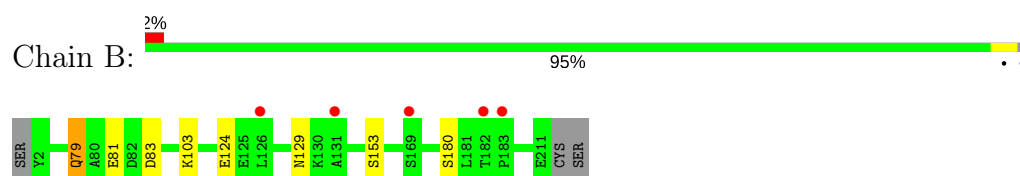
• Molecule 1: Antibody 10E8 FAB HEAVY CHAIN



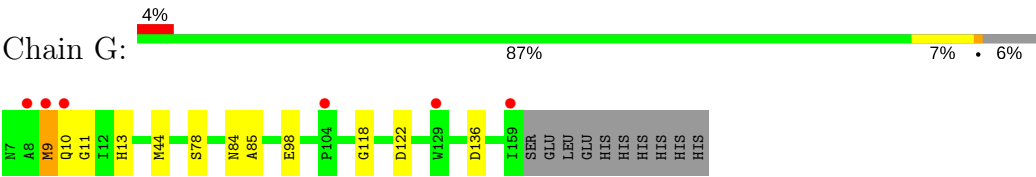
• Molecule 2: Antibody 10E8 FAB LIGHT CHAIN



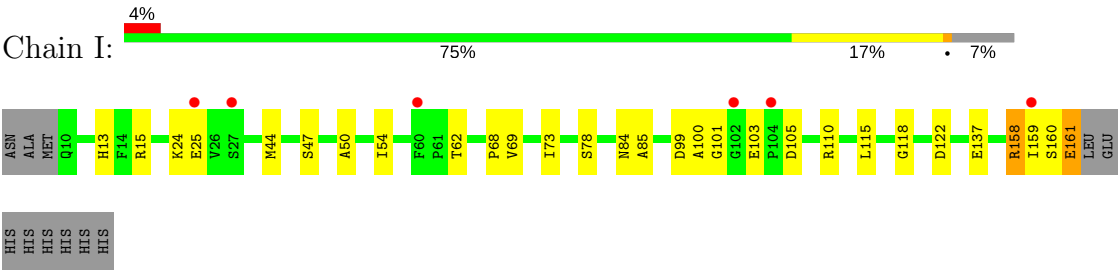
• Molecule 2: Antibody 10E8 FAB LIGHT CHAIN



● Molecule 3: 10E8 EPITOPE SCAFFOLD T117V2



● Molecule 3: 10E8 EPITOPE SCAFFOLD T117V2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.10Å 158.97Å 99.69Å 90.00° 97.98° 90.00°	Depositor
Resolution (Å)	47.14 – 2.10 47.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.14-2.10) 97.5 (47.14-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10_2155: 000)	Depositor
R, R_{free}	0.178 , 0.218 0.178 , 0.218	Depositor DCC
R_{free} test set	3623 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9545	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EPE

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	0.46	0/1731	0.58	0/2362
1	H	0.46	0/1795	0.60	1/2447 (0.0%)
2	B	0.37	0/1599	0.54	0/2185
2	L	0.41	0/1660	0.56	0/2263
3	G	0.37	0/1240	0.52	0/1695
3	I	0.33	0/1236	0.49	0/1694
All	All	0.41	0/9261	0.55	1/12646 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	50	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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	1678	0	1545	19	0
1	H	1744	0	1665	30	0
2	B	1563	0	1468	2	0
2	L	1624	0	1538	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1209	0	1179	7	0
3	I	1205	0	1158	15	0
4	A	42	0	56	6	0
4	B	18	0	24	1	0
4	G	12	0	16	0	0
4	H	18	0	24	3	0
4	L	12	0	16	1	0
5	L	15	0	17	0	0
6	A	87	0	0	1	0
6	B	65	0	0	1	0
6	G	35	0	0	1	0
6	H	110	0	0	3	0
6	I	19	0	0	0	0
6	L	89	0	0	0	0
All	All	9545	0	8706	83	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 5.

All (83) 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:H:163:VAL:HG12	1:H:182:VAL:HB	1.64	0.79
3:I:78:SER:HB2	3:I:118:GLY:HA2	1.75	0.69
3:G:78:SER:HB2	3:G:118:GLY:HA2	1.75	0.68
1:H:159:LEU:HD21	1:H:182:VAL:HG21	1.75	0.66
3:G:84:ASN:ND2	3:G:122:ASP:OD2	2.29	0.66
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.78	0.64
1:H:171:GLN:NE2	6:H:404:HOH:O	2.31	0.64
1:A:63:VAL:HG13	1:A:67:PHE:HB2	1.79	0.63
1:H:169:VAL:HG21	2:L:161:GLU:HB3	1.81	0.63
1:H:123:PRO:HD3	1:H:209:LYS:HE3	1.82	0.62
2:L:128:ALA:O	2:L:130:LYS:N	2.33	0.62
1:H:50:ARG:HD3	1:H:100(J):GLU:OE1	2.03	0.59
1:H:19:ARG:NH1	6:H:407:HOH:O	2.36	0.58
1:H:50:ARG:NH2	1:H:58:ASP:OD2	2.31	0.58
2:B:83:ASP:OD1	2:B:103:LYS:NZ	2.33	0.57
1:A:52(C):GLY:N	4:A:301:GOL:O1	2.37	0.57
2:L:95(B):ARG:HE	4:L:303:GOL:H31	1.70	0.57
1:A:19[B]:ARG:HG2	1:A:81:GLU:HG2	1.88	0.56
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:160:SER:O	3:I:161:GLU:HB2	2.06	0.55
1:A:50:ARG:HD3	1:A:100(J):GLU:OE1	2.07	0.55
3:G:44:MET:HE2	3:G:85:ALA:HB2	1.88	0.55
3:I:73[A]:ILE:HD11	3:I:115:LEU:HD11	1.88	0.54
3:G:13:HIS:HB2	3:G:44:MET:HE2	1.90	0.54
1:A:19[A]:ARG:NH1	4:A:306:GOL:O2	2.41	0.53
1:H:191:THR:OG1	1:H:192:GLN:N	2.40	0.53
3:I:69:VAL:HG23	3:I:110:ARG:HB2	1.90	0.53
3:I:13:HIS:HD2	3:I:15:ARG:HH12	1.56	0.52
1:A:165:THR:HA	1:A:180:SER:HA	1.92	0.52
1:H:139:GLY:HA3	1:H:181:VAL:HG12	1.90	0.52
1:H:126:PRO:HD3	1:H:138:LEU:HB3	1.93	0.51
1:H:105:ARG:HH21	1:A:19[B]:ARG:NE	2.10	0.49
1:H:4:LEU:HB3	1:H:92[A]:CYS:SG	2.53	0.49
1:A:52(C):GLY:HA3	3:G:118:GLY:O	2.13	0.49
3:I:44:MET:HE2	3:I:85:ALA:HB2	1.95	0.48
3:I:68:PRO:HD3	3:I:137:GLU:HG2	1.95	0.48
2:L:195:GLN:NE2	2:L:204:GLU:OE1	2.47	0.48
1:A:105:ARG:NE	6:A:405:HOH:O	2.46	0.48
4:B:302:GOL:H2	6:B:447:HOH:O	2.13	0.47
1:H:33:TRP:CE2	1:H:97:LYS:HD3	2.50	0.47
1:A:53:GLU:OE2	4:A:301:GOL:O3	2.25	0.47
1:A:19[A]:ARG:HG2	4:A:306:GOL:H2	1.96	0.47
3:I:99:ASP:OD1	3:I:101:GLY:N	2.42	0.46
1:H:135:THR:HA	1:H:185:PRO:HA	1.97	0.46
2:L:168:GLN:HG2	2:L:172:LYS:O	2.15	0.46
1:H:63:VAL:HG13	1:H:67:PHE:HB2	1.98	0.46
3:I:13:HIS:HD2	3:I:15:ARG:NH1	2.12	0.46
1:A:82:MET:HB3	1:A:82(C):LEU:HD21	1.98	0.46
3:I:50:ALA:O	3:I:54:ILE:HG13	2.15	0.45
3:I:84:ASN:ND2	3:I:122:ASP:OD2	2.50	0.45
2:L:4:LEU:HB3	2:L:23[A]:CYS:SG	2.56	0.45
1:A:19[A]:ARG:NE	4:A:302:GOL:O1	2.48	0.45
1:H:200:HIS:NE2	1:H:202:PRO:HG2	2.32	0.45
1:H:52(C):GLY:N	4:H:301:GOL:O2	2.48	0.45
1:H:160:THR:O	1:H:163:VAL:HG22	2.17	0.44
1:H:52(A):GLY:HA3	4:H:301:GOL:H12	1.99	0.44
1:A:85:GLU:N	1:A:85:GLU:OE1	2.50	0.44
2:L:17:ARG:HD3	2:L:17:ARG:HA	1.79	0.44
4:H:301:GOL:H32	3:I:118:GLY:O	2.18	0.44
3:I:62:THR:HA	3:I:100:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:9:MET:HE3	3:G:9:MET:HB2	1.89	0.43
1:H:52(B):PRO:HB3	1:H:55:TRP:CZ2	2.54	0.43
2:L:123:SER:O	2:L:127:GLN:HG3	2.18	0.43
1:H:163:VAL:HG23	1:H:163:VAL:O	2.18	0.43
2:B:79:GLN:HB3	2:B:81:GLU:HG2	2.00	0.43
3:G:136:ASP:OD2	6:G:301:HOH:O	2.22	0.43
1:H:146:PHE:HA	1:H:147:PRO:HA	1.84	0.43
1:A:33:TRP:CE2	1:A:97:LYS:HD3	2.54	0.43
2:L:114:PRO:HB3	2:L:140:PHE:HB3	2.01	0.43
1:H:171:GLN:HB3	6:H:412:HOH:O	2.19	0.42
1:A:19[A]:ARG:HG3	1:A:20:LEU:N	2.34	0.42
3:I:69:VAL:CG2	3:I:110:ARG:HB2	2.48	0.42
1:H:6:GLU:HG3	1:H:92[A]:CYS:SG	2.59	0.42
2:L:131:ALA:HB3	2:L:181:LEU:HD12	2.02	0.42
2:L:150:LYS:HB2	2:L:193:SER:HB2	2.02	0.42
1:H:29:PHE:O	1:H:71:ARG:NH2	2.53	0.42
1:H:23:SER:HB2	1:H:77:PHE:CZ	2.55	0.41
3:I:158:ARG:HG2	3:I:158:ARG:H	1.63	0.40
1:A:19[B]:ARG:HB2	4:A:306:GOL:H2	2.02	0.40
1:H:168:ALA:HB2	1:H:178:LEU:HB3	2.04	0.40
2:L:145:VAL:CG1	2:L:196:VAL:HG13	2.51	0.40
1:A:50:ARG:NH2	1:A:58:ASP:OD2	2.44	0.40
1:H:72:LEU:HD23	1:H:72:LEU:HA	1.94	0.40

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	223/236 (94%)	218 (98%)	4 (2%)	1 (0%)	36 34
1	H	224/236 (95%)	212 (95%)	12 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	210/215 (98%)	201 (96%)	9 (4%)	0	100	100
2	L	217/215 (101%)	202 (93%)	12 (6%)	3 (1%)	12	7
3	G	151/163 (93%)	146 (97%)	3 (2%)	2 (1%)	13	8
3	I	154/163 (94%)	147 (96%)	5 (3%)	2 (1%)	13	8
All	All	1179/1228 (96%)	1126 (96%)	45 (4%)	8 (1%)	24	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	129	ASN
1	A	188	SER
3	I	24	LYS
2	L	152	ASP
3	G	10	GLN
2	L	185	GLN
3	I	25	GLU
3	G	11	GLY

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	173/198 (87%)	166 (96%)	7 (4%)	34	34
1	H	191/198 (96%)	183 (96%)	8 (4%)	32	32
2	B	167/180 (93%)	162 (97%)	5 (3%)	44	47
2	L	177/180 (98%)	174 (98%)	3 (2%)	63	70
3	G	131/145 (90%)	129 (98%)	2 (2%)	67	73
3	I	128/145 (88%)	122 (95%)	6 (5%)	29	27
All	All	967/1046 (92%)	936 (97%)	31 (3%)	42	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	50	ARG
1	H	63	VAL
1	H	72	LEU
1	H	135	THR
1	H	138	LEU
1	H	182	VAL
1	H	183	THR
1	H	206	LYS
2	L	136[A]	LEU
2	L	136[B]	LEU
2	L	181	LEU
1	A	50	ARG
1	A	63	VAL
1	A	120	SER
1	A	140	CYS
1	A	164	HIS
1	A	165	THR
1	A	196	CYS
2	B	79	GLN
2	B	124	GLU
2	B	129	ASN
2	B	153	SER
2	B	180	SER
3	G	9	MET
3	G	98	GLU
3	I	47	SER
3	I	103	GLU
3	I	105	ASP
3	I	158	ARG
3	I	159	ILE
3	I	161	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	13	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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	301	-	5,5,5	0.51	0	5,5,5	1.02	0
4	GOL	A	302	-	5,5,5	0.32	0	5,5,5	0.39	0
4	GOL	A	303	-	5,5,5	0.37	0	5,5,5	0.38	0
4	GOL	A	304	-	5,5,5	0.40	0	5,5,5	0.56	0
4	GOL	A	305	-	5,5,5	0.32	0	5,5,5	0.39	0
4	GOL	A	306	-	5,5,5	0.34	0	5,5,5	0.29	0
4	GOL	A	307	-	5,5,5	0.41	0	5,5,5	0.35	0
4	GOL	B	301	-	5,5,5	0.32	0	5,5,5	0.34	0
4	GOL	B	302	-	5,5,5	0.42	0	5,5,5	0.44	0
4	GOL	B	303	-	5,5,5	0.34	0	5,5,5	0.41	0
4	GOL	G	201	-	5,5,5	0.35	0	5,5,5	0.56	0
4	GOL	G	202	-	5,5,5	0.40	0	5,5,5	0.22	0
4	GOL	H	301	-	5,5,5	0.46	0	5,5,5	0.49	0
4	GOL	H	302	-	5,5,5	0.34	0	5,5,5	0.32	0
4	GOL	H	303	-	5,5,5	0.36	0	5,5,5	0.44	0
5	EPE	L	301	-	15,15,15	0.88	1 (6%)	18,20,20	1.68	5 (27%)
4	GOL	L	302	-	5,5,5	0.41	0	5,5,5	0.36	0
4	GOL	L	303	-	5,5,5	0.33	0	5,5,5	0.44	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	301	-	-	0/4/4/4	0/0/0/0
4	GOL	A	302	-	-	0/4/4/4	0/0/0/0
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
4	GOL	A	304	-	-	0/4/4/4	0/0/0/0
4	GOL	A	305	-	-	0/4/4/4	0/0/0/0
4	GOL	A	306	-	-	0/4/4/4	0/0/0/0
4	GOL	A	307	-	-	0/4/4/4	0/0/0/0
4	GOL	B	301	-	-	0/4/4/4	0/0/0/0
4	GOL	B	302	-	-	0/4/4/4	0/0/0/0
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0
4	GOL	G	201	-	-	0/4/4/4	0/0/0/0
4	GOL	G	202	-	-	0/4/4/4	0/0/0/0
4	GOL	H	301	-	-	0/4/4/4	0/0/0/0
4	GOL	H	302	-	-	0/4/4/4	0/0/0/0
4	GOL	H	303	-	-	0/4/4/4	0/0/0/0
5	EPE	L	301	-	-	0/9/19/19	0/1/1/1
4	GOL	L	302	-	-	0/4/4/4	0/0/0/0
4	GOL	L	303	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	301	EPE	C10-S	2.76	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	301	EPE	C6-N1-C2	2.21	113.76	108.87
5	L	301	EPE	C7-N4-C5	2.63	118.09	111.24
5	L	301	EPE	C7-N4-C3	2.71	118.31	111.24
5	L	301	EPE	O3S-S-C10	3.15	110.87	105.77
5	L	301	EPE	C5-N4-C3	3.67	116.98	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	GOL	1	0
4	A	306	GOL	3	0
4	B	302	GOL	1	0
4	H	301	GOL	3	0
4	L	303	GOL	1	0

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	223/236 (94%)	0.48	20 (8%) 9 12	21, 37, 111, 143	2 (0%)
1	H	224/236 (94%)	0.70	33 (14%) 2 3	20, 36, 121, 153	0
2	B	212/215 (98%)	0.13	5 (2%) 59 64	26, 55, 88, 128	0
2	L	212/215 (98%)	0.46	12 (5%) 24 29	21, 43, 105, 126	0
3	G	153/163 (93%)	0.00	6 (3%) 39 46	29, 47, 80, 127	0
3	I	152/163 (93%)	0.31	6 (3%) 39 46	31, 58, 92, 124	0
All	All	1176/1228 (95%)	0.37	82 (6%) 16 21	20, 49, 109, 153	2 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	184	VAL	6.6
1	H	137	ALA	6.6
1	A	196	CYS	5.6
1	A	185	PRO	5.5
1	H	138	LEU	5.3
2	L	188	SER	4.7
1	H	124	LEU	4.6
1	H	122	PHE	4.4
1	H	194	TYR	4.1
1	H	125	ALA	4.0
1	H	159	LEU	3.8
1	H	214	LYS	3.8
1	A	182	VAL	3.7
1	H	189	LEU	3.6
2	L	182	THR	3.6
1	A	194	TYR	3.6
1	H	211	VAL	3.5
1	A	208	ASP	3.5
1	H	139	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	121	VAL	3.4
3	G	104	PRO	3.3
2	L	134	VAL	3.3
2	L	129	ASN	3.3
2	L	184	GLU	3.3
1	H	195	ILE	3.2
1	A	126	PRO	3.2
1	H	162	GLY	3.2
1	H	136	ALA	3.2
1	A	155	ASN	3.2
1	A	188	SER	3.1
1	H	158	ALA	3.1
1	H	161	SER	3.1
1	H	188	SER	3.0
3	G	10	GLN	3.0
3	I	27	SER	3.0
1	A	140	CYS	3.0
1	H	123	PRO	3.0
3	G	8	ALA	3.0
1	A	139	GLY	2.9
1	H	135	THR	2.9
1	A	193	THR	2.9
1	H	210	ARG	2.9
2	B	131	ALA	2.9
3	I	104	PRO	2.9
1	H	164[A]	HIS	2.8
1	A	154	TRP	2.7
2	B	169	SER	2.7
1	A	181	VAL	2.7
1	A	190	GLY	2.7
2	L	208	ALA	2.7
2	L	119	PHE	2.6
1	A	163	VAL	2.6
2	L	135	CYS	2.6
2	B	183	PRO	2.6
1	H	163	VAL	2.6
3	I	159	ILE	2.6
2	L	181	LEU	2.6
3	I	102	GLY	2.5
1	H	182	VAL	2.5
1	H	187	SER	2.5
3	I	60	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	151	THR	2.5
1	A	121	VAL	2.4
1	A	187	SER	2.4
1	H	185	PRO	2.4
1	A	158	ALA	2.4
2	B	182	THR	2.4
3	G	129	TRP	2.3
1	A	213	PRO	2.3
2	L	136[A]	LEU	2.3
1	H	153	SER	2.3
3	I	25	GLU	2.3
2	L	183	PRO	2.2
3	G	9	MET	2.2
1	H	190	GLY	2.2
1	H	157	GLY	2.2
3	G	159	ILE	2.2
1	H	141	LEU	2.1
2	L	210	THR	2.1
1	H	169	VAL	2.1
1	A	137	ALA	2.0
2	B	126	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	303	6/6	0.74	0.17	51,64,69,69	0
4	GOL	A	306	6/6	0.74	0.21	67,70,75,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	301	6/6	0.77	0.14	75,75,76,77	0
4	GOL	G	202	6/6	0.80	0.18	67,70,71,72	0
4	GOL	L	303	6/6	0.82	0.22	83,83,84,87	0
4	GOL	A	304	6/6	0.84	0.28	42,53,55,62	0
4	GOL	A	305	6/6	0.85	0.23	63,67,73,76	0
4	GOL	A	302	6/6	0.85	0.15	62,67,70,70	0
4	GOL	H	302	6/6	0.86	0.19	71,72,72,73	0
4	GOL	B	303	6/6	0.86	0.17	79,82,82,84	0
4	GOL	H	303	6/6	0.87	0.17	54,61,66,69	0
4	GOL	H	301	6/6	0.87	0.22	49,50,53,55	0
4	GOL	G	201	6/6	0.89	0.21	53,65,68,71	0
5	EPE	L	301	15/15	0.90	0.15	59,66,72,73	0
4	GOL	A	301	6/6	0.92	0.17	33,45,47,48	0
4	GOL	B	302	6/6	0.93	0.11	45,55,62,63	0
4	GOL	L	302	6/6	0.93	0.14	46,58,62,62	0
4	GOL	A	307	6/6	0.95	0.17	63,68,71,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.