



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:50 AM UTC

PDB ID : 7KIB / pdb_00007kib
Title : PRMT5:MEP50 Complexed with 5,5-Bicyclic Inhibitor Compound 4
Authors : Palte, R.L.; Hayes, R.P.
Deposited on : 2020-10-23
Resolution : 2.52 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

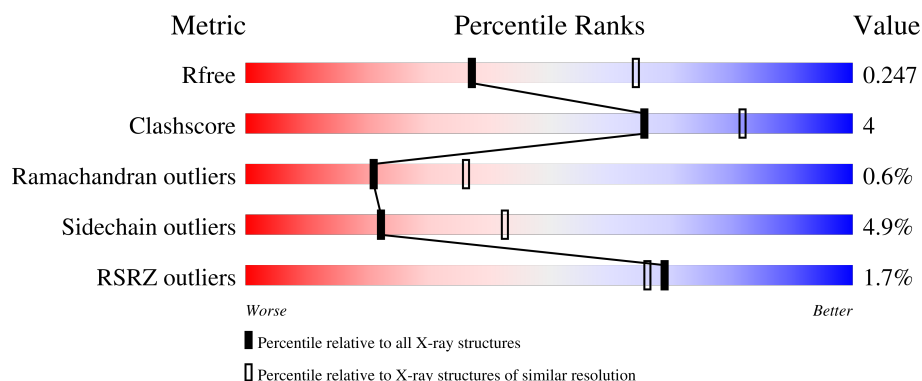
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	645	
2	B	350	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7922 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	1	0
			5069	3242	870	932	25			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O14744
A	-6	ASP	-	expression tag	UNP O14744
A	-5	TYR	-	expression tag	UNP O14744
A	-4	LYS	-	expression tag	UNP O14744
A	-3	ASP	-	expression tag	UNP O14744
A	-2	ASP	-	expression tag	UNP O14744
A	-1	ASP	-	expression tag	UNP O14744
A	0	ASP	-	expression tag	UNP O14744
A	1	LYS	-	expression tag	UNP O14744

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	310	Total	C	N	O	S	0	0	0
			2339	1468	400	457	14			

There are 9 discrepancies between the modelled and reference sequences:

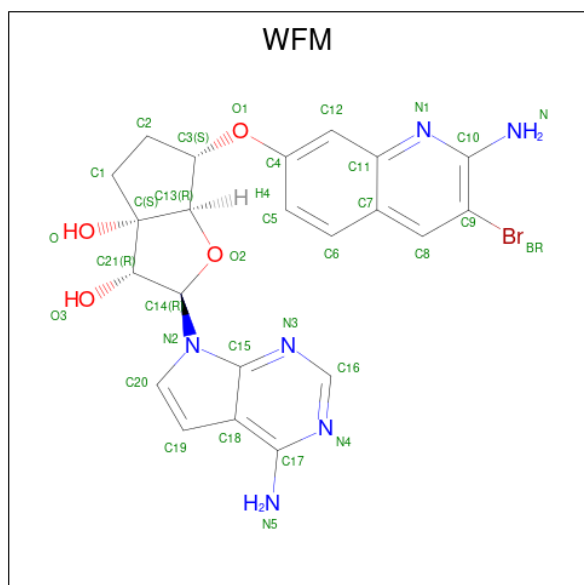
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag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

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

- Molecule 3 is (2R,3R,3aS,6S,6aR)-6-[(2-amino-3-bromoquinolin-7-yl)oxy]-2-(4-amino-7H-pyrrolo[2,3-d]pyrimidin-7-yl)hexahydro-3aH-cyclopenta[b]furan-3,3a-diol (CCD ID: WFM) (formula: C₂₂H₂₁BrN₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			33	1	22	6	4		

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

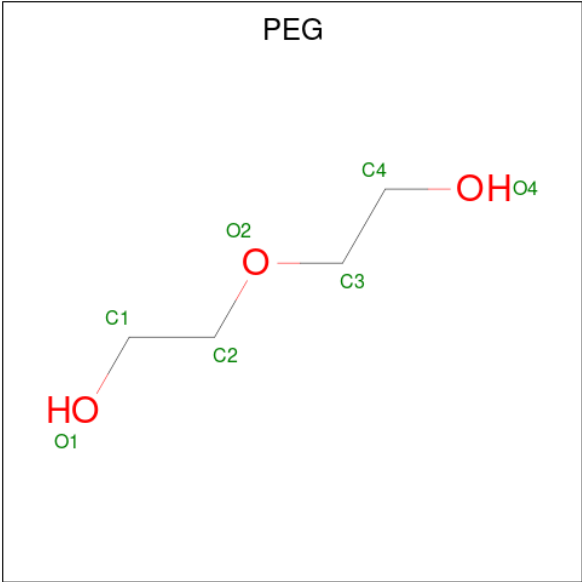


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

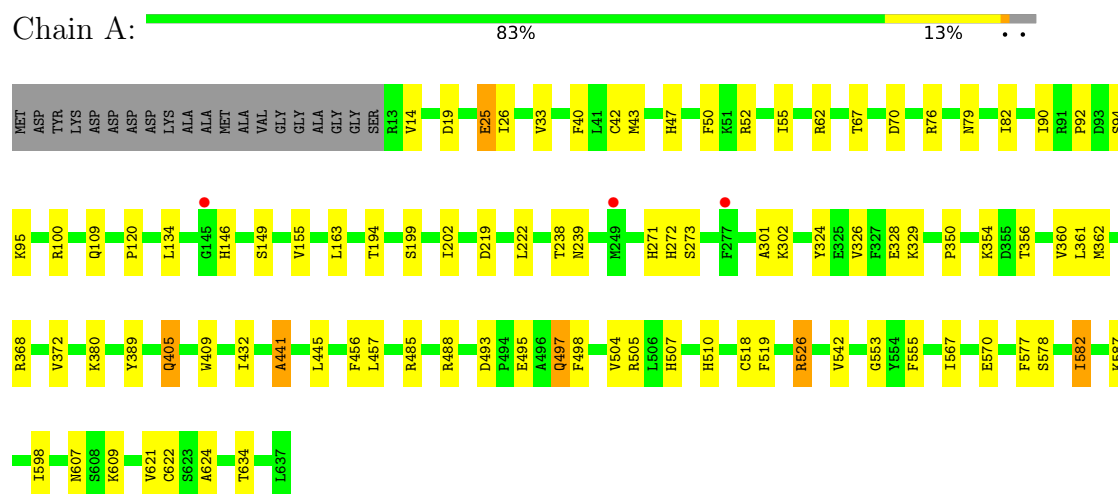
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	328	Total	O	0	0
			328	328		
7	B	96	Total	O	0	0
			96	96		

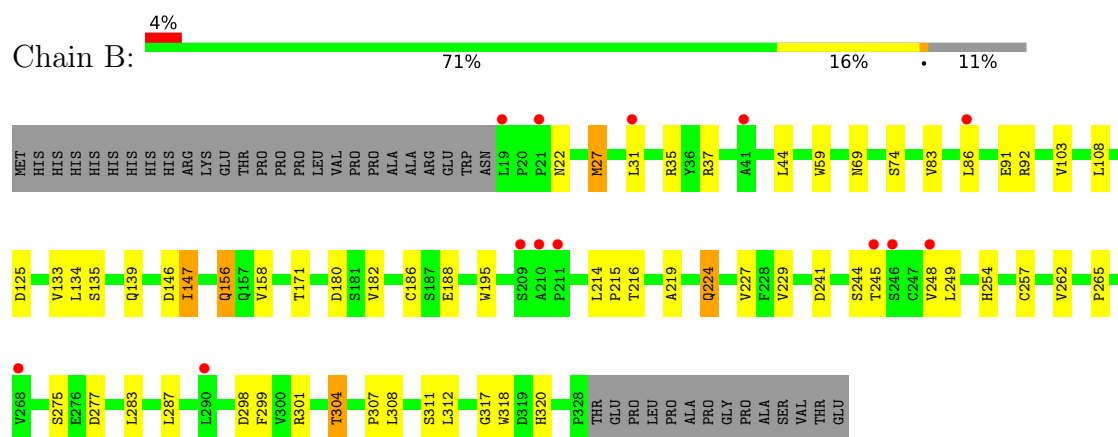
3 Residue-property plots [i](#)

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



- Molecule 2: Methylosome protein 50



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.80Å 138.95Å 179.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.52 46.55 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.55-2.52) 99.9 (46.55-2.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.193 , 0.245 0.193 , 0.247	Depositor DCC
R_{free} test set	2171 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7922	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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.*

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: CL, PEG, EDO, WFM

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	0.88	2/5211 (0.0%)	1.28	23/7088 (0.3%)
2	B	0.88	2/2396 (0.1%)	1.31	11/3275 (0.3%)
All	All	0.88	4/7607 (0.1%)	1.29	34/10363 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	MET	SD-CE	-5.48	1.65	1.79
1	A	518	CYS	CA-C	5.43	1.55	1.52
1	A	507	HIS	CA-C	5.30	1.57	1.52
2	B	147	ILE	CA-C	5.08	1.59	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	ASP	CA-CB-CG	8.19	120.79	112.60
2	B	69	ASN	CA-C-N	7.13	130.14	120.38
2	B	69	ASN	C-N-CA	7.13	130.14	120.38
1	A	456	PHE	CA-CB-CG	7.01	120.81	113.80
1	A	79	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	239	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	67	THR	CA-C-N	5.95	129.73	120.75
1	A	67	THR	C-N-CA	5.95	129.73	120.75
1	A	43	MET	N-CA-C	5.93	115.13	108.25
1	A	272	HIS	CA-C-N	5.90	129.00	120.38
1	A	272	HIS	C-N-CA	5.90	129.00	120.38
1	A	134	LEU	N-CA-C	-5.61	105.08	111.14
1	A	493	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	634	THR	CA-C-N	5.52	130.30	123.12
1	A	634	THR	C-N-CA	5.52	130.30	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	265	PRO	CA-C-N	5.52	128.93	120.82
2	B	265	PRO	C-N-CA	5.52	128.93	120.82
2	B	146	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	372	VAL	N-CA-C	-5.42	105.56	110.82
1	A	70	ASP	CA-CB-CG	5.39	118.00	112.60
2	B	133	VAL	N-CA-CB	5.37	116.58	110.72
1	A	25	GLU	CA-C-N	5.31	128.01	120.53
1	A	25	GLU	C-N-CA	5.31	128.01	120.53
2	B	244	SER	CA-C-N	5.30	131.66	121.54
2	B	244	SER	C-N-CA	5.30	131.66	121.54
2	B	299	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	350	PRO	CA-C-N	5.26	128.05	120.38
1	A	350	PRO	C-N-CA	5.26	128.05	120.38
1	A	90	ILE	CB-CA-C	5.17	116.81	111.23
1	A	194	THR	N-CA-C	-5.15	105.58	111.14
1	A	519	PHE	CA-CB-CG	5.09	118.89	113.80
2	B	22	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	567	ILE	N-CA-C	-5.03	108.22	113.10
1	A	624	ALA	N-CA-C	-5.02	103.90	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5069	0	4960	36	0
2	B	2339	0	2256	22	0
3	A	33	0	0	1	0
4	A	32	0	48	4	0
4	B	8	0	12	0	0
5	A	3	0	0	0	0
6	A	14	0	20	1	0
7	A	328	0	0	1	0
7	B	96	0	0	1	0
All	All	7922	0	7296	56	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 4.

All (56) 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:324:TYR:HB2	1:A:368:ARG:HD2	1.74	0.68
1:A:324:TYR:CB	1:A:368:ARG:HD2	2.23	0.67
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.77	0.66
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.12	0.64
1:A:485:ARG:HG3	1:A:498:PHE:HZ	1.63	0.63
1:A:94:SER:O	1:A:100:ARG:HD3	1.99	0.63
1:A:329:LYS:O	1:A:577:PHE:HE1	1.81	0.63
2:B:35:ARG:HA	2:B:304:THR:HG21	1.84	0.59
1:A:301:ALA:HB1	1:A:505:ARG:HG2	1.85	0.58
1:A:82:ILE:O	1:A:120:PRO:HD2	2.05	0.55
1:A:109:GLN:HE21	4:A:706:EDO:H21	1.71	0.55
1:A:199:SER:HB3	1:A:202:ILE:HD12	1.89	0.55
2:B:188:GLU:HG2	2:B:214:LEU:HD13	1.92	0.52
1:A:92:PRO:O	1:A:100:ARG:HG3	2.11	0.51
1:A:432:ILE:HG12	1:A:457:LEU:HD13	1.92	0.51
1:A:109:GLN:NE2	4:A:706:EDO:H21	2.26	0.51
2:B:224:GLN:HB2	2:B:227:VAL:HG22	1.93	0.51
2:B:182:VAL:HA	2:B:195:TRP:O	2.10	0.51
1:A:405:GLN:HA	1:A:409:TRP:HB2	1.95	0.49
1:A:497:GLN:H	1:A:497:GLN:CD	2.21	0.47
1:A:328:GLU:OE2	1:A:368:ARG:HD3	2.14	0.47
1:A:495:GLU:HB3	1:A:587:LYS:HE2	1.97	0.47
1:A:607:ASN:HB3	1:A:609:LYS:H	1.81	0.46
1:A:368:ARG:NH2	4:A:705:EDO:H22	2.31	0.46
2:B:44:LEU:HB2	2:B:59:TRP:HB2	1.96	0.46
1:A:55:ILE:HD13	7:A:967:HOH:O	2.16	0.45
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.98	0.45
2:B:31:LEU:HB2	2:B:317:GLY:O	2.17	0.45
1:A:324:TYR:HB3	1:A:368:ARG:HD2	1.98	0.45
2:B:254:HIS:CG	2:B:275:SER:HB2	2.51	0.45
2:B:37:ARG:O	2:B:307:PRO:HG3	2.16	0.44
2:B:219:ALA:HB3	2:B:229:VAL:CG2	2.47	0.44
1:A:26:ILE:HG22	7:B:504:HOH:O	2.16	0.44
2:B:171:THR:HG21	2:B:216:THR:HA	1.99	0.44
1:A:271:HIS:HE1	2:B:125:ASP:OD1	2.00	0.44
1:A:149:SER:HB2	4:A:707:EDO:O2	2.17	0.44
2:B:92:ARG:O	2:B:108:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:VAL:HG23	2:B:249:LEU:H	1.83	0.43
1:A:19:ASP:HA	1:A:42:CYS:HB2	2.01	0.43
1:A:578:SER:O	3:A:701:WFM:BR	2.91	0.43
2:B:27:MET:HE3	2:B:31:LEU:HD21	2.01	0.43
2:B:186:CYS:HB2	2:B:215:PRO:HG2	2.01	0.43
2:B:227:VAL:HG12	2:B:241:ASP:HA	2.01	0.43
1:A:526:ARG:H	1:A:526:ARG:HG2	1.60	0.42
1:A:553:GLY:HA3	1:A:582:ILE:HG22	2.01	0.42
1:A:40:PHE:HB3	6:A:713:PEG:H32	2.00	0.42
1:A:219:ASP:O	1:A:222:LEU:HB2	2.19	0.42
1:A:222:LEU:HB3	1:A:510:HIS:HB2	2.01	0.42
2:B:86:LEU:HD12	2:B:86:LEU:HA	1.86	0.41
1:A:441:ALA:HB2	1:A:555:PHE:HB2	2.02	0.41
2:B:27:MET:HG2	2:B:320:HIS:HE1	1.85	0.41
2:B:134:LEU:HD12	2:B:139:GLN:HB3	2.02	0.41
1:A:542:VAL:HG21	1:A:598:ILE:HD12	2.02	0.41
1:A:380:LYS:HA	1:A:380:LYS:HD2	1.96	0.40
1:A:62:ARG:HD3	2:B:298:ASP:OD2	2.21	0.40
2:B:156:GLN:HB3	2:B:158:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	624/645 (97%)	597 (96%)	25 (4%)	2 (0%)	36	53
2	B	308/350 (88%)	287 (93%)	17 (6%)	4 (1%)	9	17
All	All	932/995 (94%)	884 (95%)	42 (4%)	6 (1%)	21	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
2	B	135	SER
1	A	354	LYS
2	B	245	THR
1	A	441	ALA
2	B	308	LEU

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	559/570 (98%)	533 (95%)	26 (5%)	23	44
2	B	263/298 (88%)	249 (95%)	14 (5%)	20	39
All	All	822/868 (95%)	782 (95%)	40 (5%)	22	43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	25	GLU
1	A	33	VAL
1	A	52	ARG
1	A	76	ARG
1	A	95	LYS
1	A	146	HIS
1	A	155	VAL
1	A	163	LEU
1	A	238	THR
1	A	273	SER
1	A	302	LYS
1	A	326	VAL
1	A	356	THR
1	A	360	VAL
1	A	361	LEU
1	A	405	GLN
1	A	445	LEU

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Mol	Chain	Res	Type
1	A	488	ARG
1	A	497	GLN
1	A	504	VAL
1	A	526	ARG
1	A	570	GLU
1	A	582	ILE
1	A	621	VAL
1	A	622	CYS
2	B	74	SER
2	B	83	VAL
2	B	91	GLU
2	B	103	VAL
2	B	156	GLN
2	B	180	ASP
2	B	224	GLN
2	B	257	CYS
2	B	262	VAL
2	B	283	LEU
2	B	287	LEU
2	B	304	THR
2	B	311	SER
2	B	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	271	HIS
1	A	313	GLN
1	A	336	GLN
1	A	359	GLN
1	A	511	GLN
1	A	533	ASN
2	B	223	GLN
2	B	256	GLN
2	B	309	ASN
2	B	310	HIS

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](#)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	$\# Z > 2$
4	EDO	A	709	-	3,3,3	0.55	0	2,2,2	0.33	0
4	EDO	A	705	-	3,3,3	0.38	0	2,2,2	0.68	0
4	EDO	A	702	-	3,3,3	0.37	0	2,2,2	0.74	0
3	WFM	A	701	-	36,38,38	0.33	0	46,59,59	0.89	3 (6%)
4	EDO	A	704	-	3,3,3	0.57	0	2,2,2	0.19	0
4	EDO	A	706	-	3,3,3	0.55	0	2,2,2	0.36	0
4	EDO	A	703	-	3,3,3	0.56	0	2,2,2	0.37	0
4	EDO	A	708	-	3,3,3	0.49	0	2,2,2	0.46	0
6	PEG	A	714	-	6,6,6	0.22	0	5,5,5	0.19	0
4	EDO	B	402	-	3,3,3	0.72	0	2,2,2	0.13	0
4	EDO	A	707	-	3,3,3	0.62	0	2,2,2	0.19	0
4	EDO	B	401	-	3,3,3	0.61	0	2,2,2	0.21	0
6	PEG	A	713	-	6,6,6	0.18	0	5,5,5	0.11	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
4	EDO	A	709	-	-	1/1/1/1	-
4	EDO	A	705	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	702	-	-	0/1/1/1	-
3	WFM	A	701	-	-	1/8/38/38	0/6/6/6
4	EDO	A	704	-	-	0/1/1/1	-
4	EDO	A	706	-	-	1/1/1/1	-
4	EDO	A	703	-	-	0/1/1/1	-
4	EDO	A	708	-	-	0/1/1/1	-
6	PEG	A	714	-	-	1/4/4/4	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	A	707	-	-	0/1/1/1	-
4	EDO	B	401	-	-	1/1/1/1	-
6	PEG	A	713	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	WFM	C13-C-C21	3.19	104.61	101.49
3	A	701	WFM	C-C13-C3	3.04	110.81	104.45
3	A	701	WFM	C2-C1-C	2.44	107.18	102.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	WFM	C2-C3-O1-C4
4	B	401	EDO	O1-C1-C2-O2
6	A	714	PEG	C4-C3-O2-C2
4	A	706	EDO	O1-C1-C2-O2
4	A	709	EDO	O1-C1-C2-O2

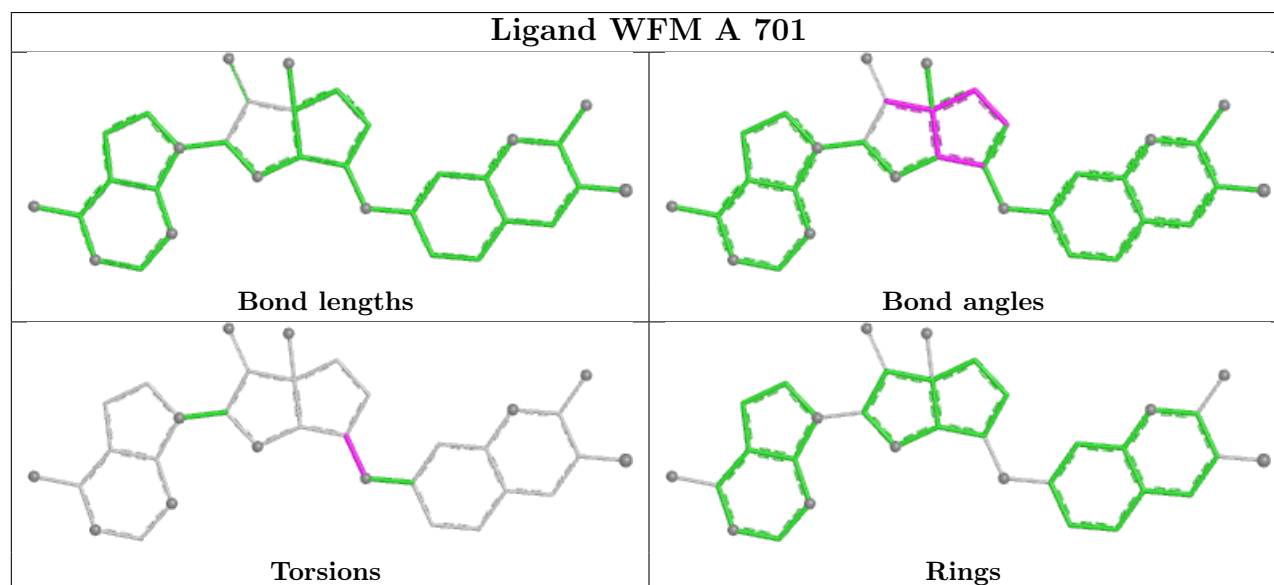
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	EDO	1	0
3	A	701	WFM	1	0
4	A	706	EDO	2	0
4	A	707	EDO	1	0
6	A	713	PEG	1	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	625/645 (96%)	-0.10	3 (0%) 87 85	29, 57, 97, 132	1 (0%)
2	B	310/350 (88%)	0.51	13 (4%) 40 37	51, 73, 110, 140	0
All	All	935/995 (93%)	0.10	16 (1%) 69 66	29, 63, 102, 140	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	PHE	3.8
2	B	210	ALA	2.9
2	B	248	VAL	2.8
2	B	245	THR	2.8
2	B	41	ALA	2.6
2	B	19	LEU	2.5
1	A	249	MET	2.4
2	B	268	VAL	2.4
2	B	211	PRO	2.3
2	B	21	PRO	2.3
2	B	86	LEU	2.2
2	B	290	LEU	2.2
1	A	145	GLY	2.1
2	B	31	LEU	2.1
2	B	209	SER	2.1
2	B	246	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates ⓘ

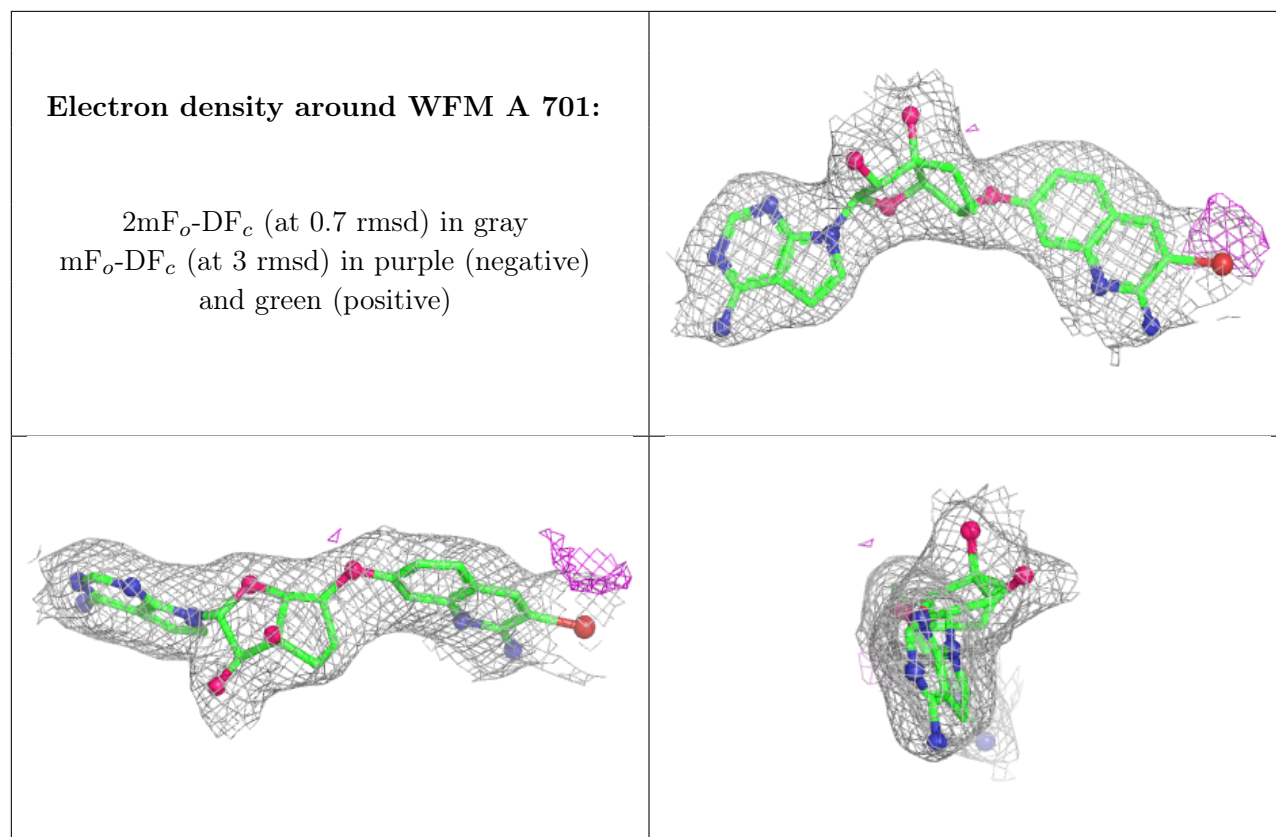
There are no oligosaccharides in this entry.

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
4	EDO	A	703	4/4	0.77	0.19	80,81,81,82	0
4	EDO	A	709	4/4	0.78	0.19	80,81,82,82	0
6	PEG	A	714	7/7	0.79	0.20	62,78,84,84	0
4	EDO	B	401	4/4	0.85	0.18	74,75,76,76	0
4	EDO	A	708	4/4	0.85	0.13	87,87,88,89	0
4	EDO	A	704	4/4	0.86	0.14	98,99,101,102	0
4	EDO	A	707	4/4	0.87	0.25	71,71,72,73	0
6	PEG	A	713	7/7	0.90	0.14	76,82,92,92	0
4	EDO	A	706	4/4	0.90	0.19	62,63,63,63	0
4	EDO	B	402	4/4	0.92	0.16	68,69,69,70	0
5	CL	A	712	1/1	0.93	0.09	82,82,82,82	0
4	EDO	A	705	4/4	0.93	0.12	59,59,61,64	0
5	CL	A	711	1/1	0.93	0.13	92,92,92,92	0
5	CL	A	710	1/1	0.94	0.11	81,81,81,81	0
4	EDO	A	702	4/4	0.96	0.07	41,42,45,47	0
3	WFM	A	701	33/33	0.98	0.06	45,49,52,59	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.