



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:28 AM UTC

PDB ID : 3WZU / pdb_00003wzu
Title : THE STRUCTURE OF MAP2K7 IN COMPLEX WITH 5Z-7-oxozeaenol
Authors : Sogabe, Y.; Hashimoto, Y.; Matsumoto, T.; Kinoshita, T.
Deposited on : 2014-10-07
Resolution : 3.01 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

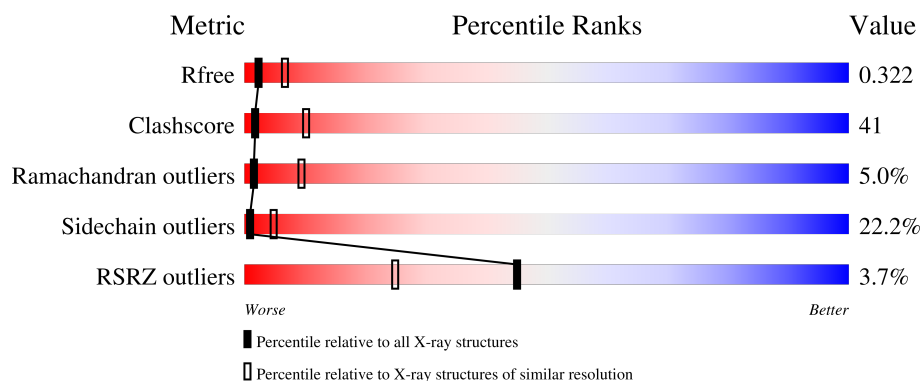
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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 $\leq 5\%$. 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	324	

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
2	1FM	A	600	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2200 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.

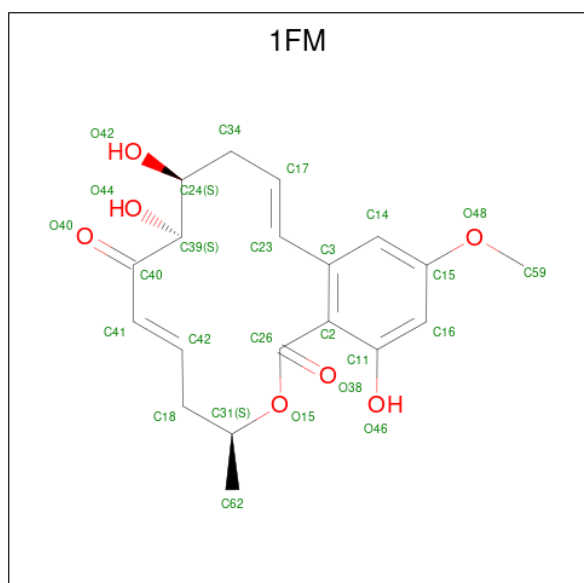
- Molecule 1 is a protein called Dual specificity mitogen-activated protein kinase kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2150	1374	371	387	18	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	MET	-	expression tag	UNP O14733
A	436	HIS	-	expression tag	UNP O14733
A	437	HIS	-	expression tag	UNP O14733
A	438	HIS	-	expression tag	UNP O14733
A	439	HIS	-	expression tag	UNP O14733
A	440	HIS	-	expression tag	UNP O14733
A	441	HIS	-	expression tag	UNP O14733

- Molecule 2 is (3S,5Z,8S,9S,11E)-8,9,16-trihydroxy-14-methoxy-3-methyl-3,4,9,10-tetrahydro-1H-2-benzoxacyclotetradecine-1,7(8H)-dione (CCD ID: 1FM) (formula: C₁₉H₂₂O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			26	19	7		

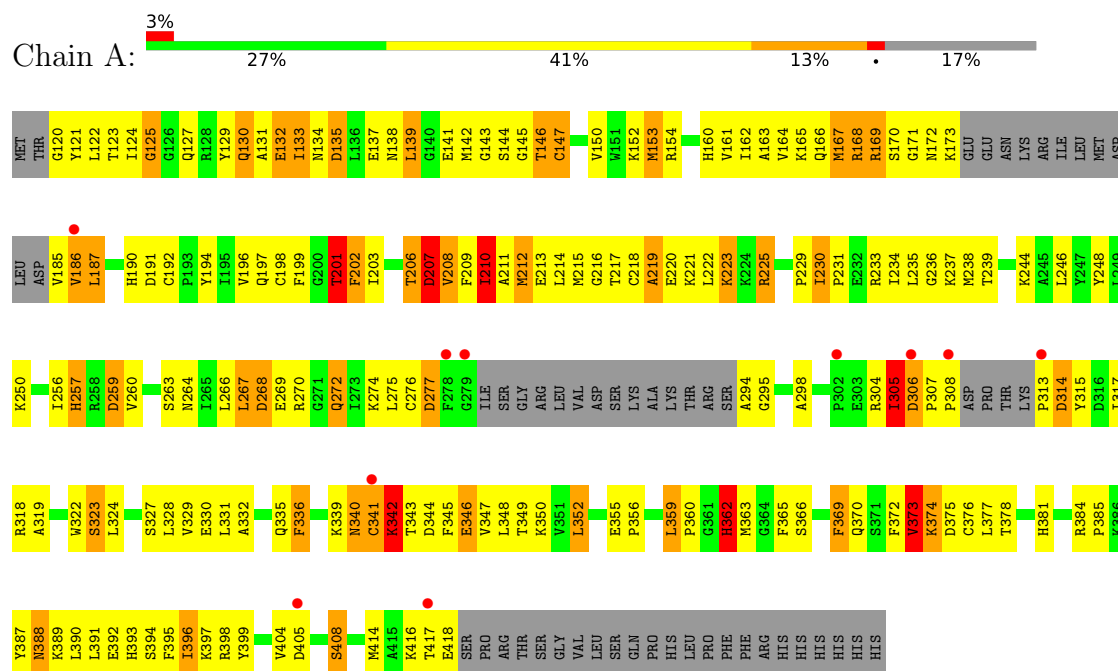
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		

3 Residue-property plots

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: Dual specificity mitogen-activated protein kinase kinase 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	71.39Å 71.39Å 268.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.28 – 3.01 36.28 – 3.01	Depositor EDS
% Data completeness (in resolution range)	82.9 (36.28-3.01) 83.1 (36.28-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.236 , 0.322 0.232 , 0.322	Depositor DCC
R_{free} test set	339 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2200	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: 1FM

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	0.84	0/2194	1.21	23/2948 (0.8%)

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	3

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASP	CA-C-N	7.83	135.80	121.70
1	A	207	ASP	C-N-CA	7.83	135.80	121.70
1	A	207	ASP	N-CA-C	-7.72	97.26	109.23
1	A	230	ILE	CA-C-N	7.48	129.19	119.84
1	A	230	ILE	C-N-CA	7.48	129.19	119.84
1	A	219	ALA	N-CA-C	-6.41	103.91	111.03
1	A	153	MET	N-CA-C	5.61	117.60	109.07
1	A	259	ASP	N-CA-C	5.58	118.68	107.41
1	A	201	THR	CA-C-N	5.41	131.44	121.70
1	A	201	THR	C-N-CA	5.41	131.44	121.70
1	A	210	ILE	N-CA-C	5.38	115.73	107.77
1	A	341	CYS	CA-C-N	5.35	131.33	121.70
1	A	341	CYS	C-N-CA	5.35	131.33	121.70
1	A	336	PHE	CA-C-N	5.34	126.52	119.84
1	A	336	PHE	C-N-CA	5.34	126.52	119.84
1	A	342	LYS	CA-C-N	5.27	131.18	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	LYS	C-N-CA	5.27	131.18	121.70
1	A	208	VAL	N-CA-C	5.19	125.52	111.00
1	A	272	GLN	N-CA-C	5.18	116.98	110.24
1	A	160	HIS	N-CA-C	5.13	117.32	110.35
1	A	207	ASP	CA-C-O	-5.13	115.11	121.06
1	A	362	HIS	N-CA-C	5.02	119.43	112.45
1	A	171	GLY	N-CA-C	-5.01	103.56	112.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	MET	Peptide
1	A	201	THR	Peptide
1	A	207	ASP	Peptide

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	2150	0	2173	174	0
2	A	26	0	20	10	0
3	A	24	0	0	1	0
All	All	2200	0	2193	177	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 41.

All (177) 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:359:LEU:HD12	1:A:360:PRO:HD2	1.29	1.07
1:A:342:LYS:HG2	1:A:343:THR:HB	1.37	1.06
1:A:120:GLY:HA3	1:A:121:TYR:HB2	1.34	1.05
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:MET:HA	1:A:168:ARG:HG2	1.33	1.03
1:A:341:CYS:HB3	1:A:342:LYS:HA	1.43	1.00
1:A:143:GLY:HA2	1:A:144:SER:HB2	1.46	0.97
1:A:212:MET:HE2	2:A:600:1FM:H14	1.46	0.95
1:A:186:VAL:HA	1:A:187:LEU:O	1.67	0.94
1:A:359:LEU:CD1	1:A:360:PRO:HD2	1.98	0.93
1:A:150:VAL:HG23	1:A:165:LYS:HD3	1.50	0.92
1:A:186:VAL:HA	1:A:187:LEU:C	1.95	0.92
1:A:186:VAL:HB	3:A:720:HOH:O	1.73	0.89
1:A:306:ASP:HB2	1:A:307:PRO:HD2	1.55	0.86
1:A:229:PRO:HB3	1:A:332:ALA:O	1.75	0.86
1:A:201:THR:HA	1:A:202:PHE:HB2	1.56	0.85
1:A:294:ALA:HB3	1:A:295:GLY:HA2	1.57	0.85
1:A:359:LEU:HD12	1:A:360:PRO:CD	2.07	0.84
1:A:342:LYS:CG	1:A:343:THR:HB	2.07	0.84
1:A:167:MET:HA	1:A:168:ARG:CG	2.07	0.84
1:A:256:ILE:HG22	1:A:256:ILE:O	1.76	0.84
2:A:600:1FM:H39	2:A:600:1FM:H23	1.62	0.81
1:A:342:LYS:HG2	1:A:343:THR:CB	2.10	0.81
1:A:221:LYS:HG3	2:A:600:1FM:H18A	1.64	0.80
1:A:137:GLU:O	1:A:153:MET:HB2	1.81	0.80
1:A:212:MET:CE	2:A:600:1FM:H59B	2.15	0.76
1:A:345:PHE:C	1:A:347:VAL:H	1.91	0.76
1:A:143:GLY:HA2	1:A:144:SER:CB	2.18	0.74
1:A:335:GLN:HB3	1:A:339:LYS:HE3	1.68	0.74
1:A:201:THR:HG22	1:A:210:ILE:HB	1.69	0.74
1:A:304:ARG:O	1:A:305:ILE:HG13	1.88	0.74
1:A:201:THR:CG2	1:A:210:ILE:HB	2.19	0.72
1:A:169:ARG:HB2	1:A:206:THR:O	1.90	0.72
1:A:150:VAL:CG2	1:A:165:LYS:HD3	2.20	0.71
1:A:212:MET:HE2	2:A:600:1FM:H59B	1.71	0.70
1:A:340:ASN:HB2	1:A:350:LYS:NZ	2.06	0.70
1:A:167:MET:HB3	1:A:168:ARG:HB2	1.73	0.69
1:A:167:MET:O	1:A:207:ASP:HA	1.93	0.69
2:A:600:1FM:H39	2:A:600:1FM:C23	2.21	0.68
1:A:322:TRP:HE3	1:A:384:ARG:NH1	1.92	0.67
1:A:256:ILE:O	1:A:256:ILE:CG2	2.43	0.67
1:A:213:GLU:O	2:A:600:1FM:H59	1.95	0.66
1:A:374:LYS:HD3	1:A:374:LYS:C	2.20	0.66
1:A:341:CYS:CB	1:A:342:LYS:HA	2.23	0.66
1:A:130:GLN:HE21	1:A:131:ALA:N	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:HG3	1:A:385:PRO:HD2	1.77	0.66
1:A:215:MET:HE2	1:A:268:ASP:HB3	1.78	0.65
1:A:163:ALA:HB3	1:A:212:MET:HG3	1.78	0.65
1:A:212:MET:CE	2:A:600:1FM:H14	2.23	0.64
1:A:162:ILE:HG22	1:A:199:PHE:HE2	1.60	0.64
1:A:147:CYS:H	1:A:165:LYS:HZ1	1.43	0.64
1:A:130:GLN:NE2	1:A:131:ALA:O	2.30	0.64
1:A:260:VAL:HB	1:A:323:SER:HB2	1.80	0.63
1:A:169:ARG:HG2	1:A:169:ARG:NH1	1.98	0.62
1:A:132:GLU:O	1:A:135:ASP:N	2.32	0.61
1:A:143:GLY:CA	1:A:144:SER:HB2	2.27	0.61
1:A:341:CYS:SG	1:A:347:VAL:HG22	2.41	0.61
1:A:345:PHE:C	1:A:347:VAL:N	2.56	0.61
1:A:139:LEU:HD22	1:A:153:MET:HA	1.81	0.61
1:A:201:THR:CA	1:A:202:PHE:HB2	2.30	0.61
1:A:202:PHE:HB3	1:A:209:PHE:HB2	1.82	0.61
1:A:277:ASP:OD2	1:A:277:ASP:N	2.31	0.61
1:A:363:MET:HB2	1:A:365:PHE:CE2	2.36	0.60
1:A:388:ASN:HD22	1:A:389:LYS:H	1.47	0.60
1:A:162:ILE:HG22	1:A:199:PHE:CE2	2.36	0.60
1:A:225:ARG:NH2	1:A:414:MET:HA	2.17	0.60
1:A:229:PRO:CB	1:A:332:ALA:O	2.48	0.59
1:A:322:TRP:CE3	1:A:384:ARG:NH1	2.69	0.59
1:A:327:SER:O	1:A:331:LEU:HB2	2.03	0.59
1:A:340:ASN:HB2	1:A:350:LYS:HZ1	1.66	0.58
1:A:186:VAL:O	1:A:198:CYS:HB3	2.02	0.58
1:A:405:ASP:HB3	1:A:408:SER:OG	2.04	0.58
2:A:600:1FM:H23	2:A:600:1FM:C39	2.32	0.58
1:A:190:HIS:HA	1:A:197:GLN:HE21	1.68	0.58
1:A:133:ILE:HG23	1:A:202:PHE:HD2	1.69	0.57
1:A:388:ASN:HD22	1:A:389:LYS:N	2.03	0.57
1:A:233:ARG:HA	1:A:399:TYR:OH	2.04	0.57
1:A:133:ILE:HG23	1:A:202:PHE:CD2	2.40	0.57
1:A:120:GLY:HA3	1:A:121:TYR:CB	2.17	0.57
1:A:294:ALA:HA	1:A:344:ASP:HB3	1.88	0.56
1:A:246:LEU:HB3	1:A:387:TYR:CZ	2.41	0.56
1:A:373:VAL:O	1:A:373:VAL:CG1	2.52	0.56
1:A:306:ASP:CB	1:A:307:PRO:HD2	2.30	0.55
1:A:244:LYS:HG2	1:A:391:LEU:HD21	1.88	0.55
1:A:387:TYR:HA	1:A:390:LEU:HD12	1.88	0.55
1:A:162:ILE:CG2	1:A:199:PHE:CE2	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:C	1:A:202:PHE:HD1	2.15	0.55
1:A:374:LYS:HD3	1:A:375:ASP:N	2.22	0.54
1:A:186:VAL:CA	1:A:187:LEU:C	2.78	0.53
1:A:294:ALA:HB3	1:A:295:GLY:CA	2.36	0.53
1:A:355:GLU:HB3	1:A:356:PRO:HD2	1.90	0.53
1:A:163:ALA:HB3	1:A:212:MET:CG	2.39	0.52
1:A:365:PHE:O	1:A:366:SER:C	2.52	0.52
1:A:221:LYS:O	1:A:225:ARG:HB2	2.09	0.52
1:A:322:TRP:HB2	1:A:384:ARG:NH2	2.24	0.52
1:A:237:LYS:HE2	1:A:404:VAL:HG23	1.91	0.52
1:A:143:GLY:CA	1:A:145:GLY:H	2.23	0.51
1:A:130:GLN:NE2	1:A:131:ALA:N	2.59	0.51
1:A:268:ASP:OD1	1:A:268:ASP:C	2.53	0.51
1:A:392:GLU:OE2	1:A:397:LYS:HE2	2.10	0.51
1:A:132:GLU:O	1:A:135:ASP:HB2	2.11	0.50
1:A:341:CYS:HB3	1:A:342:LYS:CA	2.28	0.50
1:A:360:PRO:C	1:A:362:HIS:H	2.19	0.50
1:A:384:ARG:CG	1:A:385:PRO:HD2	2.40	0.50
1:A:341:CYS:SG	1:A:347:VAL:CG2	3.00	0.49
1:A:169:ARG:HB3	1:A:170:SER:HB2	1.93	0.49
1:A:161:VAL:HG12	1:A:214:LEU:HD22	1.93	0.49
1:A:202:PHE:HB2	1:A:209:PHE:O	2.12	0.48
1:A:238:MET:O	1:A:239:THR:C	2.57	0.48
1:A:256:ILE:O	1:A:257:HIS:C	2.57	0.48
1:A:130:GLN:NE2	1:A:131:ALA:H	2.12	0.47
1:A:124:ILE:O	1:A:125:GLY:C	2.58	0.47
1:A:340:ASN:HB2	1:A:350:LYS:HZ3	1.77	0.47
1:A:257:HIS:CD2	1:A:277:ASP:HA	2.50	0.47
1:A:342:LYS:HG2	1:A:343:THR:CG2	2.44	0.47
1:A:349:THR:O	1:A:350:LYS:C	2.58	0.47
1:A:143:GLY:C	1:A:145:GLY:H	2.23	0.47
1:A:212:MET:HE3	2:A:600:1FM:H59B	1.93	0.47
1:A:139:LEU:HD11	1:A:154:ARG:HH12	1.80	0.47
1:A:186:VAL:CA	1:A:187:LEU:O	2.53	0.46
1:A:344:ASP:HA	1:A:346:GLU:OE1	2.15	0.46
1:A:142:MET:HE1	1:A:214:LEU:HD11	1.97	0.46
1:A:376:CYS:C	1:A:378:THR:H	2.23	0.46
1:A:139:LEU:HD11	1:A:154:ARG:NH1	2.31	0.46
1:A:417:THR:O	1:A:418:GLU:HB2	2.16	0.46
1:A:230:ILE:HA	1:A:231:PRO:HD2	1.66	0.45
1:A:315:TYR:HD1	1:A:381:HIS:HE2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HB2	1:A:398:ARG:NH1	2.31	0.45
1:A:329:VAL:O	1:A:330:GLU:C	2.59	0.45
1:A:294:ALA:CB	1:A:295:GLY:HA2	2.30	0.45
1:A:381:HIS:HA	1:A:384:ARG:HB2	1.99	0.45
1:A:397:LYS:HD3	1:A:397:LYS:HA	1.80	0.45
1:A:393:HIS:ND1	1:A:394:SER:N	2.65	0.45
1:A:259:ASP:O	1:A:264:ASN:ND2	2.50	0.45
1:A:235:LEU:HA	1:A:238:MET:HB2	1.97	0.45
1:A:313:PRO:HA	1:A:314:ASP:HA	1.79	0.45
1:A:306:ASP:HB2	1:A:307:PRO:CD	2.39	0.45
1:A:138:ASN:HA	1:A:153:MET:HB3	1.99	0.44
1:A:150:VAL:HG22	1:A:165:LYS:HB2	2.00	0.44
1:A:133:ILE:HG21	1:A:209:PHE:CG	2.52	0.44
1:A:146:THR:HA	1:A:147:CYS:HA	1.78	0.44
1:A:172:ASN:HA	1:A:173:LYS:C	2.43	0.44
1:A:215:MET:HE1	1:A:274:LYS:HG3	1.99	0.43
1:A:307:PRO:HA	1:A:308:PRO:HD3	1.92	0.43
1:A:396:ILE:HG22	1:A:397:LYS:N	2.32	0.43
1:A:239:THR:HG21	1:A:372:PHE:CE2	2.53	0.43
1:A:298:ALA:CB	1:A:336:PHE:HZ	2.31	0.43
1:A:266:LEU:HD13	1:A:276:CYS:HB2	1.99	0.43
1:A:340:ASN:OD1	1:A:340:ASN:N	2.52	0.43
1:A:246:LEU:HD23	1:A:387:TYR:CE2	2.54	0.42
1:A:219:ALA:O	1:A:222:LEU:N	2.41	0.42
1:A:162:ILE:HD12	1:A:211:ALA:HB1	2.01	0.42
1:A:362:HIS:ND1	1:A:362:HIS:C	2.77	0.42
1:A:192:CYS:HB2	1:A:248:TYR:CD1	2.54	0.42
1:A:201:THR:C	1:A:202:PHE:CD1	2.96	0.42
1:A:223:LYS:C	1:A:223:LYS:HD3	2.45	0.42
1:A:416:LYS:HA	1:A:417:THR:HA	1.74	0.42
1:A:127:GLN:HB3	1:A:129:TYR:CZ	2.55	0.42
1:A:257:HIS:C	1:A:257:HIS:ND1	2.78	0.42
1:A:305:ILE:HD13	1:A:352:LEU:HD12	2.02	0.41
1:A:372:PHE:C	1:A:374:LYS:N	2.79	0.41
1:A:372:PHE:CE1	1:A:396:ILE:CD1	3.03	0.41
1:A:236:GLY:HA2	1:A:395:PHE:CZ	2.56	0.41
1:A:374:LYS:C	1:A:374:LYS:CD	2.89	0.41
1:A:166:GLN:HE21	1:A:207:ASP:CG	2.28	0.41
1:A:173:LYS:C	1:A:173:LYS:HD3	2.45	0.41
1:A:122:LEU:HD12	1:A:199:PHE:O	2.20	0.41
1:A:138:ASN:HB2	1:A:153:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TYR:O	1:A:274:LYS:HA	2.21	0.41
1:A:222:LEU:HD12	1:A:267:LEU:CD2	2.51	0.41
1:A:230:ILE:CG2	1:A:234:ILE:HB	2.51	0.41
1:A:359:LEU:HA	1:A:360:PRO:HD2	1.83	0.41
1:A:317:ILE:O	1:A:319:ALA:N	2.54	0.40
1:A:328:LEU:O	1:A:332:ALA:N	2.42	0.40
1:A:169:ARG:NH1	1:A:169:ARG:CG	2.76	0.40
1:A:298:ALA:HB1	1:A:336:PHE:HZ	1.87	0.40
1:A:369:PHE:O	1:A:370:GLN:C	2.64	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	262/324 (81%)	217 (83%)	32 (12%)	13 (5%)	1 9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	THR
1	A	187	LEU
1	A	202	PHE
1	A	216	GLY
1	A	125	GLY
1	A	168	ARG
1	A	208	VAL
1	A	373	VAL
1	A	305	ILE
1	A	377	LEU
1	A	257	HIS
1	A	306	ASP

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Mol	Chain	Res	Type
1	A	369	PHE

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	A	234/285 (82%)	182 (78%)	52 (22%)	1 5

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	THR
1	A	130	GLN
1	A	132	GLU
1	A	133	ILE
1	A	134	ASN
1	A	135	ASP
1	A	139	LEU
1	A	141	GLU
1	A	147	CYS
1	A	152	LYS
1	A	164	VAL
1	A	169	ARG
1	A	185	VAL
1	A	186	VAL
1	A	191	ASP
1	A	196	VAL
1	A	203	ILE
1	A	206	THR
1	A	207	ASP
1	A	210	ILE
1	A	212	MET
1	A	217	THR
1	A	218	CYS
1	A	220	GLU
1	A	223	LYS

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	250	LYS
1	A	263	SER
1	A	267	LEU
1	A	268	ASP
1	A	269	GLU
1	A	270	ARG
1	A	272	GLN
1	A	275	LEU
1	A	277	ASP
1	A	305	ILE
1	A	314	ASP
1	A	318	ARG
1	A	323	SER
1	A	324	LEU
1	A	340	ASN
1	A	342	LYS
1	A	346	GLU
1	A	348	LEU
1	A	352	LEU
1	A	359	LEU
1	A	362	HIS
1	A	373	VAL
1	A	374	LYS
1	A	388	ASN
1	A	396	ILE
1	A	408	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	197	GLN
1	A	353	GLN
1	A	388	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	1FM	A	600	-	27,27,27	2.65	5 (18%)	33,37,37	2.40	9 (27%)

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	1FM	A	600	-	-	8/30/30/30	0/1/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	1FM	C41-C42	8.02	1.54	1.32
2	A	600	1FM	O15-C26	6.62	1.48	1.34
2	A	600	1FM	C2-C3	6.55	1.50	1.42
2	A	600	1FM	C2-C11	4.37	1.48	1.41
2	A	600	1FM	C24-C39	2.88	1.56	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	1FM	C18-C42-C41	-7.00	110.79	125.93
2	A	600	1FM	C42-C41-C40	-6.08	113.11	124.40
2	A	600	1FM	C34-C17-C23	-5.54	117.17	124.31
2	A	600	1FM	O15-C26-O38	-4.17	116.78	123.55
2	A	600	1FM	C3-C2-C11	-3.43	115.24	118.73
2	A	600	1FM	O15-C26-C2	3.27	121.74	113.53
2	A	600	1FM	C59-O48-C15	2.51	122.88	117.50
2	A	600	1FM	C24-C34-C17	-2.23	109.39	112.88
2	A	600	1FM	C11-C16-C15	2.14	121.95	119.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

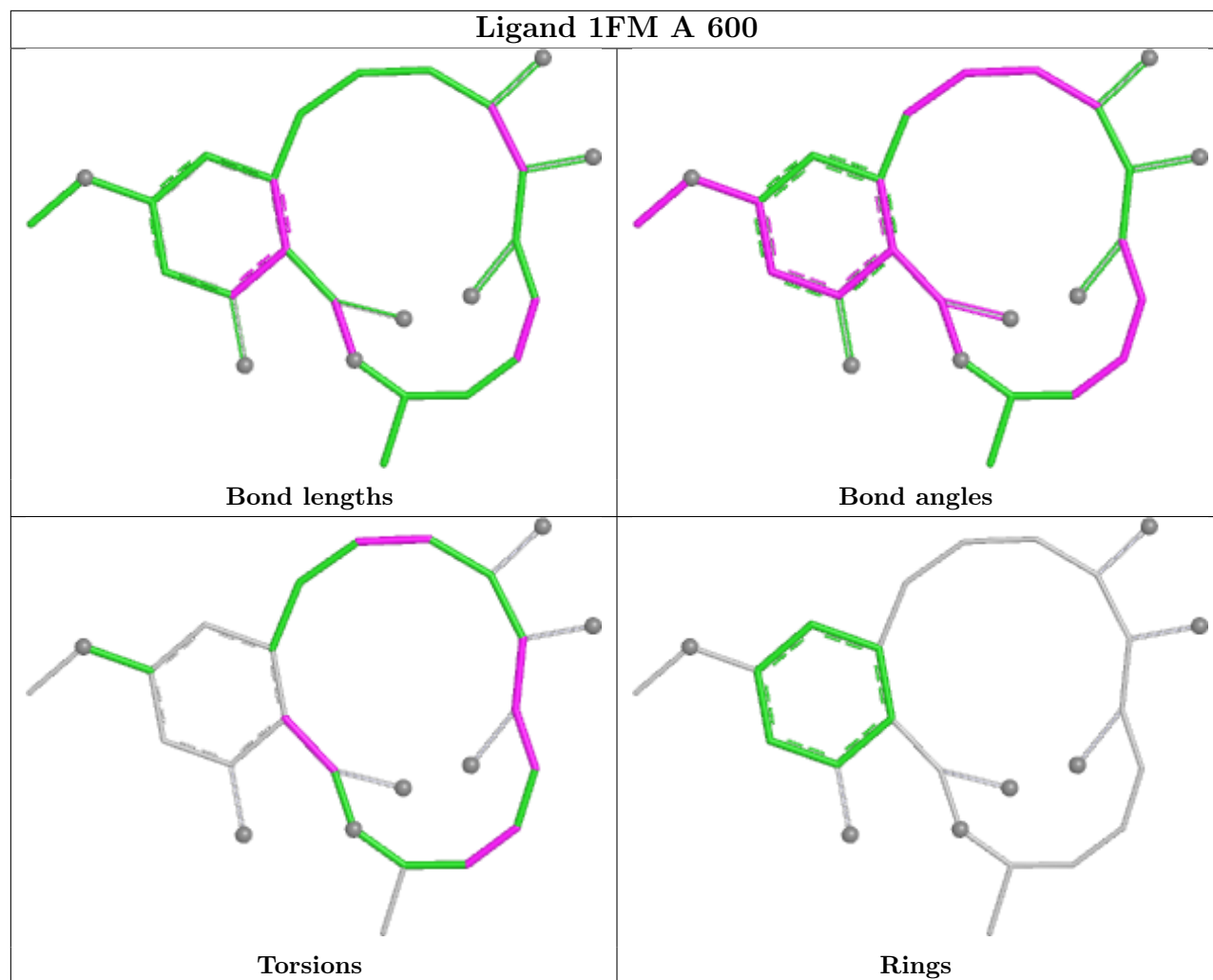
Mol	Chain	Res	Type	Atoms
2	A	600	1FM	C24-C39-C40-C41
2	A	600	1FM	O44-C39-C40-O40
2	A	600	1FM	O44-C39-C40-C41
2	A	600	1FM	O40-C40-C41-C42
2	A	600	1FM	C39-C40-C41-C42
2	A	600	1FM	C31-C18-C42-C41
2	A	600	1FM	C23-C17-C34-C24
2	A	600	1FM	C11-C2-C26-O15

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	1FM	10	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 than 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.



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	270/324 (83%)	0.18	10 (3%) 45 25	20, 52, 109, 131	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	3.3
1	A	308	PRO	3.0
1	A	278	PHE	2.8
1	A	405	ASP	2.7
1	A	417	THR	2.6
1	A	186	VAL	2.5
1	A	313	PRO	2.5
1	A	302	PRO	2.5
1	A	341	CYS	2.3
1	A	306	ASP	2.2

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](#)

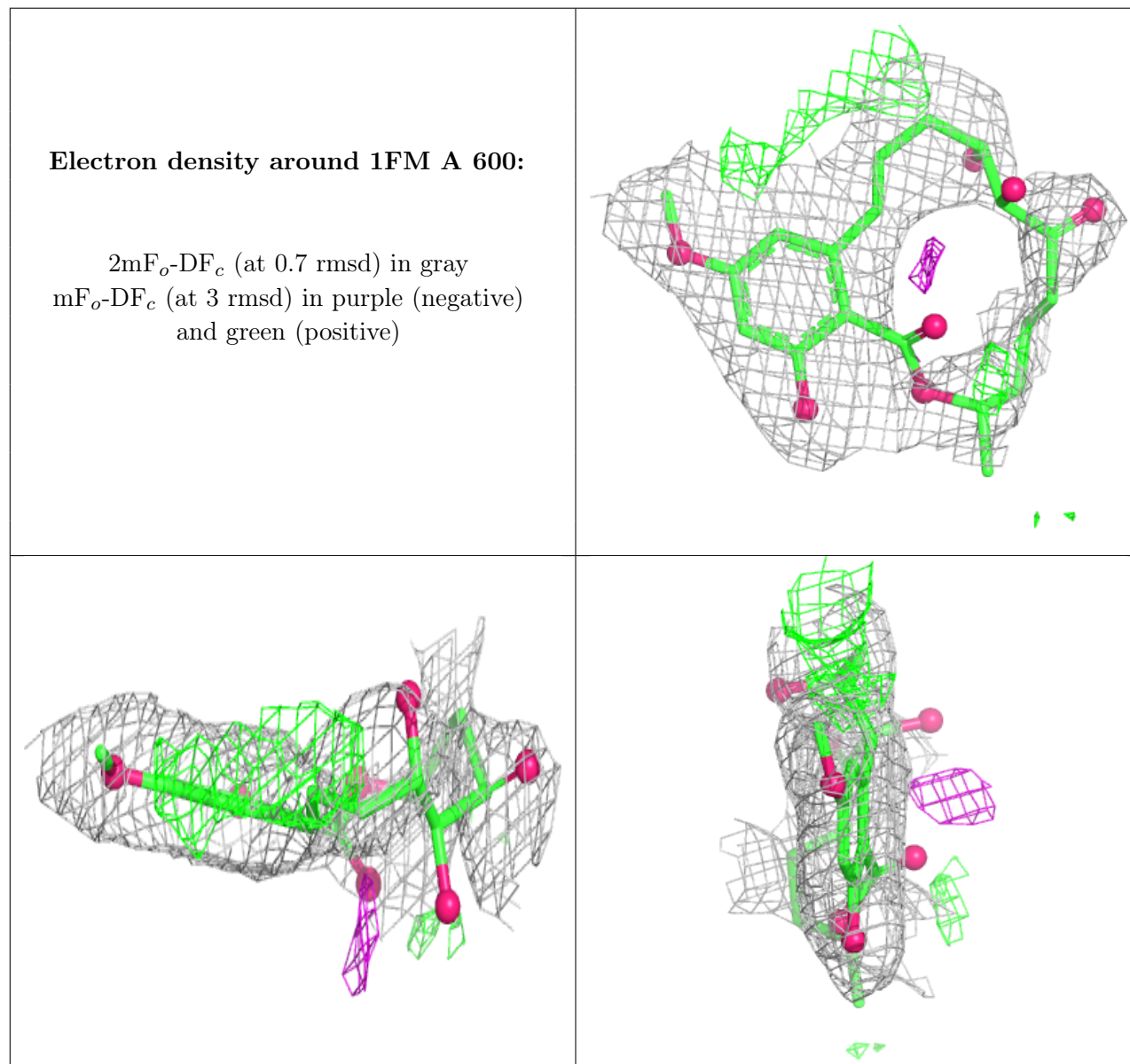
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	1FM	A	600	26/26	0.77	0.18	53,86,99,114	0

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.