



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:49 PM UTC

PDB ID : 9M25 / pdb_00009m25
Title : Type I diterpene synthase from Streptomyces
Authors : Bai, Z.Y.; Ma, M.
Deposited on : 2025-02-27
Resolution : 2.50 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
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

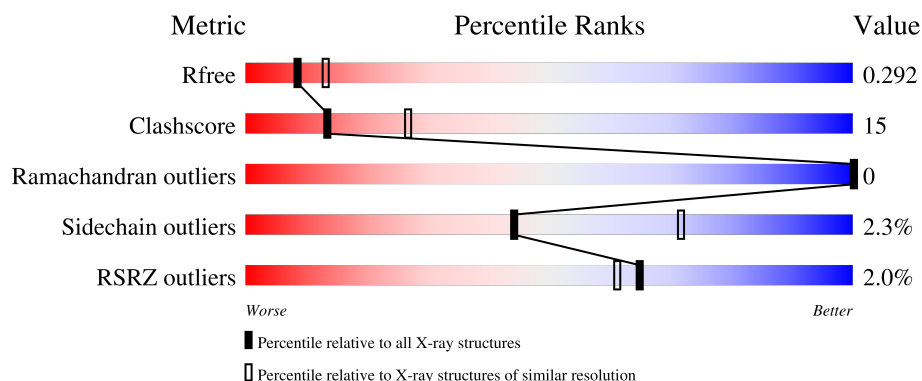
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

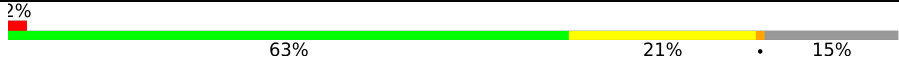

The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	363	
1	B	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	402	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5070 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 Terpene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2439	1528	461	438	12			
1	B	306	Total	C	N	O	S	0	0	0
			2426	1520	462	432	12			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7K3HBY9
A	2	ASP	-	expression tag	UNP A0A7K3HBY9
A	3	ALA	-	expression tag	UNP A0A7K3HBY9
A	4	VAL	-	expression tag	UNP A0A7K3HBY9
A	5	HIS	-	expression tag	UNP A0A7K3HBY9
A	6	GLY	-	expression tag	UNP A0A7K3HBY9
A	7	PRO	-	expression tag	UNP A0A7K3HBY9
A	8	GLU	-	expression tag	UNP A0A7K3HBY9
A	9	ASP	-	expression tag	UNP A0A7K3HBY9
A	10	GLY	-	expression tag	UNP A0A7K3HBY9
A	11	SER	-	expression tag	UNP A0A7K3HBY9
A	12	GLY	-	expression tag	UNP A0A7K3HBY9
A	13	PRO	-	expression tag	UNP A0A7K3HBY9
A	14	GLY	-	expression tag	UNP A0A7K3HBY9
A	15	SER	-	expression tag	UNP A0A7K3HBY9
A	16	GLU	-	expression tag	UNP A0A7K3HBY9
A	17	SER	-	expression tag	UNP A0A7K3HBY9
A	18	GLY	-	expression tag	UNP A0A7K3HBY9
A	19	SER	-	expression tag	UNP A0A7K3HBY9
A	20	ALA	-	expression tag	UNP A0A7K3HBY9
A	21	SER	-	expression tag	UNP A0A7K3HBY9
A	22	ARG	-	expression tag	UNP A0A7K3HBY9
A	23	PRO	-	expression tag	UNP A0A7K3HBY9
A	24	GLY	-	expression tag	UNP A0A7K3HBY9
A	25	ALA	-	expression tag	UNP A0A7K3HBY9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	-	expression tag	UNP A0A7K3HBY9
A	27	GLN	-	expression tag	UNP A0A7K3HBY9
A	28	PRO	-	expression tag	UNP A0A7K3HBY9
A	29	PRO	-	expression tag	UNP A0A7K3HBY9
A	30	GLU	-	expression tag	UNP A0A7K3HBY9
A	31	ILE	-	expression tag	UNP A0A7K3HBY9
A	32	HIS	-	expression tag	UNP A0A7K3HBY9
A	33	CYS	-	expression tag	UNP A0A7K3HBY9
A	34	PRO	-	expression tag	UNP A0A7K3HBY9
A	35	PHE	-	expression tag	UNP A0A7K3HBY9
A	36	PRO	-	expression tag	UNP A0A7K3HBY9
A	37	SER	-	expression tag	UNP A0A7K3HBY9
A	38	GLU	-	expression tag	UNP A0A7K3HBY9
B	1	MET	-	initiating methionine	UNP A0A7K3HBY9
B	2	ASP	-	expression tag	UNP A0A7K3HBY9
B	3	ALA	-	expression tag	UNP A0A7K3HBY9
B	4	VAL	-	expression tag	UNP A0A7K3HBY9
B	5	HIS	-	expression tag	UNP A0A7K3HBY9
B	6	GLY	-	expression tag	UNP A0A7K3HBY9
B	7	PRO	-	expression tag	UNP A0A7K3HBY9
B	8	GLU	-	expression tag	UNP A0A7K3HBY9
B	9	ASP	-	expression tag	UNP A0A7K3HBY9
B	10	GLY	-	expression tag	UNP A0A7K3HBY9
B	11	SER	-	expression tag	UNP A0A7K3HBY9
B	12	GLY	-	expression tag	UNP A0A7K3HBY9
B	13	PRO	-	expression tag	UNP A0A7K3HBY9
B	14	GLY	-	expression tag	UNP A0A7K3HBY9
B	15	SER	-	expression tag	UNP A0A7K3HBY9
B	16	GLU	-	expression tag	UNP A0A7K3HBY9
B	17	SER	-	expression tag	UNP A0A7K3HBY9
B	18	GLY	-	expression tag	UNP A0A7K3HBY9
B	19	SER	-	expression tag	UNP A0A7K3HBY9
B	20	ALA	-	expression tag	UNP A0A7K3HBY9
B	21	SER	-	expression tag	UNP A0A7K3HBY9
B	22	ARG	-	expression tag	UNP A0A7K3HBY9
B	23	PRO	-	expression tag	UNP A0A7K3HBY9
B	24	GLY	-	expression tag	UNP A0A7K3HBY9
B	25	ALA	-	expression tag	UNP A0A7K3HBY9
B	26	ALA	-	expression tag	UNP A0A7K3HBY9
B	27	GLN	-	expression tag	UNP A0A7K3HBY9
B	28	PRO	-	expression tag	UNP A0A7K3HBY9
B	29	PRO	-	expression tag	UNP A0A7K3HBY9

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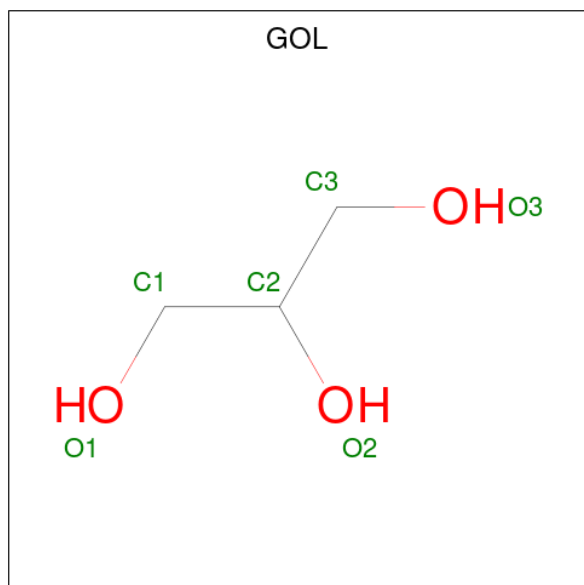
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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	GLU	-	expression tag	UNP A0A7K3HBY9
B	31	ILE	-	expression tag	UNP A0A7K3HBY9
B	32	HIS	-	expression tag	UNP A0A7K3HBY9
B	33	CYS	-	expression tag	UNP A0A7K3HBY9
B	34	PRO	-	expression tag	UNP A0A7K3HBY9
B	35	PHE	-	expression tag	UNP A0A7K3HBY9
B	36	PRO	-	expression tag	UNP A0A7K3HBY9
B	37	SER	-	expression tag	UNP A0A7K3HBY9
B	38	GLU	-	expression tag	UNP A0A7K3HBY9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	0
			95	95		
5	B	98	Total	O	0	0
			98	98		

- Molecule 1: Terpene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.29Å 110.26Å 156.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.51 – 2.50 26.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (26.51-2.50) 94.6 (26.51-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.90 (at 2.50Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.211 , 0.297 0.214 , 0.292	Depositor DCC
R_{free} test set	1108 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.5	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	0.93	EDS
Total number of atoms	5070	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2808e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, GOL

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	0.55	0/2504	0.68	1/3407 (0.0%)
1	B	0.52	0/2489	0.63	2/3384 (0.1%)
All	All	0.54	0/4993	0.65	3/6791 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ALA	N-CA-C	-8.44	101.71	112.93
1	B	68	ARG	N-CA-C	-5.43	105.28	111.14
1	B	47	GLU	CA-CB-CG	5.07	124.24	114.10

There are no chirality outliers.

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	A	2439	0	2347	83	0
1	B	2426	0	2341	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	8	1	0
4	B	4	0	6	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	95	0	0	12	0
5	B	98	0	0	7	0
All	All	5070	0	4702	141	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 15.

All (141) 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:B:129:VAL:HG13	4:B:402:EDO:H21	1.39	1.04
1:A:300:ARG:HG3	5:A:506:HOH:O	1.63	0.97
1:A:303:LEU:HD21	1:A:314:LEU:HD22	1.64	0.79
1:B:116:ILE:HG22	1:B:118:SER:H	1.49	0.77
1:A:236:ALA:HB1	1:A:299:HIS:CD2	2.20	0.77
1:B:152:ARG:HG3	4:B:402:EDO:H22	1.67	0.77
1:A:295:ARG:O	1:A:299:HIS:ND1	2.20	0.74
1:A:300:ARG:CG	1:A:318:LEU:HD13	2.17	0.74
1:A:264:HIS:HD2	5:A:504:HOH:O	1.72	0.73
1:A:314:LEU:O	1:A:318:LEU:HG	1.91	0.71
1:A:159:ALA:HB1	1:A:167:ARG:HE	1.55	0.70
1:A:300:ARG:HD2	1:A:318:LEU:HD13	1.74	0.70
1:A:33:CYS:HB3	1:A:326:ARG:HH11	1.58	0.68
1:B:152:ARG:CG	4:B:402:EDO:H22	2.23	0.68
1:A:279:ARG:NE	5:A:505:HOH:O	2.26	0.67
1:A:104:ASP:HB3	5:A:545:HOH:O	1.92	0.67
1:A:299:HIS:HD2	1:A:302:ARG:NH2	1.94	0.66
1:B:31:ILE:O	1:B:333:ARG:NH2	2.29	0.66
1:B:116:ILE:HD13	1:B:122:ALA:HA	1.80	0.63
1:B:152:ARG:CB	4:B:402:EDO:H22	2.28	0.63
1:A:300:ARG:CD	1:A:318:LEU:HD13	2.29	0.62
1:B:116:ILE:N	5:B:507:HOH:O	2.34	0.60
1:B:123:MET:SD	1:B:179:GLU:HG2	2.42	0.60
1:B:49:HIS:CE1	1:B:91:ASP:HB3	2.37	0.59
1:B:31:ILE:HD11	1:B:251:TRP:CD2	2.36	0.59
1:B:254:LEU:HD22	1:B:282:LEU:HD21	1.83	0.59
1:A:237:VAL:HG23	1:A:321:MET:HE1	1.85	0.58
1:B:128:ARG:NH1	5:B:509:HOH:O	2.36	0.58
1:A:46:ALA:HA	1:A:91:ASP:OD1	2.04	0.58
1:A:275:ARG:NH2	1:B:123:MET:HE1	2.18	0.57
1:B:337:ARG:HH11	1:B:337:ARG:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:CD2	5:A:504:HOH:O	2.53	0.57
1:A:234:PHE:N	1:A:303:LEU:HD12	2.19	0.57
1:A:56:ARG:HD3	5:A:528:HOH:O	2.03	0.57
1:A:224:LEU:HD21	1:A:313:ALA:HB3	1.87	0.56
1:A:295:ARG:HB3	1:A:299:HIS:HE1	1.70	0.56
1:A:31:ILE:HD11	1:A:251:TRP:CD2	2.41	0.56
1:A:199:TYR:OH	1:A:250:ASP:OD2	2.22	0.56
1:A:232:GLU:HB3	5:A:518:HOH:O	2.04	0.56
1:A:275:ARG:O	1:B:121:ARG:HD3	2.06	0.56
1:B:290:SER:O	1:B:294:ARG:HG2	2.06	0.56
1:A:234:PHE:HD1	1:A:303:LEU:HD11	1.70	0.55
1:A:184:GLU:HG3	1:A:264:HIS:ND1	2.22	0.55
1:A:33:CYS:HB3	1:A:326:ARG:NH1	2.22	0.55
1:A:287:ALA:O	1:A:291:ALA:HB2	2.07	0.54
1:A:184:GLU:HG3	1:A:264:HIS:CG	2.42	0.54
1:B:64:VAL:O	1:B:68:ARG:HG3	2.07	0.54
1:B:108:ASP:OD2	1:B:188:ARG:NH2	2.39	0.54
1:B:108:ASP:OD2	1:B:188:ARG:NH1	2.41	0.54
1:B:126:LEU:O	1:B:129:VAL:HB	2.08	0.53
1:A:290:SER:O	1:A:294:ARG:NH1	2.41	0.53
1:A:299:HIS:CD2	1:A:302:ARG:HH21	2.25	0.53
1:A:295:ARG:HB3	1:A:299:HIS:CE1	2.45	0.52
1:A:318:LEU:HD22	5:A:506:HOH:O	2.10	0.52
1:A:299:HIS:CD2	1:A:302:ARG:NH2	2.76	0.51
1:A:204:ARG:HH21	1:A:243:ASP:CG	2.18	0.51
1:A:204:ARG:NH1	1:A:239:ARG:HH21	2.08	0.51
1:A:253:SER:HA	1:A:256:LYS:HD2	1.93	0.51
1:A:254:LEU:HD13	1:A:267:VAL:HB	1.93	0.51
1:A:204:ARG:HH12	1:A:239:ARG:HH21	1.59	0.51
1:B:296:TYR:HE1	1:B:321:MET:CE	2.23	0.50
1:A:257:GLU:HG3	1:A:265:ASN:HD22	1.76	0.50
1:A:133:GLU:HG2	5:A:531:HOH:O	2.12	0.50
1:B:204:ARG:HD3	1:B:210:TYR:OH	2.12	0.49
1:B:108:ASP:OD2	1:B:188:ARG:CZ	2.59	0.49
1:B:140:ARG:HD2	1:B:144:GLU:O	2.12	0.49
1:B:123:MET:HG3	1:B:178:LEU:HB3	1.94	0.49
1:A:295:ARG:NH2	5:A:512:HOH:O	2.44	0.49
1:A:82:TYR:CD1	1:A:93:VAL:HG11	2.48	0.49
1:A:119:ALA:HB1	1:A:182:CYS:SG	2.53	0.49
1:A:234:PHE:HA	1:A:303:LEU:CD1	2.43	0.48
1:B:267:VAL:HG11	1:B:282:LEU:CD2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:O	1:A:228:VAL:HG22	2.14	0.48
1:A:31:ILE:HD11	1:A:251:TRP:CG	2.48	0.48
1:B:60:VAL:HG12	1:B:66:ARG:HG2	1.95	0.48
1:B:179:GLU:OE1	5:B:501:HOH:O	2.20	0.48
1:B:152:ARG:HD2	4:B:402:EDO:O1	2.14	0.48
1:A:209:ILE:HG21	1:A:242:SER:HB3	1.96	0.47
1:B:291:ALA:O	1:B:295:ARG:HG3	2.15	0.47
1:A:326:ARG:HD2	1:A:326:ARG:HA	1.46	0.47
1:B:33:CYS:SG	1:B:35:PHE:HD2	2.37	0.47
1:A:300:ARG:HG2	1:A:318:LEU:HD13	1.93	0.47
1:B:49:HIS:HE1	1:B:95:ASP:OD2	1.98	0.47
1:B:67:GLU:OE2	1:B:67:GLU:HA	2.15	0.47
1:A:318:LEU:HB3	5:A:506:HOH:O	2.14	0.47
1:A:274:ARG:HB3	1:A:276:LEU:HG	1.97	0.46
1:A:290:SER:O	1:A:294:ARG:CZ	2.62	0.46
1:A:30:GLU:OE1	1:A:31:ILE:N	2.34	0.46
1:A:37:SER:HB3	1:A:330:ASP:OD2	2.15	0.46
1:B:123:MET:HB3	1:B:123:MET:HE2	1.35	0.46
1:B:168:ARG:NH1	5:B:513:HOH:O	2.43	0.46
1:A:184:GLU:HG3	1:A:264:HIS:CE1	2.50	0.46
1:B:124:ASP:O	1:B:128:ARG:HG3	2.16	0.46
1:B:31:ILE:HG13	1:B:252:TYR:HE1	1.80	0.46
1:A:189:ILE:O	1:A:190:ALA:HB3	2.16	0.46
1:A:210:TYR:OH	1:A:239:ARG:HG2	2.16	0.45
1:B:82:TYR:CD1	1:B:93:VAL:HG11	2.51	0.45
1:B:129:VAL:HG13	4:B:402:EDO:C2	2.29	0.45
1:B:296:TYR:HE1	1:B:321:MET:HE3	1.82	0.45
1:A:224:LEU:HD21	1:A:313:ALA:CB	2.45	0.44
1:B:44:GLU:OE1	1:B:44:GLU:N	2.49	0.44
1:B:116:ILE:HG22	1:B:117:ASP:N	2.31	0.44
1:B:318:LEU:HD23	1:B:321:MET:CE	2.48	0.44
1:A:204:ARG:HD3	1:A:210:TYR:OH	2.18	0.44
1:A:237:VAL:CG2	1:A:321:MET:HE1	2.48	0.44
1:B:130:LEU:HD23	1:B:171:THR:HG23	1.99	0.44
1:A:236:ALA:HB1	1:A:299:HIS:HD2	1.77	0.43
1:B:136:ALA:HB3	1:B:153:ASP:HB2	2.00	0.43
1:A:228:VAL:HG12	1:A:307:HIS:CD2	2.53	0.43
1:A:296:TYR:HD2	1:A:297:LEU:HD23	1.84	0.43
1:A:273:ALA:HB2	5:A:542:HOH:O	2.19	0.43
1:B:267:VAL:HG11	1:B:282:LEU:HD23	1.99	0.43
1:B:116:ILE:CG2	1:B:117:ASP:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:NH1	1:A:262:GLU:OE1	2.52	0.43
1:A:275:ARG:HH22	1:B:123:MET:HE1	1.84	0.42
1:A:204:ARG:NE	1:A:243:ASP:OD1	2.44	0.42
1:B:262:GLU:HB3	5:B:547:HOH:O	2.19	0.42
1:A:173:HIS:ND1	1:A:214:ASP:OD2	2.46	0.42
1:B:288:ALA:O	5:B:502:HOH:O	2.22	0.42
1:A:289:ILE:C	1:A:291:ALA:H	2.26	0.42
1:B:152:ARG:HB2	4:B:402:EDO:H22	1.98	0.42
1:A:42:HIS:NE2	3:A:402:GOL:H32	2.35	0.42
1:B:152:ARG:HG3	4:B:402:EDO:C2	2.45	0.42
1:A:253:SER:O	1:A:257:GLU:HG2	2.20	0.41
1:A:295:ARG:C	1:A:299:HIS:HD1	2.26	0.41
1:B:60:VAL:CG1	1:B:66:ARG:HG2	2.49	0.41
1:A:296:TYR:CD2	1:A:297:LEU:HD23	2.56	0.41
1:A:234:PHE:HA	1:A:303:LEU:HD13	2.03	0.41
1:A:116:ILE:HB	1:A:122:ALA:HB2	2.03	0.41
1:B:49:HIS:ND1	1:B:91:ASP:HB3	2.35	0.41
1:B:272:HIS:HB2	5:B:524:HOH:O	2.21	0.41
1:A:258:MET:HE1	1:A:278:LEU:HD21	2.03	0.41
1:B:188:ARG:HD3	1:B:262:GLU:OE1	2.20	0.41
1:B:59:VAL:HG22	1:B:102:LEU:HD13	2.02	0.41
1:A:232:GLU:N	1:A:233:PRO:HD2	2.36	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.85	0.41
1:B:300:ARG:HG3	1:B:318:LEU:HD22	2.02	0.41
1:A:224:LEU:HA	1:A:225:PRO:HD3	1.87	0.41
1:B:296:TYR:CE1	1:B:321:MET:HE3	2.56	0.41
1:A:257:GLU:HG3	1:A:265:ASN:ND2	2.35	0.40
1:A:234:PHE:CA	1:A:303:LEU:CD1	2.98	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	306/363 (84%)	301 (98%)	5 (2%)	0	100	100
1	B	302/363 (83%)	300 (99%)	2 (1%)	0	100	100
All	All	608/726 (84%)	601 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	240/276 (87%)	233 (97%)	7 (3%)	37	65
1	B	238/276 (86%)	234 (98%)	4 (2%)	53	78
All	All	478/552 (87%)	467 (98%)	11 (2%)	44	72

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	112	VAL
1	A	178	LEU
1	A	189	ILE
1	A	235	GLN
1	A	326	ARG
1	A	336	LEU
1	B	37	SER
1	B	67	GLU
1	B	260	LEU
1	B	336	LEU

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

Mol	Chain	Res	Type
1	A	229	HIS
1	A	249	ASN

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Mol	Chain	Res	Type
1	A	299	HIS
1	B	49	HIS
1	B	76	GLN
1	B	156	HIS
1	B	264	HIS
1	B	307	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	GOL	A	402	-	5,5,5	1.07	0	5,5,5	1.33	1 (20%)
4	EDO	B	402	-	3,3,3	0.30	0	2,2,2	0.46	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	GOL	A	402	-	-	1/4/4/4	-
4	EDO	B	402	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	402	GOL	C3-C2-C1	-2.03	104.34	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-O2
4	B	402	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	1	0
4	B	402	EDO	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	308/363 (84%)	0.37	9 (2%) 53 49	28, 46, 76, 103	0
1	B	306/363 (84%)	0.22	3 (0%) 79 76	29, 43, 68, 105	0
All	All	614/726 (84%)	0.30	12 (1%) 65 61	28, 44, 74, 105	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	GLU	4.0
1	A	290	SER	3.8
1	A	234	PHE	3.5
1	B	67	GLU	2.9
1	A	198	GLU	2.6
1	A	223	ASP	2.5
1	A	227	ALA	2.4
1	A	86	ASP	2.4
1	A	44	GLU	2.2
1	B	133	GLU	2.1
1	B	116	ILE	2.1
1	A	168	ARG	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 oligosaccharides in this entry.

6.4 Ligands

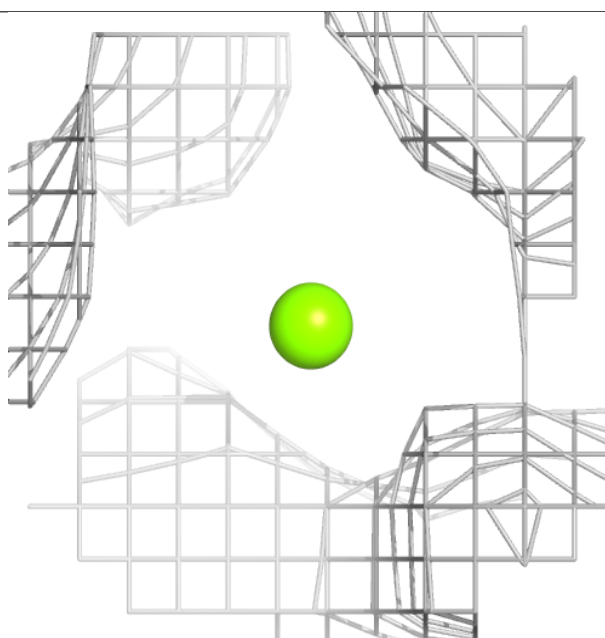
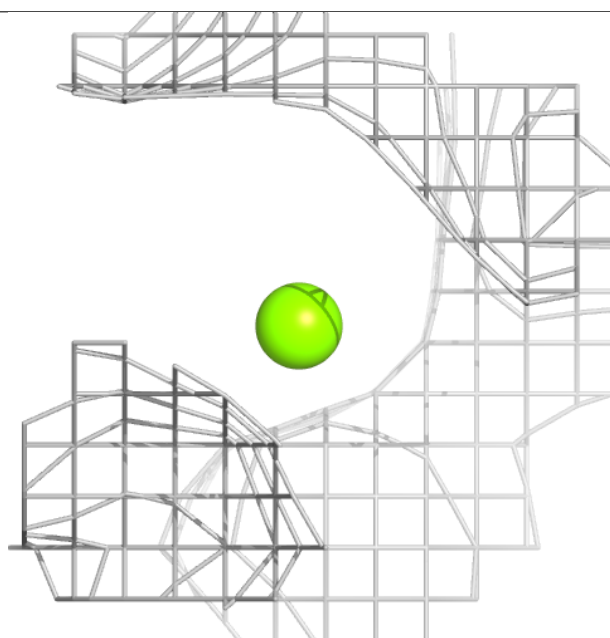
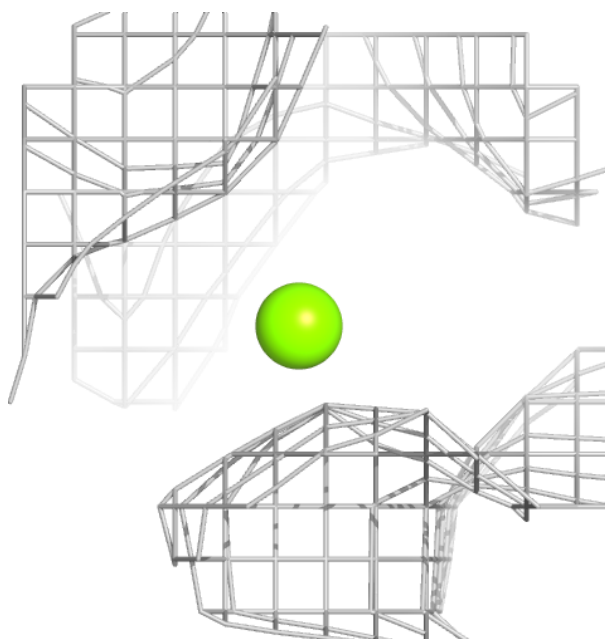
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

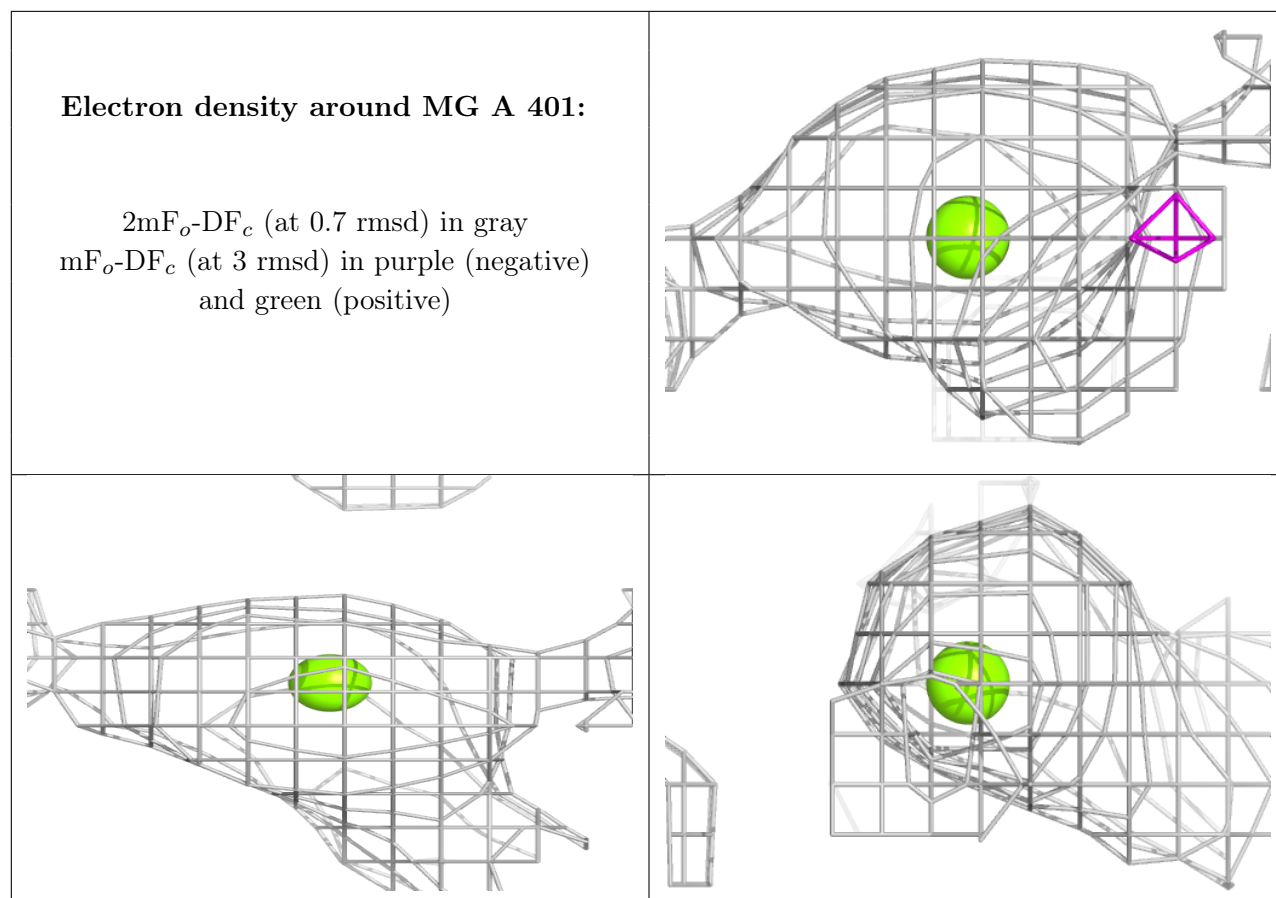
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	401	1/1	0.78	0.23	75,75,75,75	0
3	GOL	A	402	6/6	0.81	0.20	44,50,53,55	0
4	EDO	B	402	4/4	0.89	0.16	35,36,42,42	0
2	MG	A	401	1/1	0.96	0.09	77,77,77,77	0

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.

Electron density around MG B 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.