



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:31 PM GMT

PDB ID : 1TZG
Title : Crystal structure of HIV-1 neutralizing human Fab 4E10 in complex with a 13-residue peptide containing the 4E10 epitope on gp41
Authors : Cardoso, R.M.F.; Zwick, M.B.; Stanfield, R.L.; Kunert, R.; Binley, J.M.; Katinger, H.; Burton, D.R.; Wilson, I.A.
Deposited on : 2004-07-09
Resolution : 2.20 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 ⓘ 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 (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

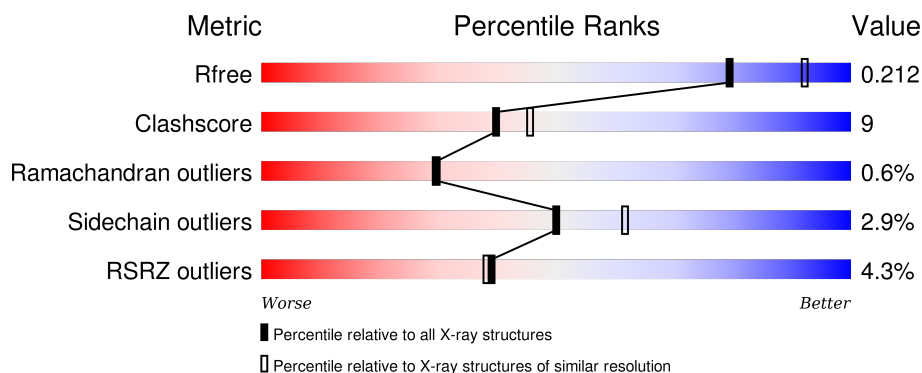
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	L	214	<div> <div style="width: 15%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 1%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div> <div>6% 84% 15% .</div>
1	M	214	<div> <div style="width: 6%; background-color: red;"></div> <div style="width: 75%; background-color: green;"></div> <div style="width: 22%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div> <div>6% 75% 22% .</div>
2	H	232	<div> <div style="width: 4%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div> <div>4% 84% 15% .</div>
2	I	232	<div> <div style="width: 7%; background-color: red;"></div> <div style="width: 78%; background-color: green;"></div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>7% 78% 20% ..</div>
3	P	13	<div> <div style="width: 77%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 8%; background-color: grey;"></div> </div> <div>77% 15% 8%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	13	 <div>69% 23% 8%</div>

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
4	GOL	L	701	-	X	-	X
4	GOL	L	702	-	X	-	X
4	GOL	L	703	-	X	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7535 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 Fab 4E10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			
1	M	214	Total	C	N	O	S	0	0	0
			1639	1017	284	334	4			

- Molecule 2 is a protein called Fab 4E10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	232	Total	C	N	O	S	0	1	0
			1720	1085	294	335	6			
2	I	228	Total	C	N	O	S	0	0	0
			1689	1069	289	326	5			

- Molecule 3 is a protein called Envelope polypeptide GP160.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O	0	0	0
			109	74	18	17			
3	Q	12	Total	C	N	O	0	0	0
			109	74	18	17			

- 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	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

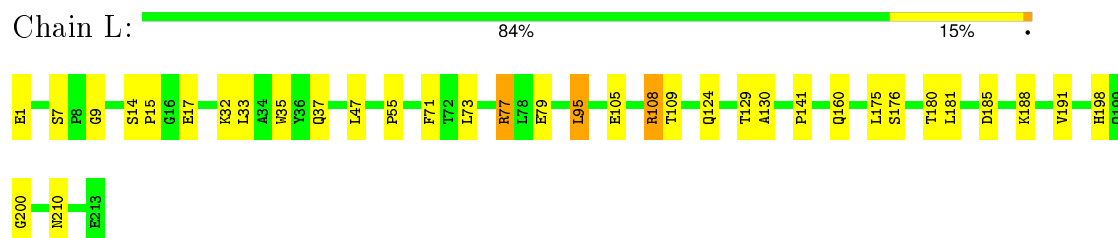
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	231	Total	O	0	0
			231	231		
5	I	91	Total	O	0	0
			91	91		
5	L	226	Total	O	0	0
			226	226		
5	M	50	Total	O	0	0
			50	50		
5	P	9	Total	O	0	0
			9	9		
5	Q	5	Total	O	0	0
			5	5		

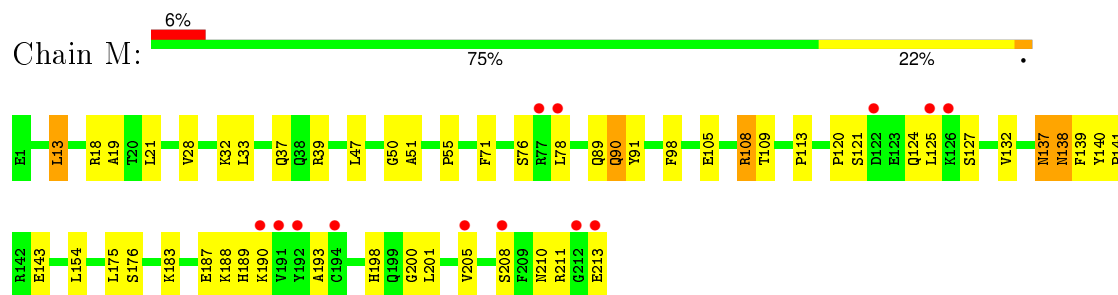
3 Residue-property plots

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.

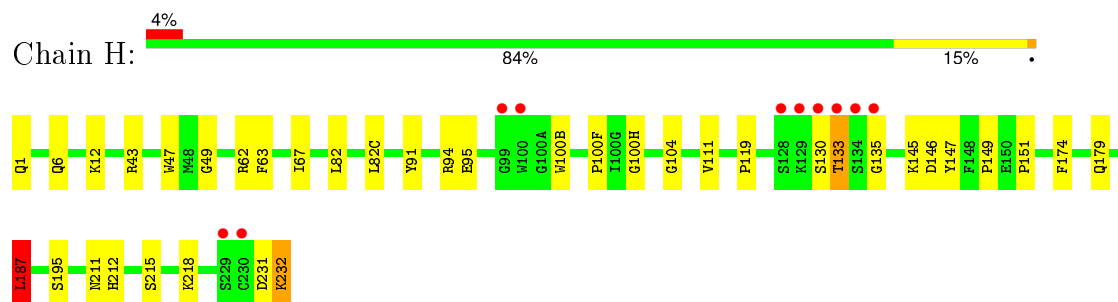
- Molecule 1: Fab 4E10



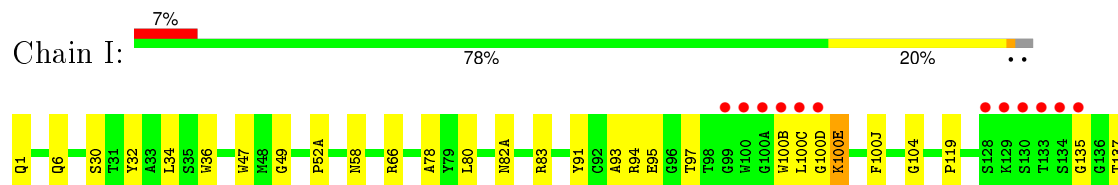
- Molecule 1: Fab 4E10

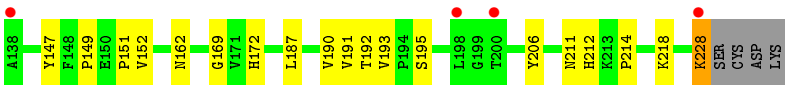


- Molecule 2: Fab 4E10



- Molecule 2: Fab 4E10





● Molecule 3: Envelope polypeptide GP160



● Molecule 3: Envelope polypeptide GP160



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.30 Å 45.10 Å 198.50 Å 90.00° 113.80° 90.00°	Depositor
Resolution (Å)	43.00 – 2.20 43.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.2 (43.00-2.20) 93.3 (43.04-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.20 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.260 0.216 , 0.212	Depositor DCC
R_{free} test set	3098 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 61322 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7535	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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, 0.375 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

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	L	0.36	0/1672	0.65	0/2266
1	M	0.28	0/1672	0.54	0/2266
2	H	0.36	0/1768	0.68	1/2412 (0.0%)
2	I	0.29	0/1732	0.60	0/2366
3	P	0.45	0/115	0.47	0/157
3	Q	0.42	0/115	0.45	0/157
All	All	0.33	0/7074	0.61	1/9624 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	187	LEU	CA-CB-CG	5.71	128.44	115.30

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	L	1639	0	1589	24	0
1	M	1639	0	1589	42	0
2	H	1720	0	1707	27	0
2	I	1689	0	1679	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	109	0	91	1	0
3	Q	109	0	91	2	0
4	L	18	0	12	4	0
5	H	231	0	0	1	1
5	I	91	0	0	0	0
5	L	226	0	0	2	0
5	M	50	0	0	0	0
5	P	9	0	0	0	0
5	Q	5	0	0	0	0
All	All	7535	0	6758	121	1

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 9.

All (121) 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:L:9:GLY:H	4:L:703:GOL:H11	1.39	0.88
1:M:211:ARG:HH11	1:M:211:ARG:HB3	1.47	0.78
1:M:113:PRO:HB3	1:M:139:PHE:HB3	1.66	0.78
2:I:119:PRO:HB3	2:I:147:TYR:HB3	1.66	0.76
1:L:160:GLN:HE22	2:H:179:GLN:HA	1.51	0.75
1:L:32:LYS:HE3	3:P:674:ASP:OD1	1.89	0.73
1:L:180:THR:C	1:L:181:LEU:HD12	2.10	0.71
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.72	0.70
1:M:211:ARG:HB3	1:M:211:ARG:NH1	2.08	0.69
1:L:185:ASP:HA	1:L:188:LYS:HD3	1.75	0.68
1:M:175:LEU:HD23	1:M:176:SER:N	2.10	0.67
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.78	0.66
1:L:7:SER:HB3	5:L:787:HOH:O	1.96	0.63
1:L:198:HIS:CD2	1:L:200:GLY:H	2.16	0.63
2:H:211:ASN:HD21	2:H:218:LYS:HE2	1.65	0.62
2:H:231:ASP:O	2:H:232:LYS:HB2	1.99	0.62
2:I:30:SER:HA	2:I:52(A):PRO:HB2	1.81	0.62
1:M:18:ARG:HG3	1:M:76:SER:HA	1.83	0.60
1:M:137:ASN:HD22	1:M:138:ASN:H	1.50	0.59
1:M:188:LYS:HE3	1:M:189:HIS:HE1	1.68	0.58
1:M:108:ARG:HD3	1:M:109:THR:O	2.04	0.58
2:H:212:HIS:HD2	2:H:215:SER:OG	1.85	0.58
1:M:39:ARG:HH21	1:M:39:ARG:HG3	1.68	0.58
1:M:143:GLU:CD	1:M:143:GLU:H	2.07	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:PHE:O	2:H:67:ILE:HG22	2.05	0.57
1:M:32:LYS:HE3	3:Q:674:ASP:OD1	2.05	0.56
2:I:100(D):GLY:O	2:I:100(E):LYS:HB2	2.05	0.56
2:H:1:GLN:CD	2:H:1:GLN:N	2.60	0.56
2:H:95:GLU:OE1	2:H:100(F):PRO:HB2	2.05	0.55
1:M:121:SER:O	1:M:125:LEU:HD23	2.05	0.55
2:I:1:GLN:N	2:I:100(B):TRP:CE2	2.75	0.54
1:M:89:GLN:HB2	1:M:98:PHE:CE1	2.42	0.54
1:M:201:LEU:HD13	1:M:205:VAL:HG23	1.88	0.54
1:M:210:ASN:HB2	1:M:213:GLU:OE2	2.07	0.54
1:L:108:ARG:HD3	1:L:109:THR:O	2.08	0.53
1:L:141:PRO:O	1:L:198:HIS:HE1	1.92	0.53
2:I:211:ASN:ND2	2:I:218:LYS:HG2	2.24	0.53
1:M:37:GLN:HB2	1:M:47:LEU:HD11	1.91	0.53
1:M:113:PRO:CB	1:M:139:PHE:HB3	2.38	0.53
2:I:6:GLN:HE21	2:I:104:GLY:HA3	1.74	0.53
2:I:187:LEU:HD12	2:I:187:LEU:C	2.29	0.52
1:L:9:GLY:N	4:L:703:GOL:H11	2.17	0.52
1:M:198:HIS:CD2	1:M:200:GLY:H	2.28	0.52
1:M:211:ARG:HH11	1:M:211:ARG:CB	2.19	0.52
2:I:34:LEU:HD13	2:I:78:ALA:HB2	1.92	0.52
1:L:77:ARG:HD3	1:L:79:GLU:OE2	2.09	0.52
1:M:39:ARG:NH2	1:M:39:ARG:HG3	2.25	0.51
1:L:15:PRO:HB3	5:L:821:HOH:O	2.10	0.51
1:M:28:VAL:HG13	1:M:90:GLN:HG2	1.93	0.51
1:M:137:ASN:HD22	1:M:138:ASN:N	2.09	0.50
1:M:21:LEU:N	1:M:21:LEU:HD12	2.27	0.50
2:H:6:GLN:HE22	2:H:91:TYR:HA	1.76	0.50
1:M:47:LEU:O	1:M:55:PRO:HD2	2.12	0.49
2:H:1:GLN:H3	2:H:1:GLN:CD	2.15	0.49
2:I:66:ARG:HD2	2:I:82(A):ASN:O	2.12	0.49
2:I:137:THR:CG2	2:I:192:THR:HB	2.43	0.49
2:I:94:ARG:HG2	2:I:95:GLU:N	2.27	0.48
2:H:149:PRO:O	2:H:212:HIS:HE1	1.95	0.48
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.78	0.48
1:M:13:LEU:HD23	1:M:19:ALA:HB2	1.95	0.48
1:L:124:GLN:HG2	1:L:129:THR:O	2.13	0.48
1:M:189:HIS:O	1:M:211:ARG:NH1	2.47	0.48
2:I:147:TYR:CE2	2:I:152:VAL:HG23	2.49	0.48
1:M:175:LEU:HD23	1:M:175:LEU:C	2.34	0.48
2:H:212:HIS:CD2	2:H:215:SER:OG	2.65	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:89:GLN:HB2	1:M:98:PHE:CD1	2.48	0.47
4:L:701:GOL:O3	2:H:174:PHE:HB2	2.13	0.47
2:I:135:GLY:O	2:I:195:SER:HB3	2.15	0.47
1:M:154:LEU:HD23	1:M:154:LEU:C	2.34	0.47
2:I:32:TYR:OH	2:I:100(C):LEU:HA	2.13	0.47
1:M:188:LYS:HE3	1:M:189:HIS:CE1	2.49	0.47
2:I:97:THR:HA	2:I:100(E):LYS:O	2.15	0.46
2:H:95:GLU:CG	2:H:100(H):GLY:H	2.28	0.46
2:H:12:LYS:O	2:H:111:VAL:HA	2.15	0.46
1:L:14:SER:HB2	1:L:17:GLU:HG3	1.98	0.46
2:I:1:GLN:HG3	2:I:100(B):TRP:CZ2	2.50	0.46
2:I:137:THR:HG21	2:I:192:THR:HB	1.98	0.46
2:H:133:THR:O	2:H:195:SER:HB3	2.16	0.46
2:H:62:ARG:CZ	5:H:358:HOH:O	2.64	0.46
2:I:212:HIS:CE1	2:I:214:PRO:HB2	2.51	0.45
2:I:34:LEU:HD13	2:I:78:ALA:CB	2.47	0.45
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.51	0.45
1:L:175:LEU:C	1:L:175:LEU:HD23	2.37	0.45
2:H:145:LYS:HD3	2:H:146:ASP:CG	2.37	0.45
1:M:33:LEU:HD13	1:M:71:PHE:CD1	2.53	0.44
1:M:137:ASN:ND2	1:M:138:ASN:N	2.65	0.44
2:H:95:GLU:HG3	2:H:100(H):GLY:CA	2.48	0.44
2:I:228:LYS:HD2	2:I:228:LYS:C	2.38	0.43
2:I:93:ALA:HB1	2:I:100(J):PHE:HB3	2.00	0.43
2:I:193:VAL:HG11	2:I:206:TYR:CE1	2.52	0.43
1:M:120:PRO:HD3	1:M:132:VAL:HG22	2.00	0.43
1:L:191:VAL:HG22	1:L:210:ASN:ND2	2.32	0.43
2:H:1:GLN:HA	2:H:100(B):TRP:CE2	2.53	0.43
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.53	0.43
1:M:190:LYS:O	1:M:210:ASN:HA	2.19	0.43
1:M:125:LEU:O	1:M:183:LYS:HD2	2.19	0.43
2:H:187:LEU:C	2:H:187:LEU:HD12	2.39	0.43
2:I:36:TRP:CE2	2:I:80:LEU:HB2	2.54	0.43
2:I:47:TRP:CZ2	2:I:49:GLY:HA2	2.53	0.43
4:L:701:GOL:C3	2:H:187:LEU:HA	2.49	0.43
1:M:193:ALA:CB	1:M:208:SER:HB3	2.49	0.43
2:I:6:GLN:HE22	2:I:91:TYR:HA	1.83	0.42
1:L:1:GLU:HG3	1:L:95:LEU:HD13	2.01	0.42
1:L:47:LEU:O	1:L:55:PRO:HD2	2.19	0.42
1:M:140:TYR:CG	1:M:141:PRO:HA	2.55	0.42
1:M:187:GLU:HA	1:M:211:ARG:NE	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:LEU:HD23	1:L:176:SER:N	2.34	0.41
1:L:181:LEU:N	1:L:181:LEU:HD12	2.35	0.41
1:M:124:GLN:O	1:M:127:SER:HB2	2.20	0.41
2:I:172:HIS:HB2	2:I:190:VAL:HG23	2.00	0.41
2:I:58:ASN:HB2	3:Q:672:TRP:CD1	2.55	0.41
2:I:169:GLY:O	2:I:191:VAL:HA	2.20	0.41
2:H:211:ASN:ND2	2:H:218:LYS:HE2	2.34	0.41
2:H:94:ARG:HG2	2:H:95:GLU:N	2.35	0.41
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.55	0.41
1:L:129:THR:HG22	1:L:130:ALA:N	2.36	0.41
2:H:43:ARG:HH21	2:H:43:ARG:HG3	1.85	0.41
2:I:162:ASN:HD21	2:I:206:TYR:HA	1.86	0.41
1:M:33:LEU:HD13	1:M:71:PHE:CG	2.57	0.41
1:M:137:ASN:ND2	1:M:138:ASN:H	2.18	0.40
1:M:50:GLY:O	1:M:51:ALA:HB3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:462:HOH:O	5:H:462:HOH:O 2_555	1.59	0.61

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	L	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
1	M	212/214 (99%)	198 (93%)	13 (6%)	1 (0%)	34	35
2	H	231/232 (100%)	222 (96%)	6 (3%)	3 (1%)	15	11
2	I	226/232 (97%)	209 (92%)	16 (7%)	1 (0%)	39	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	10/13 (77%)	10 (100%)	0	0	100	100
3	Q	10/13 (77%)	10 (100%)	0	0	100	100
All	All	901/918 (98%)	857 (95%)	39 (4%)	5 (1%)	30	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	133	THR
2	H	135	GLY
1	M	138	ASN
2	H	130	SER
2	I	100(E)	LYS

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	L	184/184 (100%)	180 (98%)	4 (2%)	60	72
1	M	184/184 (100%)	177 (96%)	7 (4%)	40	49
2	H	192/191 (100%)	187 (97%)	5 (3%)	54	66
2	I	187/191 (98%)	183 (98%)	4 (2%)	61	74
3	P	10/11 (91%)	9 (90%)	1 (10%)	9	8
3	Q	10/11 (91%)	9 (90%)	1 (10%)	9	8
All	All	767/772 (99%)	745 (97%)	22 (3%)	50	62

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	77	ARG
1	L	95	LEU
1	L	105	GLU
1	L	108	ARG
2	H	82	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	82(C)	LEU
2	H	151	PRO
2	H	187	LEU
2	H	232	LYS
1	M	13	LEU
1	M	78	LEU
1	M	90	GLN
1	M	91	TYR
1	M	105	GLU
1	M	108	ARG
1	M	137	ASN
2	I	83	ARG
2	I	149	PRO
2	I	151	PRO
2	I	228	LYS
3	P	671	ASN
3	Q	671	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	11	GLN
1	L	31	ASN
1	L	37	GLN
1	L	42	GLN
1	L	93	GLN
1	L	160	GLN
1	L	198	HIS
1	L	210	ASN
2	H	6	GLN
2	H	58	ASN
2	H	82(A)	ASN
2	H	211	ASN
2	H	212	HIS
1	M	30	ASN
1	M	31	ASN
1	M	37	GLN
1	M	42	GLN
1	M	93	GLN
1	M	124	GLN
1	M	137	ASN
1	M	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	189	HIS
1	M	198	HIS
2	I	6	GLN
2	I	58	ASN
2	I	64	GLN
2	I	102	HIS
2	I	162	ASN
2	I	179	GLN
2	I	211	ASN
3	P	671	ASN
3	P	677	ASN
3	Q	671	ASN
3	Q	677	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	L	701	-	5,5,5	4.91	5 (100%)	5,5,5	5.79	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	L	702	-	5,5,5	4.82	5 (100%)	5,5,5	5.66	3 (60%)
4	GOL	L	703	-	5,5,5	4.77	5 (100%)	5,5,5	5.71	3 (60%)

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	L	701	-	-	0/4/4/4	0/0/0/0
4	GOL	L	702	-	-	0/4/4/4	0/0/0/0
4	GOL	L	703	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	701	GOL	C3-C2	-8.50	1.19	1.52
4	L	702	GOL	C3-C2	-8.21	1.21	1.52
4	L	703	GOL	C3-C2	-7.99	1.21	1.52
4	L	701	GOL	O2-C2	-3.25	1.33	1.43
4	L	702	GOL	C1-C2	-3.25	1.39	1.52
4	L	701	GOL	C1-C2	-3.19	1.40	1.52
4	L	703	GOL	C1-C2	-3.17	1.40	1.52
4	L	702	GOL	O2-C2	-2.82	1.35	1.43
4	L	703	GOL	O2-C2	-2.78	1.35	1.43
4	L	701	GOL	O3-C3	2.81	1.54	1.42
4	L	702	GOL	O3-C3	3.29	1.56	1.42
4	L	703	GOL	O3-C3	3.42	1.57	1.42
4	L	702	GOL	O1-C1	4.39	1.61	1.42
4	L	701	GOL	O1-C1	4.42	1.61	1.42
4	L	703	GOL	O1-C1	4.51	1.61	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	701	GOL	O1-C1-C2	3.07	125.08	110.18
4	L	702	GOL	O1-C1-C2	3.17	125.55	110.18
4	L	703	GOL	O1-C1-C2	3.31	126.22	110.18
4	L	701	GOL	O2-C2-C3	6.38	137.92	108.65
4	L	702	GOL	O2-C2-C3	6.62	138.99	108.65
4	L	703	GOL	O2-C2-C3	6.62	139.02	108.65
4	L	702	GOL	O3-C3-C2	10.28	160.05	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	703	GOL	O3-C3-C2	10.39	160.58	110.18
4	L	701	GOL	O3-C3-C2	10.83	162.69	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	701	GOL	2	0
4	L	703	GOL	2	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	L	214/214 (100%)	-0.38	0 100 100	10, 18, 30, 45	0
1	M	214/214 (100%)	0.51	13 (6%) 25 24	26, 46, 62, 75	0
2	H	232/232 (100%)	-0.06	10 (4%) 39 38	10, 18, 45, 67	0
2	I	228/232 (98%)	0.37	16 (7%) 19 19	19, 38, 71, 88	0
3	P	12/13 (92%)	0.04	0 100 100	16, 24, 42, 43	0
3	Q	12/13 (92%)	0.18	0 100 100	21, 34, 43, 47	0
All	All	912/918 (99%)	0.11	39 (4%) 39 38	10, 28, 62, 88	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	THR	11.8
2	I	133	THR	6.8
2	I	100(B)	TRP	6.4
2	I	100	TRP	6.1
2	I	100(D)	GLY	6.1
2	I	135	GLY	6.0
2	H	130	SER	5.5
2	I	130	SER	5.2
2	I	134	SER	5.2
2	I	99	GLY	5.1
2	I	129	LYS	4.8
2	I	228	LYS	4.7
2	H	134	SER	4.6
2	I	100(C)	LEU	4.4
2	I	100(A)	GLY	3.5
1	M	190	LYS	3.4
1	M	126	LYS	3.3
1	M	212	GLY	3.3
2	H	230	CYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	129	LYS	3.1
1	M	213	GLU	3.0
2	H	128	SER	3.0
1	M	191	VAL	2.9
2	H	135	GLY	2.9
1	M	205	VAL	2.9
1	M	77	ARG	2.7
2	I	128	SER	2.6
2	I	198	LEU	2.6
1	M	194	CYS	2.6
2	I	200	THR	2.6
1	M	125	LEU	2.4
1	M	208	SER	2.4
1	M	122	ASP	2.3
2	H	100	TRP	2.2
2	I	138	ALA	2.2
2	H	99	GLY	2.1
1	M	78	LEU	2.0
1	M	192	TYR	2.0
2	H	229	SER	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	L	703	6/6	0.74	0.20	10.44	40,46,47,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	L	701	6/6	0.89	0.22	7.05	20,26,27,32	0
4	GOL	L	702	6/6	0.87	0.17	4.62	43,44,46,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.