

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2025 – 04:52 PM EST

PDB ID	:	9MGQ
Title	:	Crystal structure of PRMT5:MEP50 in complex with sinefungin and com-
		pound 47
Authors	:	Whittington, D.A.
Deposited on	:	2024-12-11
Resolution	:	1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.85 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	А	645	90%		7%	•				
2	В	350	11%	8%	13%	-				



9MGQ

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8134 atoms, of which 193 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	624	Total 5063	C 3240	N 866	O 932	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	0	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-7	MET	-	initiating methionine	UNP 014744
А	-6	ASP	-	expression tag	UNP 014744
А	-5	TYR	-	expression tag	UNP 014744
А	-4	LYS	-	expression tag	UNP 014744
А	-3	ASP	-	expression tag	UNP 014744
А	-2	ASP	-	expression tag	UNP 014744
А	-1	ASP	-	expression tag	UNP 014744
А	0	ASP	-	expression tag	UNP 014744
A	1	LYS	-	expression tag	UNP 014744

• Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	306	Total 2318	C 1456	N 396	O 452	S 14	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-7	MET	-	initiating methionine	UNP Q9BQA1
В	-6	HIS	-	expression tag	UNP Q9BQA1
В	-5	HIS	-	expression tag	UNP Q9BQA1
В	-4	HIS	-	expression tag	UNP Q9BQA1
В	-3	HIS	-	expression tag	UNP Q9BQA1
В	-2	HIS	-	expression tag	UNP Q9BQA1
В	-1	HIS	-	expression tag	UNP Q9BQA1



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Chain	Residue	Modelled	Actual	Comment	Reference
В	0	HIS	-	expression tag	UNP Q9BQA1
В	1	HIS	-	expression tag	UNP Q9BQA1

• Molecule 3 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	А	1	Total 50	C 15	Н 23	N 7	O 5	0	0

• Molecule 4 is 2-(cyclobutylamino)-N-{(2R)-2-hydroxy-2-[(3S)-1,2,3,4-tetrahydroisoquino lin-3-yl]ethyl}pyridine-4-carboxamide (three-letter code: A1BLG) (formula: C₂₁H₂₆N₄O₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	А	1	Total 53	C 21	Н 26	N 4	0 2	0	0

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{cccc} \mathrm{Total} & \mathrm{C} & \mathrm{H} & \mathrm{O} \\ 10 & 2 & 6 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 10 & 2 & 6 & 2 \end{array}$	0	0
5	А	1	Total C H O 10 2 6 2	0	0

Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
E	٨	1	Total	С	Н	0	0	0
5	A	L	10	2	6	2	0	0
Б	Δ	1	Total	С	Η	0	0	0
0	A	L	10	2	6	2	0	0
F	Δ	1	Total	С	Η	0	0	0
0	A	L	10	2	6	2	0	0
5	Λ	1	Total	С	Н	0	0	0
0	Л	T	10	2	6	2	0	0
5	Δ	1	Total	С	Η	0	0	0
0	Π	T	10	2	6	2	0	0
5	Δ	1	Total	С	Η	0	0	0
0	Π	T	10	2	6	2	0	0
5	Δ	1	Total	С	Η	0	0	0
0	11	I	10	2	6	2	0	0
5	Δ	1	Total	С	Η	Ο	0	0
0	11	I	10	2	6	2	0	0
5	Δ	1	Total	С	Η	Ο	0	0
0	11	I	10	2	6	2	0	0
5	Δ	1	Total	С	Η	Ο	0	0
0	Π	T	10	2	6	2	0	0
5	Δ	1	Total	С	Η	Ο	0	0
0	11	I	10	2	6	2	0	0
5	Δ	1	Total	С	Η	Ο	0	0
0	11	T	10	2	6	2	0	0
5	А	1	Total	С	Н	Ο	0	0
0	11	T	10	2	6	2	0	0
5	Δ	1	Total	С	Η	Ο	0	0
0		1	10	2	6	2	0	0
5	В	1	Total	С	Η	Ο	0	0
		*	10	2	6	2		
5	В	1	Total	С	Η	Ο	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Λ	1	Total O S	0	0
0	Л	1	5 4 1	0	0
6	Δ	1	Total O S	0	0
0	Π	1	5 4 1	0	0
6	Δ	1	Total O S	0	0
0	Π	T	5 4 1	0	U
6	Δ	1	Total O S	0	0
0	Π	T	5 4 1	0	
6	Δ	1	Total O S	0	0
0	Π	1	5 4 1	0	0
6	Δ	1	Total O S	0	0
0	11	1	5 4 1	0	0
6	Δ	1	Total O S	0	0
0	Л	T	5 4 1	0	0
6	B	1	Total O S	0	0
0	D	1	5 4 1	0	

• Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	А	1	Total C 17 4	H 10	0 3	0	0
7	А	1	TotalC174	H 10	0 3	0	0
7	А	1	Total C 17 4	H 10	O 3	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	281	Total O 281 281	0	0
8	В	88	Total O 88 88	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: Protein arginine N-methyltransferase 5





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	101.66Å 137.70Å 178.00Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(Å)	37.00 - 1.85	Depositor
Resolution (A)	37.00 - 1.85	EDS
% Data completeness	70.3 (37.00-1.85)	Depositor
(in resolution range)	70.4 (37.00-1.85)	EDS
R_{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 1.85 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
P. P.	0.199 , 0.242	Depositor
n, n_{free}	0.210 , 0.251	DCC
R_{free} test set	3690 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	29.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 31.0	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8134	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: SFG, EDO, A1BLG, PEG, SO4 $\,$

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	А	0.42	0/5208	0.61	0/7086	
2	В	0.40	0/2377	0.66	0/3247	
All	All	0.42	0/7585	0.62	0/10333	

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 (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	А	5063	0	4953	30	0
2	В	2318	0	2239	14	0
3	А	27	23	22	0	0
4	А	27	26	0	0	0
5	А	68	102	102	8	0
5	В	8	12	12	2	0
6	А	35	0	0	0	0
6	В	5	0	0	0	0
7	А	21	30	30	5	0
8	А	281	0	0	0	0
8	В	88	0	0	0	0
All	All	7941	193	7358	42	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 3.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:109:GLN:HE21	7:A:729:PEG:H22	1.36	0.91
1:A:112:ASN:HB2	5:A:712:EDO:H22	1.58	0.86
1:A:202:ILE:HB	5:A:710:EDO:H12	1.77	0.67
1:A:147:HIS:HD2	1:A:201:ARG:HH22	1.45	0.65
1:A:200:LYS:H	5:A:707:EDO:H12	1.62	0.64
2:B:240:VAL:HG22	2:B:247:CYS:HB3	1.80	0.64
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.87	0.57
1:A:131:ASN:H	7:A:727:PEG:H32	1.71	0.56
1:A:485:ARG:HG3	1:A:498:PHE:HZ	1.72	0.54
1:A:202:ILE:HB	5:A:710:EDO:C1	2.37	0.53
1:A:361:LEU:HD11	1:A:431:ILE:HD12	1.90	0.53
1:A:157:LEU:HB2	5:A:704:EDO:H12	1.92	0.52
1:A:147:HIS:CD2	1:A:201:ARG:HH22	2.27	0.51
1:A:109:GLN:HG3	7:A:729:PEG:H22	1.94	0.50
1:A:109:GLN:NE2	7:A:729:PEG:H22	2.17	0.49
1:A:567:ILE:HG21	1:A:579:TRP:HB2	1.94	0.49
2:B:284:ASP:HB3	2:B:290:LEU:HD11	1.95	0.48
1:A:333:LYS:HE3	1:A:435:GLU:HG3	1.96	0.47
2:B:96:VAL:HB	2:B:104:GLU:HG3	1.96	0.47
1:A:183:GLU:OE2	1:A:216:HIS:HD2	1.98	0.47
1:A:209:GLY:N	5:A:704:EDO:H11	2.30	0.47
2:B:44:LEU:HB2	2:B:59:TRP:HB2	1.97	0.46
2:B:220:TRP:H	5:B:401:EDO:H21	1.79	0.46
1:A:209:GLY:O	1:A:250:HIS:HE1	1.98	0.46
2:B:206:ILE:HG23	2:B:245:THR:HG23	1.97	0.46
1:A:82:ILE:O	1:A:120:PRO:HD2	2.16	0.46
1:A:553:GLY:HA3	1:A:582:ILE:HG22	1.98	0.45
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.99	0.45
2:B:24:PRO:HG3	2:B:78:GLN:HE21	1.82	0.45
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.32	0.45
2:B:309:ASN:HB3	2:B:312:LEU:HD12	1.99	0.45
2:B:27:MET:HG3	2:B:59:TRP:NE1	2.32	0.43
1:A:198:TYR:HA	5:A:710:EDO:C2	2.49	0.43
1:A:131:ASN:HB2	7:A:727:PEG:H41	2.01	0.43
1:A:167:ILE:HB	2:B:202:PRO:HD2	2.01	0.43
1:A:621:VAL:HA	5:A:719:EDO:H21	2.02	0.42
1:A:68:ARG:HB3	2:B:51:GLY:O	2.20	0.42



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104[A]:GLU:HG2	1:A:137:VAL:HG21	2.03	0.41
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.85	0.40
2:B:303:ALA:HB1	2:B:313:LEU:HD11	2.03	0.40
2:B:24:PRO:HG3	2:B:78:GLN:HG2	2.02	0.40
1:A:96:VAL:HG11	5:B:402:EDO:H21	2.03	0.40

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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	Perce	entiles
1	А	624/645~(97%)	611 (98%)	13~(2%)	0	100	100
2	В	303/350~(87%)	292~(96%)	10 (3%)	1 (0%)	37	25
All	All	927/995~(93%)	903~(97%)	23~(2%)	1 (0%)	48	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	147	ILE

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 side chain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	559/570~(98%)	551 (99%)	8 (1%)	62 53	
2	В	261/298~(88%)	256~(98%)	5(2%)	52 39	
All	All	820/868~(94%)	807~(98%)	13~(2%)	58 46	

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All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	193	ARG
1	А	214	SER
1	А	275	LYS
1	А	351	GLU
1	А	393	LYS
1	А	435	GLU
1	А	544	VAL
1	А	570	GLU
2	В	111	ASN
2	В	187	SER
2	В	205	GLN
2	В	225	SER
2	В	274	LEU

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

Mol	Chain	Res	Type
1	А	131	ASN
1	А	147	HIS
1	А	216	HIS
1	А	250	HIS
1	А	508	ASN
1	А	532	ASN
2	В	78	GLN
2	В	111	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

32 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).

Mal	Tune	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	SO4	А	723	-	4,4,4	0.26	0	$6,\!6,\!6$	0.07	0
5	EDO	В	401	-	3,3,3	0.57	0	2,2,2	0.25	0
5	EDO	А	704	-	3,3,3	0.67	0	2,2,2	0.05	0
6	SO4	А	726	-	4,4,4	0.24	0	6,6,6	0.10	0
5	EDO	А	719	-	3,3,3	0.57	0	$2,\!2,\!2$	0.33	0
5	EDO	А	716	-	3, 3, 3	0.50	0	$2,\!2,\!2$	0.38	0
5	EDO	А	703	-	3,3,3	0.44	0	2,2,2	0.33	0
5	EDO	А	712	-	3,3,3	0.41	0	$2,\!2,\!2$	0.47	0
7	PEG	А	729	-	6,6,6	0.15	0	$5,\!5,\!5$	0.35	0
5	EDO	А	717	-	3, 3, 3	0.51	0	$2,\!2,\!2$	0.34	0
4	A1BLG	А	702	-	30,30,30	0.20	0	33,41,41	0.54	1 (3%)
6	SO4	А	721	-	4,4,4	0.25	0	6,6,6	0.17	0
5	EDO	А	718	-	3,3,3	0.35	0	2,2,2	0.47	0
5	EDO	А	715	-	3,3,3	0.42	0	$2,\!2,\!2$	0.44	0
6	SO4	А	724	-	4,4,4	0.20	0	$6,\!6,\!6$	0.13	0
5	EDO	А	714	-	3, 3, 3	0.50	0	$2,\!2,\!2$	0.43	0
5	EDO	А	713	-	3, 3, 3	0.50	0	$2,\!2,\!2$	0.15	0
3	SFG	А	701	-	24,29,29	0.73	0	20,42,42	0.74	1(5%)
7	PEG	А	728	-	6,6,6	0.19	0	$5,\!5,\!5$	0.29	0
5	EDO	В	402	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	A	709	-	3,3,3	0.41	0	2,2,2	0.40	0
5	EDO	А	710	-	3,3,3	0.66	0	2,2,2	0.16	0



Mal	Tune	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	В	ond ang	les
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	В	403	-	4,4,4	0.24	0	$6,\!6,\!6$	0.11	0
6	SO4	А	720	-	4,4,4	0.20	0	6,6,6	0.17	0
5	EDO	А	711	-	3,3,3	0.49	0	$2,\!2,\!2$	0.47	0
6	SO4	А	725	-	4,4,4	0.24	0	6,6,6	0.11	0
5	EDO	А	705	-	3,3,3	0.60	0	$2,\!2,\!2$	0.25	0
5	EDO	А	708	-	3,3,3	0.56	0	$2,\!2,\!2$	0.20	0
6	SO4	А	722	-	4,4,4	0.24	0	$6,\!6,\!6$	0.06	0
5	EDO	А	707	-	3,3,3	0.67	0	2,2,2	0.10	0
5	EDO	А	706	-	3,3,3	0.62	0	2,2,2	0.38	0
7	PEG	А	727	-	6,6,6	0.25	0	$5,\!5,\!5$	0.18	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
5	EDO	В	401	-	-	1/1/1/1	-
5	EDO	А	704	-	-	0/1/1/1	-
5	EDO	А	719	-	-	0/1/1/1	-
5	EDO	А	716	-	-	0/1/1/1	-
5	EDO	А	703	-	-	1/1/1/1	-
5	EDO	А	712	-	-	1/1/1/1	-
7	PEG	А	729	-	-	2/4/4/4	-
5	EDO	А	717	-	-	0/1/1/1	-
4	A1BLG	А	702	-	-	4/17/32/32	0/4/4/4
5	EDO	А	718	-	-	0/1/1/1	-
5	EDO	А	715	-	-	0/1/1/1	-
5	EDO	А	714	-	-	1/1/1/1	-
5	EDO	А	713	-	-	1/1/1/1	-
3	SFG	А	701	-	-	2/13/33/33	0/3/3/3
7	PEG	А	728	-	-	2/4/4/4	-
5	EDO	В	402	-	-	0/1/1/1	-
5	EDO	А	709	-	-	0/1/1/1	-
5	EDO	А	710	-	-	1/1/1/1	-
5	EDO	А	711	-	-	0/1/1/1	-
5	EDO	А	705	-	-	0/1/1/1	-
5	EDO	А	708	-	-	0/1/1/1	-
5	EDO	А	707	-	-	0/1/1/1	-
5	EDO	A	706	-	-	0/1/1/1	-
7	PEG	A	727	-	-	2/4/4/4	-



There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	702	A1BLG	C-C12-N3	-2.20	107.06	110.85
3	А	701	SFG	C5-C6-N6	2.14	123.57	120.31

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	701	SFG	NE-CD-CG-CB
3	А	701	SFG	C5'-CD-CG-CB
7	А	727	PEG	O1-C1-C2-O2
7	А	728	PEG	O2-C3-C4-O4
7	А	729	PEG	O1-C1-C2-O2
5	А	703	EDO	O1-C1-C2-O2
5	В	401	EDO	O1-C1-C2-O2
7	А	728	PEG	C4-C3-O2-C2
4	А	702	A1BLG	O1-C2-C3-C11
4	А	702	A1BLG	N-C2-C3-C11
5	А	713	EDO	O1-C1-C2-O2
4	А	702	A1BLG	C12-C-C1-N
5	А	710	EDO	O1-C1-C2-O2
5	А	714	EDO	O1-C1-C2-O2
7	А	727	PEG	C4-C3-O2-C2
4	А	702	A1BLG	O-C-C1-N
7	А	729	PEG	C4-C3-O2-C2
5	А	712	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	401	EDO	1	0
5	А	704	EDO	2	0
5	А	719	EDO	1	0
5	А	712	EDO	1	0
7	А	729	PEG	3	0
5	В	402	EDO	1	0
5	А	710	EDO	3	0
5	А	707	EDO	1	0
7	А	727	PEG	2	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 sufficient 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	624/645~(96%)	0.33	36 (5%) 30 32	11, 30, 59, 86	2 (0%)
2	В	306/350~(87%)	1.00	40 (13%) 8 8	23, 39, 70, 95	1 (0%)
All	All	930/995~(93%)	0.55	76 (8%) 19 20	11, 33, 64, 95	3~(0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	206	ILE	8.2
2	В	21	PRO	5.7
2	В	248	VAL	5.7
2	В	247	CYS	4.9
2	В	211	PRO	4.7
2	В	246	SER	4.7
2	В	20	PRO	4.4
2	В	210	ALA	4.1
1	А	174	THR	4.0
1	А	243	PHE	3.7
1	А	176	THR	3.7
1	А	146	HIS	3.6
2	В	23	ALA	3.5
2	В	249	LEU	3.4
2	В	245	THR	3.4
2	В	72	PHE	3.2
1	А	529	MET	3.1
2	В	108	LEU	3.0
1	А	175	HIS	3.0
1	А	275	LYS	3.0
2	В	328	PRO	2.8
1	А	284	LEU	2.8
1	A	249	MET	2.8
1	А	281	LEU	2.8



Mol	Chain	Res	Type	RSRZ
2	В	22	ASN	2.8
2	В	25	ALA	2.7
2	В	225	SER	2.7
2	В	24	PRO	2.7
1	А	290	ASN	2.6
1	А	148	SER	2.6
1	А	277	PHE	2.6
2	В	62	LYS	2.6
2	В	111	ASN	2.6
1	А	349	VAL	2.6
1	А	292	PRO	2.6
1	А	361	LEU	2.6
2	В	148	CYS	2.5
2	В	89	VAL	2.5
2	В	118	LYS	2.5
2	В	244	SER	2.4
2	В	243	LYS	2.4
2	В	26	CYS	2.4
1	А	240	LYS	2.4
1	А	273	SER	2.4
2	В	242	THR	2.4
1	А	530	ILE	2.3
1	А	357	ASN	2.3
1	А	637	LEU	2.3
2	В	327	VAL	2.3
2	В	308	LEU	2.3
2	В	41	ALA	2.2
2	В	212	GLY	2.2
1	А	14	VAL	2.2
2	В	268	VAL	2.2
2	В	267	SER	2.2
1	А	241	LYS	2.2
1	А	285	GLU	2.2
1	A	356	THR	2.2
2	В	313	LEU	2.2
2	В	155	ALA	2.2
1	А	316	MET	2.2
2	В	290	LEU	2.2
1	А	528	PRO	2.2
1	А	274	GLU	2.1
1	А	404	TRP	2.1
1	А	147	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	А	411	SER	2.1
1	А	259	LYS	2.1
2	В	61	PHE	2.1
1	А	296	ALA	2.0
1	А	527	ASP	2.0
2	В	109	ASP	2.0
1	А	278	CYS	2.0
2	В	257	CYS	2.0
2	В	312	LEU	2.0
1	А	406	PHE	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	SO4	А	726	5/5	0.48	0.18	123,123,123,123	0
7	PEG	А	728	7/7	0.58	0.28	73,75,80,80	0
5	EDO	А	715	4/4	0.63	0.26	81,82,83,83	0
7	PEG	А	729	7/7	0.67	0.26	$66,\!67,\!68,\!68$	0
6	SO4	А	725	5/5	0.68	0.26	$139,\!139,\!139,\!139,\!139$	0
5	EDO	А	708	4/4	0.69	0.28	58,60,66,66	0
6	SO4	В	403	5/5	0.70	0.20	$105,\!106,\!106,\!107$	0
5	EDO	А	719	4/4	0.71	0.27	83,84,85,85	0
6	SO4	А	722	5/5	0.72	0.22	$151,\!151,\!151,\!151,\!151$	0
5	EDO	А	717	4/4	0.73	0.17	74,74,75,75	0
6	SO4	А	724	5/5	0.74	0.20	$129,\!129,\!129,\!129$	0
5	EDO	А	716	4/4	0.74	0.19	74,75,75,75	0
5	EDO	A	707	4/4	0.74	0.17	43,44,45,45	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	А	712	4/4	0.76	0.33	30,38,43,43	0
5	EDO	А	703	4/4	0.77	0.30	40,43,46,46	0
6	SO4	А	720	5/5	0.78	0.21	79,79,79,79	0
5	EDO	А	710	4/4	0.80	0.38	39,41,46,46	0
6	SO4	А	723	5/5	0.82	0.19	$114,\!115,\!115,\!115$	0
5	EDO	В	401	4/4	0.83	0.22	33,37,38,38	0
5	EDO	В	402	4/4	0.84	0.28	48,49,50,50	0
7	PEG	А	727	7/7	0.84	0.13	36,45,51,51	0
5	EDO	А	705	4/4	0.85	0.26	39,43,43,43	0
5	EDO	А	709	4/4	0.86	0.27	43,45,47,48	0
5	EDO	А	714	4/4	0.86	0.12	$55,\!55,\!56,\!56$	0
5	EDO	А	713	4/4	0.87	0.14	$53,\!54,\!55,\!55$	0
5	EDO	А	706	4/4	0.87	0.28	30,35,36,37	0
6	SO4	А	721	5/5	0.90	0.15	82,84,84,86	0
5	EDO	А	704	4/4	0.91	0.23	34,35,37,37	0
5	EDO	А	718	4/4	0.91	0.13	37,39,40,40	0
5	EDO	А	711	4/4	0.94	0.11	31,32,32,32	0
3	SFG	А	701	27/27	0.95	0.07	15,23,32,34	0
4	A1BLG	А	702	27/27	0.97	0.05	19,23,25,26	0

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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.

