



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 PM UTC

PDB ID : 5EMJ / pdb_00005emj
Title : Crystal structure of PRMT5:MEP50 with Compound 8 and sinefungin
Authors : Boriack-Sjodin, P.A.; Jin, L.
Deposited on : 2015-11-06
Resolution : 2.27 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

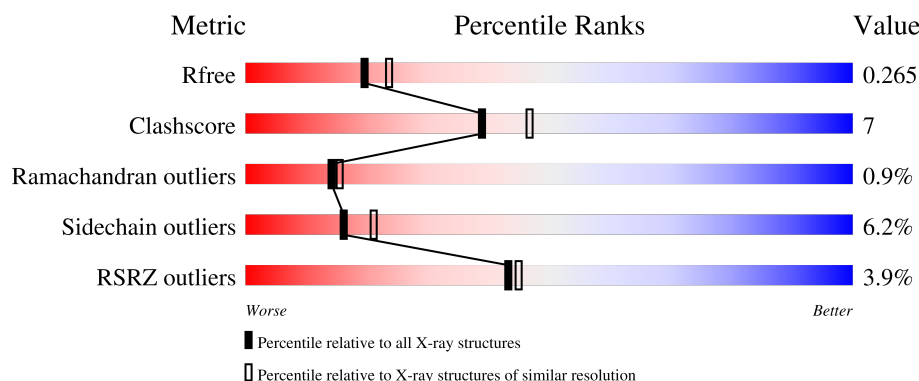
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

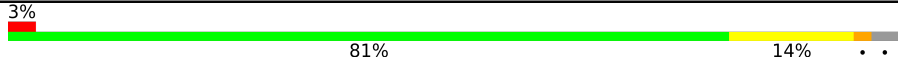
The reported resolution of this entry is 2.27 Å.

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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	705	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7774 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	5188	3315	896	952	25	0	16	0

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
			Total	C	N	O	S			
2	B	303	2301	1442	393	450	16	0	2	0

There are 9 discrepancies between the modelled and reference sequences:

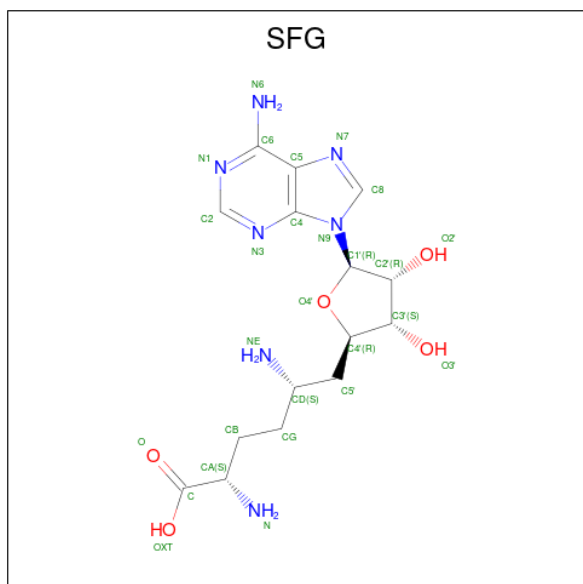
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag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

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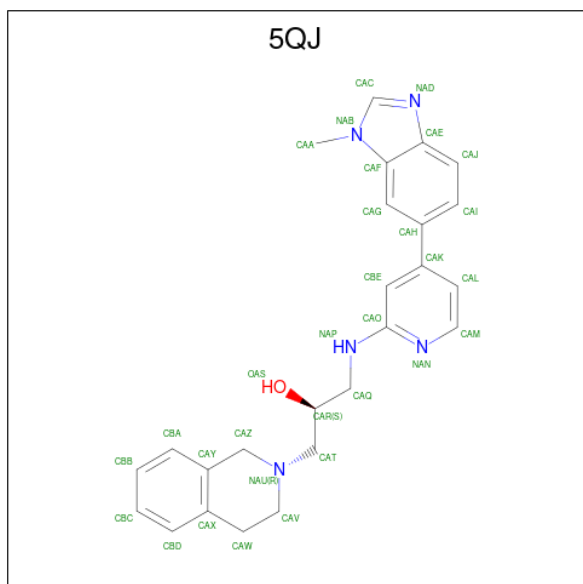
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is SINEFUNGIN (CCD ID: SFG) (formula: $\text{C}_{15}\text{H}_{23}\text{N}_7\text{O}_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 4 is (2 {S})-1-(3,4-dihydro-1 {H}-isoquinolin-2-yl)-3-[[4-(3-methylbenzimidazol-5-yl)pyridin-2-yl]amino]propan-2-ol (CCD ID: 5QJ) (formula: C₂₅H₂₇N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			31	25	5	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

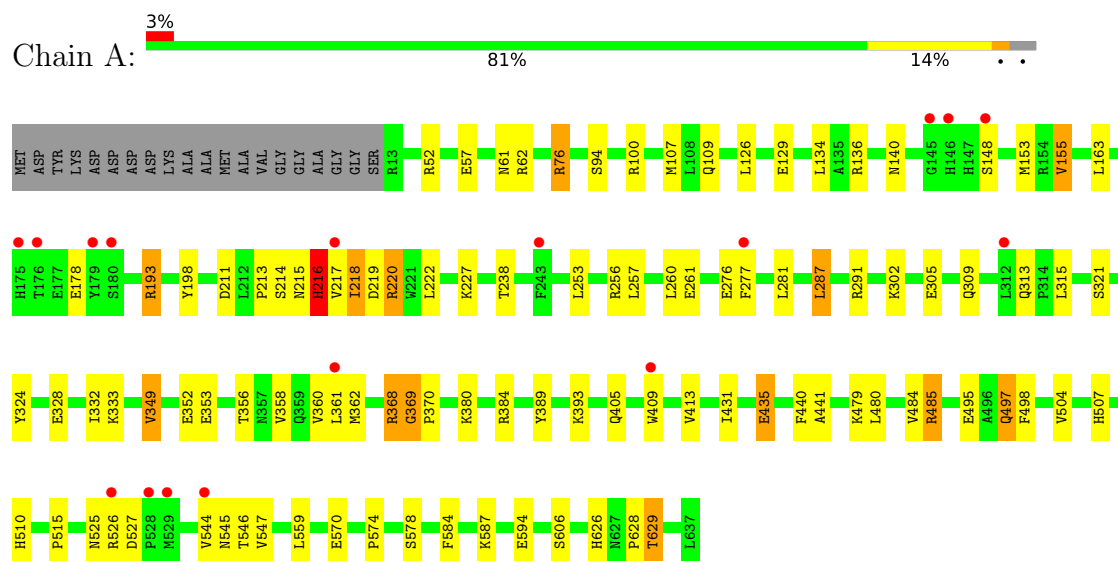
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	163	Total	O	0	0
			163	163		
6	B	40	Total	O	0	0
			40	40		

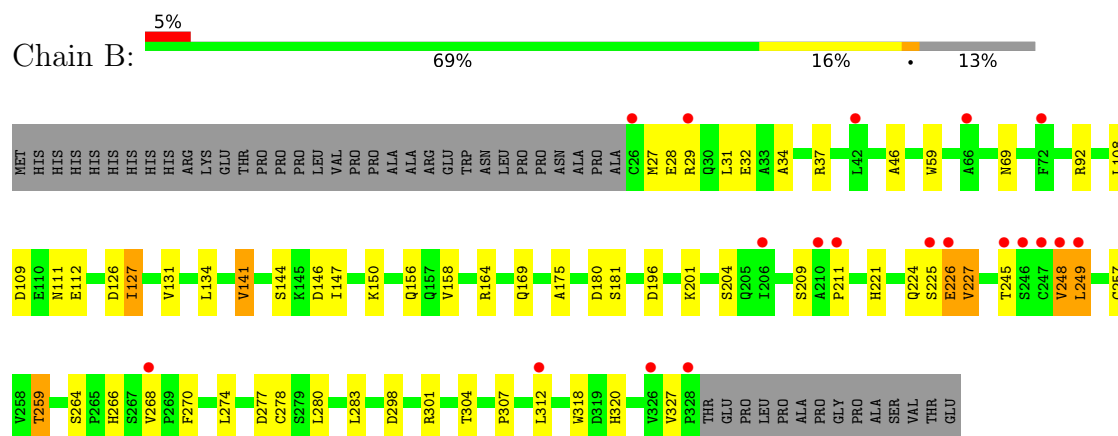
3 Residue-property plots [i](#)

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	104.24Å 138.83Å 179.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.05 – 2.27 61.05 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.7 (61.05-2.27) 98.7 (61.05-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.209 , 0.266 0.208 , 0.265	Depositor DCC
R_{free} test set	2996 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7774	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5QJ, GOL, SFG

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	0.71	2/5335 (0.0%)	0.97	9/7258 (0.1%)
2	B	0.62	0/2358	0.94	3/3219 (0.1%)
All	All	0.68	2/7693 (0.0%)	0.96	12/10477 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	584	PHE	C-O	-6.39	1.18	1.24
1	A	626	HIS	CA-C	-5.05	1.46	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	LYS	CA-C-N	7.33	127.35	119.28
2	B	201	LYS	C-N-CA	7.33	127.35	119.28
1	A	349	VAL	CA-C-N	5.90	125.81	119.85
1	A	349	VAL	C-N-CA	5.90	125.81	119.85
1	A	369	GLY	N-CA-C	5.79	124.15	112.34
2	B	327	VAL	N-CA-C	5.50	113.49	107.60
1	A	155	VAL	CB-CA-C	-5.47	101.41	111.36
1	A	606	SER	N-CA-C	5.20	116.70	108.96
1	A	313	GLN	CA-C-N	5.17	124.67	119.19
1	A	313	GLN	C-N-CA	5.17	124.67	119.19
1	A	440	PHE	N-CA-C	-5.08	105.56	112.26
1	A	129	GLU	N-CA-C	5.06	116.48	111.07

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	5188	0	5064	72	0
2	B	2301	0	2217	31	0
3	A	27	0	22	0	0
4	A	31	0	0	0	0
5	A	18	0	24	4	0
5	B	6	0	8	1	0
6	A	163	0	0	6	0
6	B	40	0	0	5	0
All	All	7774	0	7335	102	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 (102) 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:215[B]:ASN:O	1:A:217[B]:VAL:N	1.64	1.28
1:A:220[B]:ARG:NH1	1:A:220[B]:ARG:HB3	1.88	0.88
1:A:218[B]:ILE:HG22	1:A:256:ARG:HH21	1.38	0.87
1:A:220[B]:ARG:HB3	1:A:220[B]:ARG:HH11	1.43	0.80
1:A:215[B]:ASN:C	1:A:217[B]:VAL:N	2.39	0.78
1:A:222[A]:LEU:HB3	1:A:510:HIS:HB2	1.66	0.78
1:A:215[A]:ASN:O	1:A:216[A]:HIS:HB3	1.82	0.77
1:A:215[B]:ASN:O	1:A:217[B]:VAL:HG22	1.84	0.77
1:A:215[B]:ASN:C	1:A:217[B]:VAL:H	1.93	0.74
2:B:69:ASN:HB2	6:B:535:HOH:O	1.88	0.74
1:A:546:THR:OG1	1:A:547:VAL:N	2.24	0.71
1:A:109:GLN:HE22	5:A:705:GOL:C3	2.03	0.70
1:A:218[B]:ILE:CG2	1:A:256:ARG:HH21	2.04	0.70
1:A:52:ARG:HD2	5:A:705:GOL:O3	1.93	0.69
1:A:215[B]:ASN:O	1:A:218[B]:ILE:N	2.26	0.68
1:A:215[B]:ASN:O	1:A:216[B]:HIS:C	2.36	0.67
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.77	0.66
1:A:215[B]:ASN:O	1:A:217[B]:VAL:CG2	2.44	0.66
2:B:32:GLU:OE2	2:B:301:ARG:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HG3	1:A:498:PHE:HZ	1.62	0.64
1:A:324:TYR:CB	1:A:368:ARG:HD2	2.27	0.64
1:A:215[B]:ASN:O	1:A:217[B]:VAL:CA	2.45	0.64
1:A:525:ASN:HD21	1:A:527:ASP:HB2	1.63	0.64
1:A:109:GLN:HE22	5:A:705:GOL:H31	1.64	0.63
1:A:218[B]:ILE:HG22	1:A:256:ARG:NH2	2.10	0.63
1:A:349:VAL:HG23	1:A:384:ARG:HE	1.64	0.61
1:A:220[B]:ARG:HG2	6:A:801:HOH:O	1.99	0.61
1:A:215[B]:ASN:OD1	1:A:216[B]:HIS:N	2.33	0.61
1:A:479:LYS:NZ	6:A:804:HOH:O	2.32	0.61
1:A:219[A]:ASP:O	1:A:222[A]:LEU:HB2	2.01	0.61
1:A:544:VAL:HG22	1:A:545:ASN:O	2.01	0.60
1:A:215[A]:ASN:O	1:A:216[A]:HIS:CB	2.50	0.59
1:A:628:PRO:O	1:A:629:THR:HB	2.00	0.59
2:B:156:GLN:HB3	2:B:158:VAL:HG22	1.83	0.59
2:B:259:THR:HG21	2:B:301:ARG:NH2	2.18	0.58
1:A:193:ARG:HH21	1:A:193:ARG:HG3	1.70	0.57
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.04	0.57
1:A:525:ASN:ND2	1:A:527:ASP:HB2	2.20	0.56
1:A:305:GLU:HG2	1:A:507:HIS:CG	2.41	0.56
2:B:111:ASN:HA	6:B:521:HOH:O	2.06	0.56
2:B:277:ASP:O	2:B:278:CYS:HB2	2.09	0.53
1:A:57:GLU:HG2	1:A:61:ASN:ND2	2.25	0.52
2:B:27:MET:HG3	2:B:59:TRP:NE1	2.24	0.52
2:B:181:SER:O	2:B:196:ASP:HA	2.11	0.51
1:A:324:TYR:HB2	1:A:368:ARG:HD2	1.92	0.51
1:A:332:ILE:HG13	1:A:574:PRO:O	2.12	0.50
1:A:140:ASN:ND2	6:A:807:HOH:O	2.44	0.50
1:A:333:LYS:HE3	1:A:435:GLU:HG2	1.92	0.50
2:B:29:ARG:HG3	2:B:320:HIS:HB2	1.93	0.50
1:A:215[A]:ASN:HA	1:A:218[A]:ILE:HG23	1.94	0.50
1:A:328:GLU:OE2	1:A:368:ARG:HB2	2.13	0.49
1:A:328:GLU:OE2	1:A:368:ARG:HD3	2.13	0.48
2:B:221:HIS:HB2	2:B:227:VAL:HG22	1.95	0.48
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.28	0.48
1:A:222[B]:LEU:HD11	1:A:256:ARG:HB3	1.95	0.48
2:B:221:HIS:HB2	2:B:227:VAL:CG2	2.44	0.48
2:B:34:ALA:O	2:B:304:THR:HB	2.15	0.47
1:A:220[B]:ARG:HG3	6:A:806:HOH:O	2.15	0.46
1:A:495:GLU:HB3	1:A:587:LYS:HE2	1.97	0.46
2:B:224:GLN:C	2:B:226:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HB3	5:A:705:GOL:O3	2.16	0.45
1:A:480:LEU:O	1:A:484:VAL:HG23	2.15	0.45
2:B:164:ARG:NH2	6:B:501:HOH:O	2.27	0.45
1:A:544:VAL:HG22	1:A:545:ASN:N	2.32	0.45
2:B:141:VAL:HA	2:B:150:LYS:O	2.17	0.45
2:B:92:ARG:O	2:B:108:LEU:HB2	2.17	0.45
1:A:62:ARG:HD3	2:B:298:ASP:OD2	2.16	0.44
2:B:248:VAL:HG12	2:B:249:LEU:HD13	1.99	0.44
1:A:193:ARG:HG3	1:A:193:ARG:NH2	2.29	0.44
1:A:260:LEU:O	1:A:261:GLU:HB2	2.17	0.44
1:A:107:MET:SD	1:A:134:LEU:HD12	2.58	0.44
2:B:169:GLN:HG2	6:B:528:HOH:O	2.17	0.44
1:A:126:LEU:HD21	1:A:153:MET:HE2	1.98	0.43
1:A:349:VAL:HG23	1:A:349:VAL:O	2.18	0.43
1:A:352:GLU:H	1:A:352:GLU:CD	2.26	0.43
1:A:515:PRO:HD2	1:A:570:GLU:OE1	2.18	0.43
1:A:497:GLN:H	1:A:497:GLN:CD	2.25	0.43
2:B:109:ASP:HB3	2:B:112:GLU:H	1.84	0.43
2:B:126:ASP:O	2:B:127:ILE:C	2.62	0.43
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.84	0.43
1:A:361:LEU:HD23	1:A:431:ILE:HB	2.00	0.43
2:B:37:ARG:O	2:B:307:PRO:HG3	2.19	0.43
2:B:92:ARG:HD3	6:B:532:HOH:O	2.18	0.43
1:A:409:TRP:HB3	1:A:413:VAL:CG2	2.49	0.42
2:B:134:LEU:HA	2:B:175:ALA:HB1	2.00	0.42
1:A:253:LEU:HG	1:A:257:LEU:HD12	2.00	0.42
1:A:276:GLU:HG2	1:A:277:PHE:H	1.84	0.42
2:B:31:LEU:HD23	2:B:46:ALA:HB2	2.01	0.42
1:A:222[B]:LEU:CD1	1:A:256:ARG:HB3	2.49	0.42
1:A:211:ASP:HB2	6:A:813:HOH:O	2.20	0.42
2:B:221:HIS:CB	2:B:227:VAL:HG22	2.50	0.42
1:A:193:ARG:HD3	1:A:198:TYR:CE2	2.55	0.42
1:A:222[A]:LEU:HD13	1:A:510:HIS:CD2	2.54	0.41
2:B:264:SER:OG	2:B:270:PHE:N	2.53	0.41
1:A:76:ARG:HB2	1:A:76:ARG:HH11	1.85	0.41
1:A:94:SER:O	1:A:100:ARG:NH1	2.49	0.41
1:A:510:HIS:ND1	6:A:806:HOH:O	2.37	0.41
2:B:264:SER:HB2	2:B:266:HIS:HD2	1.86	0.41
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.96	0.40
1:A:369:GLY:N	1:A:370:PRO:HD2	2.36	0.40
2:B:211:PRO:HA	5:B:401:GOL:H31	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	639/645 (99%)	601 (94%)	32 (5%)	6 (1%)	14	15
2	B	303/350 (87%)	286 (94%)	13 (4%)	4 (1%)	9	9
All	All	942/995 (95%)	887 (94%)	45 (5%)	10 (1%)	14	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214[A]	SER
1	A	214[B]	SER
1	A	216[A]	HIS
1	A	216[B]	HIS
2	B	147	ILE
2	B	209	SER
2	B	127	ILE
1	A	441	ALA
2	B	248	VAL
1	A	213	PRO

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	572/570 (100%)	534 (93%)	38 (7%)	15	19
2	B	260/298 (87%)	243 (94%)	17 (6%)	15	20
All	All	832/868 (96%)	777 (93%)	55 (7%)	16	19

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	136	ARG
1	A	148[A]	SER
1	A	148[B]	SER
1	A	155	VAL
1	A	163	LEU
1	A	178	GLU
1	A	193	ARG
1	A	216[A]	HIS
1	A	216[B]	HIS
1	A	218[A]	ILE
1	A	218[B]	ILE
1	A	220[A]	ARG
1	A	220[B]	ARG
1	A	238	THR
1	A	287	LEU
1	A	291	ARG
1	A	302	LYS
1	A	309	GLN
1	A	315	LEU
1	A	321	SER
1	A	353	GLU
1	A	356	THR
1	A	358	VAL
1	A	360	VAL
1	A	368	ARG
1	A	380	LYS
1	A	393	LYS
1	A	405	GLN
1	A	435	GLU
1	A	485	ARG
1	A	497	GLN
1	A	504	VAL

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Mol	Chain	Res	Type
1	A	526	ARG
1	A	559	LEU
1	A	578	SER
1	A	594	GLU
1	A	629	THR
2	B	28	GLU
2	B	131	VAL
2	B	141	VAL
2	B	180	ASP
2	B	204	SER
2	B	225	SER
2	B	226	GLU
2	B	227	VAL
2	B	245	THR
2	B	249	LEU
2	B	257	CYS
2	B	259	THR
2	B	268	VAL
2	B	274	LEU
2	B	280	LEU
2	B	283	LEU
2	B	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	56	GLN
1	A	61	ASN
1	A	66	GLN
1	A	79	ASN
1	A	109	GLN
1	A	140	ASN
1	A	263	GLN
1	A	289	GLN
1	A	318	ASN
1	A	405	GLN
1	A	511	GLN
1	A	525	ASN
1	A	533	ASN
2	B	78	GLN
2	B	178	HIS

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 ⓘ

6 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	5QJ	A	702	-	35,35,35	2.13	10 (28%)	48,49,49	1.92	9 (18%)
5	GOL	A	704	-	5,5,5	0.34	0	5,5,5	0.44	0
5	GOL	A	705	-	5,5,5	0.27	0	5,5,5	0.86	0
5	GOL	A	703	-	5,5,5	0.36	0	5,5,5	0.36	0
3	SFG	A	701	-	28,29,29	1.52	4 (14%)	34,42,42	2.07	9 (26%)
5	GOL	B	401	-	5,5,5	0.24	0	5,5,5	0.67	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	5QJ	A	702	-	-	6/13/22/22	0/5/5/5
5	GOL	A	704	-	-	1/4/4/4	-
5	GOL	A	705	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	703	-	-	2/4/4/4	-
3	SFG	A	701	-	-	3/17/33/33	0/3/3/3
5	GOL	B	401	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	5QJ	CAZ-CAY	-5.50	1.39	1.51
4	A	702	5QJ	CAW-CAX	-5.13	1.42	1.51
3	A	701	SFG	C5-C4	5.10	1.48	1.39
4	A	702	5QJ	CAM-NAN	3.82	1.42	1.34
4	A	702	5QJ	CAE-NAD	-3.76	1.32	1.39
4	A	702	5QJ	CAJ-CAE	-3.73	1.34	1.40
4	A	702	5QJ	CAF-CAE	-2.98	1.35	1.40
4	A	702	5QJ	CAH-CAK	-2.98	1.42	1.49
4	A	702	5QJ	CAG-CAF	-2.71	1.35	1.39
3	A	701	SFG	C8-N7	2.59	1.36	1.31
4	A	702	5QJ	CAF-NAB	-2.41	1.34	1.38
3	A	701	SFG	C5-N7	-2.32	1.34	1.39
3	A	701	SFG	C5-C6	2.30	1.47	1.41
4	A	702	5QJ	CAO-NAP	-2.17	1.33	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	SFG	C5-C4-N3	-5.90	118.59	126.72
4	A	702	5QJ	CAA-NAB-CAF	5.43	130.72	125.69
4	A	702	5QJ	NAB-CAC-NAD	-4.55	107.88	114.27
3	A	701	SFG	N3-C4-N9	4.43	134.70	127.17
3	A	701	SFG	N3-C2-N1	-3.90	122.68	128.58
4	A	702	5QJ	CAL-CAM-NAN	-3.88	119.22	123.97
3	A	701	SFG	C2-N3-C4	3.88	121.31	111.83
3	A	701	SFG	C4-C5-N7	-3.79	106.25	110.58
4	A	702	5QJ	CAZ-NAU-CAV	3.62	115.08	110.03
4	A	702	5QJ	CAA-NAB-CAC	-3.62	120.76	126.89
4	A	702	5QJ	NAP-CAO-NAN	3.53	122.30	116.98
4	A	702	5QJ	CAE-NAD-CAC	3.53	108.73	104.40
4	A	702	5QJ	CAZ-NAU-CAT	-3.06	106.52	111.26
3	A	701	SFG	C5-N7-C8	2.60	107.54	103.45
4	A	702	5QJ	CBE-CAO-NAP	-2.56	116.64	120.79
3	A	701	SFG	C4-N9-C8	2.30	108.15	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	SFG	C2-N1-C6	2.22	122.37	118.73
3	A	701	SFG	O4'-C1'-C2'	-2.04	102.25	106.62

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	SFG	NE-CD-CG-CB
3	A	701	SFG	C5'-CD-CG-CB
4	A	702	5QJ	CBE-CAO-NAP-CAQ
4	A	702	5QJ	NAN-CAO-NAP-CAQ
5	A	703	GOL	C1-C2-C3-O3
5	A	703	GOL	O2-C2-C3-O3
5	A	705	GOL	O1-C1-C2-C3
5	B	401	GOL	C1-C2-C3-O3
5	B	401	GOL	O2-C2-C3-O3
4	A	702	5QJ	CAI-CAH-CAK-CAL
5	A	705	GOL	O1-C1-C2-O2
4	A	702	5QJ	CAG-CAH-CAK-CBE
4	A	702	5QJ	CAG-CAH-CAK-CAL
4	A	702	5QJ	CAI-CAH-CAK-CBE
5	A	704	GOL	O1-C1-C2-C3
3	A	701	SFG	N-CA-CB-CG

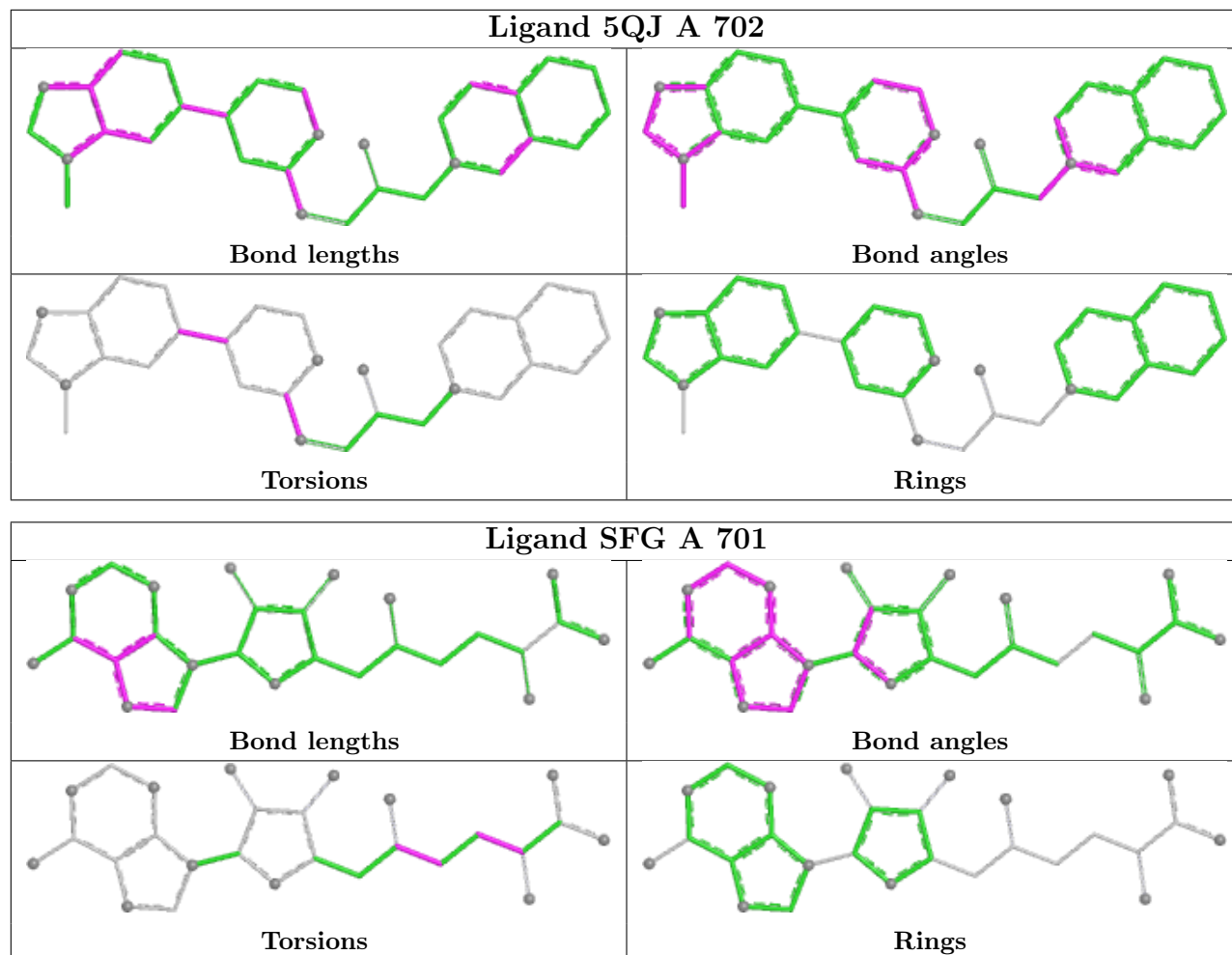
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	GOL	4	0
5	B	401	GOL	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%)	0.04	17 (2%) 56 58	13, 47, 84, 144	16 (2%)
2	B	303/350 (86%)	0.47	19 (6%) 26 27	25, 60, 93, 130	2 (0%)
All	All	928/995 (93%)	0.18	36 (3%) 43 45	13, 52, 88, 144	18 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146[A]	HIS	5.9
1	A	148[A]	SER	4.5
1	A	277	PHE	4.4
2	B	72	PHE	4.2
1	A	529	MET	4.2
2	B	248	VAL	3.3
2	B	210	ALA	3.1
2	B	26	CYS	3.0
2	B	247	CYS	2.7
2	B	29	ARG	2.7
1	A	312	LEU	2.7
2	B	268	VAL	2.7
2	B	326	VAL	2.7
2	B	246	SER	2.7
2	B	211	PRO	2.6
2	B	312	LEU	2.6
1	A	180	SER	2.5
1	A	145[A]	GLY	2.5
2	B	206	ILE	2.4
2	B	245	THR	2.4
1	A	528	PRO	2.4
2	B	249	LEU	2.4
2	B	66	ALA	2.3
1	A	176	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	225	SER	2.3
1	A	544	VAL	2.3
2	B	42	LEU	2.3
2	B	328	PRO	2.3
1	A	217[A]	VAL	2.3
1	A	243	PHE	2.2
1	A	179	TYR	2.2
1	A	361	LEU	2.1
1	A	409	TRP	2.1
2	B	226	GLU	2.1
1	A	175	HIS	2.1
1	A	526	ARG	2.1

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

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 ⓘ

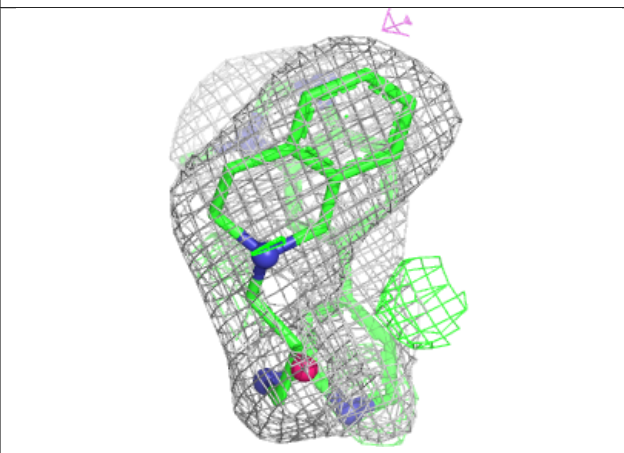
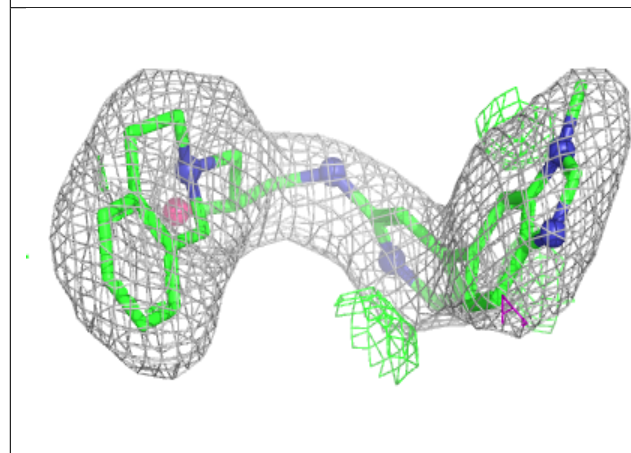
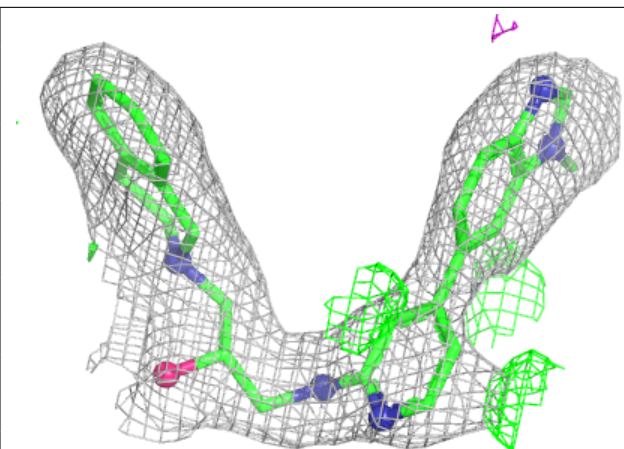
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	705	6/6	0.87	0.12	57,63,65,73	0
5	GOL	A	703	6/6	0.88	0.12	66,68,71,76	0
5	GOL	B	401	6/6	0.90	0.12	63,68,70,78	0
4	5QJ	A	702	31/31	0.92	0.12	37,56,74,78	0
5	GOL	A	704	6/6	0.93	0.10	47,53,60,64	0
3	SFG	A	701	27/27	0.97	0.05	32,35,42,43	0

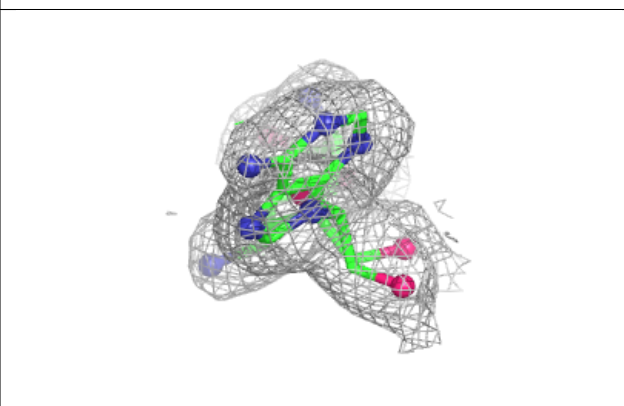
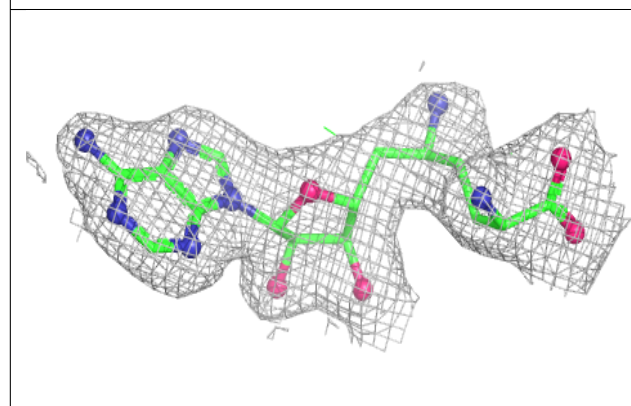
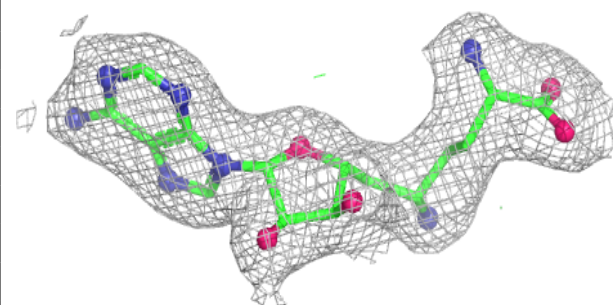
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 5QJ A 702:

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

**Electron density around SFG A 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.