



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:49 AM UTC

PDB ID : 6RLL / pdb_00006rll
Title : CRYSTAL STRUCTURE OF THE HUMAN PRMT5:MEP50 COMPLEX
with JNJ44064146
Authors : Brown, D.G.; Robinson, C.M.; Pande, V.
Deposited on : 2019-05-02
Resolution : 2.22 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

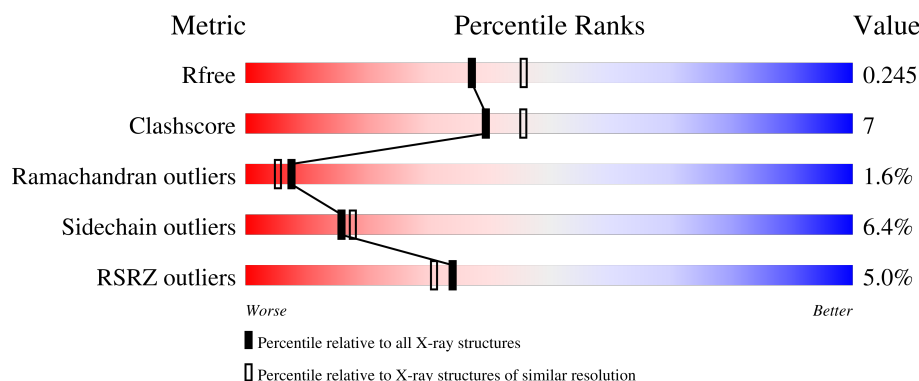
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	5% 76% 18% • •
2	B	348	4% 67% 18% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7408 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
			5017	3208	858	927	24			

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

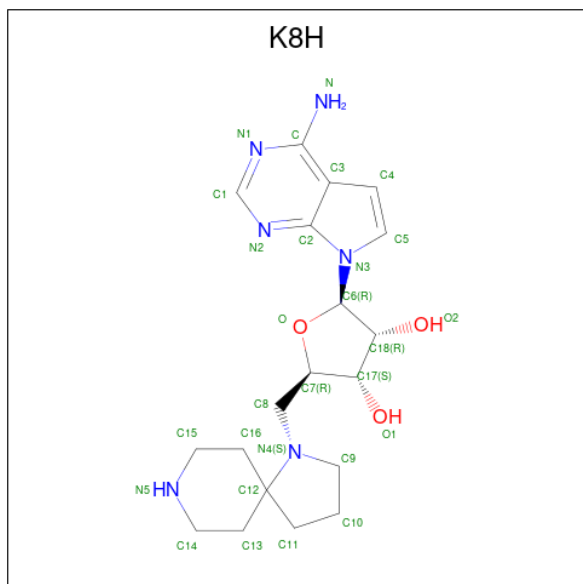
- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2269	1427	387	443	12			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	initiating methionine	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
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is (2 {R},3 {R},4 {S},5 {R})-2-(4-azanylpyrrolo[2,3-d]pyrimidin-7-yl)-5-(1,8-diazaspiro[4.5]decan-1-ylmethyl)oxolane-3,4-diol (CCD ID: K8H) (formula: C₁₉H₂₈N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	6	3		

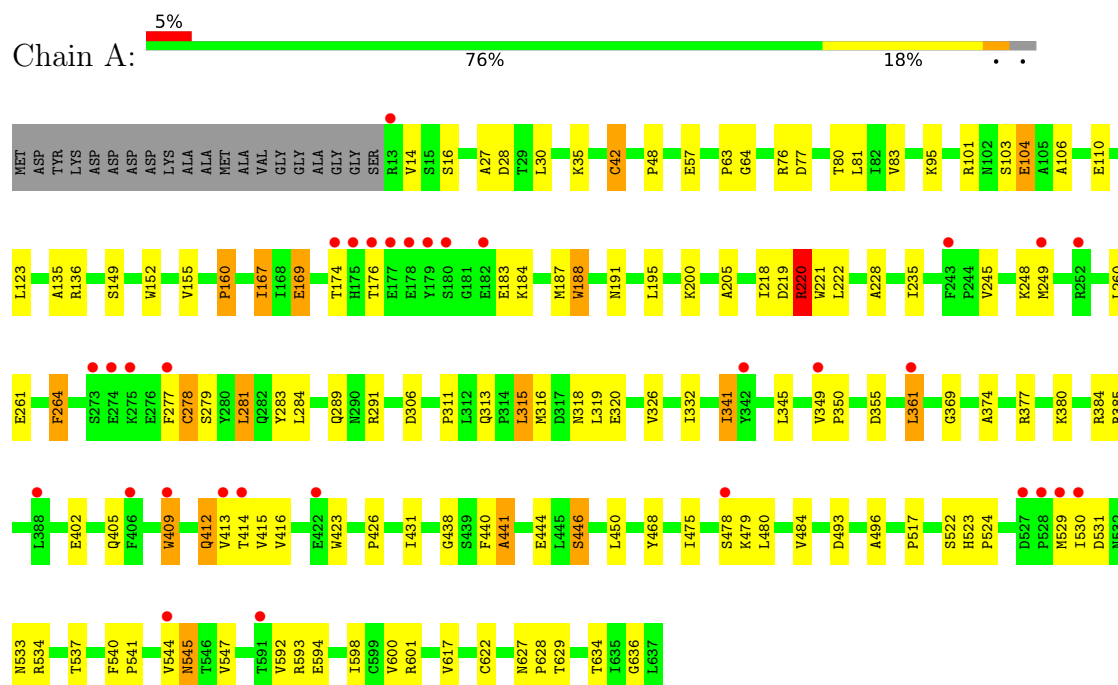
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	26	Total	O	0	0
			26	26		

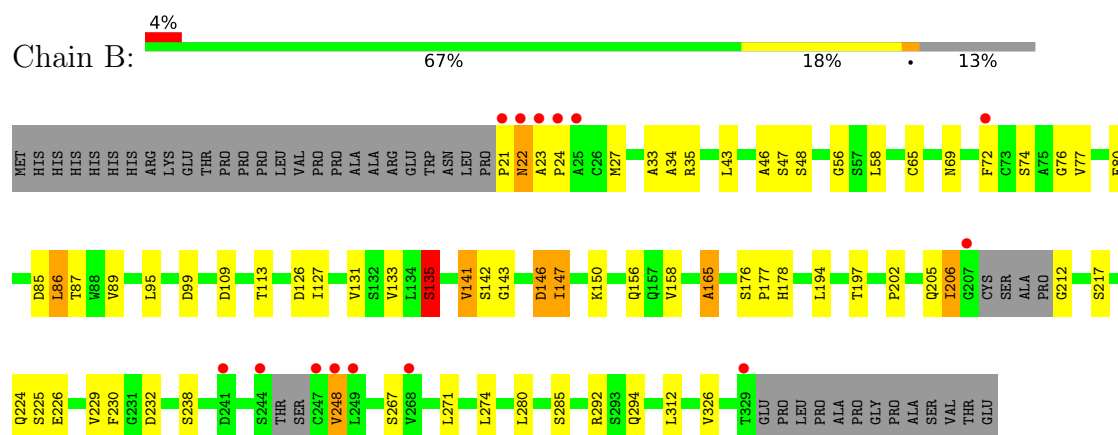
3 Residue-property plots [i](#)

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	102.96Å 136.05Å 179.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.44 – 2.22 89.44 – 2.22	Depositor EDS
% Data completeness (in resolution range)	96.4 (89.44-2.22) 96.4 (89.44-2.22)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.251 , 0.291 (Not available) , 0.245	Depositor DCC
R_{free} test set	3010 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.9	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	0.94	EDS
Total number of atoms	7408	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: K8H

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	1.20	5/5159 (0.1%)	1.57	42/7029 (0.6%)
2	B	1.22	1/2322 (0.0%)	1.48	19/3173 (0.6%)
All	All	1.21	6/7481 (0.1%)	1.54	61/10202 (0.6%)

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	2
2	B	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	PRO	C-O	-5.75	1.16	1.24
1	A	600	VAL	C-O	5.52	1.29	1.24
2	B	176	SER	C-O	5.35	1.31	1.24
1	A	219	ASP	C-O	5.27	1.30	1.24
1	A	517	PRO	C-O	-5.09	1.18	1.23
1	A	135	ALA	C-O	-5.01	1.18	1.24

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ARG	N-CA-CB	8.60	122.48	110.01
1	A	545	ASN	CB-CA-C	7.10	121.42	109.84
1	A	167	ILE	N-CA-C	-7.00	106.48	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	PHE	CB-CA-C	6.95	124.26	110.42
2	B	232	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	634	THR	CA-CB-OG1	-6.76	99.47	109.60
2	B	143	GLY	CA-C-O	-6.64	115.79	121.57
1	A	160	PRO	CA-C-N	6.42	129.52	120.28
1	A	160	PRO	C-N-CA	6.42	129.52	120.28
1	A	188	TRP	CA-C-N	6.34	128.68	120.44
1	A	188	TRP	C-N-CA	6.34	128.68	120.44
2	B	65	CYS	CA-C-N	6.17	129.05	120.29
2	B	65	CYS	C-N-CA	6.17	129.05	120.29
1	A	478	SER	N-CA-C	-6.10	104.55	112.23
1	A	318	ASN	CB-CA-C	6.06	120.81	110.81
1	A	320	GLU	CA-C-N	6.00	128.64	120.54
1	A	320	GLU	C-N-CA	6.00	128.64	120.54
1	A	522	SER	CA-C-O	-5.95	114.44	121.16
1	A	219	ASP	CA-C-O	-5.94	114.58	120.82
1	A	478	SER	CB-CA-C	5.94	122.50	110.38
2	B	126	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	315	LEU	CA-C-N	5.76	128.47	120.29
1	A	315	LEU	C-N-CA	5.76	128.47	120.29
2	B	248	VAL	CA-C-N	5.67	132.13	122.37
2	B	248	VAL	C-N-CA	5.67	132.13	122.37
2	B	165	ALA	N-CA-C	-5.65	106.06	113.12
2	B	146	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	57	GLU	CB-CG-CD	5.46	121.88	112.60
1	A	184	LYS	CA-C-O	-5.45	114.77	120.55
2	B	176	SER	O-C-N	5.44	126.91	121.30
1	A	264	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	438	GLY	CA-C-N	5.41	128.06	120.28
1	A	438	GLY	C-N-CA	5.41	128.06	120.28
2	B	87	THR	CA-CB-OG1	-5.39	101.52	109.60
1	A	319	LEU	CA-C-N	5.34	128.67	120.82
1	A	319	LEU	C-N-CA	5.34	128.67	120.82
2	B	142	SER	CA-C-N	5.29	125.68	121.61
2	B	142	SER	C-N-CA	5.29	125.68	121.61
1	A	28	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	69	ASN	CA-C-N	5.20	128.62	120.82
2	B	69	ASN	C-N-CA	5.20	128.62	120.82
1	A	188	TRP	O-C-N	5.18	127.48	122.09
1	A	64	GLY	N-CA-C	-5.18	101.78	112.34
1	A	104	GLU	CB-CG-CD	5.17	121.39	112.60
2	B	77	VAL	CA-C-N	5.17	128.89	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	VAL	C-N-CA	5.17	128.89	121.50
1	A	402	GLU	CB-CG-CD	5.16	121.37	112.60
1	A	479	LYS	N-CA-CB	5.14	117.47	110.01
1	A	311	PRO	CA-C-N	5.14	128.15	120.90
1	A	311	PRO	C-N-CA	5.14	128.15	120.90
1	A	341	ILE	CA-C-N	5.14	127.93	120.79
1	A	341	ILE	C-N-CA	5.14	127.93	120.79
1	A	195	LEU	O-C-N	5.10	127.96	122.15
1	A	103	SER	CA-C-O	-5.10	115.45	120.70
1	A	369	GLY	O-C-N	-5.09	116.67	121.77
1	A	320	GLU	CB-CG-CD	5.08	121.23	112.60
1	A	350	PRO	CA-C-N	5.03	127.02	120.28
1	A	350	PRO	C-N-CA	5.03	127.02	120.28
1	A	48	PRO	CB-CA-C	5.03	118.96	111.62
2	B	85	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	27	ALA	CA-C-O	-5.00	115.75	120.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	426	PRO	Peptide
1	A	63	PRO	Peptide
2	B	212	GLY	Peptide
2	B	248	VAL	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	5017	0	4846	67	0
2	B	2269	0	2157	31	0
3	A	28	0	0	1	0
4	A	68	0	0	13	0
4	B	26	0	0	3	0
All	All	7408	0	7003	96	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 7.

All (96) 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:416:VAL:HG11	1:A:423:TRP:HE1	1.37	0.86
1:A:77:ASP:HA	1:A:81:LEU:HD23	1.59	0.83
1:A:416:VAL:HG11	1:A:423:TRP:NE1	1.96	0.81
1:A:187[B]:MET:HE3	1:A:191:ASN:ND2	2.03	0.73
1:A:277:PHE:O	1:A:279:SER:N	2.24	0.71
2:B:21:PRO:N	4:B:401:HOH:O	2.25	0.68
1:A:629:THR:HG22	1:A:629:THR:O	1.97	0.65
1:A:277:PHE:C	1:A:279:SER:H	2.04	0.64
1:A:221:TRP:CD1	4:A:816:HOH:O	2.52	0.63
1:A:413:VAL:O	1:A:415:VAL:N	2.32	0.62
1:A:187[B]:MET:HE3	1:A:191:ASN:HD22	1.63	0.61
1:A:416:VAL:CG2	4:A:868:HOH:O	2.47	0.61
1:A:80:THR:OG1	1:A:81:LEU:CD2	2.49	0.61
1:A:220:ARG:NH1	1:A:545:ASN:O	2.35	0.60
1:A:533:ASN:O	1:A:534:ARG:HG2	2.01	0.60
1:A:349:VAL:O	1:A:384:ARG:NH1	2.35	0.59
1:A:220:ARG:HD2	4:A:816:HOH:O	2.02	0.58
1:A:220:ARG:CD	4:A:816:HOH:O	2.51	0.57
1:A:260:LEU:O	1:A:261:GLU:C	2.50	0.55
1:A:416:VAL:HG22	4:A:868:HOH:O	2.05	0.55
1:A:80:THR:OG1	1:A:81:LEU:HD22	2.07	0.55
1:A:409:TRP:HB3	4:A:801:HOH:O	2.06	0.54
1:A:278:CYS:HA	4:A:858:HOH:O	2.07	0.54
1:A:355:ASP:O	1:A:385:ARG:NH1	2.41	0.54
1:A:361:LEU:HD11	1:A:431:ILE:HD12	1.89	0.53
2:B:89:VAL:HG22	2:B:133:VAL:HG21	1.89	0.53
1:A:205:ALA:HA	1:A:228:ALA:O	2.09	0.52
1:A:16:SER:HA	1:A:264:PHE:O	2.10	0.52
2:B:141:VAL:HA	2:B:150:LYS:O	2.09	0.52
1:A:101:ARG:HG2	1:A:101:ARG:HH11	1.74	0.51
1:A:416:VAL:HG21	4:A:868:HOH:O	2.10	0.51
1:A:149:SER:HB2	4:A:821:HOH:O	2.12	0.50
2:B:33:ALA:HB1	2:B:86:LEU:HD11	1.93	0.50
1:A:627:ASN:N	1:A:628:PRO:CD	2.75	0.50
1:A:187[B]:MET:HE2	1:A:188:TRP:HA	1.95	0.49
2:B:23:ALA:HA	4:B:426:HOH:O	2.12	0.49
2:B:35:ARG:NH2	2:B:86:LEU:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ALA:O	1:A:110:GLU:HG3	2.12	0.49
1:A:440:PHE:O	1:A:441:ALA:HB3	2.13	0.48
1:A:450:LEU:HD12	1:A:523:HIS:CD2	2.48	0.48
1:A:617:VAL:O	1:A:622:CYS:HA	2.14	0.48
1:A:405:GLN:NE2	1:A:413:VAL:O	2.47	0.48
1:A:629:THR:O	1:A:629:THR:CG2	2.62	0.48
1:A:160:PRO:HD2	4:A:818:HOH:O	2.14	0.47
2:B:146:ASP:O	2:B:147:ILE:HB	2.15	0.47
1:A:104:GLU:HB3	4:A:864:HOH:O	2.15	0.47
1:A:277:PHE:C	1:A:277:PHE:CD1	2.94	0.46
1:A:277:PHE:C	1:A:279:SER:N	2.70	0.46
2:B:197:THR:HA	2:B:202:PRO:HB3	1.96	0.46
2:B:21:PRO:O	2:B:22:ASN:CB	2.63	0.46
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.83	0.45
1:A:592:VAL:HG21	1:A:598:ILE:HD11	1.98	0.45
1:A:245:VAL:HG12	1:A:283:TYR:CE1	2.52	0.45
1:A:446:SER:HB3	1:A:468:TYR:OH	2.16	0.45
2:B:33:ALA:CB	2:B:86:LEU:HD11	2.46	0.45
2:B:99:ASP:HA	2:B:127:ILE:HG12	1.98	0.44
2:B:177:PRO:HB2	2:B:178:HIS:CD2	2.52	0.44
1:A:628:PRO:O	1:A:629:THR:HB	2.17	0.44
2:B:194:LEU:HB2	2:B:206:ILE:HD11	2.00	0.44
1:A:183:GLU:HA	4:A:861:HOH:O	2.16	0.44
1:A:444:GLU:OE1	3:A:701:K8H:N5	2.51	0.44
2:B:229:VAL:HG11	2:B:271:LEU:HD22	2.00	0.43
2:B:23:ALA:HB1	2:B:24:PRO:HD2	2.00	0.43
2:B:135:SER:OG	2:B:178:HIS:C	2.61	0.43
2:B:156:GLN:O	2:B:158:VAL:HG13	2.18	0.43
2:B:86:LEU:C	2:B:86:LEU:CD1	2.92	0.43
2:B:86:LEU:HA	2:B:95:LEU:O	2.18	0.43
1:A:123:LEU:HA	1:A:152:TRP:O	2.19	0.43
1:A:480:LEU:O	1:A:484:VAL:HG23	2.19	0.43
1:A:533:ASN:C	1:A:534:ARG:HG2	2.44	0.43
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.87	0.42
1:A:341:ILE:O	1:A:345:LEU:HG	2.18	0.42
2:B:46:ALA:O	2:B:56:GLY:HA2	2.19	0.42
1:A:169:GLU:CD	1:A:169:GLU:C	2.87	0.42
1:A:493:ASP:HB3	1:A:496:ALA:HB2	2.01	0.42
1:A:523:HIS:HA	1:A:524:PRO:C	2.45	0.42
2:B:205:GLN:C	2:B:206:ILE:HG13	2.45	0.42
1:A:167:ILE:HB	2:B:202:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:LEU:C	2:B:86:LEU:HD12	2.45	0.42
1:A:545:ASN:HD22	1:A:593:ARG:HH11	1.68	0.42
2:B:58:LEU:O	2:B:76:GLY:HA2	2.19	0.42
2:B:194:LEU:CB	2:B:206:ILE:HD11	2.50	0.42
1:A:374:ALA:HA	1:A:377:ARG:NH1	2.35	0.42
2:B:24:PRO:HD3	4:B:426:HOH:O	2.19	0.41
1:A:42:CYS:HA	1:A:83:VAL:O	2.21	0.41
1:A:218:ILE:O	1:A:222:LEU:HG	2.20	0.41
1:A:537:THR:HG23	1:A:601:ARG:HD3	2.02	0.41
1:A:167:ILE:HD11	2:B:165:ALA:HB2	2.03	0.41
2:B:217:SER:O	2:B:230:PHE:HA	2.21	0.41
2:B:89:VAL:HG22	2:B:133:VAL:CG2	2.51	0.41
2:B:229:VAL:HA	2:B:238:SER:O	2.21	0.41
1:A:540:PHE:HA	1:A:541:PRO:HD2	1.93	0.41
1:A:313:GLN:HE22	1:A:636:GLY:H	1.69	0.40
1:A:220:ARG:HH22	1:A:545:ASN:HB2	1.86	0.40
1:A:220:ARG:HD3	4:A:816:HOH:O	2.20	0.40
2:B:34:ALA:HA	2:B:43:LEU:O	2.22	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%)	579 (93%)	34 (5%)	11 (2%)	6	4
2	B	297/348 (85%)	279 (94%)	14 (5%)	4 (1%)	9	7
All	All	921/993 (93%)	858 (93%)	48 (5%)	15 (2%)	7	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	THR
2	B	135	SER
2	B	147	ILE
1	A	278	CYS
1	A	529	MET
1	A	530	ILE
2	B	22	ASN
2	B	225	SER
1	A	176	THR
1	A	531	ASP
1	A	409	TRP
1	A	441	ALA
1	A	174	THR
1	A	306	ASP
1	A	412	GLN

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	546/570 (96%)	517 (95%)	29 (5%)	20	24
2	B	248/296 (84%)	226 (91%)	22 (9%)	9	9
All	All	794/866 (92%)	743 (94%)	51 (6%)	16	18

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	30	LEU
1	A	35	LYS
1	A	42	CYS
1	A	76	ARG
1	A	95	LYS
1	A	136	ARG
1	A	155	VAL
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	200	LYS
1	A	220	ARG
1	A	235	ILE
1	A	248	LYS
1	A	249	MET
1	A	281	LEU
1	A	289	GLN
1	A	291	ARG
1	A	315	LEU
1	A	316	MET
1	A	326	VAL
1	A	332	ILE
1	A	361	LEU
1	A	380	LYS
1	A	412	GLN
1	A	446	SER
1	A	475	ILE
1	A	544	VAL
1	A	547	VAL
1	A	594	GLU
2	B	27	MET
2	B	47	SER
2	B	48	SER
2	B	74	SER
2	B	80	GLU
2	B	86	LEU
2	B	109	ASP
2	B	113	THR
2	B	131	VAL
2	B	135	SER
2	B	141	VAL
2	B	206	ILE
2	B	224	GLN
2	B	226	GLU
2	B	267	SER
2	B	274	LEU
2	B	280	LEU
2	B	285	SER
2	B	292	ARG
2	B	294	GLN
2	B	312	LEU
2	B	326	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	61	ASN
1	A	66	GLN
1	A	140	ASN
1	A	270	ASN
1	A	271	HIS
1	A	313	GLN
1	A	339	GLN
1	A	507	HIS
1	A	511	GLN
1	A	525	ASN
1	A	545	ASN
2	B	178	HIS
2	B	224	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	K8H	A	701	-	31,32,32	0.48	0	35,48,48	0.90	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	K8H	A	701	-	-	0/8/47/47	0/5/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

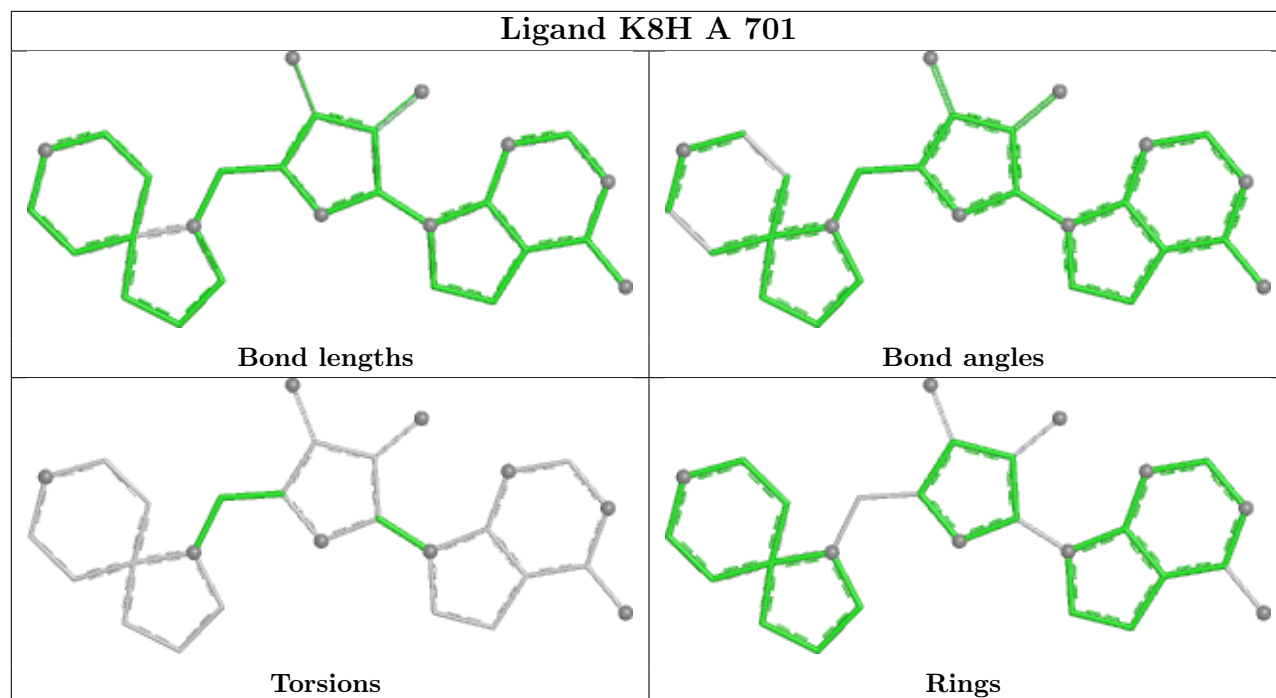
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	K8H	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

6.1 Protein, DNA and RNA chains

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%)	0.34	32 (5%) 33 30	15, 35, 66, 122	1 (0%)
2	B	303/348 (87%)	0.47	14 (4%) 37 34	24, 34, 54, 95	0
All	All	928/993 (93%)	0.38	46 (4%) 34 31	15, 34, 63, 122	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	CYS	7.0
2	B	21	PRO	6.2
1	A	413	VAL	4.9
1	A	409	TRP	4.3
2	B	248	VAL	4.3
1	A	179	TYR	4.0
2	B	207	GLY	3.7
1	A	176	THR	3.5
1	A	530	ILE	3.4
2	B	72	PHE	3.4
2	B	244	SER	3.4
1	A	591	THR	3.3
1	A	414	THR	3.2
1	A	243	PHE	3.2
2	B	329	THR	3.2
2	B	24	PRO	3.2
1	A	406	PHE	3.1
1	A	249	MET	3.1
2	B	22	ASN	3.0
1	A	273	SER	2.8
1	A	478	SER	2.7
1	A	277	PHE	2.7
1	A	527	ASP	2.7
2	B	25	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	241	ASP	2.6
1	A	13	ARG	2.6
1	A	544	VAL	2.6
1	A	342	TYR	2.6
1	A	529	MET	2.5
1	A	274	GLU	2.4
1	A	177	GLU	2.4
2	B	23	ALA	2.4
1	A	175	HIS	2.4
1	A	180	SER	2.3
1	A	361	LEU	2.3
2	B	249	LEU	2.2
2	B	268	VAL	2.3
1	A	252	ARG	2.2
1	A	388	LEU	2.2
1	A	275	LYS	2.2
1	A	174	THR	2.2
1	A	178	GLU	2.1
1	A	528	PRO	2.1
1	A	349	VAL	2.1
1	A	182	GLU	2.0
1	A	422	GLU	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 [i](#)

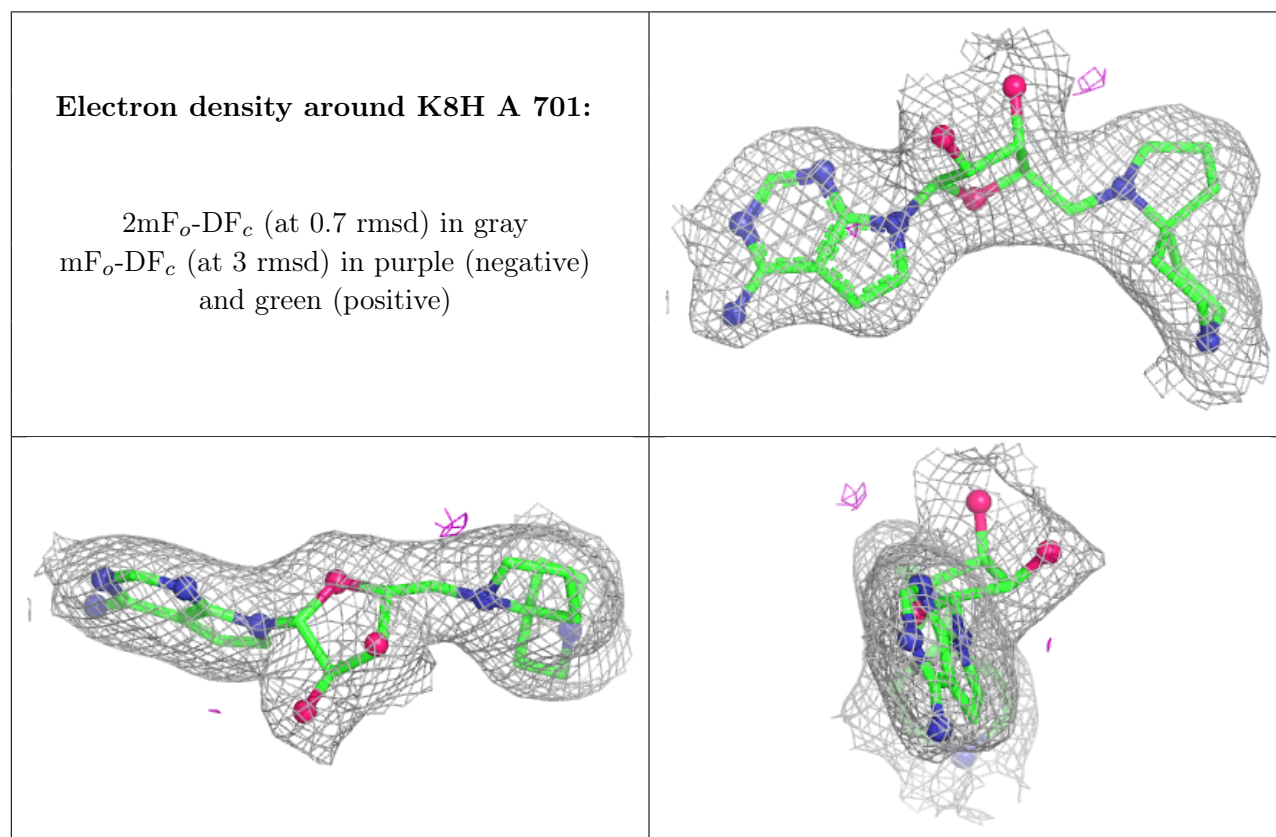
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	K8H	A	701	28/28	0.96	0.06	21,26,27,28	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.