



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:06 am BST

PDB ID : 5T5B
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF 10E8 FAB LIGHT CHAIN MUTANT5 AND T117V2 HIV-1 MPER SCAFFOLD
Authors : Irimia, A.; Wilson, I.A.
Deposited on : 2016-08-30
Resolution : 2.07 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

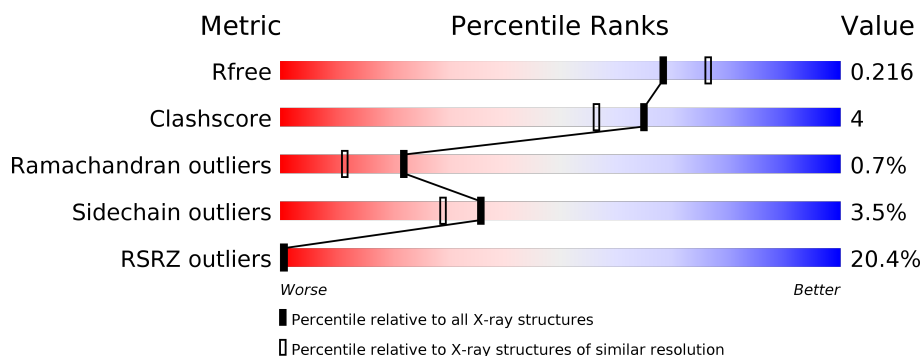
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 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	236	<div> <div>17%</div> <div>78%</div> <div>8%</div> <div>13%</div> </div>
1	H	236	<div> <div>20%</div> <div>77%</div> <div>10%</div> <div>13%</div> </div>
2	B	215	<div> <div>25%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
2	L	215	<div> <div>24%</div> <div>84%</div> <div>13%</div> <div>••</div> </div>
3	E	163	<div> <div>13%</div> <div>83%</div> <div>9%</div> <div>• 7%</div> </div>
3	O	163	<div> <div>11%</div> <div>84%</div> <div>7%</div> <div>• 8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8819 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	206	Total	C	N	O	S	0	2	0
			1548	988	258	295	7			
1	A	205	Total	C	N	O	S	0	4	0
			1581	1008	264	301	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	7	0
			1573	984	271	312	6			
2	B	210	Total	C	N	O	S	0	8	0
			1564	975	267	316	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	150	Total	C	N	O	S	0	0	0
			1156	748	191	213	4			
3	E	152	Total	C	N	O	S	0	0	0
			1152	747	192	209	4			

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



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

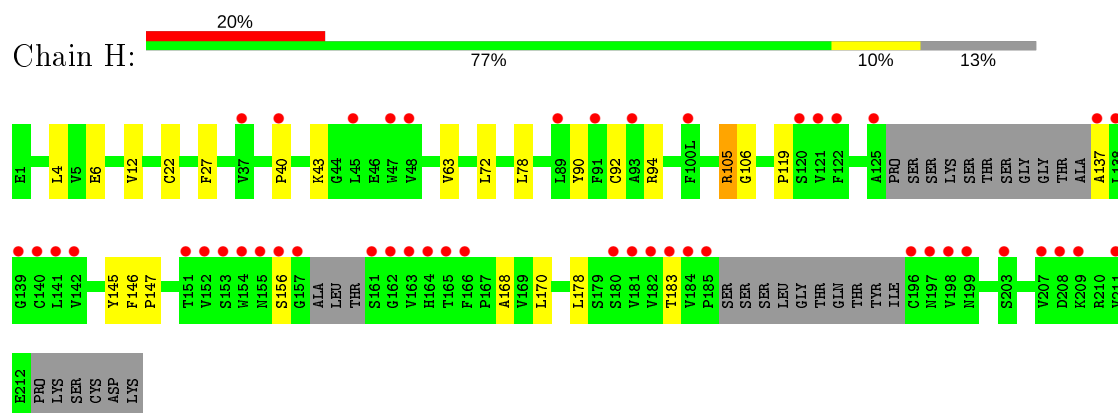
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	72	Total	O	0	0
			72	72		
5	L	28	Total	O	0	0
			28	28		
5	A	70	Total	O	0	0
			70	70		
5	B	27	Total	O	0	0
			27	27		
5	O	9	Total	O	0	0
			9	9		
5	E	3	Total	O	0	0
			3	3		

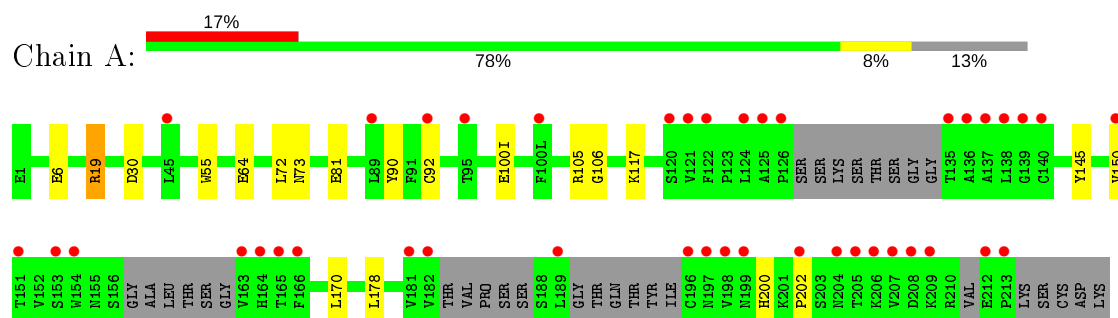
3 Residue-property plots [i](#)

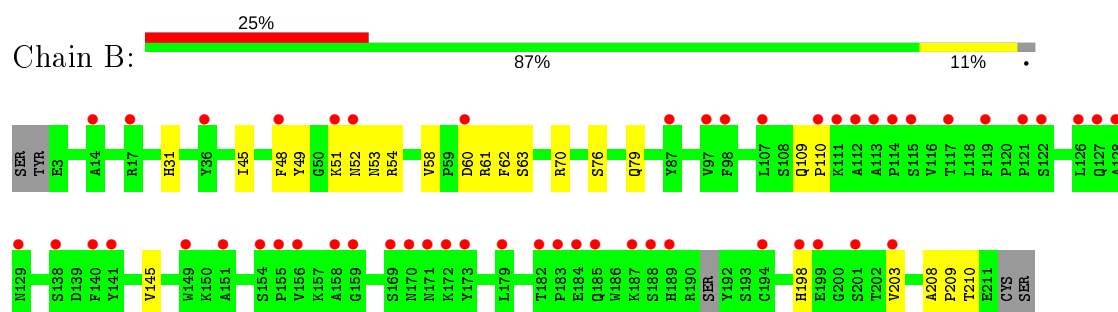
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

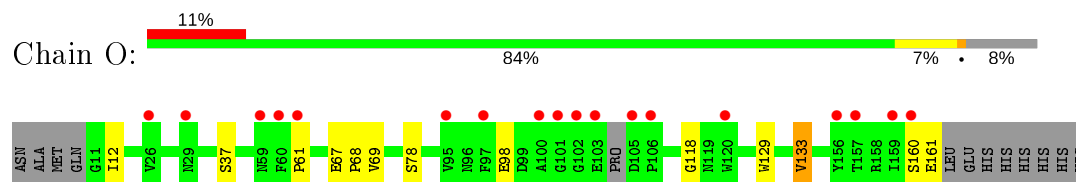


- Molecule 1: Antibody 10E8 FAB HEAVY CHAIN

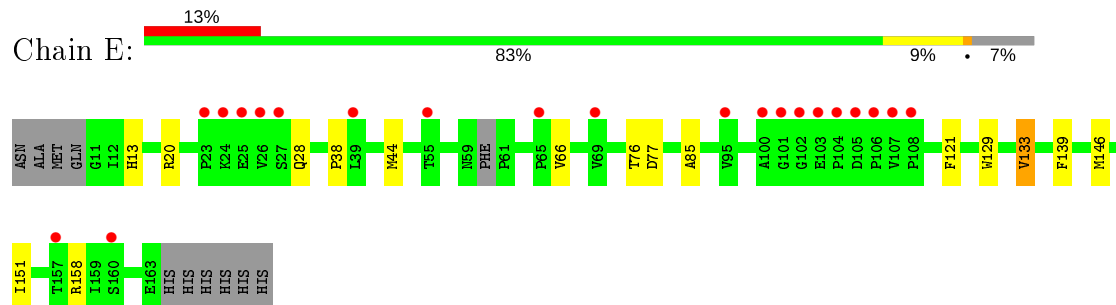




• Molecule 3: 10E8 EPITOPE SCAFFOLD T117V2



• 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	40.93Å 159.05Å 100.61Å 90.00° 95.17° 90.00°	Depositor
Resolution (Å)	37.88 – 2.07 37.88 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.6 (37.88-2.07) 94.6 (37.88-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.06Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.178 , 0.216 0.178 , 0.216	Depositor DCC
R_{free} test set	3696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.2	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	8819	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/1627	0.61	0/2211
1	H	0.50	0/1597	0.63	0/2175
2	B	0.40	0/1599	0.55	0/2185
2	L	0.38	0/1610	0.54	0/2205
3	E	0.35	0/1181	0.47	0/1620
3	O	0.35	0/1185	0.50	0/1623
All	All	0.42	0/8799	0.56	0/12019

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	51[B]	LYS	Peptide

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	1581	0	1453	11	0
1	H	1548	0	1418	16	0
2	B	1564	0	1442	13	0
2	L	1573	0	1446	20	0
3	E	1152	0	1100	9	0
3	O	1156	0	1105	4	0
4	A	18	0	24	1	0
4	B	6	0	8	0	0
4	E	6	0	8	0	0
4	L	6	0	8	0	0
5	A	70	0	0	0	0
5	B	27	0	0	0	0
5	E	3	0	0	1	0
5	H	72	0	0	1	0
5	L	28	0	0	1	0
5	O	9	0	0	0	0
All	All	8819	0	8012	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (68) 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:105:ARG:HH21	1:A:19[A]:ARG:HH21	1.24	0.83
3:E:20:ARG:HH21	3:E:38:PRO:HG3	1.52	0.74
2:L:182:THR:HG22	2:L:185:GLN:HG2	1.67	0.74
3:O:78:SER:HB2	3:O:118:GLY:HA2	1.74	0.69
2:L:133:LEU:HD12	2:L:179:LEU:HD23	1.79	0.64
2:L:48[B]:PHE:CE2	2:L:64:GLY:HA3	2.36	0.61
2:L:48[B]:PHE:HE1	2:L:73:LEU:HD13	1.67	0.59
1:H:40:PRO:HB2	1:H:43:LYS:HD3	1.85	0.59
3:E:158:ARG:NH1	5:E:301:HOH:O	2.21	0.58
2:L:55:PRO:HG2	2:L:58:VAL:HG21	1.86	0.58
1:H:27:PHE:CE2	1:H:94:ARG:HD3	2.39	0.58
1:H:94:ARG:HD2	5:H:366:HOH:O	2.04	0.58
2:L:151:ALA:HB1	2:L:189:HIS:CD2	2.39	0.57
1:H:27:PHE:CD2	1:H:94:ARG:HD3	2.39	0.57
2:B:49:TYR:O	2:B:53[A]:ASN:HB2	2.05	0.57
2:L:114:PRO:HB3	2:L:140:PHE:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48[A]:PHE:HE2	2:B:62:PHE:HB3	1.71	0.56
2:L:48[B]:PHE:CZ	2:L:64:GLY:HA3	2.40	0.56
2:L:21:ILE:HD11	2:L:73:LEU:HD23	1.88	0.55
3:O:61:PRO:HB3	3:O:98:GLU:HB3	1.88	0.54
2:L:76:SER:O	2:L:78:ALA:N	2.41	0.54
2:B:49:TYR:CE1	2:B:53[A]:ASN:HB3	2.44	0.53
3:E:44:MET:HE2	3:E:85:ALA:HB2	1.92	0.52
1:H:137:ALA:HA	1:H:183:THR:HA	1.91	0.51
2:L:120:PRO:HA	2:L:133:LEU:HD23	1.94	0.50
2:L:208:ALA:O	2:L:210:THR:N	2.39	0.49
2:L:24:ARG:NH1	2:L:70:ARG:HG3	2.28	0.49
2:B:48[B]:PHE:CE2	2:B:52[B]:ASN:HA	2.48	0.48
3:O:129:TRP:CZ2	3:O:133:VAL:HG21	2.49	0.48
2:B:49:TYR:CZ	2:B:53[A]:ASN:HB3	2.48	0.48
2:B:109:GLN:HB2	2:B:110:PRO:HD2	1.95	0.48
1:A:200:HIS:NE2	1:A:202:PRO:HG2	2.29	0.47
2:B:208:ALA:O	2:B:210:THR:N	2.47	0.47
2:B:54:ARG:HD3	2:B:58:VAL:O	2.15	0.47
1:A:90:TYR:O	1:A:106:GLY:HA2	2.15	0.46
2:B:48[A]:PHE:HZ	2:B:62:PHE:O	1.98	0.46
1:H:105:ARG:NH2	1:A:19[A]:ARG:HH21	2.02	0.46
2:B:145:VAL:HG12	2:B:198:HIS:HB2	1.97	0.45
1:H:168:ALA:HA	1:H:178:LEU:HB3	1.99	0.45
1:H:6:GLU:HG3	1:H:92[A]:CYS:SG	2.57	0.44
1:H:105:ARG:HH11	1:H:105:ARG:HB2	1.81	0.44
3:E:129:TRP:CZ2	3:E:133:VAL:HG21	2.53	0.44
2:L:182:THR:HG23	2:L:184:GLU:H	1.82	0.44
1:H:146:PHE:HA	1:H:147:PRO:HA	1.76	0.44
3:O:68:PRO:HD2	3:O:69:VAL:HG23	1.99	0.44
1:A:145:TYR:OH	1:A:178:LEU:HD23	2.19	0.43
2:L:76:SER:O	2:L:77:GLY:C	2.57	0.43
1:A:100(I):GLU:HG3	2:B:31:HIS:HB3	2.00	0.42
2:L:48[B]:PHE:HE1	2:L:73:LEU:CD1	2.31	0.42
1:A:6:GLU:HG3	1:A:92[A]:CYS:SG	2.60	0.42
3:E:13:HIS:HB2	3:E:44:MET:HE2	2.01	0.42
3:E:76:THR:OG1	3:E:77:ASP:N	2.52	0.42
2:L:95(B):ARG:HD2	3:E:121:PHE:CE1	2.54	0.42
3:E:133:VAL:HG13	3:E:139:PHE:CD2	2.55	0.42
2:L:38:LYS:NZ	5:L:402:HOH:O	2.49	0.42
1:H:90:TYR:O	1:H:106:GLY:HA2	2.21	0.41
2:L:39:LYS:HD3	2:L:84:ALA:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:TRP:CD1	4:A:303:GOL:H11	2.55	0.41
1:H:22:CYS:HB3	1:H:78:LEU:HB3	2.03	0.41
1:A:30:ASP:OD1	1:A:73:ASN:HB3	2.21	0.41
1:H:119:PRO:HB3	1:H:145:TYR:HB3	2.03	0.41
1:H:105:ARG:HD3	1:A:19[B]:ARG:NH2	2.36	0.40
3:E:146:MET:HE3	3:E:151:ILE:HG12	2.04	0.40
2:B:45:ILE:HG13	2:B:45:ILE:O	2.20	0.40
2:B:61:ARG:CZ	2:B:79:GLN:HG3	2.51	0.40
1:H:4:LEU:HB3	1:H:92[A]:CYS:SG	2.61	0.40
2:L:48[B]:PHE:CE1	2:L:73:LEU:HD13	2.52	0.40
1:A:19[B]:ARG:HD3	1:A:81[B]:GLU:HG2	2.03	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	197/236 (84%)	193 (98%)	4 (2%)	0	100	100
1	H	200/236 (85%)	197 (98%)	3 (2%)	0	100	100
2	B	215/215 (100%)	206 (96%)	6 (3%)	3 (1%)	11	3
2	L	218/215 (101%)	203 (93%)	10 (5%)	5 (2%)	6	1
3	E	148/163 (91%)	146 (99%)	2 (1%)	0	100	100
3	O	146/163 (90%)	142 (97%)	3 (2%)	1 (1%)	22	11
All	All	1124/1228 (92%)	1087 (97%)	28 (2%)	9 (1%)	22	9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51[A]	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	51[B]	LYS
3	O	12	ILE
2	L	76	SER
2	L	77	GLY
2	L	107	LEU
2	L	128	ALA
2	L	129	ASN
2	B	209	PRO

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	165/198 (83%)	157 (95%)	8 (5%)	25	18
1	H	159/198 (80%)	153 (96%)	6 (4%)	33	26
2	B	162/178 (91%)	157 (97%)	5 (3%)	40	34
2	L	159/178 (89%)	155 (98%)	4 (2%)	47	41
3	E	120/145 (83%)	117 (98%)	3 (2%)	47	41
3	O	123/145 (85%)	118 (96%)	5 (4%)	30	23
All	All	888/1042 (85%)	857 (96%)	31 (4%)	36	29

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

Mol	Chain	Res	Type
1	H	12	VAL
1	H	63	VAL
1	H	72	LEU
1	H	105	ARG
1	H	156	SER
1	H	170	LEU
2	L	1	TYR
2	L	95(B)	ARG
2	L	107	LEU
2	L	182	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	19[A]	ARG
1	A	19[B]	ARG
1	A	64	GLU
1	A	72	LEU
1	A	105	ARG
1	A	117	LYS
1	A	150	VAL
1	A	170	LEU
2	B	60	ASP
2	B	63	SER
2	B	70	ARG
2	B	76	SER
2	B	203	VAL
3	O	37	SER
3	O	67	GLU
3	O	133	VAL
3	O	160	SER
3	O	161	GLU
3	E	28	GLN
3	E	66	VAL
3	E	133	VAL

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	0.37	0	5,5,5	0.40	0
4	GOL	B	301	-	5,5,5	0.39	0	5,5,5	0.29	0
4	GOL	A	303	-	5,5,5	0.33	0	5,5,5	0.55	0
4	GOL	L	301	-	5,5,5	0.35	0	5,5,5	0.38	0
4	GOL	E	201	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	A	302	-	5,5,5	0.49	0	5,5,5	0.69	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	-	-	2/4/4/4	-
4	GOL	B	301	-	-	2/4/4/4	-
4	GOL	A	303	-	-	4/4/4/4	-
4	GOL	L	301	-	-	2/4/4/4	-
4	GOL	E	201	-	-	3/4/4/4	-
4	GOL	A	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O1-C1-C2-C3
4	B	301	GOL	O1-C1-C2-C3
4	A	303	GOL	O1-C1-C2-C3
4	A	303	GOL	C1-C2-C3-O3
4	E	201	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	303	GOL	O1-C1-C2-O2
4	L	301	GOL	O1-C1-C2-O2
4	L	301	GOL	O1-C1-C2-C3
4	B	301	GOL	O1-C1-C2-O2
4	E	201	GOL	O2-C2-C3-O3
4	A	303	GOL	O2-C2-C3-O3
4	E	201	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	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	205/236 (86%)	1.33	41 (20%) 1 0	30, 46, 129, 156	0
1	H	206/236 (87%)	1.37	47 (22%) 0 0	30, 47, 125, 148	0
2	B	210/215 (97%)	1.20	53 (25%) 0 0	34, 77, 122, 153	0
2	L	212/215 (98%)	1.33	52 (24%) 0 0	33, 84, 126, 140	0
3	E	152/163 (93%)	0.81	21 (13%) 2 2	43, 75, 112, 124	0
3	O	150/163 (92%)	0.65	18 (12%) 4 4	41, 72, 101, 123	0
All	All	1135/1228 (92%)	1.15	232 (20%) 1 0	30, 69, 124, 156	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	TRP	9.2
1	A	136	ALA	7.7
1	A	208	ASP	7.6
1	H	184	VAL	7.6
2	B	183	PRO	7.2
2	L	123	SER	6.8
2	L	131	ALA	6.8
1	A	198	VAL	6.2
1	H	209	LYS	6.2
1	H	198	VAL	6.1
1	A	139	GLY	6.1
2	L	112	ALA	5.6
1	A	207	VAL	5.5
1	A	213	PRO	5.5
1	H	185	PRO	5.5
1	A	126	PRO	5.5
2	B	156	VAL	5.5
1	H	125	ALA	5.4
3	O	102	GLY	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	122	PHE	5.2
2	L	169	SER	5.1
2	L	203	VAL	5.1
1	A	196	CYS	5.1
1	H	196	CYS	5.0
1	H	208	ASP	5.0
2	L	156	VAL	4.9
1	H	199	ASN	4.9
2	L	132	THR	4.9
1	H	157	GLY	4.9
1	H	121	VAL	4.8
1	H	165	THR	4.7
1	H	154	TRP	4.7
1	H	163	VAL	4.7
2	B	113	ALA	4.7
1	H	156	SER	4.7
2	B	122	SER	4.6
2	B	52[A]	ASN	4.6
1	A	163	VAL	4.6
2	B	151	ALA	4.5
1	H	152	VAL	4.5
2	L	48[A]	PHE	4.5
2	L	119	PHE	4.4
3	O	60	PHE	4.3
1	A	138	LEU	4.3
1	H	138	LEU	4.3
1	H	120	SER	4.2
1	H	142	VAL	4.2
1	A	153	SER	4.2
1	A	140	CYS	4.2
3	O	106	PRO	4.2
2	B	126	LEU	4.2
2	L	115	SER	4.1
2	B	128	ALA	4.1
2	L	126	LEU	4.1
2	B	182	THR	4.1
1	A	150	VAL	4.1
3	O	159	ILE	4.1
2	L	128	ALA	4.0
1	A	199	ASN	4.0
3	E	65	PRO	4.0
2	L	159	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	106	PRO	3.9
1	A	212	GLU	3.9
2	B	188	SER	3.9
2	B	170	ASN	3.9
2	B	14	ALA	3.8
1	A	151	THR	3.8
1	A	189	LEU	3.8
2	B	115	SER	3.8
2	L	200	GLY	3.8
2	L	127	GLN	3.7
3	E	104	PRO	3.7
2	L	149	TRP	3.7
1	H	207	VAL	3.7
1	H	153	SER	3.7
3	E	26	VAL	3.7
2	L	113	ALA	3.6
1	A	120	SER	3.6
1	A	204	ASN	3.6
2	L	1	TYR	3.6
1	A	197	ASN	3.6
1	A	205	THR	3.5
2	B	119	PHE	3.5
2	B	48[A]	PHE	3.5
2	L	181	LEU	3.5
1	A	125	ALA	3.5
3	O	100	ALA	3.5
1	A	182	VAL	3.5
1	H	139	GLY	3.5
2	L	136	LEU	3.4
3	E	69	VAL	3.4
3	E	102	GLY	3.4
3	E	105	ASP	3.3
1	A	121	VAL	3.3
2	L	97	VAL	3.3
3	E	160	SER	3.2
1	H	197	ASN	3.2
2	B	112	ALA	3.2
1	A	122	PHE	3.2
2	L	194	CYS	3.2
3	E	103	GLU	3.2
2	B	127	GLN	3.2
3	E	95	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	180	SER	3.1
1	A	164	HIS	3.1
1	A	135	THR	3.1
2	L	173	TYR	3.1
2	B	173	TYR	3.1
3	O	26	VAL	3.1
2	B	184	GLU	3.1
3	E	157	THR	3.1
3	O	105	ASP	3.0
1	H	45	LEU	3.0
1	H	183	THR	3.0
2	L	52[A]	ASN	3.0
2	L	183	PRO	3.0
2	L	201	SER	3.0
2	L	198	HIS	3.0
2	B	138[A]	SER	3.0
2	L	98	PHE	3.0
2	L	141	TYR	2.9
2	L	199	GLU	2.9
2	L	87	TYR	2.9
2	B	158	ALA	2.9
1	H	164	HIS	2.9
3	E	100	ALA	2.9
2	B	111	LYS	2.9
1	H	137	ALA	2.9
1	A	137	ALA	2.9
2	B	149	TRP	2.9
1	H	182	VAL	2.9
1	H	181	VAL	2.8
3	E	107	VAL	2.8
2	L	182	THR	2.8
2	L	143	GLY	2.8
1	H	141	LEU	2.8
3	O	160	SER	2.7
1	H	37	VAL	2.7
1	A	206	LYS	2.7
2	L	140	PHE	2.7
3	O	103	GLU	2.7
1	H	161	SER	2.7
2	L	186	TRP	2.7
2	L	155	PRO	2.7
3	E	24	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	130	LYS	2.6
2	L	158	ALA	2.6
1	H	151	THR	2.6
2	L	14	ALA	2.6
2	B	155	PRO	2.6
1	H	166	PHE	2.6
3	E	25	GLU	2.5
2	L	139	ASP	2.5
2	B	129	ASN	2.5
3	O	101	GLY	2.5
2	B	187	LYS	2.5
1	A	100(L)	PHE	2.4
1	A	165	THR	2.4
2	L	114	PRO	2.4
3	O	61	PRO	2.4
2	L	4	LEU	2.4
1	H	162	GLY	2.4
2	B	172	LYS	2.4
2	B	117	THR	2.4
3	E	55	THR	2.4
2	B	97	VAL	2.4
2	L	142	PRO	2.4
2	B	189	HIS	2.4
1	A	209	LYS	2.4
3	E	101	GLY	2.4
2	L	184	GLU	2.3
2	B	199	GLU	2.3
3	E	23	PRO	2.3
2	B	87	TYR	2.3
1	H	47	TRP	2.3
2	B	110	PRO	2.3
1	H	93	ALA	2.3
2	B	159	GLY	2.3
2	B	17	ARG	2.3
1	A	166	PHE	2.3
2	L	88[A]	CYS	2.3
1	H	89	LEU	2.3
3	E	39	LEU	2.3
3	O	97	PHE	2.3
1	H	48	VAL	2.3
2	B	171	ASN	2.3
2	B	107	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	108	SER	2.2
3	E	27	SER	2.2
2	B	98	PHE	2.2
2	B	169	SER	2.2
2	B	201	SER	2.2
1	A	89	LEU	2.2
2	B	51[A]	LYS	2.2
1	A	202	PRO	2.2
2	L	188	SER	2.2
1	A	45	LEU	2.2
2	B	154	SER	2.2
3	E	108	PRO	2.2
2	L	129	ASN	2.2
2	L	202	THR	2.2
1	H	100(L)	PHE	2.2
2	B	140	PHE	2.2
3	O	157	THR	2.2
2	B	114	PRO	2.2
1	A	124	LEU	2.1
2	L	116	VAL	2.1
2	B	185	GLN	2.1
3	O	156	TYR	2.1
1	A	95	THR	2.1
2	B	121	PRO	2.1
1	H	155	ASN	2.1
2	B	179	LEU	2.1
1	H	211	VAL	2.1
2	B	36	TYR	2.1
1	H	140	CYS	2.1
1	A	92[A]	CYS	2.1
2	B	194	CYS	2.1
1	A	181	VAL	2.1
3	O	95	VAL	2.1
1	H	40	PRO	2.1
3	O	29	ASN	2.1
2	B	60	ASP	2.1
2	B	198	HIS	2.1
2	B	141	TYR	2.1
3	O	120	TRP	2.1
1	H	203	SER	2.0
2	B	203	VAL	2.0
1	H	91	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	99	GLY	2.0
3	O	59	ASN	2.0
2	L	197	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 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. 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
4	GOL	A	302	6/6	0.70	0.29	51,71,82,87	0
4	GOL	A	301	6/6	0.83	0.16	60,77,85,89	0
4	GOL	B	301	6/6	0.85	0.26	69,76,78,81	0
4	GOL	A	303	6/6	0.88	0.18	63,85,88,93	0
4	GOL	E	201	6/6	0.93	0.22	84,87,88,90	0
4	GOL	L	301	6/6	0.94	0.32	80,84,86,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.