



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2017 – 12:27 PM EDT

PDB ID : 5XR8
Title : Crystal structure of the human CB1 in complex with agonist AM841
Authors : Hua, T.; Vemuri, K.; Nikas, P.S.; Laprairie, R.B.; Wu, Y.; Qu, L.; Pu, M.; Korde, A.; Shan, J.; Ho, J.H.; Han, G.W.; Ding, K.; Li, X.; Liu, H.; Hanson, M.A.; Zhao, S.; Bohn, L.M.; Makriyannis, A.; Stevens, R.C.; Liu, Z.J.
Deposited on : unknown
Resolution : 2.95 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 : rb-20030345
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) : rb-20030345

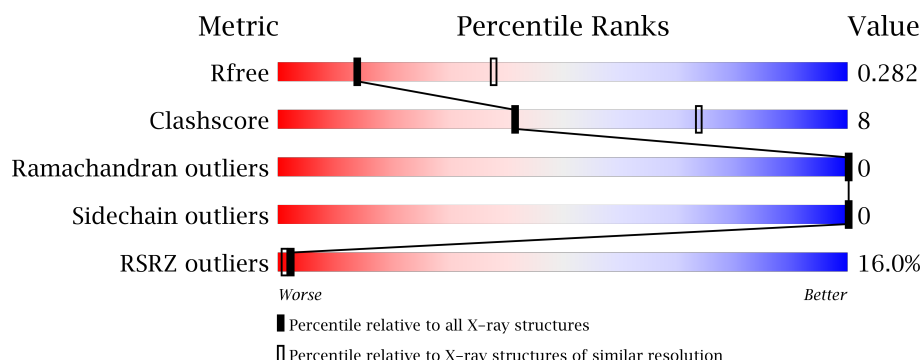
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	<div> <div>16%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3410 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.

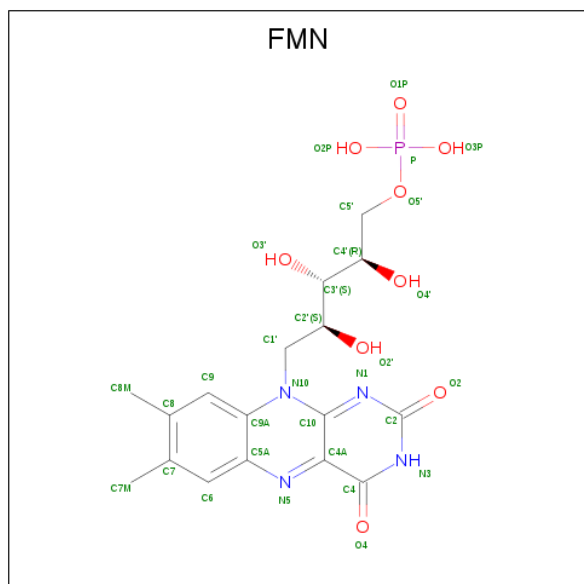
- Molecule 1 is a protein called Cannabinoid receptor 1,Flavodoxin,Cannabinoid receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3314	2163	535	594	22			

There are 6 discrepancies between the modelled and reference sequences:

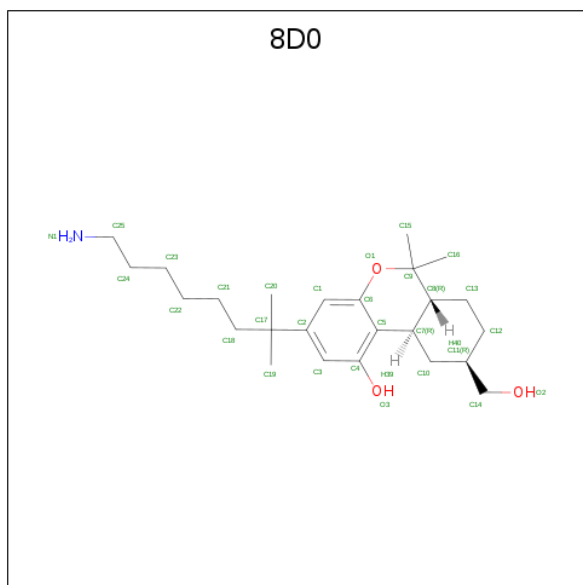
Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	THR	engineered mutation	UNP P21554
A	273	LYS	GLU	engineered mutation	UNP P21554
A	283	VAL	THR	engineered mutation	UNP P21554
A	1002	ALA	-	linker	UNP P21554
A	1098	TRP	TYR	engineered mutation	UNP P00323
A	340	GLU	ARG	engineered mutation	UNP P21554

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



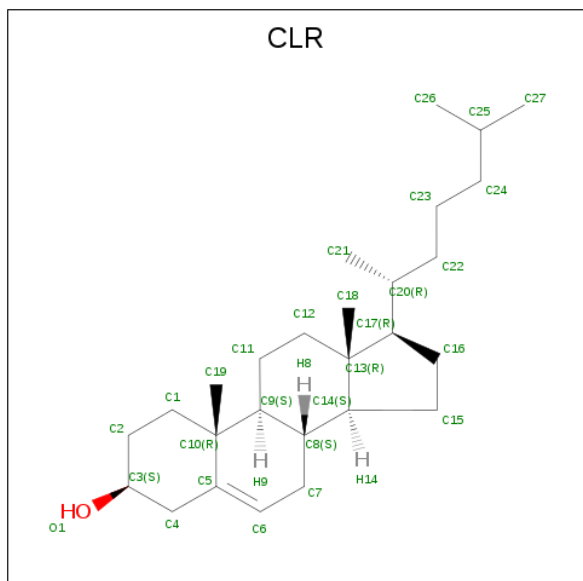
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is (6aR,9R,10aR)-3-(8-azanyl-2-methyl-octan-2-yl)-9-(hydroxymethyl)-6,6-dimethyl-6a,7,8,9,10,10a-hexahydrobenzo[c]chromen-1-ol (three-letter code: 8D0) (formula: $C_{25}H_{41}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	25	1	3		

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

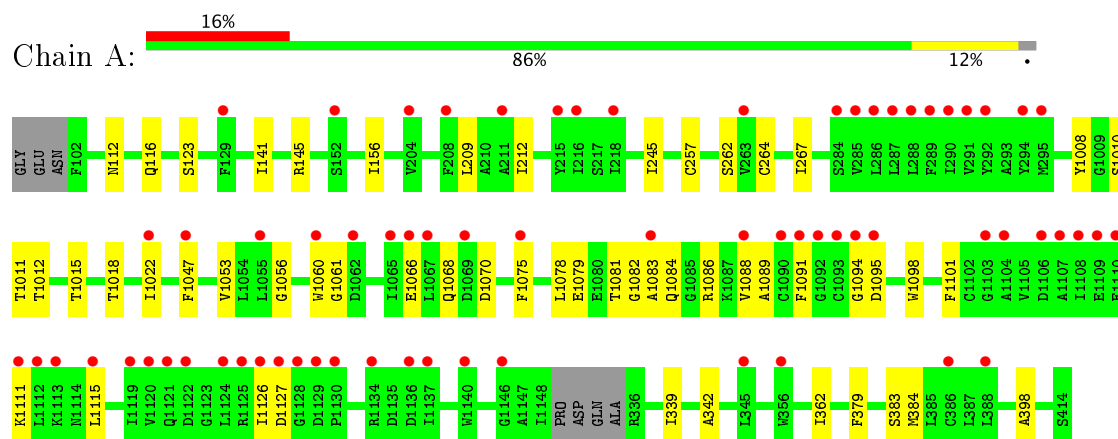
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

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: Cannabinoid receptor 1,Flavodoxin,Cannabinoid receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	66.83 Å 73.61 Å 139.64 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 2.95 49.48 – 2.95	Depositor EDS
% Data completeness (in resolution range)	88.2 (49.48-2.95) 85.6 (49.48-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.96 Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.255 , 0.274 0.259 , 0.282	Depositor DCC
R_{free} test set	598 reflections (4.63%)	DCC
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3410	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: FMN, PEG, CLR, 8D0

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	0.26	0/3389	0.40	0/4613

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3314	0	3298	54	0
2	A	31	0	19	3	0
3	A	29	0	0	1	0
4	A	28	0	46	1	0
5	A	7	0	10	0	0
6	A	1	0	0	0	0
All	All	3410	0	3373	54	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 8.

All (54) 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:A:257:CYS:SG	1:A:264:CYS:SG	1.34	1.16
1:A:257:CYS:CB	1:A:264:CYS:SG	2.36	1.14
1:A:1078:LEU:HD12	1:A:1111:LYS:HD3	1.67	0.77
1:A:257:CYS:SG	1:A:264:CYS:CB	2.75	0.72
1:A:362:ILE:HG21	1:A:379:PHE:HB2	1.73	0.71
1:A:1083:ALA:HB1	1:A:1115:LEU:HD12	1.72	0.70
1:A:1082:GLY:HA3	1:A:1086:ARG:HH21	1.57	0.70
1:A:1075:PHE:O	1:A:1078:LEU:HG	1.93	0.69
1:A:1078:LEU:O	1:A:1081:THR:N	2.27	0.67
1:A:1083:ALA:O	1:A:1084:GLN:HG3	1.95	0.65
1:A:1083:ALA:HB1	1:A:1115:LEU:CD1	2.25	0.65
1:A:1047:PHE:O	1:A:1086:ARG:NH1	2.30	0.64
1:A:1078:LEU:HD12	1:A:1111:LYS:CD	2.26	0.64
1:A:257:CYS:HB3	1:A:264:CYS:SG	2.36	0.63
1:A:1078:LEU:O	1:A:1081:THR:HB	1.99	0.61
1:A:1101:PHE:HE1	1:A:1127:ASP:HB3	1.67	0.59
1:A:1101:PHE:CE1	1:A:1127:ASP:HB3	2.40	0.57
1:A:1061:GLY:N	2:A:1201:FMN:N5	2.52	0.57
1:A:1083:ALA:O	1:A:1084:GLN:CG	2.53	0.56
1:A:1010:SER:HB3	1:A:1015:THR:HB	1.87	0.56
1:A:112:ASN:O	1:A:116:GLN:N	2.37	0.55
1:A:1082:GLY:HA3	1:A:1086:ARG:HE	1.72	0.54
1:A:1012:THR:HB	2:A:1201:FMN:O3P	2.11	0.51
1:A:156:ILE:HD11	1:A:398:ALA:HB2	1.92	0.51
1:A:1127:ASP:N	1:A:1127:ASP:OD1	2.44	0.50
1:A:1008:TYR:HA	1:A:1056:GLY:O	2.11	0.50
1:A:1011:THR:HB	1:A:1060:TRP:CZ2	2.47	0.50
1:A:1095:ASP:HB3	1:A:1098:TRP:HD1	1.77	0.49
1:A:379:PHE:O	1:A:383:SER:N	2.44	0.49
1:A:267:ILE:O	3:A:1202:8D0:O2	2.30	0.49
1:A:141:ILE:O	1:A:145:ARG:N	2.39	0.49
1:A:257:CYS:HA	1:A:262:SER:HB2	1.95	0.48
1:A:1082:GLY:HA3	1:A:1086:ARG:NH2	2.24	0.47
1:A:1095:ASP:HB3	1:A:1098:TRP:CD1	2.50	0.46
1:A:1083:ALA:C	1:A:1084:GLN:HG3	2.36	0.46
1:A:245:ILE:HD11	4:A:1203:CLR:H232	1.96	0.46
1:A:1078:LEU:O	1:A:1081:THR:CB	2.63	0.45
1:A:1053:VAL:O	1:A:1088:VAL:HG23	2.16	0.45
1:A:1094:GLY:N	1:A:1126:ILE:O	2.50	0.45
1:A:257:CYS:SG	1:A:264:CYS:CA	3.05	0.45
1:A:1088:VAL:HG22	1:A:1089:ALA:N	2.31	0.44
1:A:1068:GLN:HG3	1:A:1070:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:O	1:A:212:ILE:HG13	2.18	0.44
1:A:339:ILE:HA	1:A:342:ALA:HB3	1.99	0.43
1:A:1018:THR:O	1:A:1022:ILE:N	2.43	0.43
1:A:1056:GLY:HA3	1:A:1091:PHE:CE2	2.53	0.43
1:A:1078:LEU:O	1:A:1079:GLU:C	2.58	0.42
1:A:1088:VAL:CG2	1:A:1089:ALA:N	2.82	0.41
1:A:1056:GLY:HA2	1:A:1091:PHE:O	2.20	0.41
1:A:1060:TRP:O	1:A:1066:GLU:HB2	2.21	0.41
1:A:1011:THR:OG1	1:A:1068:GLN:OE1	2.32	0.40
1:A:1047:PHE:HB3	1:A:1086:ARG:HD3	2.01	0.40
1:A:123:SER:HA	1:A:384:MET:HE1	2.04	0.40
1:A:1010:SER:HA	2:A:1201:FMN:O2P	2.21	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	427/438 (98%)	412 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	351/369 (95%)	351 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
2	FMN	A	1201	-	31,33,33	1.13	4 (12%)	38,50,50	2.64	6 (15%)
3	8D0	A	1202	-	31,31,31	0.97	1 (3%)	43,46,46	0.97	1 (2%)
4	CLR	A	1203	-	31,31,31	0.62	1 (3%)	48,48,48	1.35	5 (10%)
5	PEG	A	1204	-	6,6,6	0.50	0	5,5,5	0.28	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
2	FMN	A	1201	-	-	0/16/18/18	0/3/3/3
3	8D0	A	1202	-	-	0/16/44/44	0/3/3/3
4	CLR	A	1203	-	-	0/10/68/68	0/4/4/4
5	PEG	A	1204	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	CLR	C10-C9	-2.14	1.52	1.56
3	A	1202	8D0	O1-C9	-2.13	1.43	1.47
2	A	1201	FMN	C4-C4A	2.25	1.45	1.41
2	A	1201	FMN	C4A-C10	2.32	1.45	1.41
2	A	1201	FMN	C5A-N5	2.54	1.39	1.35
2	A	1201	FMN	C4-N3	3.06	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	FMN	C4A-C4-N3	-6.73	113.90	123.48
2	A	1201	FMN	C4A-C10-N10	-5.57	116.66	120.52
2	A	1201	FMN	C4-C4A-C10	-3.24	117.34	119.96
4	A	1203	CLR	C19-C10-C9	-3.12	107.82	111.68
4	A	1203	CLR	C13-C17-C20	-2.75	115.06	119.47
4	A	1203	CLR	C14-C8-C9	-2.43	105.79	109.09
4	A	1203	CLR	C3-C4-C5	-2.14	108.18	111.98
4	A	1203	CLR	C13-C14-C8	-2.08	111.22	114.39
2	A	1201	FMN	P-O5'-C5'	2.27	124.54	118.30
3	A	1202	8D0	C4-C5-C6	2.27	118.40	116.37
2	A	1201	FMN	C10-C4A-N5	3.28	124.37	120.59
2	A	1201	FMN	C4-N3-C2	12.37	125.97	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	FMN	3	0
3	A	1202	8D0	1	0
4	A	1203	CLR	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	431/438 (98%)	0.81	69 (16%) 2 1	80, 126, 184, 207	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1112	LEU	8.0
1	A	1128	GLY	7.8
1	A	1083	ALA	6.9
1	A	1120	VAL	6.5
1	A	1067	LEU	6.5
1	A	1140	TRP	6.2
1	A	1060	TRP	5.6
1	A	1127	ASP	5.5
1	A	1075	PHE	5.4
1	A	1093	CYS	5.2
1	A	1108	ILE	5.0
1	A	287	LEU	5.0
1	A	1094	GLY	5.0
1	A	356	TRP	4.8
1	A	292	TYR	4.7
1	A	1110	GLU	4.7
1	A	1107	ALA	4.5
1	A	1124	LEU	4.4
1	A	290	ILE	4.3
1	A	1126	ILE	4.1
1	A	1091	PHE	4.0
1	A	1129	ASP	3.9
1	A	1119	ILE	3.9
1	A	1146	GLY	3.8
1	A	1022	ILE	3.8
1	A	1066	GLU	3.7
1	A	1137	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1062	ASP	3.6
1	A	1109	GLU	3.5
1	A	1130	PRO	3.4
1	A	1111	LYS	3.4
1	A	289	PHE	3.4
1	A	1088	VAL	3.3
1	A	1134	ARG	3.2
1	A	1104	ALA	3.2
1	A	1115	LEU	3.2
1	A	291	VAL	3.2
1	A	1121	GLN	3.1
1	A	1065	ILE	3.1
1	A	204	VAL	3.1
1	A	288	LEU	3.1
1	A	1106	ASP	3.1
1	A	1122	ASP	3.0
1	A	284	SER	2.9
1	A	1113	LYS	2.9
1	A	1136	ASP	2.8
1	A	286	LEU	2.8
1	A	263	VAL	2.8
1	A	1095	ASP	2.7
1	A	285	VAL	2.7
1	A	211	ALA	2.7
1	A	1090	CYS	2.6
1	A	294	TYR	2.5
1	A	1069	ASP	2.4
1	A	1125	ARG	2.4
1	A	216	ILE	2.3
1	A	1047	PHE	2.3
1	A	1055	LEU	2.3
1	A	218	ILE	2.3
1	A	152	SER	2.2
1	A	295	MET	2.2
1	A	388	LEU	2.2
1	A	208	PHE	2.1
1	A	386	CYS	2.1
1	A	1103	GLY	2.1
1	A	215	TYR	2.1
1	A	1092	GLY	2.1
1	A	129	PHE	2.1
1	A	345	LEU	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(\AA^2)	Q<0.9
3	8D0	A	1202	29/29	0.92	0.28	1.58	79,92,102,105	0
4	CLR	A	1203	28/28	0.94	0.25	0.67	91,103,110,116	0
5	PEG	A	1204	7/7	0.79	0.26	0.52	84,109,114,116	0
2	FMN	A	1201	31/31	0.92	0.29	-0.22	98,104,123,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.