



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:02 AM UTC

PDB ID : 6RLQ / pdb_00006rlq
Title : CRYSTAL STRUCTURE OF THE HUMAN PRMT5:MEP50 COMPLEX
with JNJ45031882
Authors : Brown, D.G.; Robinson, C.M.; Pande, V.
Deposited on : 2019-05-02
Resolution : 2.53 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

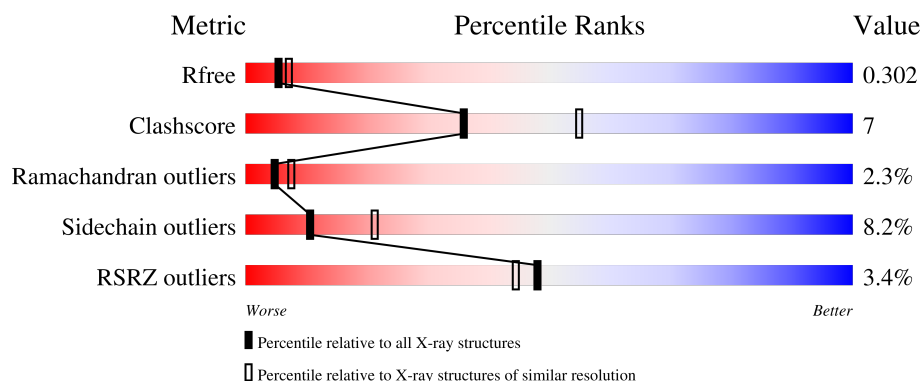
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	644	3% 71% 22% • •
2	B	348	4% 61% 23% • • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7351 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
			Total	C	N	O	S			
1	A	625	5017	3208	858	927	24	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

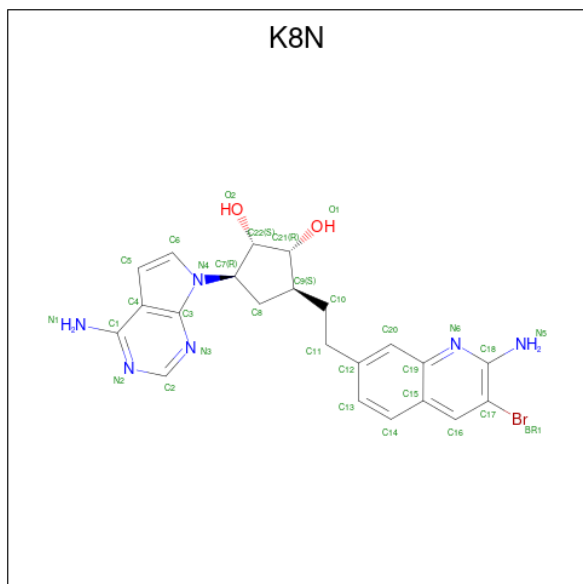
- Molecule 2 is a protein called Methylosome protein 50.

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

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 (1 {S},2 {R},3 {S},5 {R})-3-[2-(2-azanyl-3-bromanyl-quinolin-7-yl)ethyl]-5-(4-azanylpyrrolo[2,3-d]pyrimidin-7-yl)cyclopentane-1,2-diol (CCD ID: K8N) (formula: $C_{22}H_{23}BrN_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			31	1	22	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	4	Total	O	0	0
			4	4		

GLU
PRO
LEU
PRO
ALA
PRO
GLY
PRO
ALA
SER
VAL
THR
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.13Å 137.85Å 178.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.30 – 2.53 89.30 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.1 (89.30-2.53) 98.2 (89.30-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.230 , 0.299 0.233 , 0.302	Depositor DCC
R_{free} test set	2087 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.941	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7351	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: K8N

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	1.19	11/5159 (0.2%)	1.54	29/7029 (0.4%)
2	B	1.27	4/2322 (0.2%)	1.50	12/3173 (0.4%)
All	All	1.22	15/7481 (0.2%)	1.53	41/10202 (0.4%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	ASP	CG-OD1	7.30	1.39	1.25
2	B	215	PRO	C-O	-6.48	1.16	1.23
1	A	321	SER	C-O	6.26	1.31	1.24
1	A	515	PRO	C-O	-6.25	1.15	1.24
1	A	137	VAL	C-O	-6.16	1.16	1.24
2	B	267	SER	C-O	6.01	1.31	1.24
2	B	263	PHE	C-O	5.95	1.31	1.23
1	A	474	PRO	C-O	-5.94	1.17	1.23
1	A	501	PRO	C-O	-5.74	1.17	1.23
1	A	530	ILE	C-O	5.61	1.30	1.24
1	A	467	GLU	CD-OE2	5.59	1.35	1.25
1	A	116	TYR	C-O	5.37	1.30	1.24
2	B	178	HIS	ND1-CE1	-5.26	1.27	1.32
1	A	325	GLU	C-O	5.14	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	HIS	C-O	5.01	1.29	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	HIS	CA-C-N	6.47	128.94	120.60
1	A	216	HIS	C-N-CA	6.47	128.94	120.60
1	A	329	LYS	N-CA-C	-6.45	106.13	112.97
1	A	216	HIS	CB-CA-C	6.45	121.00	110.88
2	B	329	THR	CA-C-O	6.43	131.74	120.80
1	A	621	VAL	CA-C-O	-6.36	114.92	121.67
1	A	414	THR	CB-CA-C	6.27	120.35	110.19
1	A	523	HIS	CA-CB-CG	-6.21	107.59	113.80
2	B	304	THR	CB-CA-C	5.99	118.73	110.34
1	A	140	ASN	CA-CB-CG	-5.95	106.65	112.60
2	B	266	HIS	CA-C-N	5.93	128.51	120.44
2	B	266	HIS	C-N-CA	5.93	128.51	120.44
1	A	357	ASN	CA-C-N	5.93	130.49	122.90
1	A	357	ASN	C-N-CA	5.93	130.49	122.90
1	A	222	LEU	CB-CA-C	5.74	120.03	109.46
1	A	188	TRP	CA-C-N	5.73	128.24	120.44
1	A	188	TRP	C-N-CA	5.73	128.24	120.44
1	A	482	ASN	CA-C-N	5.71	127.86	120.44
1	A	482	ASN	C-N-CA	5.71	127.86	120.44
1	A	188	TRP	O-C-N	5.67	127.91	122.07
1	A	545	ASN	CA-C-O	-5.62	115.01	121.47
2	B	24	PRO	N-CA-C	5.45	123.69	112.47
1	A	456	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	136	ARG	N-CA-C	-5.33	105.37	111.07
1	A	296	ALA	CA-C-O	-5.31	115.25	120.82
2	B	72	PHE	CA-CB-CG	5.22	119.02	113.80
2	B	135	SER	CA-C-N	5.21	127.52	120.38
2	B	135	SER	C-N-CA	5.21	127.52	120.38
1	A	100	ARG	N-CA-C	-5.19	105.52	111.07
1	A	220	ARG	CA-C-N	5.17	130.76	121.66
1	A	220	ARG	C-N-CA	5.17	130.76	121.66
1	A	607	ASN	CB-CA-C	5.16	120.69	110.42
2	B	284	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	57	GLU	CB-CG-CD	5.13	121.32	112.60
1	A	239	ASN	CA-CB-CG	5.13	117.73	112.60
2	B	69	ASN	CA-C-N	5.11	127.38	120.38
2	B	69	ASN	C-N-CA	5.11	127.38	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	PRO	CA-C-O	-5.06	115.75	121.98
1	A	70	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	525	ASN	CA-C-N	5.02	127.77	120.79
1	A	525	ASN	C-N-CA	5.02	127.77	120.79

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Peptide
1	A	410	GLY	Peptide
2	B	23	ALA	Peptide
2	B	24	PRO	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	39	0
3	A	31	0	0	2	0
4	A	30	0	0	1	0
4	B	4	0	0	0	0
All	All	7351	0	7003	104	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 (104) 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:219:ASP:O	1:A:222:LEU:HD22	1.63	0.97
1:A:349:VAL:O	1:A:384:ARG:NH1	2.17	0.78
1:A:592:VAL:HG21	1:A:598:ILE:HD11	1.66	0.78
1:A:533:ASN:O	1:A:534:ARG:HG3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD21	1:A:510:HIS:CG	2.20	0.76
2:B:241:ASP:O	2:B:243:LYS:N	2.19	0.75
2:B:275:SER:HB3	2:B:277:ASP:OD1	1.90	0.71
1:A:269:THR:HG22	1:A:271:HIS:CE1	2.28	0.69
1:A:629:THR:HG22	1:A:629:THR:O	1.94	0.68
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.24	0.68
1:A:371:LEU:HD13	1:A:433:VAL:HG12	1.78	0.66
2:B:169:GLN:HB2	2:B:188:GLU:HG3	1.80	0.64
2:B:264:SER:HA	2:B:305:TRP:CD1	2.33	0.64
2:B:224:GLN:O	2:B:226:GLU:N	2.32	0.62
1:A:153:MET:HE2	1:A:192:PHE:CE2	2.36	0.61
1:A:361:LEU:HD11	1:A:431:ILE:HD12	1.83	0.60
1:A:94:SER:O	1:A:100:ARG:HD3	2.03	0.59
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.86	0.58
2:B:284:ASP:HB3	2:B:290:LEU:HD11	1.86	0.58
2:B:153:ASP:OD2	2:B:156:GLN:HB2	2.04	0.57
1:A:168:ILE:CG2	1:A:171:ALA:HB3	2.35	0.56
1:A:302:LYS:HA	1:A:305:GLU:OE2	2.05	0.56
1:A:442:ASP:OD2	1:A:604:ARG:NE	2.39	0.56
1:A:222:LEU:C	1:A:222:LEU:HD23	2.31	0.55
2:B:264:SER:HB2	2:B:305:TRP:CD2	2.42	0.55
2:B:86:LEU:C	2:B:86:LEU:HD12	2.31	0.55
2:B:141:VAL:HA	2:B:150:LYS:O	2.07	0.54
1:A:26:ILE:HD11	1:A:73:LEU:HD11	1.90	0.53
1:A:300:PHE:CD2	1:A:577:PHE:HB2	2.44	0.53
1:A:161:GLU:CD	2:B:191:ARG:HH22	2.17	0.52
1:A:179:TYR:O	1:A:216:HIS:HE1	1.93	0.51
1:A:327:PHE:CD2	3:A:701:K8N:C14	2.93	0.51
1:A:32:ALA:O	1:A:36:GLN:HG3	2.10	0.51
1:A:512:LEU:HD13	1:A:546:THR:HG21	1.91	0.51
2:B:187:SER:HB3	2:B:189:ASP:OD1	2.11	0.51
2:B:35:ARG:NH1	2:B:302:ASP:OD2	2.45	0.50
2:B:70:GLU:H	2:B:70:GLU:CD	2.20	0.50
1:A:578:SER:O	3:A:701:K8N:BR1	2.85	0.49
2:B:34:ALA:HA	2:B:43:LEU:O	2.13	0.48
1:A:465:PRO:HB3	1:A:559:LEU:HD23	1.96	0.48
1:A:454:GLN:OE1	1:A:525:ASN:N	2.35	0.48
2:B:256:GLN:O	2:B:275:SER:OG	2.31	0.48
1:A:333:LYS:HE3	4:A:806:HOH:O	2.13	0.48
1:A:74:SER:O	1:A:77:ASP:N	2.47	0.48
1:A:197:ASP:O	1:A:485:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:ALA:HB1	2:B:313:LEU:HD11	1.97	0.47
1:A:629:THR:O	1:A:629:THR:CG2	2.62	0.47
1:A:369:GLY:N	1:A:370:PRO:CD	2.78	0.47
1:A:416:VAL:HG21	1:A:423:TRP:CZ2	2.50	0.46
1:A:610:LYS:HD2	1:A:634:THR:OG1	2.15	0.46
1:A:619:ALA:HA	1:A:620:PRO:C	2.41	0.46
1:A:334:TYR:OH	1:A:435:GLU:OE1	2.26	0.46
1:A:472:LEU:O	1:A:515:PRO:HA	2.16	0.46
2:B:264:SER:CB	2:B:305:TRP:CE2	2.99	0.46
1:A:121:ALA:HA	1:A:150:MET:O	2.16	0.45
2:B:289:GLU:OE2	2:B:292:ARG:HD2	2.17	0.45
1:A:446:SER:HB3	1:A:447:PRO:HD3	1.99	0.45
1:A:163:LEU:C	1:A:163:LEU:HD12	2.41	0.45
1:A:359:GLN:OE1	1:A:430:ASP:HB3	2.16	0.45
1:A:53:GLU:O	1:A:60:LYS:HA	2.17	0.44
1:A:322:GLN:O	1:A:326:VAL:HG13	2.18	0.44
2:B:309:ASN:HB3	2:B:312:LEU:HD12	1.98	0.44
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.88	0.44
1:A:315:LEU:HD23	1:A:636:GLY:O	2.18	0.44
2:B:41:ALA:HB1	2:B:60:LEU:HD11	2.00	0.43
1:A:341:ILE:O	1:A:345:LEU:HG	2.19	0.43
2:B:224:GLN:C	2:B:226:GLU:H	2.27	0.43
1:A:437:LEU:HD21	1:A:468:TYR:CD2	2.54	0.43
1:A:277:PHE:C	1:A:279:SER:N	2.75	0.43
2:B:37:ARG:NE	2:B:39:ASP:OD1	2.50	0.43
1:A:74:SER:O	1:A:75:GLY:C	2.62	0.43
1:A:401:LEU:O	1:A:405:GLN:HB2	2.19	0.42
2:B:89:VAL:CG2	2:B:95:LEU:HB2	2.50	0.42
2:B:264:SER:HA	2:B:305:TRP:CG	2.54	0.42
1:A:312:LEU:HD12	1:A:312:LEU:HA	1.80	0.42
1:A:222:LEU:HD23	1:A:510:HIS:HB2	2.00	0.42
1:A:627:ASN:N	1:A:628:PRO:CD	2.82	0.42
1:A:184:LYS:O	1:A:187[B]:MET:HB3	2.19	0.42
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.20	0.42
1:A:228:ALA:HA	1:A:263:GLN:O	2.20	0.41
1:A:361:LEU:HD23	1:A:375:SER:HB3	2.02	0.41
2:B:171:THR:HG21	2:B:216:THR:HA	2.02	0.41
2:B:320:HIS:CG	2:B:320:HIS:O	2.73	0.41
1:A:222:LEU:HD21	1:A:510:HIS:CD2	2.54	0.41
1:A:260:LEU:O	1:A:261:GLU:C	2.62	0.41
1:A:446:SER:HB3	1:A:468:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:HIS:HB2	2:B:269:PRO:HA	2.01	0.41
1:A:222:LEU:CD2	1:A:510:HIS:HB2	2.51	0.41
2:B:134:LEU:HD12	2:B:139:GLN:CB	2.50	0.41
2:B:277:ASP:O	2:B:278:CYS:HB2	2.21	0.41
1:A:393:LYS:O	1:A:395:PRO:HD3	2.21	0.41
2:B:264:SER:HB2	2:B:305:TRP:CE2	2.55	0.41
1:A:359:GLN:O	1:A:386:ILE:HA	2.21	0.41
2:B:221:HIS:HB2	2:B:227:VAL:HG12	2.02	0.41
1:A:277:PHE:C	1:A:279:SER:H	2.29	0.41
1:A:362:MET:SD	1:A:429:ALA:HB2	2.61	0.40
2:B:175:ALA:O	2:B:220:TRP:CD1	2.75	0.40
1:A:271:HIS:CE1	2:B:125:ASP:OD1	2.75	0.40
1:A:106:ALA:O	1:A:110:GLU:HG3	2.21	0.40
2:B:306:SER:HB3	2:B:309:ASN:O	2.22	0.40
2:B:265:PRO:HD3	2:B:305:TRP:CB	2.52	0.40
1:A:198:TYR:O	1:A:199:SER:C	2.65	0.40
1:A:301:ALA:O	1:A:302:LYS:C	2.64	0.40
1:A:479:LYS:O	1:A:479:LYS:HD2	2.21	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	624/644 (97%)	567 (91%)	45 (7%)	12 (2%)	6	10
2	B	297/348 (85%)	264 (89%)	24 (8%)	9 (3%)	3	4
All	All	921/992 (93%)	831 (90%)	69 (8%)	21 (2%)	5	7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	SER
1	A	411	SER
1	A	531	ASP
2	B	24	PRO
2	B	147	ILE
2	B	225	SER
2	B	242	THR
2	B	266	HIS
1	A	75	GLY
1	A	441	ALA
1	A	459	ASP
1	A	490	LYS
2	B	22	ASN
1	A	261	GLU
1	A	276	GLU
1	A	351	GLU
2	B	38	SER
1	A	405	GLN
2	B	25	ALA
2	B	109	ASP
1	A	14	VAL

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	546/569 (96%)	504 (92%)	42 (8%)	12	23
2	B	248/296 (84%)	225 (91%)	23 (9%)	8	17
All	All	794/865 (92%)	729 (92%)	65 (8%)	10	21

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	21	ASN
1	A	25	GLU

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Mol	Chain	Res	Type
1	A	30	LEU
1	A	57	GLU
1	A	136	ARG
1	A	140	ASN
1	A	149	SER
1	A	169	GLU
1	A	199	SER
1	A	200	LYS
1	A	208	ILE
1	A	218	ILE
1	A	222	LEU
1	A	226	ILE
1	A	238	THR
1	A	248	LYS
1	A	252	ARG
1	A	262	VAL
1	A	269	THR
1	A	289	GLN
1	A	312	LEU
1	A	322	GLN
1	A	326	VAL
1	A	328	GLU
1	A	343	LYS
1	A	376	LEU
1	A	381	GLN
1	A	384	ARG
1	A	386	ILE
1	A	387	LYS
1	A	388	LEU
1	A	411	SER
1	A	412	GLN
1	A	414	THR
1	A	424	VAL
1	A	467	GLU
1	A	490	LYS
1	A	522	SER
1	A	593	ARG
1	A	594	GLU
1	A	609	LYS
2	B	21	PRO
2	B	24	PRO
2	B	27	MET

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Mol	Chain	Res	Type
2	B	47	SER
2	B	48	SER
2	B	65	CYS
2	B	74	SER
2	B	129	SER
2	B	131	VAL
2	B	133	VAL
2	B	141	VAL
2	B	161	SER
2	B	206	ILE
2	B	217	SER
2	B	226	GLU
2	B	240	VAL
2	B	257	CYS
2	B	264	SER
2	B	274	LEU
2	B	286	SER
2	B	302	ASP
2	B	312	LEU
2	B	321	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	61	ASN
1	A	66	GLN
1	A	216	HIS
1	A	263	GLN
1	A	271	HIS
1	A	289	GLN
1	A	290	ASN
1	A	295	ASN
1	A	339	GLN
1	A	357	ASN
1	A	381	GLN
1	A	396	ASN
1	A	412	GLN
1	A	511	GLN
1	A	532	ASN
2	B	69	ASN
2	B	169	GLN

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Mol	Chain	Res	Type
2	B	190	ASN
2	B	205	GLN
2	B	266	HIS
2	B	320	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](#)

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	K8N	A	701	-	35,35,35	0.58	0	47,52,52	1.05	2 (4%)

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	K8N	A	701	-	-	0/9/25/25	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	K8N	C17-C18-N5	-3.40	120.27	122.89
3	A	701	K8N	C17-C18-N6	2.89	121.93	120.07

There are no chirality outliers.

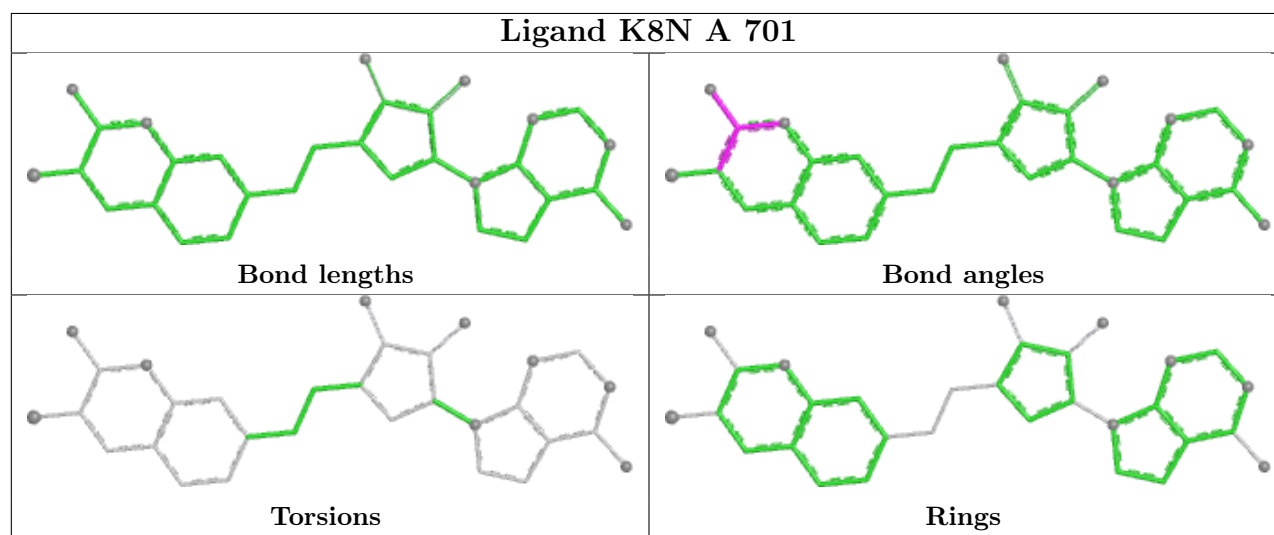
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	K8N	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 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	625/644 (97%)	0.02	19 (3%)	52	49	11, 31, 59, 114	1 (0%)
2	B	303/348 (87%)	0.45	13 (4%)	40	36	26, 40, 60, 105	0
All	All	928/992 (93%)	0.16	32 (3%)	48	44	11, 35, 60, 114	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	244	SER	5.3
1	A	13	ARG	5.2
2	B	21	PRO	4.0
2	B	24	PRO	3.8
2	B	247	CYS	3.4
2	B	23	ALA	3.3
2	B	225	SER	3.3
1	A	14	VAL	3.2
2	B	248	VAL	3.2
2	B	243	LYS	2.8
1	A	530	ILE	2.7
1	A	376	LEU	2.7
1	A	527	ASP	2.6
1	A	294	PRO	2.6
2	B	25	ALA	2.5
2	B	249	LEU	2.4
1	A	146	HIS	2.4
1	A	529	MET	2.3
1	A	299	LEU	2.3
1	A	274	GLU	2.3
2	B	72	PHE	2.3
1	A	243	PHE	2.2
1	A	292	PRO	2.2
1	A	404	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	207	GLY	2.1
1	A	249	MET	2.1
2	B	241	ASP	2.1
1	A	170	ASN	2.0
1	A	145	GLY	2.0
1	A	293	PRO	2.0
1	A	307	TYR	2.0
1	A	490	LYS	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](#)

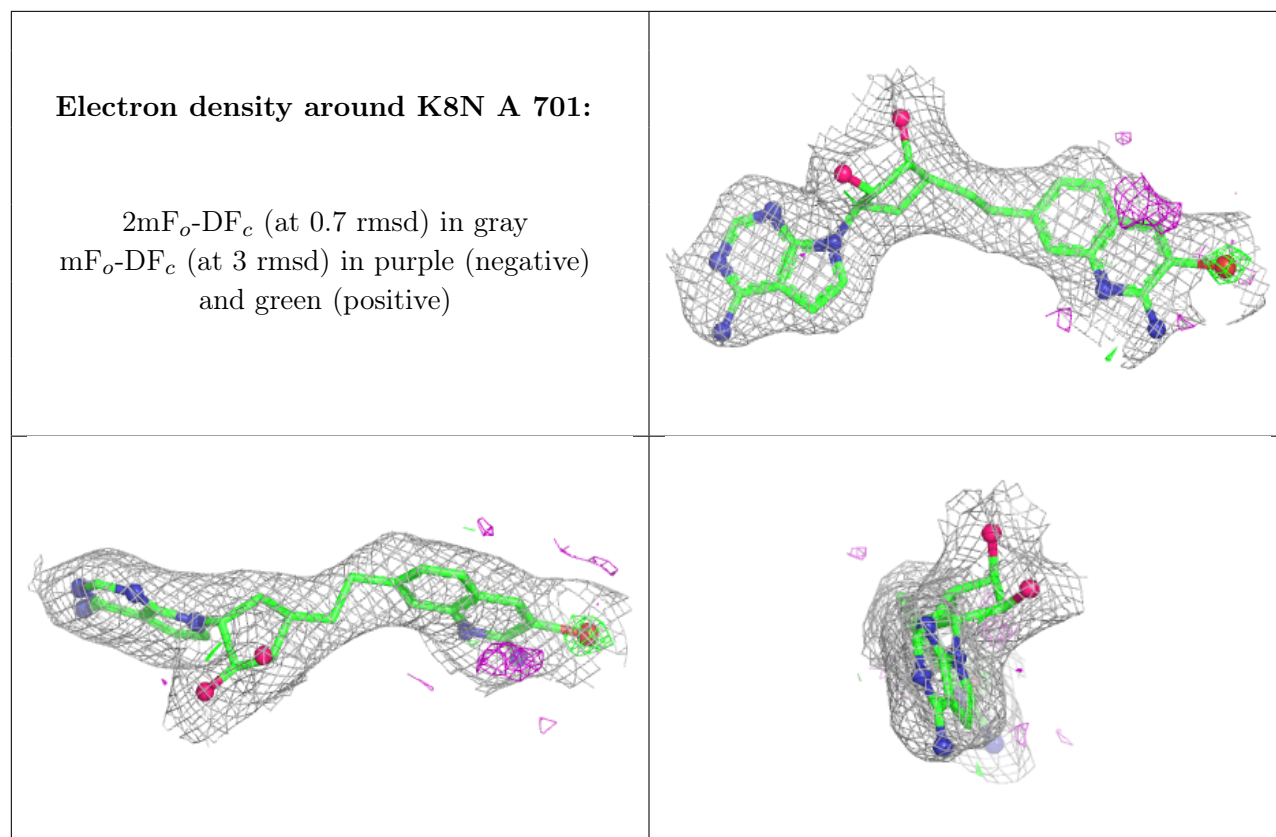
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	K8N	A	701	31/31	0.96	0.09	26,33,37,48	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.