



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:55 AM UTC

PDB ID : 5EMK / pdb_00005emk
Title : Crystal structure of PRMT5:MEP50 with Compound 9 and sinefungin
Authors : Boriack-Sjodin, P.A.; Jin, L.
Deposited on : 2015-11-06
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

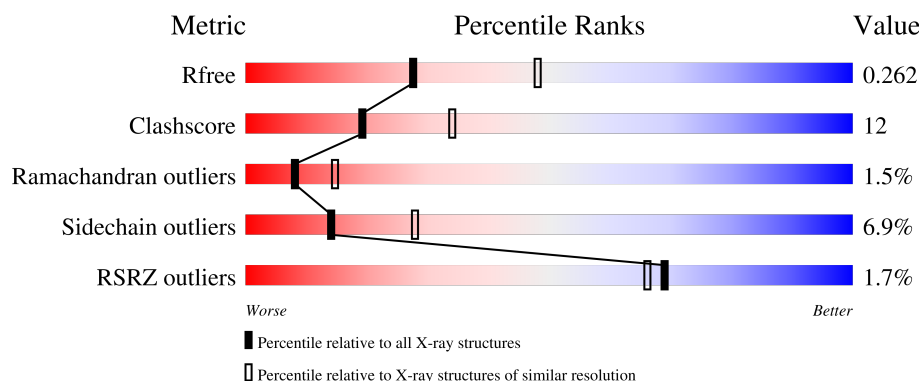
1 Overall quality at a glance

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	% 73% 20% • •
2	B	350	3% 60% 27% • 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7666 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	5144	3292	884	943	25	0	10	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	313	2376	1490	406	464	16	0	2	0

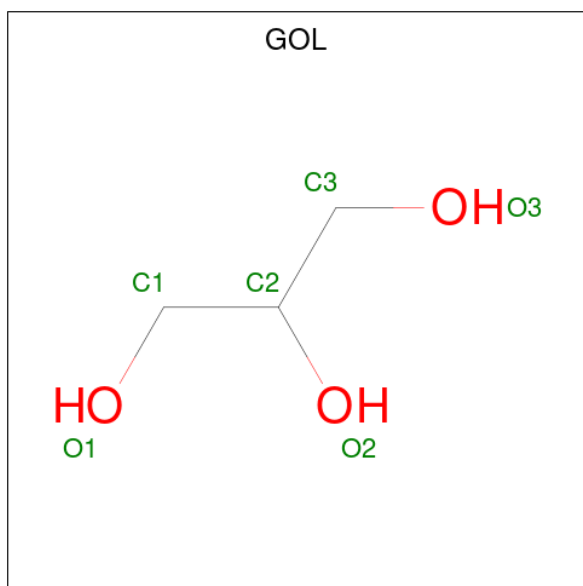
There are 9 discrepancies between the modelled and reference sequences:

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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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	24	3	2		

- 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		

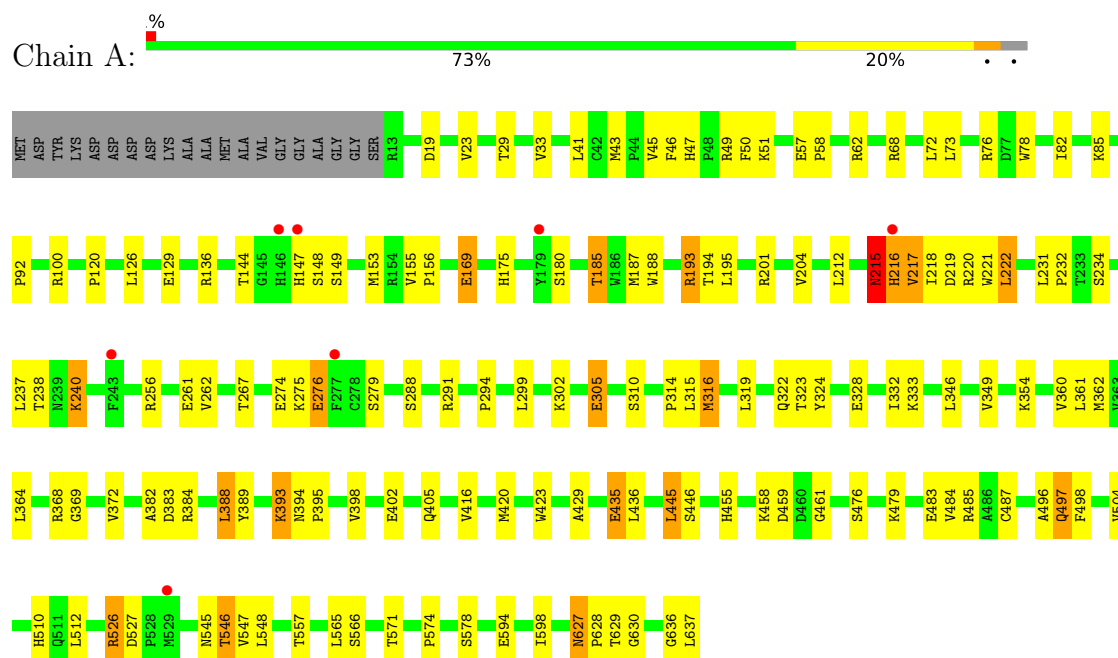
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	13	Total	O	0	0
			13	13		

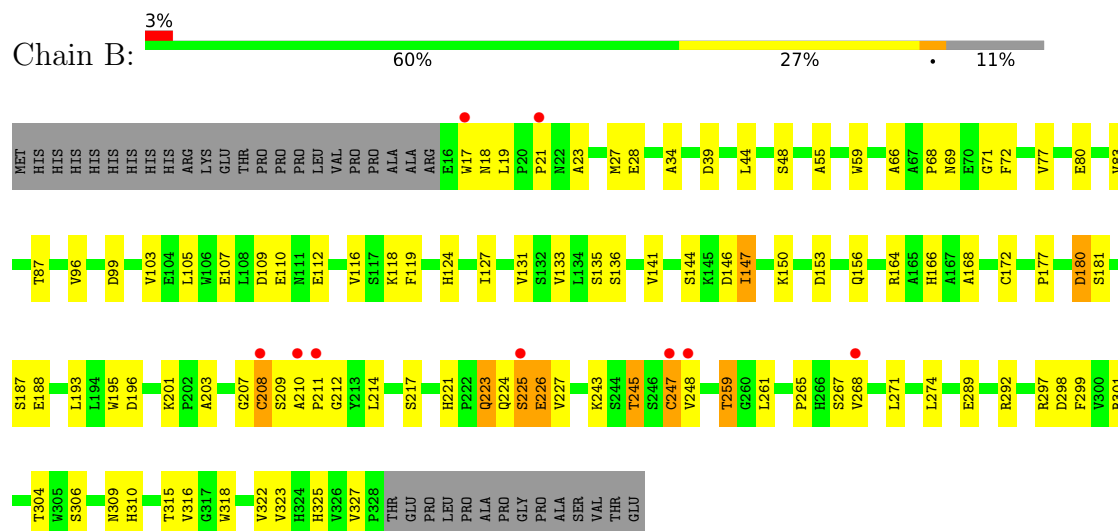
3 Residue-property plots

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	102.79Å 137.75Å 178.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.49 – 2.52 54.49 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (54.49-2.52) 99.4 (54.49-2.52)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.262 0.200 , 0.262	Depositor DCC
R_{free} test set	2161 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7666	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: GOL, 5QH, 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	0.69	0/5292	0.99	13/7200 (0.2%)
2	B	0.64	0/2438	0.99	7/3333 (0.2%)
All	All	0.68	0/7730	0.99	20/10533 (0.2%)

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	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	201	LYS	CA-C-N	7.20	126.70	118.85
2	B	201	LYS	C-N-CA	7.20	126.70	118.85
2	B	327	VAL	N-CA-C	6.61	114.68	107.60
1	A	369	GLY	CA-C-N	-6.23	113.35	119.64
1	A	369	GLY	C-N-CA	-6.23	113.35	119.64
1	A	310	SER	CA-C-N	-5.96	113.84	119.85
1	A	310	SER	C-N-CA	-5.96	113.84	119.85
2	B	19	LEU	CA-C-N	5.90	126.45	120.38
2	B	19	LEU	C-N-CA	5.90	126.45	120.38
1	A	204	VAL	N-CA-C	5.72	116.82	108.53
1	A	212	LEU	N-CA-C	-5.66	102.64	109.83
1	A	636	GLY	N-CA-C	5.59	119.35	112.14
2	B	96	VAL	N-CA-C	5.51	115.93	107.77
1	A	354	LYS	N-CA-C	5.48	118.76	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	THR	N-CA-C	5.30	115.35	107.88
1	A	175	HIS	N-CA-C	5.29	117.13	111.36
1	A	578	SER	N-CA-C	5.12	117.60	111.71
1	A	195	LEU	N-CA-C	-5.10	105.81	112.23
2	B	77	VAL	N-CA-C	5.05	114.52	108.06
1	A	388	LEU	N-CA-C	5.00	117.13	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASN	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	5144	0	5033	125	1
2	B	2376	0	2278	52	0
3	A	27	0	22	1	0
4	A	29	0	0	0	0
5	A	12	0	16	0	0
6	A	65	0	0	3	0
6	B	13	0	0	1	0
All	All	7666	0	7349	175	1

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 12.

All (175) 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:218[B]:ILE:O	1:A:222[B]:LEU:HD13	1.32	1.24
1:A:218[B]:ILE:O	1:A:218[B]:ILE:HD12	1.52	1.09
1:A:222[B]:LEU:HD12	1:A:222[B]:LEU:N	1.70	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218[B]:ILE:O	1:A:222[B]:LEU:CD1	2.16	0.92
1:A:222[B]:LEU:N	1:A:222[B]:LEU:CD1	2.30	0.91
1:A:349:VAL:HG23	1:A:384:ARG:HE	1.35	0.88
2:B:109:ASP:HB3	2:B:112:GLU:H	1.41	0.85
1:A:222[B]:LEU:CD1	1:A:222[B]:LEU:H	1.92	0.83
1:A:218[B]:ILE:HD12	1:A:222[B]:LEU:CD1	2.08	0.82
1:A:218[B]:ILE:HD12	1:A:218[B]:ILE:C	2.04	0.81
1:A:218[B]:ILE:CD1	1:A:222[B]:LEU:CD2	2.59	0.80
1:A:222[A]:LEU:HB3	1:A:510:HIS:HB2	1.65	0.78
1:A:218[B]:ILE:HD12	1:A:222[B]:LEU:HD13	1.66	0.77
1:A:23:VAL:HG22	1:A:29:THR:HG21	1.67	0.77
1:A:218[B]:ILE:HD11	1:A:222[B]:LEU:CD2	2.17	0.75
1:A:218[B]:ILE:CD1	1:A:222[B]:LEU:HD21	2.17	0.74
1:A:526:ARG:H	1:A:526:ARG:CD	2.01	0.74
1:A:215:ASN:O	1:A:217[B]:VAL:N	2.22	0.72
2:B:18:ASN:HB3	2:B:71:GLY:O	1.89	0.72
1:A:217[B]:VAL:O	1:A:217[B]:VAL:CG2	2.38	0.72
1:A:218[B]:ILE:HD11	1:A:222[B]:LEU:HD22	1.71	0.71
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.74	0.70
2:B:18:ASN:CB	2:B:71:GLY:O	2.40	0.70
1:A:217[B]:VAL:O	1:A:217[B]:VAL:HG22	1.93	0.67
2:B:109:ASP:HB3	2:B:112:GLU:N	2.10	0.66
1:A:314:PRO:O	1:A:393:LYS:HE2	1.95	0.66
1:A:222[A]:LEU:HD13	1:A:510:HIS:CD2	2.31	0.65
2:B:44:LEU:HB2	2:B:59:TRP:HB2	1.79	0.64
1:A:628:PRO:O	1:A:629:THR:HB	1.97	0.64
1:A:349:VAL:HG23	1:A:384:ARG:NE	2.11	0.63
1:A:364:LEU:HB3	1:A:420:MET:HE2	1.79	0.63
1:A:526:ARG:H	1:A:526:ARG:HD3	1.61	0.63
1:A:328:GLU:OE1	1:A:368:ARG:NH1	2.31	0.63
2:B:207:GLY:HA3	6:B:406:HOH:O	1.98	0.63
2:B:147:ILE:HG23	2:B:168:ALA:O	2.00	0.62
1:A:218[A]:ILE:O	1:A:219[A]:ASP:C	2.41	0.61
1:A:218[B]:ILE:CD1	1:A:222[B]:LEU:CD1	2.77	0.61
1:A:220[A]:ARG:HH12	1:A:546:THR:HA	1.66	0.61
1:A:222[B]:LEU:HD13	1:A:222[B]:LEU:H	1.65	0.61
2:B:27:MET:CE	2:B:68:PRO:HB2	2.31	0.60
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.83	0.60
1:A:169:GLU:HB3	6:A:846:HOH:O	2.02	0.60
2:B:221:HIS:HB2	2:B:227:VAL:HG23	1.83	0.60
1:A:219[A]:ASP:O	1:A:222[A]:LEU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:MET:HE1	1:A:436:LEU:HD11	1.85	0.59
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.04	0.58
1:A:220[A]:ARG:NH1	1:A:545:ASN:O	2.37	0.57
1:A:476:SER:HB2	1:A:512:LEU:HD21	1.85	0.57
2:B:181:SER:O	2:B:196:ASP:HA	2.04	0.57
1:A:156:PRO:O	1:A:185:THR:HG21	2.05	0.57
1:A:220[A]:ARG:NH1	1:A:546:THR:HA	2.20	0.57
1:A:526:ARG:HH21	1:A:526:ARG:HG2	1.70	0.57
1:A:218[B]:ILE:CD1	1:A:222[B]:LEU:HD11	2.35	0.56
1:A:41:LEU:HG	1:A:43:MET:HG2	1.87	0.56
2:B:315:THR:OG1	2:B:325:HIS:HE1	1.89	0.56
1:A:218[B]:ILE:HD13	1:A:222[B]:LEU:HD21	1.87	0.56
1:A:218[B]:ILE:CD1	1:A:222[B]:LEU:HD22	2.32	0.56
1:A:215:ASN:C	1:A:217[B]:VAL:H	2.13	0.55
1:A:217[A]:VAL:O	1:A:217[A]:VAL:CG2	2.54	0.55
1:A:217[A]:VAL:O	1:A:217[A]:VAL:HG23	2.06	0.55
1:A:436:LEU:O	1:A:446:SER:HB2	2.05	0.55
1:A:68:ARG:HG3	1:A:72:LEU:HD12	1.88	0.55
2:B:188:GLU:HG2	2:B:214:LEU:HD13	1.87	0.55
1:A:324:TYR:CB	1:A:368:ARG:HD2	2.36	0.55
1:A:221[B]:TRP:C	1:A:222[B]:LEU:HD12	2.29	0.54
1:A:393:LYS:O	1:A:395:PRO:HD3	2.07	0.54
1:A:51:LYS:O	1:A:62:ARG:NH1	2.39	0.54
1:A:319:LEU:HD22	1:A:323:THR:HG21	1.89	0.54
1:A:333:LYS:HE3	1:A:435:GLU:HG2	1.89	0.54
2:B:306:SER:HB3	2:B:309:ASN:O	2.07	0.54
1:A:23:VAL:HG12	1:A:23:VAL:O	2.08	0.54
1:A:416:VAL:HG21	1:A:423:TRP:CZ2	2.43	0.54
1:A:324:TYR:HB3	1:A:368:ARG:HD2	1.89	0.54
2:B:289:GLU:OE2	2:B:292:ARG:HD2	2.08	0.53
1:A:364:LEU:HB3	1:A:420:MET:CE	2.39	0.53
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.24	0.53
1:A:288:SER:O	1:A:291:ARG:HD2	2.08	0.53
2:B:135:SER:HB3	2:B:177:PRO:O	2.08	0.53
1:A:383:ASP:O	1:A:384:ARG:HD3	2.10	0.52
1:A:526:ARG:CD	1:A:526:ARG:N	2.73	0.52
1:A:218[B]:ILE:HD12	1:A:222[B]:LEU:HD11	1.88	0.52
1:A:526:ARG:HG2	1:A:526:ARG:NH2	2.24	0.52
2:B:124:HIS:CE1	2:B:150:LYS:HD2	2.44	0.52
1:A:302:LYS:O	1:A:305:GLU:OE1	2.28	0.51
2:B:17:TRP:HB3	2:B:72:PHE:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HB2	1:A:299:LEU:HG	1.92	0.51
1:A:193:ARG:HD2	1:A:193:ARG:C	2.35	0.51
2:B:66:ALA:HB1	2:B:72:PHE:HB2	1.92	0.50
2:B:136:SER:HB3	2:B:180:ASP:OD1	2.11	0.50
1:A:445:LEU:N	1:A:445:LEU:HD23	2.27	0.50
1:A:218[B]:ILE:HD11	1:A:256:ARG:CZ	2.42	0.50
1:A:19:ASP:OD1	1:A:85:LYS:HE3	2.11	0.50
1:A:240:LYS:HE2	6:A:856:HOH:O	2.12	0.50
1:A:496:ALA:O	1:A:497:GLN:C	2.55	0.49
1:A:346:LEU:HD21	1:A:382:ALA:HB1	1.94	0.49
1:A:193:ARG:HH21	1:A:193:ARG:HG2	1.78	0.49
1:A:218[B]:ILE:HD11	1:A:222[B]:LEU:HD21	1.89	0.48
2:B:87:THR:HG21	2:B:133:VAL:HG23	1.96	0.48
1:A:526:ARG:HH21	1:A:526:ARG:CG	2.26	0.48
2:B:224:GLN:C	2:B:226:GLU:H	2.21	0.48
1:A:215:ASN:HD22	1:A:216[B]:HIS:HA	1.79	0.48
2:B:259:THR:HG21	2:B:301:ARG:NH2	2.29	0.48
1:A:149:SER:HB3	1:A:201:ARG:HH21	1.79	0.47
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.79	0.47
2:B:17:TRP:HB3	2:B:72:PHE:CE1	2.49	0.47
2:B:172[B]:CYS:SG	2:B:217:SER:HA	2.55	0.47
1:A:372:VAL:HG13	1:A:388:LEU:HD13	1.98	0.46
1:A:393:LYS:O	1:A:395:PRO:CD	2.63	0.46
2:B:107:GLU:HB2	2:B:118:LYS:HD3	1.96	0.46
1:A:316:MET:O	1:A:316:MET:HG3	2.15	0.46
2:B:17:TRP:CB	2:B:72:PHE:HE1	2.29	0.46
1:A:217[B]:VAL:HG22	1:A:221[B]:TRP:CD1	2.50	0.46
1:A:275:LYS:HD3	1:A:279:SER:HB3	1.97	0.46
2:B:316:VAL:HG12	2:B:322:VAL:HG22	1.98	0.45
2:B:18:ASN:HB2	2:B:71:GLY:O	2.15	0.45
1:A:627:ASN:HD21	1:A:630:GLY:HA2	1.81	0.45
2:B:210:ALA:O	2:B:212:GLY:N	2.50	0.45
2:B:99:ASP:HA	2:B:127:ILE:HG23	1.99	0.45
1:A:275:LYS:HG2	1:A:276:GLU:H	1.81	0.45
1:A:218[B]:ILE:C	1:A:218[B]:ILE:CD1	2.68	0.44
3:A:701:SFG:H4'	3:A:701:SFG:HB1	2.00	0.44
1:A:627:ASN:ND2	1:A:630:GLY:HA2	2.33	0.44
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.53	0.44
1:A:398:VAL:O	1:A:402:GLU:HG3	2.17	0.44
1:A:217[B]:VAL:O	1:A:221[B]:TRP:CD1	2.70	0.44
1:A:455:HIS:HB3	6:A:835:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:HIS:ND1	2:B:187:SER:HB3	2.33	0.43
1:A:126:LEU:HD12	1:A:155:VAL:CG2	2.48	0.43
1:A:314:PRO:O	1:A:393:LYS:CE	2.63	0.43
2:B:193:LEU:HD13	2:B:203:ALA:HB1	2.00	0.43
2:B:208:CYS:HB2	2:B:247:CYS:HB3	1.82	0.43
1:A:49:ARG:HH21	2:B:99:ASP:CG	2.26	0.43
2:B:223:GLN:HE21	2:B:223:GLN:HA	1.84	0.43
1:A:82:ILE:O	1:A:120:PRO:HD2	2.18	0.43
1:A:458:LYS:O	1:A:461:GLY:N	2.48	0.43
2:B:261:LEU:HD22	2:B:271:LEU:HD21	2.01	0.43
1:A:332:ILE:HG13	1:A:574:PRO:O	2.19	0.42
1:A:416:VAL:HG21	1:A:423:TRP:CE2	2.53	0.42
2:B:48:SER:HB3	2:B:55:ALA:H	1.83	0.42
1:A:92:PRO:O	1:A:100:ARG:HG3	2.19	0.42
1:A:193:ARG:HG2	1:A:193:ARG:NH2	2.33	0.42
1:A:126:LEU:HD21	1:A:153:MET:HE2	2.00	0.42
2:B:136:SER:HB3	2:B:180:ASP:CG	2.44	0.42
1:A:193:ARG:HD2	1:A:194:THR:N	2.35	0.42
1:A:362:MET:SD	1:A:429:ALA:HB2	2.60	0.42
2:B:265:PRO:HB2	2:B:310:HIS:CE1	2.55	0.42
2:B:243:LYS:HE2	2:B:243:LYS:HB3	1.87	0.42
1:A:497:GLN:H	1:A:497:GLN:CD	2.26	0.42
2:B:299:PHE:CD2	2:B:318:TRP:CZ3	3.08	0.42
1:A:187[A]:MET:HE2	1:A:187[A]:MET:HB2	1.92	0.42
1:A:548:LEU:HD13	1:A:598:ILE:HD13	2.01	0.42
1:A:222[A]:LEU:HD13	1:A:510:HIS:CG	2.55	0.42
1:A:302:LYS:HD3	1:A:302:LYS:HA	1.90	0.41
2:B:34:ALA:O	2:B:304:THR:HB	2.20	0.41
2:B:193:LEU:HB2	2:B:195:TRP:HE1	1.86	0.41
2:B:21:PRO:C	2:B:23:ALA:H	2.28	0.41
1:A:126:LEU:HB2	1:A:155:VAL:HG22	2.03	0.41
2:B:153:ASP:OD1	2:B:156:GLN:HB2	2.19	0.41
1:A:58:PRO:HG3	2:B:297:ARG:HA	2.03	0.41
1:A:62:ARG:HD3	2:B:298:ASP:OD2	2.20	0.41
1:A:215:ASN:C	1:A:215:ASN:HD22	2.28	0.41
1:A:445:LEU:HD12	1:A:637:LEU:HD23	2.02	0.41
2:B:289:GLU:OE2	2:B:292:ARG:HB2	2.20	0.41
1:A:129:GLU:HA	1:A:188:TRP:CD1	2.55	0.41
1:A:557:THR:HG22	1:A:565:LEU:HB2	2.02	0.41
1:A:566:SER:HB3	1:A:571:THR:O	2.21	0.41
1:A:629:THR:HG22	1:A:629:THR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASN:C	1:A:215:ASN:ND2	2.78	0.41
1:A:232:PRO:HA	1:A:267:THR:HG23	2.01	0.41
1:A:479:LYS:O	1:A:483:GLU:HG2	2.21	0.41
1:A:496:ALA:C	1:A:498:PHE:N	2.78	0.41
1:A:546:THR:OG1	1:A:547:VAL:N	2.54	0.41
2:B:323:VAL:HG12	2:B:325:HIS:CE1	2.57	0.40
1:A:484:VAL:O	1:A:487:CYS:HB2	2.21	0.40
2:B:105:LEU:HB2	2:B:119:PHE:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:NZ	1:A:240:LYS:NZ[2_645]	2.19	0.01

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	633/645 (98%)	581 (92%)	44 (7%)	8 (1%)	9	17
2	B	313/350 (89%)	290 (93%)	16 (5%)	7 (2%)	5	8
All	All	946/995 (95%)	871 (92%)	60 (6%)	15 (2%)	8	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	A	216[A]	HIS
1	A	216[B]	HIS
1	A	261	GLU
2	B	211	PRO

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Mol	Chain	Res	Type
2	B	245	THR
2	B	247	CYS
1	A	276	GLU
2	B	208	CYS
1	A	459	ASP
1	A	234	SER
1	A	394	ASN
2	B	69	ASN
2	B	225	SER
1	A	627	ASN

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	567/570 (100%)	529 (93%)	38 (7%)	15	29
2	B	267/298 (90%)	246 (92%)	21 (8%)	11	22
All	All	834/868 (96%)	775 (93%)	59 (7%)	14	27

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	57	GLU
1	A	76	ARG
1	A	136	ARG
1	A	144	THR
1	A	147	HIS
1	A	148	SER
1	A	169	GLU
1	A	180	SER
1	A	185	THR
1	A	193	ARG
1	A	215	ASN
1	A	217[A]	VAL

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Mol	Chain	Res	Type
1	A	217[B]	VAL
1	A	222[A]	LEU
1	A	222[B]	LEU
1	A	231	LEU
1	A	237	LEU
1	A	238	THR
1	A	240	LYS
1	A	262	VAL
1	A	274	GLU
1	A	305	GLU
1	A	315	LEU
1	A	316	MET
1	A	322	GLN
1	A	360	VAL
1	A	361	LEU
1	A	393	LYS
1	A	405	GLN
1	A	435	GLU
1	A	445	LEU
1	A	485	ARG
1	A	497	GLN
1	A	504	VAL
1	A	526	ARG
1	A	527	ASP
1	A	594	GLU
2	B	28	GLU
2	B	39	ASP
2	B	80	GLU
2	B	83	VAL
2	B	103	VAL
2	B	110	GLU
2	B	116	VAL
2	B	131	VAL
2	B	141	VAL
2	B	164	ARG
2	B	180	ASP
2	B	209	SER
2	B	223	GLN
2	B	225	SER
2	B	226	GLU
2	B	245	THR
2	B	248	VAL

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Mol	Chain	Res	Type
2	B	259	THR
2	B	267	SER
2	B	268	VAL
2	B	274	LEU

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	143	HIS
1	A	215	ASN
1	A	405	GLN
1	A	455	HIS
1	A	482	ASN
1	A	511	GLN
1	A	525	ASN
1	A	545	ASN
2	B	78	GLN
2	B	178	HIS
2	B	223	GLN
2	B	254	HIS
2	B	310	HIS
2	B	325	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 ⓘ

4 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$
3	SFG	A	701	-	28,29,29	1.58	4 (14%)	34,42,42	1.81	7 (20%)
5	GOL	A	704	-	5,5,5	0.46	0	5,5,5	0.28	0
4	5QH	A	702	-	32,32,32	2.10	6 (18%)	43,43,43	1.32	6 (13%)
5	GOL	A	703	-	5,5,5	0.24	0	5,5,5	0.45	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	SFG	A	701	-	-	3/17/33/33	0/3/3/3
5	GOL	A	704	-	-	2/4/4/4	-
4	5QH	A	702	-	-	0/17/26/26	0/4/4/4
5	GOL	A	703	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	5QH	CAI-CAM	-6.06	1.39	1.49
4	A	702	5QH	CAV-CAW	-5.96	1.41	1.51
3	A	701	SFG	C5-C4	5.46	1.48	1.39
4	A	702	5QH	CAY-CAX	-4.97	1.40	1.51
4	A	702	5QH	CAG-CAE	-4.08	1.41	1.50
4	A	702	5QH	CAO-NAN	3.21	1.41	1.34
3	A	701	SFG	C8-N7	2.95	1.37	1.31
3	A	701	SFG	C5-N7	-2.55	1.34	1.39
4	A	702	5QH	CAU-CAV	-2.34	1.47	1.51
3	A	701	SFG	C5-C6	2.24	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	SFG	C5-C4-N3	-5.63	118.96	126.72
3	A	701	SFG	N3-C4-N9	4.51	134.83	127.17
4	A	702	5QH	CAY-NAT-CAU	3.92	115.50	110.03
4	A	702	5QH	CAB-CAC-NAD	-3.51	101.49	111.42
3	A	701	SFG	C2-N3-C4	3.10	119.40	111.83
4	A	702	5QH	CAP-CAO-NAN	-3.08	118.54	123.42
3	A	701	SFG	C4-C5-N7	-2.97	107.18	110.58
3	A	701	SFG	N3-C2-N1	-2.64	124.59	128.58
4	A	702	5QH	CAO-NAN-CAM	2.27	120.41	117.24
3	A	701	SFG	O4'-C1'-C2'	-2.20	101.91	106.62
3	A	701	SFG	C4-N9-C8	2.20	108.04	105.74
4	A	702	5QH	CAJ-CAI-CAM	-2.18	117.83	121.28
4	A	702	5QH	CAB-CAS-NAT	-2.03	108.54	112.23

There are no chirality outliers.

All (7) 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
5	A	704	GOL	O1-C1-C2-C3
5	A	704	GOL	O1-C1-C2-O2
5	A	703	GOL	O1-C1-C2-C3
5	A	703	GOL	O1-C1-C2-O2
3	A	701	SFG	OXT-C-CA-N

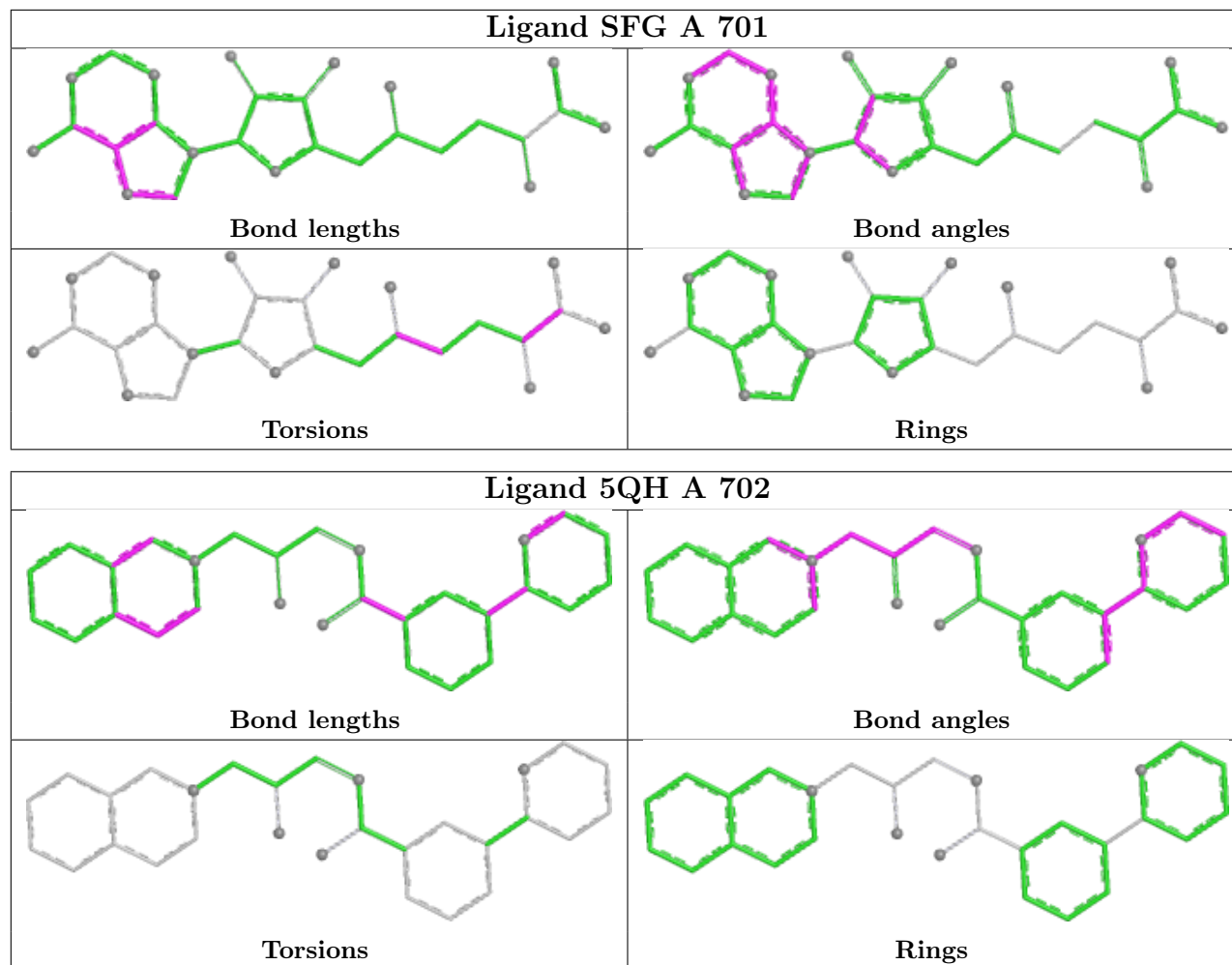
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	SFG	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%)	-0.23	7 (1%) 78 76	17, 55, 93, 145	10 (1%)
2	B	313/350 (89%)	0.17	9 (2%) 53 50	33, 69, 121, 167	2 (0%)
All	All	938/995 (94%)	-0.09	16 (1%) 69 66	17, 61, 104, 167	12 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	HIS	3.5
2	B	225	SER	3.3
1	A	277	PHE	3.2
2	B	17	TRP	3.2
2	B	268	VAL	3.1
2	B	248	VAL	3.0
2	B	247	CYS	2.9
2	B	208	CYS	2.3
1	A	146	HIS	2.2
1	A	243	PHE	2.2
2	B	21	PRO	2.2
1	A	216[A]	HIS	2.1
2	B	210	ALA	2.1
1	A	179	TYR	2.1
2	B	211	PRO	2.1
1	A	529	MET	2.1

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](#)

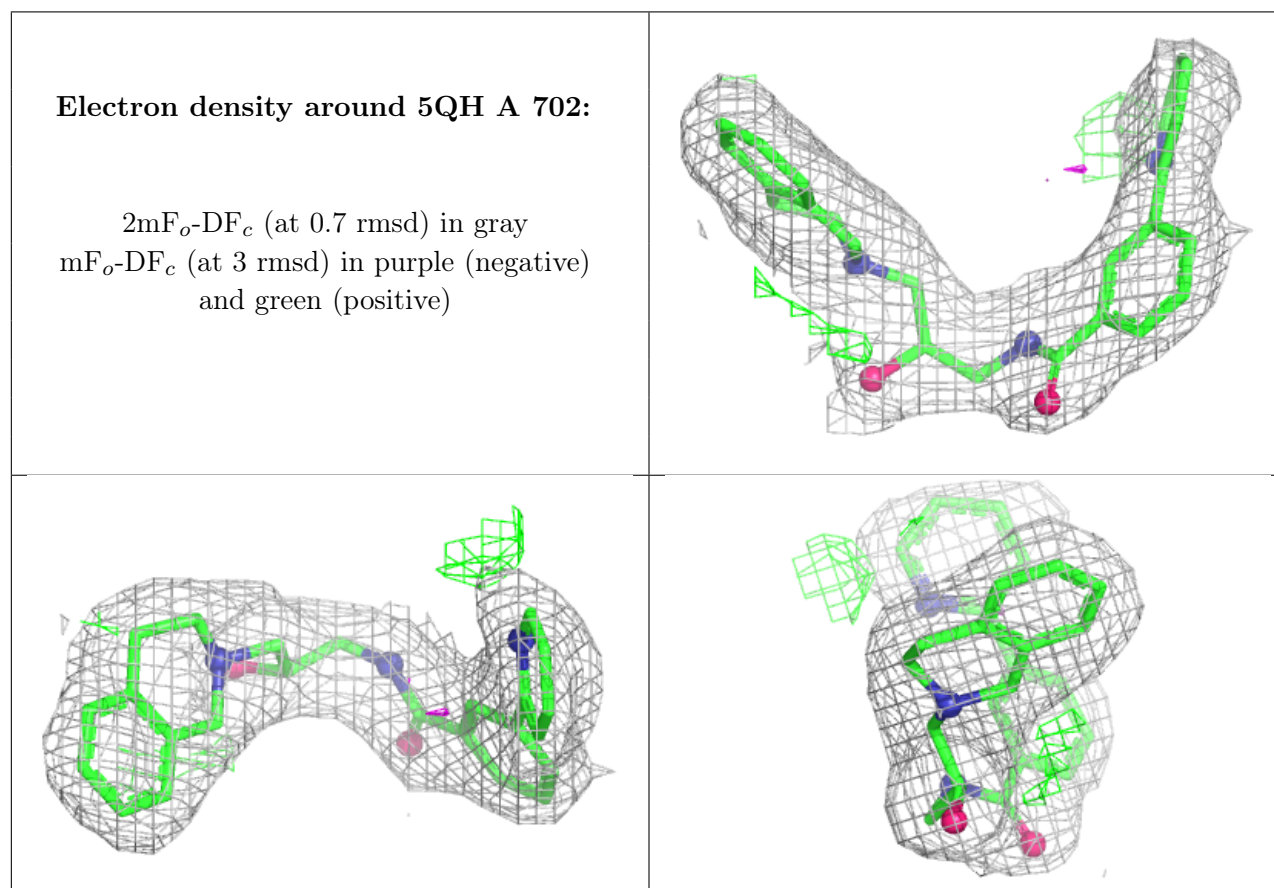
There are no oligosaccharides in this entry.

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.

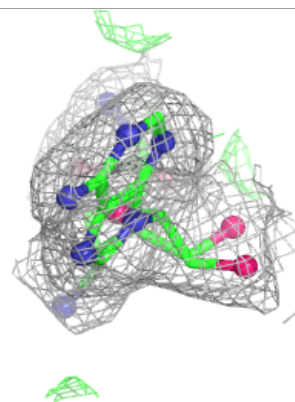
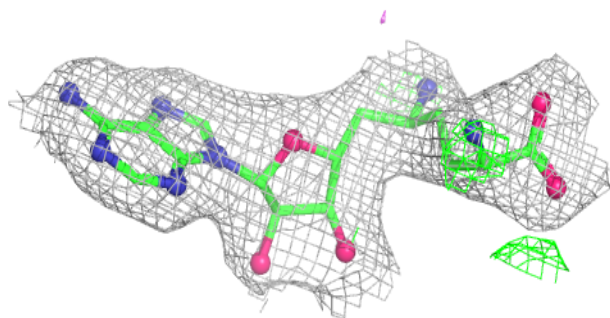
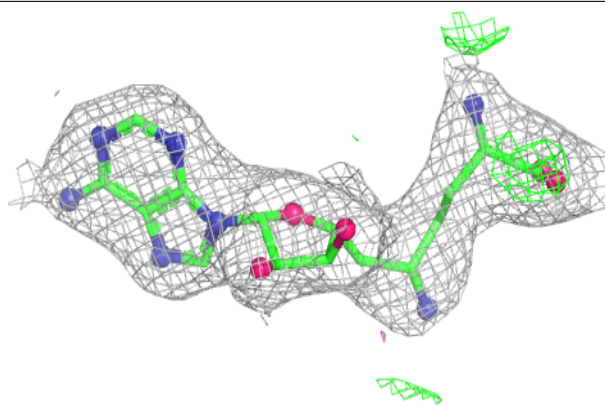
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	704	6/6	0.89	0.09	58,65,67,68	0
5	GOL	A	703	6/6	0.90	0.14	67,67,72,77	0
4	5QH	A	702	29/29	0.94	0.09	39,50,75,79	0
3	SFG	A	701	27/27	0.96	0.06	38,43,51,57	0

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 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.