Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 07:18 PM EDT

PDB ID	:	3M2J
Title	:	Crystal Structure of fluorescein-labeled Class A -lactamase PenP
Authors	:	Zhao, Y.X.; Leung, Y.C.; Wong, W.T.
Deposited on	:	2010-03-07
Resolution	:	1.80 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 (i)) were used in the production of this report:

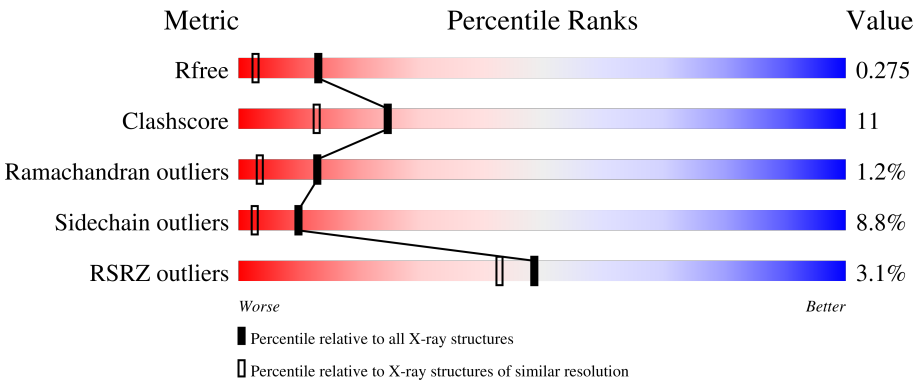
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	A	257	5% 73% 21% 5% •
1	B	257	% 79% 16% • •

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	F5M	A	292	-	X	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4303 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.

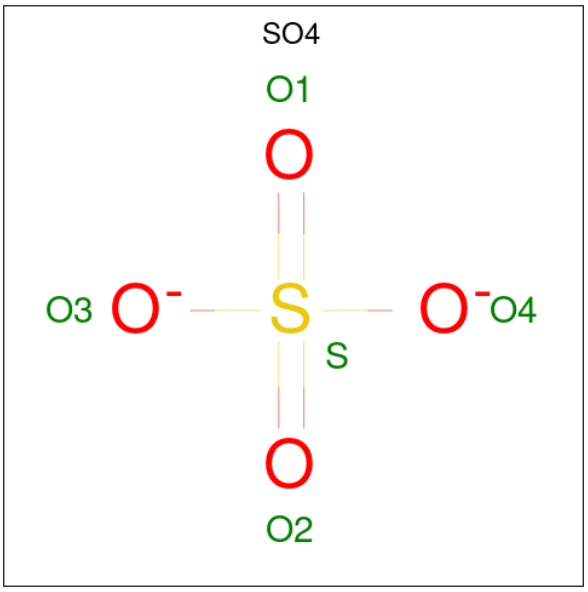
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	2001	1254	346	397	4	0	0	0
1	B	257	2006	1257	347	398	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	CYS	GLU	engineered mutation	UNP P00808
B	166	CYS	GLU	engineered mutation	UNP P00808

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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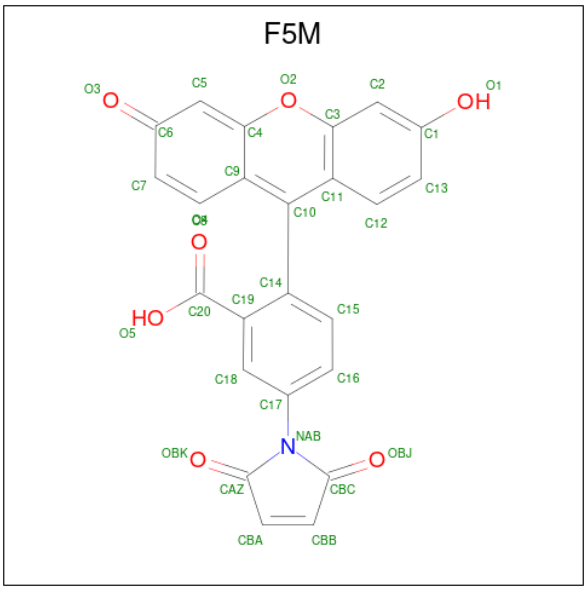
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0

- Molecule 3 is 5-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)-2-(6-hydroxy-3-oxo-3H-xanthen-9-yl) benzoic acid (three-letter code: F5M) (formula: $C_{24}H_{13}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	32	24	1	7	0	0

- Molecule 4 is water.

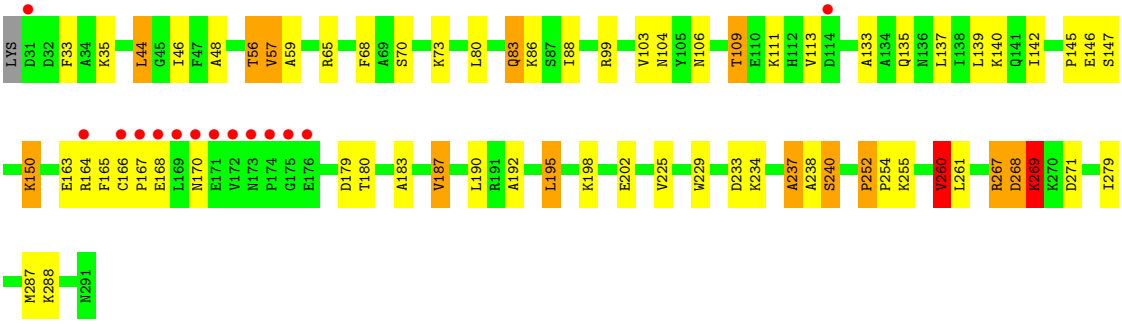
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	124	124	124	0	0
4	B	130	130	130	0	0

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.

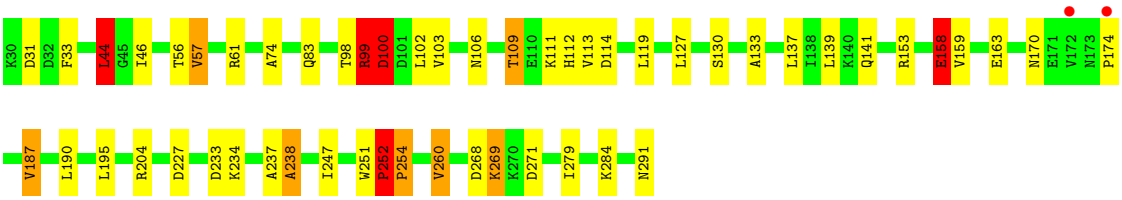
• Molecule 1: Beta-lactamase

Chain A:



• Molecule 1: Beta-lactamase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.35Å 92.34Å 66.42Å 90.00° 104.84° 90.00°	Depositor
Resolution (Å)	31.59 – 1.80 30.78 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.9 (31.59-1.80) 95.9 (30.78-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.273 0.210 , 0.275	Depositor DCC
R_{free} test set	2274 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4303	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, F5M

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	0.94	6/2031 (0.3%)	1.05	9/2749 (0.3%)
1	B	1.03	6/2036 (0.3%)	1.11	15/2756 (0.5%)
All	All	0.99	12/4067 (0.3%)	1.08	24/5505 (0.4%)

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
1	A	0	4
1	B	0	3
All	All	0	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	PRO	C-N	11.82	1.56	1.34
1	B	252	PRO	C-N	11.53	1.56	1.34
1	B	57	VAL	C-N	10.50	1.58	1.34
1	B	83	GLN	C-N	10.38	1.57	1.34
1	B	251	TRP	C-N	8.97	1.51	1.34
1	A	86	LYS	C-N	6.87	1.49	1.34
1	A	59	ALA	C-N	6.47	1.49	1.34
1	B	158	GLU	CG-CD	-6.28	1.42	1.51
1	B	237	ALA	C-N	5.71	1.47	1.34
1	A	237	ALA	C-N	5.46	1.46	1.34
1	A	234	LYS	CD-CE	5.34	1.64	1.51
1	A	240	SER	C-N	5.02	1.45	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	83	GLN	O-C-N	-14.88	98.89	122.70
1	B	238	ALA	C-N-CA	-9.19	98.73	121.70
1	B	83	GLN	CA-C-N	9.06	137.14	117.20
1	A	57	VAL	CA-C-N	-8.99	97.42	117.20
1	A	269	LYS	N-CA-C	8.79	134.74	111.00
1	A	252	PRO	O-C-N	-8.39	105.16	121.10
1	B	83	GLN	C-N-CA	8.05	141.84	121.70
1	B	252	PRO	CA-C-N	-7.49	96.12	117.10
1	B	268	ASP	N-CA-C	7.21	130.45	111.00
1	B	251	TRP	C-N-CD	7.08	143.27	128.40
1	B	204	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	99	ARG	N-CA-C	6.64	128.92	111.00
1	B	268	ASP	C-N-CA	6.63	138.27	121.70
1	A	252	PRO	CA-C-N	6.19	134.43	117.10
1	B	99	ARG	C-N-CA	6.02	136.75	121.70
1	B	254	PRO	O-C-N	5.65	131.74	122.70
1	A	83	GLN	O-C-N	-5.60	113.75	122.70
1	B	268	ASP	CA-C-N	5.48	129.27	117.20
1	A	260	VAL	CB-CA-C	5.34	121.55	111.40
1	A	56	THR	O-C-N	-5.33	114.18	122.70
1	B	44	LEU	CB-CG-CD1	5.28	119.97	111.00
1	B	99	ARG	CA-C-N	5.11	128.44	117.20
1	A	267	ARG	N-CA-C	-5.10	97.22	111.00
1	A	195	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Peptide
1	A	268	ASP	Peptide
1	A	57	VAL	Mainchain
1	A	83	GLN	Mainchain
1	B	252	PRO	Mainchain
1	B	57	VAL	Mainchain
1	B	99	ARG	Peptide

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2001	0	2015	55	0
1	B	2006	0	2017	29	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	32	0	9	22	0
4	A	124	0	0	13	0
4	B	130	0	0	10	0
All	All	4303	0	4041	88	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 11.

All (88) 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:166:CYS:SG	3:A:292:F5M:HBA	1.55	1.46
1:B:271:ASP:HB2	4:B:375:HOH:O	1.32	1.22
1:A:166:CYS:SG	3:A:292:F5M:CBA	2.27	1.21
1:A:237:ALA:O	3:A:292:F5M:H15	1.40	1.16
1:A:109:THR:HG21	1:A:133:ALA:HB3	1.22	1.12
1:A:279:ILE:HD12	4:A:239:HOH:O	1.58	1.04
1:A:80:LEU:HD13	4:A:395:HOH:O	1.57	1.03
1:B:247:ILE:HG12	4:B:390:HOH:O	1.61	1.00
1:A:167:PRO:HA	3:A:292:F5M:OBK	1.61	0.99
1:A:146:GLU:HG3	4:A:369:HOH:O	1.62	0.99
1:B:109:THR:HG21	1:B:133:ALA:HB3	1.46	0.97
1:A:237:ALA:O	3:A:292:F5M:C15	2.12	0.97
3:A:292:F5M:H13	4:A:392:HOH:O	1.65	0.96
1:B:234:LYS:HB3	4:B:390:HOH:O	1.64	0.95
3:A:292:F5M:H7	4:A:326:HOH:O	1.64	0.95
3:A:292:F5M:H16	3:A:292:F5M:OBJ	1.68	0.93
1:A:150:LYS:HB2	4:A:383:HOH:O	1.69	0.90
1:A:168:GLU:HB3	4:A:335:HOH:O	1.74	0.87
3:A:292:F5M:H16	4:A:310:HOH:O	1.76	0.85
1:A:166:CYS:HG	3:A:292:F5M:HBA	0.94	0.82
1:B:99:ARG:O	1:B:102:LEU:HB2	1.82	0.79
1:A:109:THR:HG21	1:A:133:ALA:CB	2.11	0.77
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.66	0.77
4:A:393:HOH:O	1:B:112:HIS:HE1	1.65	0.76
1:A:106:ASN:HB3	1:A:109:THR:CG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:HG3	4:A:380:HOH:O	1.88	0.73
1:A:73:LYS:HE3	1:A:135:GLN:HB2	1.70	0.73
1:A:269:LYS:HG2	1:A:271:ASP:OD1	1.91	0.71
1:B:109:THR:HG21	1:B:133:ALA:CB	2.19	0.71
1:B:187:VAL:HB	1:B:260:VAL:HG22	1.74	0.69
1:B:284:LYS:CE	4:B:376:HOH:O	2.40	0.69
1:B:98:THR:OG1	1:B:100:ASP:HB3	1.95	0.66
1:B:99:ARG:HA	1:B:102:LEU:HD13	1.78	0.66
1:A:164:ARG:HB3	1:A:168:GLU:HG2	1.78	0.65
1:B:284:LYS:HE3	4:B:376:HOH:O	1.96	0.64
1:B:291:ASN:ND2	4:B:344:HOH:O	2.29	0.64
1:B:284:LYS:NZ	4:B:376:HOH:O	2.10	0.64
1:A:187:VAL:HB	1:A:260:VAL:HG22	1.80	0.64
3:A:292:F5M:C16	4:A:310:HOH:O	2.39	0.63
1:A:254:PRO:HG3	1:B:111:LYS:HB3	1.82	0.62
1:A:33:PHE:CE1	1:A:46:ILE:HD13	2.34	0.61
1:A:70:SER:N	3:A:292:F5M:OBJ	2.34	0.61
1:B:187:VAL:HB	1:B:260:VAL:CG2	2.30	0.60
1:B:269:LYS:HG2	4:B:371:HOH:O	2.00	0.60
1:A:164:ARG:HB3	1:A:168:GLU:CG	2.32	0.59
1:A:170:ASN:HB3	1:A:238:ALA:HB1	1.86	0.57
1:A:229:TRP:HZ3	1:A:287:MET:CE	2.18	0.56
1:A:229:TRP:HZ3	1:A:287:MET:HE1	1.71	0.55
1:A:268:ASP:HB2	4:A:358:HOH:O	2.08	0.54
1:B:279:ILE:HD12	4:B:379:HOH:O	2.09	0.53
1:A:170:ASN:HB3	1:A:238:ALA:CB	2.39	0.53
1:A:252:PRO:O	1:A:254:PRO:C	2.47	0.53
3:A:292:F5M:OBJ	3:A:292:F5M:C16	2.44	0.51
1:A:240:SER:HA	3:A:292:F5M:O3	2.11	0.50
1:B:106:ASN:HB3	1:B:109:THR:HG22	1.93	0.49
1:B:119:LEU:HD21	1:B:141:GLN:HG3	1.94	0.49
1:A:183:ALA:O	1:A:187:VAL:HG13	2.13	0.49
1:A:170:ASN:OD1	3:A:292:F5M:C17	2.60	0.49
1:A:48:ALA:HB2	1:A:261:LEU:HD13	1.95	0.48
1:A:73:LYS:HE3	1:A:135:GLN:CB	2.40	0.48
1:A:166:CYS:SG	3:A:292:F5M:CAZ	3.00	0.48
1:A:139:LEU:HD23	1:A:142:ILE:HD11	1.95	0.47
1:A:170:ASN:ND2	3:A:292:F5M:C16	2.78	0.47
1:A:145:PRO:HD3	1:A:165:PHE:CE2	2.49	0.47
1:B:33:PHE:CE1	1:B:46:ILE:HD13	2.50	0.47
1:A:192:ALA:HB1	1:A:198:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:O	1:B:238:ALA:HB1	2.16	0.46
1:A:170:ASN:HD21	3:A:292:F5M:C16	2.29	0.45
1:A:254:PRO:CG	1:B:111:LYS:HB3	2.46	0.45
1:A:111:LYS:HE3	4:A:387:HOH:O	2.17	0.45
1:A:288:LYS:HE3	1:A:288:LYS:HB2	1.89	0.44
1:A:70:SER:OG	3:A:292:F5M:OBJ	2.33	0.44
1:B:74:ALA:HA	1:B:127:LEU:HD21	2.00	0.44
1:A:104:ASN:HD21	3:A:292:F5M:C20	2.31	0.43
1:B:153:ARG:CD	1:B:158:GLU:HG3	2.48	0.43
1:A:33:PHE:CD1	1:A:46:ILE:HD13	2.53	0.43
1:A:229:TRP:CZ3	1:A:287:MET:CE	3.01	0.43
1:A:65:ARG:HD3	1:A:180:THR:OG1	2.19	0.42
1:B:252:PRO:CB	1:B:254:PRO:CD	2.97	0.42
1:B:44:LEU:O	1:B:61:ARG:HD2	2.20	0.42
1:A:70:SER:HG	3:A:292:F5M:CBC	2.32	0.41
1:A:44:LEU:HG	1:A:46:ILE:HD11	2.02	0.41
1:A:70:SER:CA	3:A:292:F5M:OBJ	2.67	0.41
1:A:88:ILE:CD1	1:A:202:GLU:HB3	2.51	0.41
1:B:153:ARG:HD2	1:B:158:GLU:HG3	2.03	0.41
1:A:68:PHE:CZ	1:A:179:ASP:HA	2.56	0.40
1:A:166:CYS:HA	1:A:167:PRO:HA	1.87	0.40
1:B:269:LYS:HD2	4:B:337:HOH:O	2.22	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	254/257 (99%)	242 (95%)	10 (4%)	2 (1%)	19 7
1	B	255/257 (99%)	244 (96%)	7 (3%)	4 (2%)	9 2
All	All	509/514 (99%)	486 (96%)	17 (3%)	6 (1%)	13 3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	LYS
1	B	100	ASP
1	A	269	LYS
1	B	103	VAL
1	A	103	VAL
1	B	174	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	A	216/217 (100%)	197 (91%)	19 (9%)	10 3
1	B	216/217 (100%)	197 (91%)	19 (9%)	10 3
All	All	432/434 (100%)	394 (91%)	38 (9%)	10 3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	44	LEU
1	A	56	THR
1	A	99	ARG
1	A	109	THR
1	A	113	VAL
1	A	137	LEU
1	A	140	LYS
1	A	147	SER
1	A	150	LYS
1	A	163	GLU
1	A	187	VAL
1	A	190	LEU
1	A	195	LEU
1	A	225	VAL
1	A	233	ASP
1	A	255	LYS

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Mol	Chain	Res	Type
1	A	260	VAL
1	A	269	LYS
1	B	31	ASP
1	B	44	LEU
1	B	56	THR
1	B	100	ASP
1	B	109	THR
1	B	113	VAL
1	B	114	ASP
1	B	130	SER
1	B	137	LEU
1	B	139	LEU
1	B	158	GLU
1	B	159	VAL
1	B	163	GLU
1	B	187	VAL
1	B	190	LEU
1	B	195	LEU
1	B	227	ASP
1	B	233	ASP
1	B	260	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	93	GLN
1	A	161	ASN
1	A	173	ASN
1	B	83	GLN
1	B	112	HIS
1	B	170	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 monosaccharides 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	$\#\|Z\| > 2$
3	F5M	A	292	-	36,36,36	3.53	14 (38%)	54,54,54	5.68	28 (51%)
2	SO4	B	1	-	4,4,4	0.11	0	6,6,6	0.64	0
2	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.56	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	F5M	A	292	-	-	8/10/29/29	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	292	F5M	CBB-CBA	7.89	1.52	1.35
3	A	292	F5M	C2-C1	-7.49	1.28	1.39
3	A	292	F5M	C12-C11	-6.37	1.29	1.39
3	A	292	F5M	C13-C12	-6.11	1.27	1.38
3	A	292	F5M	O3-C6	6.10	1.43	1.24
3	A	292	F5M	C13-C1	5.95	1.50	1.38
3	A	292	F5M	C19-C14	5.74	1.50	1.40
3	A	292	F5M	CAZ-NAB	-5.24	1.31	1.40
3	A	292	F5M	C11-C3	4.59	1.49	1.40
3	A	292	F5M	C2-C3	-4.59	1.30	1.38
3	A	292	F5M	CBC-NAB	-4.39	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	292	F5M	C9-C10	3.63	1.51	1.39
3	A	292	F5M	C17-NAB	-3.52	1.39	1.44
3	A	292	F5M	CBB-CBC	2.05	1.52	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	292	F5M	C13-C12-C11	18.55	150.99	120.94
3	A	292	F5M	C3-C2-C1	18.38	148.87	119.05
3	A	292	F5M	C12-C13-C1	-16.22	102.08	119.88
3	A	292	F5M	O2-C3-C2	12.16	134.03	115.79
3	A	292	F5M	C13-C1-C2	-11.11	108.00	120.17
3	A	292	F5M	C2-C3-C11	-9.48	103.19	121.35
3	A	292	F5M	C12-C11-C3	-8.68	106.82	118.21
3	A	292	F5M	O3-C6-C5	-6.79	111.69	121.41
3	A	292	F5M	C18-C17-NAB	6.21	126.80	119.12
3	A	292	F5M	O3-C6-C7	-5.50	112.71	121.56
3	A	292	F5M	CBA-CBB-CBC	-5.13	99.62	108.67
3	A	292	F5M	C12-C11-C10	4.86	133.01	123.28
3	A	292	F5M	CBB-CBC-NAB	4.80	115.13	106.11
3	A	292	F5M	C14-C10-C11	4.04	124.65	119.94
3	A	292	F5M	CBA-CAZ-NAB	3.72	113.10	106.11
3	A	292	F5M	CBB-CBA-CAZ	-3.65	102.23	108.67
3	A	292	F5M	C7-C6-C5	-3.43	113.63	117.13
3	A	292	F5M	OBJ-CBC-CBB	-3.32	122.36	128.56
3	A	292	F5M	C19-C14-C10	3.09	127.62	123.33
3	A	292	F5M	OBK-CAZ-CBA	-3.04	122.88	128.56
3	A	292	F5M	C11-C10-C9	-2.96	114.07	119.99
3	A	292	F5M	C16-C17-NAB	-2.93	116.13	119.64
3	A	292	F5M	O1-C1-C2	2.78	127.06	119.84
3	A	292	F5M	C15-C14-C19	-2.65	116.31	119.26
3	A	292	F5M	C15-C16-C17	2.45	123.55	120.32
3	A	292	F5M	C4-C5-C6	2.37	122.85	120.76
3	A	292	F5M	O2-C4-C9	2.24	123.02	120.49
3	A	292	F5M	C8-C9-C10	-2.22	119.20	123.96

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	292	F5M	C18-C17-NAB-CBC
3	A	292	F5M	C16-C17-NAB-CBC

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Mol	Chain	Res	Type	Atoms
3	A	292	F5M	C18-C17-NAB-CAZ
3	A	292	F5M	C16-C17-NAB-CAZ
3	A	292	F5M	C18-C19-C20-O4
3	A	292	F5M	C18-C19-C20-O5
3	A	292	F5M	C14-C19-C20-O4
3	A	292	F5M	C14-C19-C20-O5

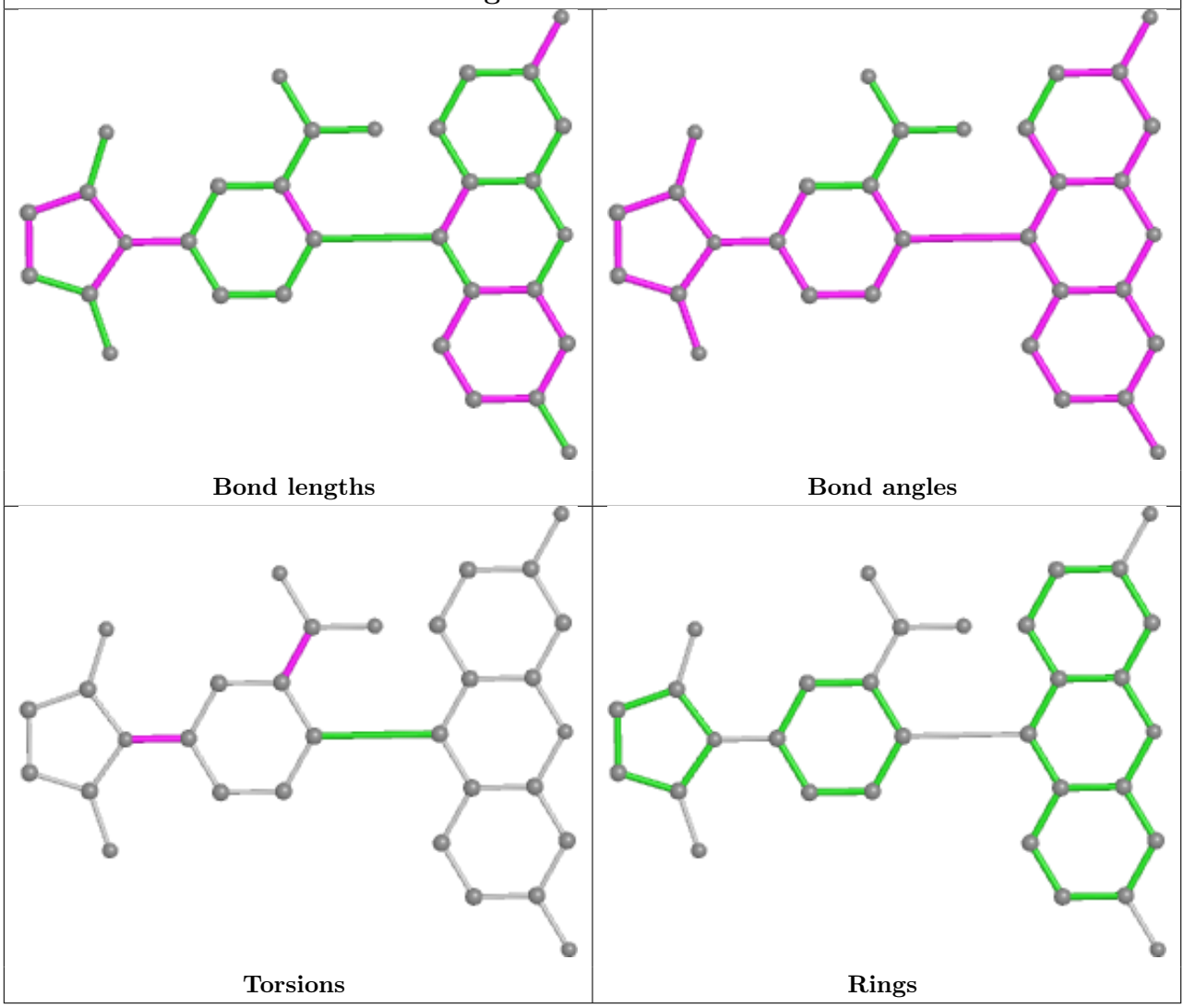
There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	292	F5M	22	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand F5M A 292



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	A	256/257 (99%)	-0.07	14 (5%)	25	20	8, 18, 42, 59	0
1	B	257/257 (100%)	-0.37	2 (0%)	86	84	10, 18, 38, 52	0
All	All	513/514 (99%)	-0.22	16 (3%)	49	43	8, 18, 40, 59	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	PRO	6.2
1	A	173	ASN	4.4
1	A	175	GLY	4.4
1	A	170	ASN	4.0
1	A	172	VAL	3.9
1	A	169	LEU	3.9
1	A	168	GLU	3.5
1	A	167	PRO	3.2
1	A	176	GLU	2.8
1	A	114	ASP	2.7
1	A	171	GLU	2.7
1	A	164	ARG	2.5
1	A	166	CYS	2.4
1	B	172	VAL	2.3
1	A	31	ASP	2.2
1	B	174	PRO	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

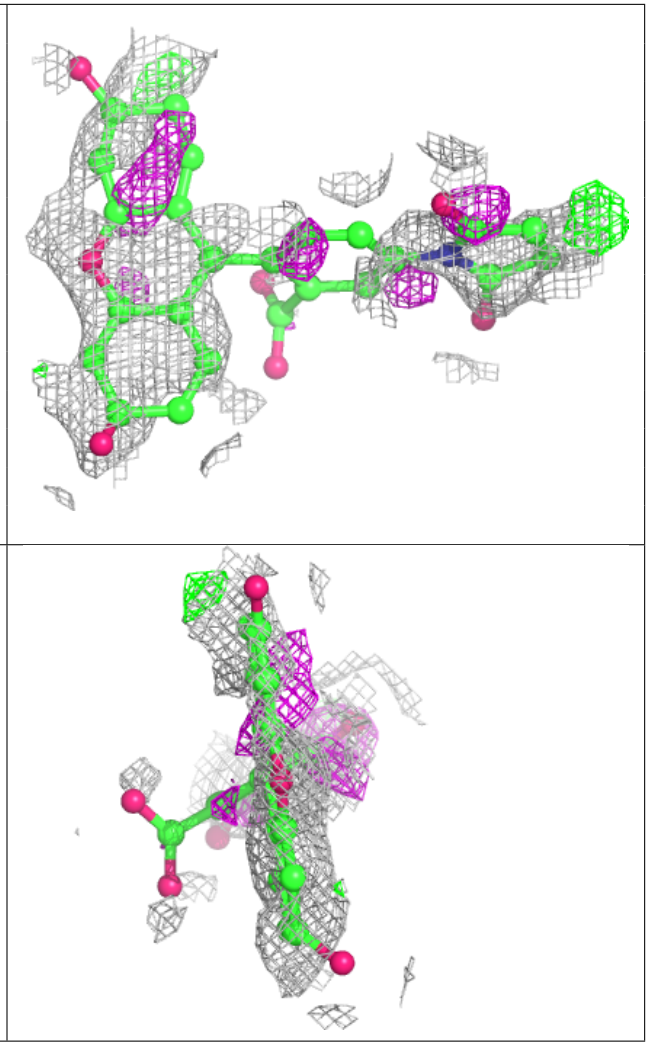
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	F5M	A	292	32/32	0.46	0.46	69,71,73,76	0
2	SO4	B	1	5/5	0.98	0.11	21,22,25,28	3
2	SO4	A	1	5/5	0.98	0.11	19,24,25,25	3

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F5M A 292:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.