Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 06:39 AM EST

PDB ID	:	1MPA
Title	:	BACTERICIDAL ANTIBODY AGAINST NEISSERIA MENINGITIDIS
Authors	:	Van Den Elsen, J.M.H.; Herron, J.N.; Kroon, J.; Gros, P.
Deposited on	:	1997-02-26
Resolution	:	2.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

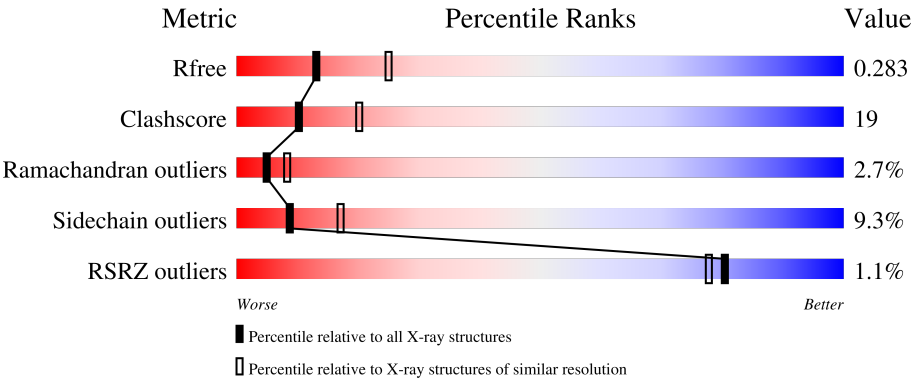
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of 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 <=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	219	53% 42% 5%
2	H	225	2% 64% 29% 5%
3	P	9	44% 44% 11%

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
3	CYF	P	9	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4279 atoms, of which 747 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 MN12H2 IGG2A-KAPPA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	219	Total	C	H	N	O	S	0	0	0
			2043	1057	348	292	339	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ILE	VAL	conflict	PIR PC4203
L	3	VAL	LEU	conflict	PIR PC4203
L	18	LYS	GLN	conflict	PIR PC4203
L	28	ALA	SER	conflict	PIR PC4203
L	29	LEU	ILE	conflict	PIR PC4203
L	32	SER	THR	conflict	PIR PC4203
L	39	HIS	GLU	conflict	PIR PC4203
L	91	PHE	TYR	conflict	PIR PC4203
L	92	PHE	TYR	conflict	PIR PC4203
L	94	SER	PHE	conflict	PIR PC4203
L	96	SER	GLY	conflict	PIR PC4203
L	97	THR	SER	conflict	PIR PC4203

- Molecule 2 is a protein called MN12H2 IGG2A-KAPPA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	225	Total	C	H	N	O	S	0	0	0
			2065	1089	348	282	338	8			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	9	THR	PRO	conflict	PIR S38950
H	10	VAL	GLU	conflict	PIR S38950
H	12	ALA	VAL	conflict	PIR S38950
H	19	ARG	LYS	conflict	PIR S38950

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Chain	Residue	Modelled	Actual	Comment	Reference
H	20	MET	ILE	conflict	PIR S38950
H	28	SER	THR	conflict	PIR S38950
H	31	SER	ASP	conflict	PIR S38950
H	33	TRP	TYR	conflict	PIR S38950
H	34	LEU	ILE	conflict	PIR S38950
H	37	ILE	VAL	conflict	PIR S38950
H	43	GLN	GLU	conflict	PIR S38950
H	50	GLY	TRP	conflict	PIR S38950
H	55	ASN	SER	conflict	PIR S38950
H	56	ARG	GLY	conflict	PIR S38950
H	57	ASP	ASN	conflict	PIR S38950
H	59	ARG	LYS	conflict	PIR S38950
H	61	THR	ASN	conflict	PIR S38950
H	62	GLN	GLU	conflict	PIR S38950
H	63	ARG	LYS	conflict	PIR S38950
H	66	ASP	GLY	conflict	PIR S38950
H	69	LYS	THR	conflict	PIR S38950
H	72	ALA	VAL	conflict	PIR S38950
H	73	VAL	ASP	conflict	PIR S38950
H	76	ALA	SER	conflict	PIR S38950
H	77	ASN	SER	conflict	PIR S38950
H	82	GLU	GLN	conflict	PIR S38950
H	88	ASN	SER	conflict	PIR S38950
H	95	TYR	PHE	conflict	PIR S38950
H	97	SER	-	insertion	PIR S38950
H	98	ILE	-	insertion	PIR S38950
H	99	ILE	-	insertion	PIR S38950
H	100	TYR	-	insertion	PIR S38950
H	101	PHE	ALA	conflict	PIR S38950
H	102	ASP	ARG	conflict	PIR S38950
H	103	TYR	GLY	conflict	PIR S38950
H	104	ALA	GLY	conflict	PIR S38950
H	105	ASP	LYS	conflict	PIR S38950
H	107	ILE	ALA	conflict	PIR S38950
H	116	THR	SER	conflict	PIR S38950

- Molecule 3 is a protein called PORA P1.16 PEPTIDE FLUORESCEIN CONJUGATE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	P	9	Total	C	H	N	O	S	0	0	0
			119	63	17	15	23	1			

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total Cd 1 1	0	0

- Molecule 5 is water.

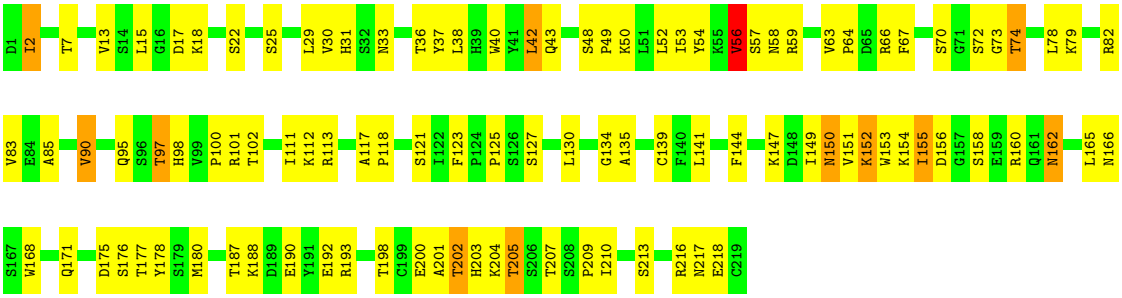
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	8	Total H O 24 16 8	0	0
5	H	8	Total H O 24 16 8	0	0
5	P	1	Total H O 3 2 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

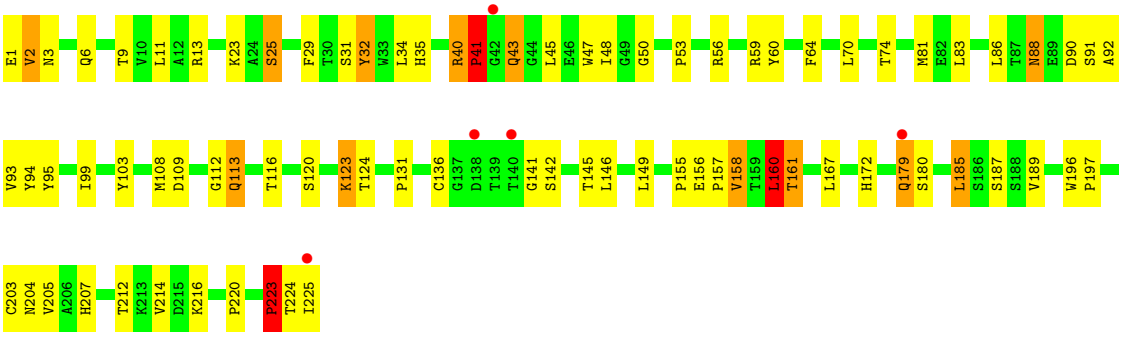
• Molecule 1: MN12H2 IGG2A-KAPPA

Chain L:



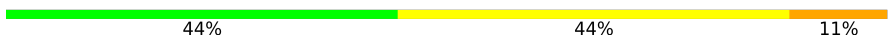
• Molecule 2: MN12H2 IGG2A-KAPPA

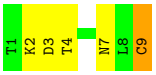
Chain H:



• Molecule 3: PORA P1.16 PEPTIDE FLUORESCEIN CONJUGATE

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.68Å 69.10Å 72.95Å 90.00° 112.01° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.3 (8.00-2.60) 92.3 (8.00-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.59Å)	Xtriage
Refinement program	X-PLOR 3.63	Depositor
R, R_{free}	0.194 , 0.309 0.182 , 0.283	Depositor DCC
R_{free} test set	1522 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4279	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 7.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CD, THC, CYF

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	0.55	0/1733	0.80	0/2348
2	H	0.54	0/1763	0.81	2/2411 (0.1%)
3	P	0.56	0/55	0.99	0/73
All	All	0.54	0/3551	0.81	2/4832 (0.0%)

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
3	P	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	156	GLU	N-CA-C	5.91	126.97	111.00
2	H	160	LEU	CA-CB-CG	5.50	127.95	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	P	9	CYF	C10

There are no planarity outliers.

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	L	1695	348	1645	78	0
2	H	1717	348	1669	57	0
3	P	102	17	73	5	0
4	L	1	0	0	0	0
5	H	8	16	0	0	0
5	L	8	16	0	1	0
5	P	1	2	0	0	0
All	All	3532	747	3387	130	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 19.

All (130) 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:37:TYR:HB2	1:L:97:THR:HG22	1.47	0.93
1:L:149:ILE:HG13	1:L:203:HIS:HB2	1.58	0.86
2:H:9:THR:HG23	2:H:116:THR:HG23	1.56	0.85
2:H:161:THR:HG23	2:H:204:ASN:HB2	1.58	0.85
1:L:18:LYS:HD2	1:L:79:LYS:NZ	1.94	0.82
2:H:123:LYS:HD2	2:H:123:LYS:H	1.48	0.78
2:H:2:VAL:HA	2:H:25:SER:O	1.85	0.77
1:L:113:ARG:HD2	1:L:176:SER:HB2	1.67	0.77
2:H:136:CYS:SG	2:H:223:PRO:HD3	2.24	0.77
1:L:29:LEU:O	1:L:97:THR:HG21	1.85	0.77
1:L:101:ARG:HD2	5:L:225:HOH:O	1.89	0.72
2:H:160:LEU:HD22	2:H:205:VAL:HG22	1.70	0.72
1:L:216:ARG:HG2	1:L:217:ASN:OD1	1.90	0.72
1:L:2:ILE:HG13	1:L:2:ILE:O	1.90	0.72
1:L:147:LYS:HD3	1:L:178:TYR:CD2	2.29	0.67
1:L:18:LYS:HD2	1:L:79:LYS:HZ1	1.60	0.66
1:L:59:ARG:HG2	1:L:63:VAL:HB	1.77	0.65
1:L:151:VAL:HG12	1:L:201:ALA:HB2	1.79	0.65
1:L:188:LYS:O	1:L:192:GLU:HG2	1.95	0.65
1:L:66:ARG:HD3	1:L:82:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ILE:CD1	1:L:25:SER:HB2	2.28	0.64
1:L:90:VAL:HG11	2:H:43:GLN:NE2	2.14	0.63
3:P:9:CYF:OL	3:P:9:CYF:HB2	1.98	0.62
2:H:35:HIS:HE1	2:H:99:ILE:HD11	1.63	0.62
1:L:160:ARG:HE	1:L:162:ASN:HB3	1.63	0.61
1:L:43:GLN:HE21	2:H:43:GLN:NE2	1.98	0.61
2:H:167:LEU:HD13	2:H:189:VAL:HG21	1.83	0.60
1:L:90:VAL:HG11	2:H:43:GLN:HE21	1.67	0.60
2:H:41:PRO:HD3	2:H:92:ALA:HA	1.85	0.58
1:L:49:PRO:HG2	2:H:45:LEU:HD11	1.86	0.58
2:H:29:PHE:CE2	2:H:53:PRO:HB3	2.39	0.58
1:L:150:ASN:N	1:L:150:ASN:HD22	2.02	0.57
2:H:197:PRO:HB3	2:H:220:PRO:HG3	1.87	0.57
1:L:37:TYR:CB	1:L:97:THR:HG22	2.27	0.57
2:H:81:MET:HE3	2:H:83:LEU:HD21	1.87	0.56
1:L:149:ILE:HG22	1:L:168:TRP:CH2	2.40	0.56
2:H:86:LEU:HA	2:H:90:ASP:OD2	2.05	0.56
1:L:121:SER:O	1:L:139:CYS:HA	2.06	0.55
2:H:32:TYR:CD1	2:H:32:TYR:N	2.73	0.55
2:H:160:LEU:HD22	2:H:205:VAL:CG2	2.37	0.55
2:H:35:HIS:CG	2:H:47:TRP:HE1	2.25	0.54
2:H:146:LEU:HD22	2:H:146:LEU:N	2.22	0.54
1:L:40:TRP:CE2	1:L:78:LEU:HB2	2.43	0.53
2:H:158:VAL:HG23	2:H:207:HIS:HD2	1.72	0.53
1:L:15:LEU:HD22	1:L:15:LEU:N	2.24	0.53
1:L:165:LEU:HD21	2:H:179:GLN:HG2	1.91	0.53
2:H:123:LYS:HD2	2:H:123:LYS:N	2.19	0.53
1:L:150:ASN:HD22	1:L:150:ASN:H	1.57	0.53
1:L:202:THR:HG23	1:L:209:PRO:HB3	1.91	0.53
2:H:99:ILE:HA	2:H:108:MET:O	2.08	0.53
2:H:94:TYR:N	2:H:94:TYR:CD1	2.77	0.53
1:L:152:LYS:HB3	1:L:200:GLU:HG3	1.92	0.52
1:L:53:ILE:HA	1:L:58:ASN:O	2.10	0.51
1:L:147:LYS:O	1:L:147:LYS:HG3	2.10	0.51
3:P:2:LYS:HA	3:P:7:ASN:O	2.09	0.51
2:H:124:THR:HG23	2:H:155:PRO:HD3	1.91	0.51
3:P:4:THR:O	3:P:4:THR:HG22	2.11	0.51
1:L:175:ASP:HB3	1:L:177:THR:HG23	1.91	0.51
1:L:149:ILE:HG22	1:L:168:TRP:HH2	1.75	0.50
1:L:150:ASN:HD21	1:L:202:THR:CB	2.24	0.50
2:H:131:PRO:HB3	2:H:216:LYS:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:THR:OG1	1:L:190:GLU:HG3	2.12	0.50
2:H:60:TYR:CE2	2:H:70:LEU:HG	2.47	0.50
2:H:6:GLN:OE1	2:H:112:GLY:HA3	2.12	0.50
1:L:48:SER:HB3	2:H:95:TYR:CE2	2.47	0.49
2:H:35:HIS:CE1	2:H:99:ILE:HD11	2.47	0.49
2:H:48:ILE:HG23	2:H:64:PHE:CG	2.48	0.49
1:L:190:GLU:O	1:L:193:ARG:HG2	2.13	0.49
1:L:85:ALA:HA	1:L:111:ILE:HD11	1.94	0.48
1:L:123:PHE:HZ	2:H:145:THR:O	1.96	0.48
1:L:171:GLN:HG2	1:L:176:SER:HA	1.96	0.48
1:L:54:TYR:O	1:L:58:ASN:HB2	2.13	0.48
2:H:123:LYS:N	2:H:123:LYS:CD	2.76	0.48
1:L:15:LEU:HD11	1:L:111:ILE:HD13	1.96	0.47
1:L:64:PRO:HD2	1:L:67:PHE:CE2	2.49	0.47
2:H:11:LEU:HD13	2:H:155:PRO:HG3	1.96	0.47
1:L:117:ALA:N	1:L:205:THR:HG21	2.29	0.47
1:L:154:LYS:HA	1:L:158:SER:O	2.14	0.47
1:L:118:PRO:CA	1:L:144:PHE:HB3	2.45	0.47
1:L:166:ASN:HB3	1:L:180:MET:HE1	1.96	0.47
2:H:123:LYS:H	2:H:123:LYS:CD	2.21	0.47
1:L:200:GLU:HA	1:L:210:ILE:O	2.15	0.46
2:H:155:PRO:C	2:H:157:PRO:HD2	2.35	0.46
3:P:3:ASP:OD2	3:P:7:ASN:HB2	2.16	0.46
1:L:111:ILE:CG2	1:L:112:LYS:N	2.79	0.46
1:L:125:PRO:HG2	1:L:135:ALA:HB1	1.97	0.46
2:H:212:THR:HG22	2:H:214:VAL:HG23	1.97	0.46
2:H:59:ARG:HD2	3:P:4:THR:OG1	2.16	0.45
2:H:223:PRO:O	2:H:225:ILE:HG22	2.16	0.45
2:H:40:ARG:HD2	2:H:91:SER:O	2.15	0.45
2:H:141:GLY:O	2:H:142:SER:HB2	2.16	0.45
1:L:52:LEU:HA	1:L:63:VAL:HG21	1.99	0.45
2:H:34:LEU:O	2:H:50:GLY:HA2	2.17	0.45
1:L:43:GLN:NE2	2:H:43:GLN:NE2	2.64	0.45
1:L:42:LEU:O	1:L:50:LYS:HG2	2.17	0.44
1:L:95:GLN:OE1	1:L:98:HIS:N	2.50	0.44
1:L:130:LEU:HD23	1:L:134:GLY:O	2.17	0.44
1:L:100:PRO:O	1:L:102:THR:HG23	2.18	0.44
2:H:6:GLN:N	2:H:113:GLN:OE1	2.45	0.44
1:L:56:VAL:CG2	1:L:57:SER:N	2.81	0.44
2:H:172:HIS:O	2:H:187:SER:HA	2.18	0.44
1:L:147:LYS:HB2	1:L:178:TYR:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:VAL:HG11	1:L:83:VAL:HG21	2.00	0.43
1:L:190:GLU:HA	1:L:193:ARG:HE	1.83	0.43
1:L:139:CYS:HB2	1:L:153:TRP:CH2	2.53	0.43
1:L:147:LYS:HD3	1:L:178:TYR:CE2	2.54	0.43
1:L:18:LYS:HD2	1:L:79:LYS:HZ2	1.78	0.43
1:L:2:ILE:HD12	1:L:25:SER:HB2	2.01	0.42
2:H:99:ILE:HG22	2:H:109:ASP:OD2	2.18	0.42
2:H:13:ARG:HD2	2:H:13:ARG:N	2.33	0.42
1:L:217:ASN:C	1:L:218:GLU:HG3	2.40	0.42
2:H:31:SER:HB2	2:H:32:TYR:CE1	2.54	0.42
1:L:123:PHE:CZ	2:H:145:THR:O	2.73	0.42
2:H:48:ILE:HG23	2:H:64:PHE:CB	2.49	0.42
1:L:155:ILE:HG22	1:L:156:ASP:N	2.35	0.42
1:L:130:LEU:HD23	1:L:130:LEU:HA	1.89	0.42
1:L:125:PRO:CG	1:L:135:ALA:HB1	2.50	0.41
1:L:118:PRO:HB3	1:L:144:PHE:HB3	2.01	0.41
2:H:56:ARG:NH2	2:H:74:THR:OG1	2.53	0.41
1:L:152:LYS:N	1:L:200:GLU:O	2.51	0.41
1:L:72:SER:O	1:L:74:THR:N	2.51	0.41
2:H:88:ASN:HD22	2:H:88:ASN:HA	1.61	0.41
2:H:196:TRP:CG	2:H:197:PRO:HA	2.55	0.41
1:L:30:VAL:HG22	1:L:36:THR:OG1	2.20	0.41
1:L:31:HIS:ND1	1:L:33:ASN:ND2	2.69	0.41
1:L:141:LEU:CD1	1:L:151:VAL:HG11	2.51	0.41
1:L:198:THR:HA	1:L:213:SER:HB3	2.02	0.41
2:H:40:ARG:HG3	2:H:41:PRO:HD2	2.03	0.40
2:H:160:LEU:HD23	2:H:185:LEU:HD23	2.02	0.40
1:L:40:TRP:CD2	1:L:78:LEU:HB2	2.56	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	217/219 (99%)	201 (93%)	10 (5%)	6 (3%)	5 7
2	H	223/225 (99%)	195 (87%)	22 (10%)	6 (3%)	5 8
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
All	All	447/453 (99%)	402 (90%)	33 (7%)	12 (3%)	5 8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	155	ILE
2	H	43	GLN
1	L	73	GLY
2	H	224	THR
1	L	162	ASN
1	L	205	THR
2	H	223	PRO
1	L	204	LYS
2	H	2	VAL
2	H	180	SER
1	L	56	VAL
2	H	41	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	196/196 (100%)	180 (92%)	16 (8%)	11 22
2	H	193/193 (100%)	172 (89%)	21 (11%)	6 11
3	P	7/7 (100%)	7 (100%)	0	100 100
All	All	396/396 (100%)	359 (91%)	37 (9%)	9 17

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE

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Mol	Chain	Res	Type
1	L	7	THR
1	L	17	ASP
1	L	22	SER
1	L	38	LEU
1	L	42	LEU
1	L	56	VAL
1	L	70	SER
1	L	74	THR
1	L	90	VAL
1	L	97	THR
1	L	127	SER
1	L	150	ASN
1	L	152	LYS
1	L	202	THR
1	L	207	THR
2	H	1	GLU
2	H	3	ASN
2	H	23	LYS
2	H	25	SER
2	H	32	TYR
2	H	40	ARG
2	H	41	PRO
2	H	88	ASN
2	H	93	VAL
2	H	103	TYR
2	H	113	GLN
2	H	120	SER
2	H	123	LYS
2	H	149	LEU
2	H	158	VAL
2	H	160	LEU
2	H	161	THR
2	H	179	GLN
2	H	185	LEU
2	H	203	CYS
2	H	223	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	58	ASN
1	L	142	ASN

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Mol	Chain	Res	Type
1	L	150	ASN
1	L	194	HIS
2	H	3	ASN
2	H	43	GLN
2	H	62	GLN
2	H	88	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	THC	P	1	3	8,9,10	0.77	0	9,11,13	0.83	0
3	CYF	P	9	3	39,39,39	2.91	10 (25%)	52,56,56	2.38	15 (28%)

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	THC	P	1	3	-	3/8/10/12	-
3	CYF	P	9	3	1/1/6/6	3/20/34/34	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	9	CYF	C14-C10	-8.54	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	9	CYF	C9-C10	-8.15	1.38	1.52
3	P	9	CYF	C11-C10	-6.74	1.40	1.52
3	P	9	CYF	O1-C1	-5.63	1.23	1.37
3	P	9	CYF	O3-C6	-5.30	1.24	1.37
3	P	9	CYF	C19-C20	-4.64	1.39	1.49
3	P	9	CYF	O2-C3	4.07	1.44	1.38
3	P	9	CYF	C17-NL	-4.06	1.33	1.41
3	P	9	CYF	C19-C14	3.38	1.44	1.40
3	P	9	CYF	CAL-CL	-2.27	1.49	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	9	CYF	C17-NL-CL	10.20	145.33	127.50
3	P	9	CYF	C11-C10-C9	9.08	119.38	105.83
3	P	9	CYF	C4-O2-C3	-3.69	110.50	118.58
3	P	9	CYF	O2-C4-C9	3.59	127.33	122.38
3	P	9	CYF	C8-C9-C10	-2.69	121.87	126.14
3	P	9	CYF	C4-C9-C10	-2.53	118.86	121.53
3	P	9	CYF	O2-C4-C5	-2.50	111.49	115.20
3	P	9	CYF	C3-C11-C10	-2.48	118.91	121.53
3	P	9	CYF	C14-C10-C9	2.43	121.42	113.32
3	P	9	CYF	C12-C11-C10	-2.41	122.32	126.14
3	P	9	CYF	OL-CL-NL	2.31	127.85	123.63
3	P	9	CYF	C18-C19-C14	-2.23	118.05	120.33
3	P	9	CYF	O5-C20-O4	-2.20	118.47	123.35
3	P	9	CYF	OL-CL-CAL	-2.02	118.10	121.58
3	P	9	CYF	O5-C20-C19	2.01	121.11	115.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	P	9	CYF	C10

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	1	THC	C-CA-CB-CG2
3	P	9	CYF	C18-C17-NL-CL
3	P	9	CYF	C16-C17-NL-CL
3	P	1	THC	N1-CA-CB-CG2
3	P	1	THC	C-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
3	P	9	CYF	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	9	CYF	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	L	219/219 (100%)	-0.58	0 100 100	6, 34, 66, 77	0
2	H	225/225 (100%)	-0.53	5 (2%) 62 56	8, 33, 69, 100	0
3	P	7/9 (77%)	-0.94	0 100 100	13, 17, 37, 37	0
All	All	451/453 (99%)	-0.56	5 (1%) 80 78	6, 33, 67, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	ASP	6.3
2	H	225	ILE	3.3
2	H	140	THR	3.3
2	H	42	GLY	2.6
2	H	179	GLN	2.3

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

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	THC	P	1	10/11	0.85	0.21	20,42,63,65	0
3	CYF	P	9	36/36	0.95	0.12	5,26,49,53	0

6.3 Carbohydrates

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CD	L	220	1/1	0.98	0.03	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.