



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:34 am GMT

PDB ID : 4NHC
Title : Crystal structure of the HIV-1 neutralizing antibody 4E10 Fab fragment in complex with a hydrocarbon-stapled peptide containing the 4e10 epitope on gp41.
Authors : Irimia, A.; Wilson, I.A.
Deposited on : 2013-11-04
Resolution : 2.91 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

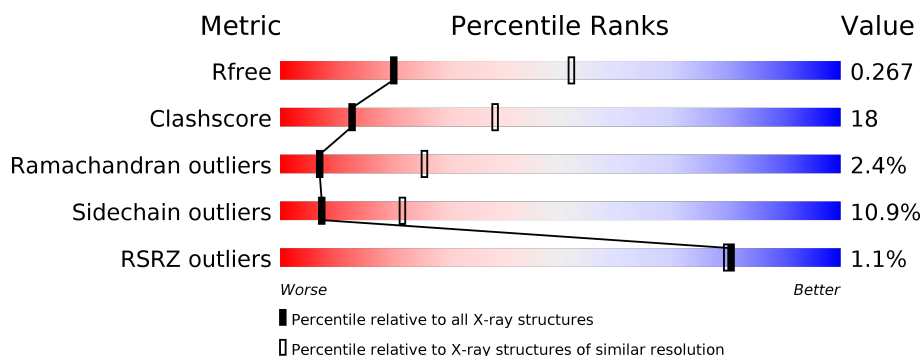
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	100719	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)

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	215	<div> <div></div> <div>69% 26% 6%</div> </div>
2	H	228	<div> <div></div> <div>59% 34% 7%</div> </div>
3	P	17	<div> <div></div> <div>29% 59% 12%</div> </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	TFA	H	302	-	-	-	X
4	TFA	L	301	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3551 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 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	2	0
			1663	1031	288	339	5			

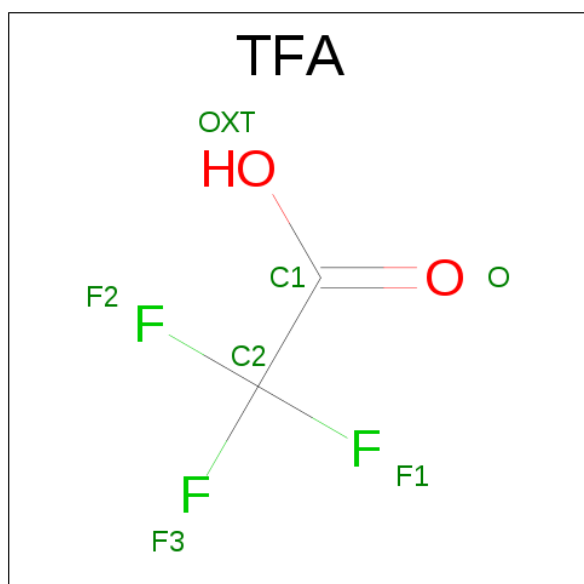
- Molecule 2 is a protein called FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1690	1069	289	327	5			

- Molecule 3 is a protein called MODIFIED FRAGMENT OF HIV GLYCOPROTEIN (GP41).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	17	Total	C	N	O	0	0	0
			150	103	25	22			

- Molecule 4 is TRIFLUOROACETIC ACID (three-letter code: TFA) (formula: $C_2HF_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	F	O	0	0
			7	2	3	2		
4	H	1	Total	C	F	O	0	0
			7	2	3	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	12	Total	O	0	0
			12	12		
6	H	16	Total	O	0	0
			16	16		
6	P	1	Total	O	0	0
			1	1		

i

- Molecule 1: FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	226.11Å 226.11Å 41.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.95 – 2.91 48.95 – 2.91	Depositor EDS
% Data completeness (in resolution range)	95.5 (48.95-2.91) 95.5 (48.95-2.91)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.210 , 0.268 0.199 , 0.267	Depositor DCC
R_{free} test set	688 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	63.8	Xtrriage
Anisotropy	0.659	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3551	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: PO4, TFA, DIV, ACE, MK8

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	0.26	0/1696	0.46	0/2297
2	H	0.26	0/1733	0.45	0/2366
3	P	0.89	2/134 (1.5%)	1.26	2/175 (1.1%)
All	All	0.31	2/3563 (0.1%)	0.51	2/4838 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	682	ILE	C-N	5.31	1.46	1.34
3	P	679	LEU	C-N	5.20	1.46	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	670	ACE	O-C-N	8.06	135.60	122.70
3	P	670	ACE	C-N-CA	-7.67	102.51	121.70

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	1663	0	1611	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1690	0	1679	78	0
3	P	150	0	160	7	0
4	H	7	0	0	0	0
4	L	7	0	0	1	0
5	H	5	0	0	0	0
6	H	16	0	0	0	0
6	L	12	0	0	2	0
6	P	1	0	0	0	0
All	All	3551	0	3450	129	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 18.

All (129) 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:213:GLU:HA	1:L:214:CYS:HB2	1.29	1.06
1:L:185:ASP:HB3	1:L:188:LYS:HE3	1.50	0.93
2:H:105:GLN:HE21	2:H:105:GLN:H	0.96	0.91
2:H:100(A):GLY:N	2:H:100(B):TRP:HA	1.85	0.89
1:L:213:GLU:HA	1:L:214:CYS:CB	2.04	0.87
2:H:100(A):GLY:HA2	2:H:100(B):TRP:CD1	2.11	0.85
2:H:126:PRO:HG3	2:H:140:LEU:HB3	1.60	0.83
1:L:213:GLU:CA	1:L:214:CYS:HB2	2.10	0.81
2:H:105:GLN:NE2	2:H:105:GLN:H	1.76	0.81
2:H:100(A):GLY:C	2:H:100(B):TRP:HD1	1.87	0.78
2:H:105:GLN:N	2:H:105:GLN:HE21	1.78	0.78
2:H:28:SER:HB3	2:H:32:TYR:HE2	1.51	0.76
1:L:12:SER:HB3	1:L:105:GLU:HG2	1.70	0.74
2:H:100:TRP:C	2:H:100(B):TRP:HA	2.09	0.72
2:H:30:SER:HA	2:H:52(A):PRO:HB2	1.72	0.71
2:H:100(D):GLY:O	2:H:100(E):LYS:HB3	1.90	0.71
2:H:52:ILE:HB	2:H:56:ILE:HG13	1.73	0.70
2:H:6:GLN:H	2:H:105:GLN:HE22	1.36	0.70
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.73	0.69
2:H:28:SER:HB3	2:H:32:TYR:CE2	2.28	0.68
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.59	0.68
2:H:100(A):GLY:CA	2:H:100(B):TRP:CD1	2.77	0.67
2:H:176:ALA:HB2	2:H:187:LEU:HD23	1.78	0.66
2:H:100(A):GLY:HA2	2:H:100(B):TRP:HD1	1.61	0.65
2:H:100(A):GLY:CA	2:H:100(B):TRP:HD1	2.07	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:117:LYS:HG3	2:H:118:GLY:O	1.98	0.64
1:L:132:VAL:HG23	1:L:179:LEU:HB3	1.81	0.62
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.81	0.61
2:H:171:VAL:HG22	2:H:191:VAL:HB	1.83	0.60
1:L:207:LYS:HE2	4:L:301:TFA:F2	1.90	0.60
3:P:678:DIV:O	3:P:682:ILE:HD12	2.01	0.59
1:L:47:LEU:O	1:L:48:ILE:HD12	2.02	0.59
2:H:98:THR:HB	2:H:100(E):LYS:HG2	1.86	0.58
2:H:117:LYS:HE2	2:H:146:ASP:O	2.03	0.58
2:H:6:GLN:NE2	2:H:92:CYS:H	2.01	0.58
1:L:183:LYS:O	1:L:186:TYR:HB3	2.04	0.58
1:L:13:LEU:HD13	1:L:78:LEU:HD11	1.86	0.57
1:L:147:GLN:HG2	1:L:154:LEU:HD11	1.87	0.56
1:L:213:GLU:HG3	1:L:214:CYS:HB2	1.87	0.56
2:H:100(A):GLY:C	2:H:100(B):TRP:CD1	2.73	0.56
2:H:41:PRO:HD3	2:H:87:THR:O	2.06	0.55
2:H:203:GLN:HG3	2:H:205:THR:N	2.23	0.54
1:L:124:GLN:HG2	1:L:129:THR:O	2.08	0.54
2:H:226:GLU:HB2	2:H:227:PRO:HD2	1.90	0.54
2:H:13:ARG:HG2	2:H:14:PRO:HD2	1.89	0.54
1:L:154:LEU:HD12	1:L:155:GLN:H	1.73	0.53
1:L:161:GLU:HA	1:L:176:SER:O	2.08	0.53
1:L:214:CYS:HA	2:H:228:LYS:HB3	1.91	0.52
1:L:159:SER:HA	1:L:178:THR:O	2.09	0.52
2:H:97:THR:HA	2:H:100(E):LYS:O	2.09	0.52
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.43	0.51
2:H:169:GLY:O	2:H:191:VAL:HA	2.12	0.50
2:H:83:ARG:HG2	2:H:86:ASP:OD2	2.11	0.50
2:H:37:VAL:O	2:H:91:TYR:HB2	2.12	0.50
3:P:671:ASN:HB3	3:P:674:ASN:OD1	2.12	0.50
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.77	0.50
2:H:63:PHE:O	2:H:66:ARG:HB3	2.13	0.49
2:H:6:GLN:H	2:H:105:GLN:NE2	2.06	0.49
2:H:19:THR:HB	2:H:81:GLU:HG3	1.93	0.49
1:L:120:PRO:HD3	1:L:132:VAL:HG13	1.94	0.49
2:H:176:ALA:HA	2:H:187:LEU:HB3	1.94	0.48
1:L:67:SER:O	1:L:69:THR:N	2.47	0.48
1:L:61:ARG:HG3	6:L:403:HOH:O	2.12	0.48
1:L:150:VAL:HG22	1:L:192:TYR:CD2	2.49	0.48
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.95	0.47
1:L:34:ALA:HA	1:L:48:ILE:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:SER:HA	2:H:133:THR:HG22	1.95	0.47
2:H:58:ASN:HB2	3:P:672:TRP:CD1	2.50	0.47
1:L:145[A]:LYS:HD2	1:L:197:THR:HB	1.95	0.47
3:P:675:ILE:O	3:P:678:DIV:HB22	2.15	0.47
2:H:56:ILE:HG12	2:H:56:ILE:H	1.44	0.47
2:H:23:LYS:HE3	2:H:75:THR:O	2.15	0.46
1:L:213:GLU:CG	1:L:214:CYS:HB2	2.45	0.46
2:H:100:TRP:HZ3	2:H:100(C):LEU:HD13	1.80	0.46
1:L:35:TRP:CD2	1:L:73:LEU:HB2	2.51	0.46
2:H:99:GLY:O	2:H:100(A):GLY:N	2.39	0.46
1:L:145[B]:LYS:HB3	1:L:197:THR:HB	1.97	0.46
1:L:59:ALA:HB1	6:L:403:HOH:O	2.16	0.46
2:H:6:GLN:HE22	2:H:91:TYR:HA	1.81	0.46
1:L:38:GLN:O	1:L:84:ALA:HB1	2.16	0.46
2:H:96:GLY:O	2:H:100(G):ILE:HG12	2.16	0.46
1:L:185:ASP:HA	1:L:188:LYS:HG2	1.98	0.45
2:H:99:GLY:C	2:H:100(A):GLY:H	2.20	0.45
2:H:13:ARG:O	2:H:16:SER:HB3	2.17	0.45
1:L:207:LYS:HD3	1:L:207:LYS:HA	1.68	0.45
1:L:13:LEU:HD13	1:L:78:LEU:CD1	2.46	0.45
2:H:100(F):PRO:HG3	3:P:676:THR:C	2.36	0.45
2:H:95:GLU:HA	2:H:100(I):ALA:O	2.17	0.44
1:L:182:SER:O	1:L:183:LYS:C	2.54	0.44
2:H:16:SER:OG	2:H:17:SER:N	2.50	0.44
2:H:198:LEU:HA	2:H:198:LEU:HD12	1.77	0.44
1:L:147:GLN:CG	1:L:154:LEU:HD11	2.48	0.44
1:L:49:TYR:O	1:L:53:SER:HB2	2.17	0.44
2:H:12:LYS:HG3	2:H:18:VAL:HB	2.00	0.44
2:H:212:HIS:CD2	2:H:214:PRO:HD2	2.53	0.44
2:H:17:SER:OG	2:H:82(A):ASN:HB3	2.17	0.44
1:L:124:GLN:HE22	1:L:131:SER:CB	2.32	0.43
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.53	0.43
2:H:87:THR:HG23	2:H:110:THR:HA	2.00	0.43
2:H:98:THR:CB	2:H:100(E):LYS:HG2	2.49	0.43
1:L:32:LYS:HB3	1:L:91:TYR:CD2	2.53	0.43
1:L:187:GLU:HA	1:L:211:ARG:NH2	2.33	0.43
1:L:32:LYS:HB3	1:L:91:TYR:CE2	2.53	0.43
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.54	0.43
2:H:207:ILE:HD12	2:H:207:ILE:N	2.34	0.42
2:H:140:LEU:CD1	2:H:191:VAL:HG13	2.50	0.42
2:H:14:PRO:HA	2:H:82(C):LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:LEU:HA	1:L:107:LYS:HE3	2.01	0.42
2:H:213:LYS:N	2:H:214:PRO:CD	2.82	0.42
2:H:70:THR:HG22	2:H:71:ALA:N	2.35	0.42
2:H:63:PHE:HB3	2:H:67:ILE:HG21	2.01	0.42
1:L:137:ASN:HD21	2:H:172:HIS:CD2	2.37	0.42
2:H:98:THR:O	2:H:99:GLY:O	2.37	0.42
1:L:7:SER:HA	1:L:8:PRO:C	2.40	0.41
3:P:685:LYS:HA	3:P:685:LYS:HD2	1.37	0.41
2:H:100(B):TRP:CD1	2:H:100(B):TRP:N	2.86	0.41
1:L:192:TYR:HE1	1:L:211:ARG:HD3	1.85	0.41
2:H:35:SER:HA	2:H:50:GLY:HA2	2.01	0.41
2:H:63:PHE:O	2:H:67:ILE:HG22	2.20	0.41
1:L:184:ALA:HA	1:L:187:GLU:H	1.86	0.41
2:H:184:LEU:N	2:H:184:LEU:HD22	2.36	0.41
1:L:175:LEU:C	1:L:175:LEU:HD23	2.40	0.41
3:P:677:ASN:O	3:P:678:DIV:C	2.69	0.41
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.61	0.40
2:H:70:THR:CG2	2:H:71:ALA:N	2.84	0.40
1:L:191:VAL:HG12	1:L:210:ASN:OD1	2.21	0.40
2:H:83:ARG:H	2:H:83:ARG:HG2	1.79	0.40
2:H:100(A):GLY:N	2:H:100(B):TRP:CA	2.68	0.40
2:H:94:ARG:HH12	2:H:100(C):LEU:HD12	1.87	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	L	215/215 (100%)	201 (94%)	10 (5%)	4 (2%)	9	32
2	H	226/228 (99%)	203 (90%)	16 (7%)	7 (3%)	5	19
3	P	13/17 (76%)	10 (77%)	3 (23%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	454/460 (99%)	414 (91%)	29 (6%)	11 (2%)	7	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	66	ARG
1	L	40	PRO
1	L	68	GLY
1	L	157	GLY
2	H	99	GLY
2	H	100(E)	LYS
2	H	53	LEU
1	L	211	ARG
2	H	227	PRO
2	H	100	TRP
2	H	2	VAL

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	187/185 (101%)	168 (90%)	19 (10%)	8	25
2	H	187/187 (100%)	165 (88%)	22 (12%)	6	18
3	P	14/14 (100%)	12 (86%)	2 (14%)	4	11
All	All	388/386 (100%)	345 (89%)	43 (11%)	7	21

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	12	SER
1	L	13	LEU
1	L	18	ARG
1	L	20	THR
1	L	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	52	SER
1	L	70	ASP
1	L	95	LEU
1	L	105	GLU
1	L	132	VAL
1	L	145[A]	LYS
1	L	145[B]	LYS
1	L	147	GLN
1	L	161	GLU
1	L	165	GLU
1	L	185	ASP
1	L	191	VAL
1	L	210	ASN
1	L	213	GLU
2	H	19	THR
2	H	22	CYS
2	H	54	LEU
2	H	56	ILE
2	H	67	ILE
2	H	68	THR
2	H	81	GLU
2	H	82(A)	ASN
2	H	94	ARG
2	H	100(E)	LYS
2	H	105	GLN
2	H	140	LEU
2	H	153	THR
2	H	167	THR
2	H	168	SER
2	H	177	VAL
2	H	198	LEU
2	H	200	THR
2	H	209	ASN
2	H	217	THR
2	H	219	VAL
2	H	228	LYS
3	P	685	LYS
3	P	686	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	ASN
1	L	124	GLN
1	L	137	ASN
1	L	138	ASN
2	H	1	GLN
2	H	6	GLN
2	H	105	GLN
2	H	179	GLN
2	H	211	ASN
3	P	677	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	DIV	P	678	3	3,6,7	0.82	0	3,8,10	2.38	2 (66%)
3	MK8	P	681	3	6,8,9	0.83	0	4,10,12	1.19	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
3	DIV	P	678	3	-	0/3/6/9	0/0/0/0
3	MK8	P	681	3	-	0/6/8/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	678	DIV	CB2-CA-CB1	-2.13	107.03	111.17
3	P	678	DIV	CG1-CB1-CA	3.52	123.83	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	678	DIV	3	0

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	$\# Z > 2$
5	PO4	H	301	-	4,4,4	0.78	0	6,6,6	0.39	0
4	TFA	H	302	-	3,6,6	0.13	0	3,9,9	1.00	0
4	TFA	L	301	-	3,6,6	0.11	0	3,9,9	0.99	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
5	PO4	H	301	-	-	0/0/0/0	0/0/0/0
4	TFA	H	302	-	-	0/0/6/6	0/0/0/0
4	TFA	L	301	-	-	0/0/6/6	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	TFA	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	215/215 (100%)	-0.10	3 (1%) 75 75	49, 68, 96, 135	0
2	H	228/228 (100%)	-0.17	2 (0%) 84 83	44, 65, 96, 163	1 (0%)
3	P	14/17 (82%)	0.17	0 100 100	56, 74, 114, 118	0
All	All	457/460 (99%)	-0.13	5 (1%) 80 80	44, 68, 97, 163	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	100(B)	TRP	2.7
1	L	214	CYS	2.5
1	L	192	TYR	2.1
2	H	100	TRP	2.1
1	L	213	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	DIV	P	678	7/8	0.96	0.15	-	68,70,73,74	0
3	MK8	P	681	9/10	0.95	0.24	-	64,73,81,84	1

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	TFA	H	302	7/7	0.77	0.53	10.11	121,122,123,124	0
4	TFA	L	301	7/7	0.78	0.34	4.85	103,106,110,116	7
5	PO4	H	301	5/5	0.95	0.14	-1.24	109,109,110,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.