



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:06 PM UTC

PDB ID : 5EMM / pdb_00005emm
Title : Crystal structure of PRMT5:MEP50 with Compound 15 and sinefungin
Authors : Boriack-Sjodin, P.A.; Jin, L.
Deposited on : 2015-11-06
Resolution : 2.37 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

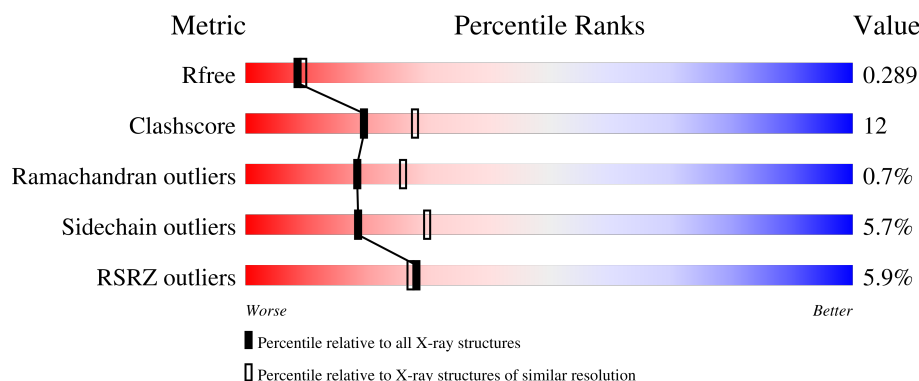
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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% 73% 21% • •
2	B	350	6% 67% 20% • 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7660 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	5153	3296	887	945	25	0	12	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	2370	1487	405	463	15	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

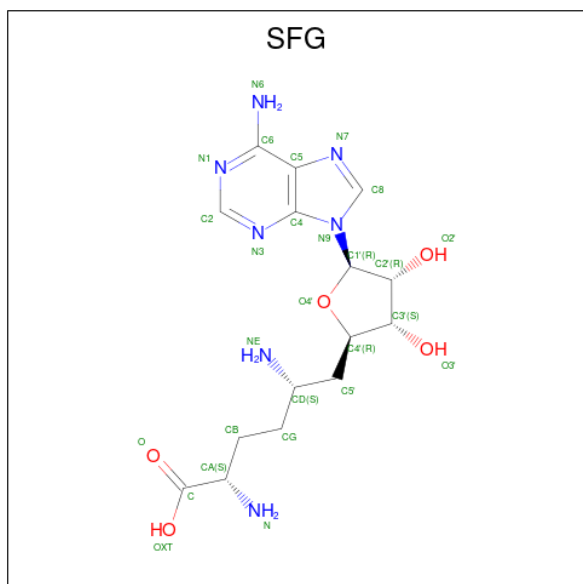
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag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

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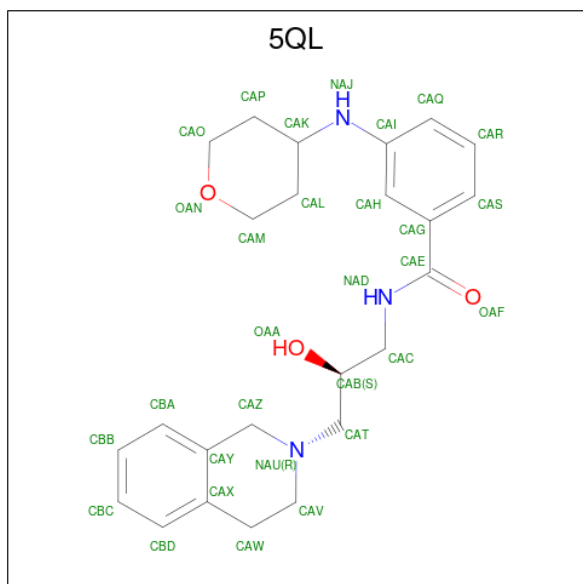
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is SINEFUNGIN (CCD ID: SFG) (formula: $C_{15}H_{23}N_7O_5$).



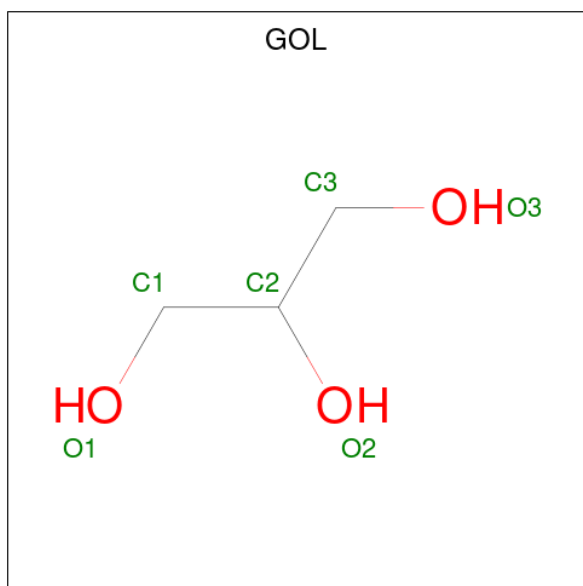
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 4 is {N}-[(2 {S})-3-(3,4-dihydro-1 {H}-isoquinolin-2-yl)-2-oxidanyl-propyl]-3-(oxan-4-ylamino)benzamide (CCD ID: 5QL) (formula: $C_{24}H_{31}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	24	3	3		

- 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		

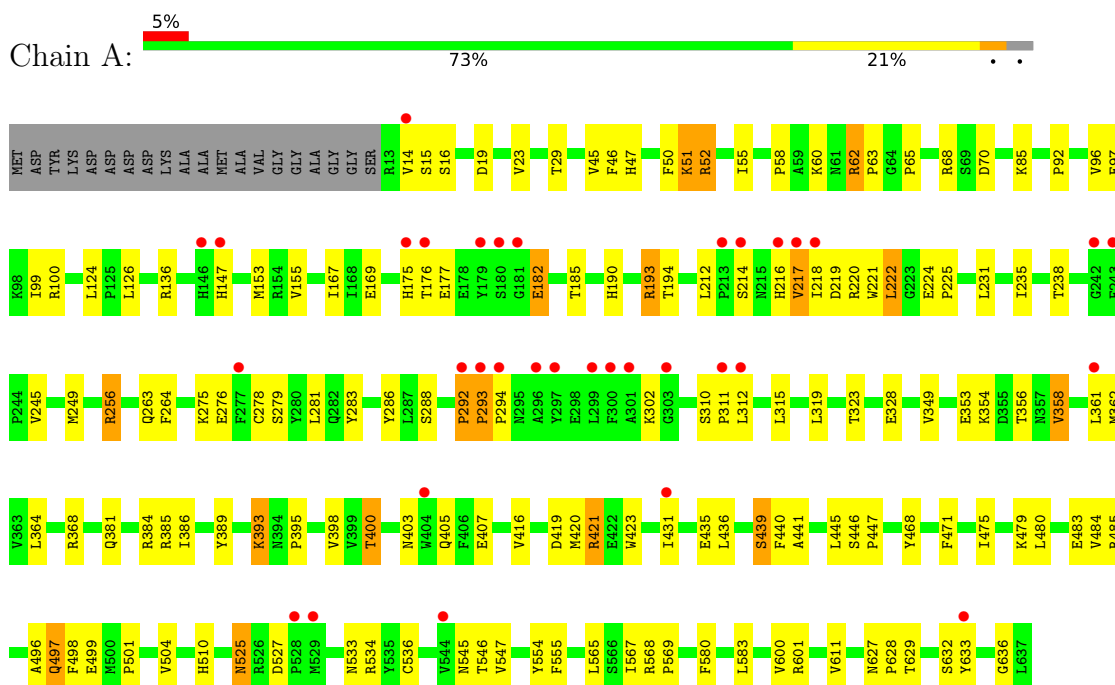
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	55	Total	O	0	0
			55	55		
6	B	13	Total	O	0	0
			13	13		

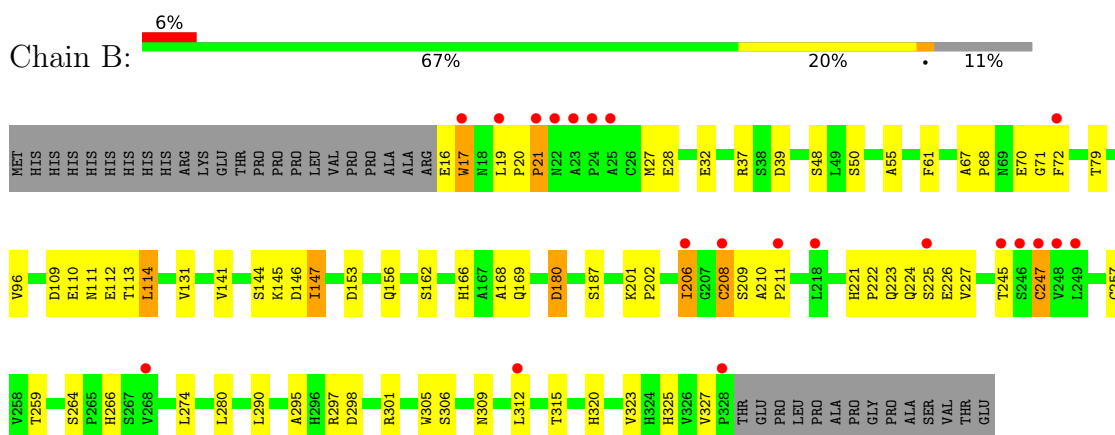
3 Residue-property plots [i](#)

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	103.53Å 138.18Å 179.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.61 – 2.37 89.61 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.61-2.37) 99.7 (89.61-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.234 , 0.293 0.232 , 0.289	Depositor DCC
R_{free} test set	2668 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.5	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	0.95	EDS
Total number of atoms	7660	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: 5QL, 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	0.66	3/5298 (0.1%)	0.99	11/7210 (0.2%)
2	B	0.76	7/2432 (0.3%)	0.99	9/3325 (0.3%)
All	All	0.69	10/7730 (0.1%)	0.99	20/10535 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	223	GLN	C-N	10.75	1.47	1.33
2	B	21	PRO	N-CD	9.09	1.60	1.47
1	A	175	HIS	CE1-NE2	8.96	1.41	1.32
2	B	19	LEU	CA-CB	7.96	1.66	1.53
2	B	114	LEU	C-N	7.35	1.42	1.33
1	A	238	THR	C-O	-7.15	1.16	1.24
2	B	222	PRO	C-N	6.77	1.43	1.33
1	A	175	HIS	CG-ND1	6.59	1.45	1.38
2	B	225	SER	C-O	5.75	1.31	1.24
2	B	19	LEU	C-N	5.10	1.39	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	THR	O-C-N	-15.84	104.74	123.27
1	A	292	PRO	CA-C-N	8.58	125.92	119.66
1	A	292	PRO	C-N-CA	8.58	125.92	119.66
2	B	201	LYS	CA-C-N	8.35	127.66	118.97
2	B	201	LYS	C-N-CA	8.35	127.66	118.97
1	A	175	HIS	N-CA-C	7.54	119.13	111.07
1	A	177	GLU	N-CA-C	7.34	120.33	110.35
1	A	238	THR	CA-C-N	6.43	133.34	122.15
1	A	238	THR	C-N-CA	6.43	133.34	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	VAL	N-CA-C	6.42	117.10	108.11
1	A	381	GLN	N-CA-C	-6.17	106.39	114.04
1	A	354	LYS	N-CA-C	6.08	118.69	111.33
2	B	327	VAL	N-CA-C	5.76	114.29	107.73
1	A	293	PRO	N-CA-C	5.60	115.84	110.47
1	A	386	ILE	N-CA-C	5.44	116.50	108.45
2	B	79	THR	CA-C-N	5.41	127.99	120.63
2	B	79	THR	C-N-CA	5.41	127.99	120.63
2	B	323	VAL	N-CA-C	5.39	115.88	108.12
2	B	113	THR	O-C-N	5.16	128.70	122.20
2	B	70	GLU	N-CA-C	5.09	116.83	111.28

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	5153	0	5042	131	0
2	B	2370	0	2274	47	0
3	A	27	0	22	1	0
4	A	30	0	0	0	0
5	A	12	0	16	0	0
6	A	55	0	0	0	0
6	B	13	0	0	2	0
All	All	7660	0	7354	174	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 12.

All (174) 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)
2:B:16:GLU:HA	2:B:71:GLY:HA3	1.25	1.11
2:B:27:MET:HE1	2:B:68:PRO:HB2	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ALA:HB1	2:B:211:PRO:HD2	1.39	1.01
1:A:218[B]:ILE:O	1:A:222[B]:LEU:HD13	1.62	1.00
1:A:222[B]:LEU:HD12	1:A:222[B]:LEU:N	1.78	0.95
1:A:218[B]:ILE:HD13	1:A:222[B]:LEU:HD11	1.57	0.85
1:A:218[B]:ILE:CG2	1:A:219[B]:ASP:N	2.41	0.83
1:A:218[B]:ILE:HG23	1:A:256:ARG:HH12	1.45	0.80
2:B:27:MET:CE	2:B:68:PRO:HB2	2.11	0.80
2:B:210:ALA:HB1	2:B:211:PRO:CD	2.13	0.79
2:B:27:MET:HE1	2:B:68:PRO:CB	2.13	0.78
1:A:218[B]:ILE:CD1	1:A:222[B]:LEU:HD11	2.14	0.78
1:A:218[B]:ILE:HG23	1:A:219[B]:ASP:N	1.98	0.78
1:A:52:ARG:HH11	1:A:52:ARG:HG3	1.48	0.77
1:A:364:LEU:HB3	1:A:420:MET:HE2	1.68	0.75
1:A:218[B]:ILE:O	1:A:222[B]:LEU:CD1	2.33	0.75
1:A:222[B]:LEU:N	1:A:222[B]:LEU:CD1	2.47	0.74
1:A:217[B]:VAL:CG2	1:A:221[B]:TRP:CD1	2.72	0.72
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.73	0.71
1:A:216[A]:HIS:HA	1:A:219[A]:ASP:OD2	1.93	0.68
2:B:224:GLN:N	2:B:224:GLN:OE1	2.28	0.67
1:A:218[B]:ILE:HG22	1:A:219[B]:ASP:H	1.59	0.67
1:A:218[B]:ILE:HD13	1:A:222[B]:LEU:CD1	2.24	0.67
1:A:218[B]:ILE:CG2	1:A:219[B]:ASP:H	2.07	0.67
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.06	0.66
1:A:275:LYS:HD3	1:A:279:SER:HB3	1.76	0.66
1:A:220[A]:ARG:NH1	1:A:546:THR:HA	2.10	0.66
2:B:224:GLN:HB2	2:B:227:VAL:HG12	1.77	0.66
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.79	0.64
1:A:62:ARG:HD3	2:B:298:ASP:OD2	1.98	0.64
1:A:328:GLU:OE1	1:A:368:ARG:NH1	2.30	0.64
2:B:210:ALA:CB	2:B:211:PRO:HD2	2.22	0.64
1:A:420:MET:HE1	1:A:436:LEU:HD11	1.81	0.63
1:A:310[B]:SER:HB2	1:A:311[B]:PRO:HD2	1.79	0.63
1:A:220[A]:ARG:HH12	1:A:546:THR:HA	1.63	0.63
1:A:193:ARG:HD2	1:A:193:ARG:C	2.24	0.62
1:A:216[A]:HIS:O	1:A:219[A]:ASP:HB2	1.99	0.62
2:B:180:ASP:HB2	6:B:413:HOH:O	2.00	0.61
1:A:218[B]:ILE:CD1	1:A:222[B]:LEU:CD1	2.79	0.61
1:A:364:LEU:HB3	1:A:420:MET:CE	2.31	0.60
1:A:217[B]:VAL:HG22	1:A:221[B]:TRP:CD1	2.35	0.60
1:A:219[A]:ASP:O	1:A:222[A]:LEU:HB2	2.01	0.60
1:A:222[A]:LEU:HB3	1:A:510:HIS:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:SER:HB3	1:A:580:PHE:O	2.02	0.60
1:A:600:VAL:C	1:A:601:ARG:HG2	2.28	0.59
1:A:220[A]:ARG:NH2	1:A:545:ASN:HB2	2.19	0.58
1:A:218[B]:ILE:HD12	1:A:256:ARG:NH1	2.18	0.58
1:A:349:VAL:HG23	1:A:384:ARG:HE	1.68	0.58
1:A:419:ASP:OD1	1:A:421:ARG:HD3	2.04	0.58
2:B:27:MET:HE3	2:B:320:HIS:CE1	2.39	0.57
1:A:193:ARG:HH21	1:A:193:ARG:HG2	1.69	0.57
2:B:306:SER:HB3	2:B:309:ASN:O	2.05	0.57
2:B:16:GLU:HA	2:B:71:GLY:CA	2.17	0.56
1:A:600:VAL:HG22	1:A:601:ARG:H	1.70	0.56
1:A:19:ASP:OD1	1:A:85:LYS:HE3	2.05	0.56
1:A:222[B]:LEU:HD12	1:A:222[B]:LEU:H	1.68	0.56
2:B:17:TRP:HB2	2:B:72:PHE:CD2	2.41	0.56
1:A:219[A]:ASP:HA	1:A:222[A]:LEU:HD12	1.87	0.56
1:A:218[B]:ILE:HG23	1:A:256:ARG:NH1	2.19	0.56
1:A:217[B]:VAL:HG22	1:A:221[B]:TRP:HD1	1.71	0.55
2:B:206:ILE:HD12	2:B:245:THR:HG23	1.89	0.55
2:B:224:GLN:C	2:B:226:GLU:H	2.13	0.55
2:B:259:THR:HG21	2:B:301:ARG:NH2	2.21	0.55
2:B:221:HIS:HB2	2:B:227:VAL:HG13	1.88	0.54
1:A:217[A]:VAL:O	1:A:217[A]:VAL:CG2	2.55	0.54
1:A:310[B]:SER:HB2	1:A:311[B]:PRO:CD	2.37	0.54
1:A:600:VAL:O	1:A:601:ARG:HG2	2.07	0.54
1:A:222[B]:LEU:CD1	1:A:222[B]:LEU:H	2.18	0.54
1:A:328:GLU:OE2	1:A:368:ARG:HB2	2.08	0.53
1:A:218[B]:ILE:O	1:A:218[B]:ILE:HD13	2.09	0.53
1:A:23:VAL:HG22	1:A:29:THR:HG21	1.91	0.52
1:A:628:PRO:O	1:A:629:THR:HB	2.10	0.52
1:A:221[B]:TRP:C	1:A:222[B]:LEU:HD12	2.33	0.52
1:A:126:LEU:HD12	1:A:155:VAL:HG22	1.91	0.52
1:A:479:LYS:O	1:A:483:GLU:HG2	2.10	0.52
2:B:37:ARG:HE	2:B:39:ASP:HB3	1.75	0.51
1:A:220[A]:ARG:HH21	1:A:545:ASN:HB2	1.75	0.51
1:A:52:ARG:HH11	1:A:52:ARG:CG	2.19	0.51
1:A:447:PRO:HD3	1:A:468:TYR:OH	2.11	0.51
2:B:153:ASP:HB3	2:B:156:GLN:HB2	1.92	0.51
1:A:185:THR:HG23	1:A:221[B]:TRP:HZ2	1.75	0.51
1:A:217[B]:VAL:HG23	1:A:220[B]:ARG:HH11	1.75	0.51
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.11	0.50
1:A:16:SER:OG	1:A:281:LEU:HD11	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:ASP:HB2	2:B:114:LEU:O	2.12	0.50
1:A:445:LEU:HD21	1:A:611:VAL:HB	1.94	0.50
2:B:16:GLU:CA	2:B:71:GLY:HA3	2.18	0.50
1:A:283:TYR:O	1:A:286:TYR:HB3	2.12	0.49
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.94	0.49
2:B:315:THR:OG1	2:B:325:HIS:HE1	1.96	0.49
1:A:58:PRO:HG2	2:B:297:ARG:HA	1.94	0.49
2:B:224:GLN:C	2:B:226:GLU:N	2.70	0.49
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.78	0.48
1:A:217[A]:VAL:O	1:A:217[A]:VAL:HG23	2.13	0.48
1:A:353:GLU:O	1:A:356:THR:HG22	2.12	0.48
1:A:600:VAL:HG22	1:A:601:ARG:N	2.28	0.48
1:A:525:ASN:ND2	1:A:527:ASP:HB2	2.28	0.48
2:B:17:TRP:HB2	2:B:72:PHE:HD2	1.79	0.48
2:B:259:THR:HG21	2:B:301:ARG:HH22	1.78	0.48
2:B:109:ASP:HB3	2:B:112:GLU:H	1.79	0.48
2:B:20:PRO:HB2	2:B:21:PRO:CD	2.44	0.47
1:A:51:LYS:O	1:A:62:ARG:NH1	2.46	0.47
1:A:193:ARG:HG2	1:A:193:ARG:NH2	2.29	0.47
1:A:245:VAL:HG12	1:A:283:TYR:CE1	2.49	0.47
1:A:368:ARG:HG2	1:A:400:THR:HG21	1.97	0.47
1:A:416:VAL:HG11	1:A:423:TRP:CD1	2.49	0.47
1:A:92:PRO:O	1:A:100:ARG:HG3	2.15	0.47
1:A:217[B]:VAL:HG23	1:A:221[B]:TRP:CD1	2.49	0.47
1:A:629:THR:HG22	1:A:629:THR:O	2.13	0.47
1:A:218[B]:ILE:CD1	1:A:218[B]:ILE:C	2.87	0.47
1:A:361:LEU:CD2	1:A:431:ILE:HB	2.45	0.47
1:A:436:LEU:HB2	1:A:446:SER:HB2	1.97	0.47
1:A:485:ARG:HG3	1:A:498:PHE:HZ	1.80	0.47
2:B:20:PRO:HB2	2:B:21:PRO:HD2	1.95	0.47
1:A:525:ASN:C	1:A:527:ASP:H	2.22	0.47
1:A:23:VAL:O	1:A:68:ARG:NH1	2.38	0.46
2:B:280:LEU:HD22	2:B:315:THR:HG21	1.96	0.46
1:A:193:ARG:HD2	1:A:194:THR:N	2.30	0.46
2:B:61:PHE:CE2	2:B:67:ALA:HA	2.50	0.46
1:A:499:GLU:HB2	1:A:632:SER:HB2	1.97	0.46
1:A:416:VAL:HG21	1:A:423:TRP:CZ2	2.51	0.46
1:A:14:VAL:HG21	1:A:264:PHE:HD2	1.80	0.46
1:A:217[B]:VAL:CG2	1:A:221[B]:TRP:NE1	2.79	0.45
1:A:361:LEU:HD23	1:A:431:ILE:HB	1.99	0.45
1:A:167:ILE:HB	2:B:202:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:HIS:CE1	1:A:547:VAL:HG21	2.52	0.45
2:B:48:SER:HB3	2:B:55:ALA:H	1.83	0.44
2:B:166:HIS:ND1	2:B:187:SER:HB3	2.33	0.44
1:A:393:LYS:O	1:A:395:PRO:HD3	2.17	0.44
1:A:554:TYR:HB3	1:A:567:ILE:HG13	2.00	0.44
1:A:501:PRO:HA	1:A:583:LEU:O	2.17	0.44
1:A:96:VAL:HB	1:A:99:ILE:HD12	2.00	0.44
1:A:217[B]:VAL:CG2	1:A:220[B]:ARG:HH11	2.31	0.43
2:B:208:CYS:HB3	2:B:247:CYS:HB2	1.69	0.43
1:A:55:ILE:O	1:A:60:LYS:HD2	2.18	0.43
1:A:403:ASN:O	1:A:407:GLU:HG3	2.19	0.43
2:B:109:ASP:HB3	2:B:112:GLU:N	2.34	0.43
1:A:220[A]:ARG:NH2	1:A:545:ASN:CB	2.82	0.43
1:A:319:LEU:HD22	1:A:323:THR:HG21	1.99	0.43
1:A:349:VAL:HG23	1:A:384:ARG:NE	2.32	0.43
1:A:420:MET:HG2	3:A:701:SFG:N1	2.34	0.43
1:A:358:VAL:HA	1:A:385:ARG:O	2.18	0.43
1:A:70:ASP:N	1:A:70:ASP:OD1	2.51	0.43
1:A:217[B]:VAL:HB	1:A:220[B]:ARG:NH1	2.34	0.42
2:B:147:ILE:HG23	2:B:168:ALA:O	2.18	0.42
1:A:293:PRO:HA	1:A:294:PRO:HD3	1.90	0.42
1:A:441:ALA:HB2	1:A:555:PHE:HB2	2.02	0.42
1:A:276:GLU:HB3	1:A:278:CYS:SG	2.59	0.42
1:A:14:VAL:HG22	1:A:15:SER:N	2.35	0.42
1:A:533:ASN:C	1:A:534:ARG:HG2	2.45	0.42
1:A:496:ALA:O	1:A:497:GLN:C	2.63	0.42
1:A:496:ALA:C	1:A:498:PHE:N	2.78	0.42
2:B:32:GLU:OE2	2:B:301:ARG:HD3	2.20	0.42
2:B:221:HIS:CB	2:B:227:VAL:HG13	2.50	0.42
1:A:568:ARG:HA	1:A:569:PRO:HD3	1.95	0.41
1:A:14:VAL:HG21	1:A:264:PHE:CD2	2.55	0.41
1:A:62:ARG:HA	1:A:63:PRO:HD2	1.77	0.41
1:A:212:LEU:HD12	1:A:249:MET:HE2	2.02	0.41
2:B:145:LYS:HA	2:B:169:GLN:HB2	2.02	0.41
1:A:545:ASN:O	1:A:546:THR:HB	2.21	0.41
2:B:305:TRP:HD1	6:B:403:HOH:O	2.03	0.41
1:A:65:PRO:O	2:B:50:SER:OG	2.38	0.41
1:A:480:LEU:O	1:A:484:VAL:HG23	2.21	0.41
1:A:628:PRO:O	1:A:629:THR:CB	2.69	0.41
1:A:218[B]:ILE:O	1:A:218[B]:ILE:CD1	2.68	0.41
1:A:315:LEU:HD12	1:A:636:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLU:HB3	1:A:217[A]:VAL:HG11	2.02	0.40
1:A:440:PHE:HE1	1:A:471:PHE:O	2.04	0.40
2:B:264:SER:HB2	2:B:266:HIS:HD2	1.86	0.40
1:A:311[B]:PRO:HG3	1:A:501:PRO:HD2	2.02	0.40
2:B:145:LYS:HA	2:B:169:GLN:CB	2.51	0.40
1:A:15:SER:HB3	1:A:263:GLN:HG2	2.02	0.40
1:A:124:LEU:O	1:A:153:MET:HA	2.22	0.40
1:A:216[A]:HIS:CG	1:A:217[A]:VAL:N	2.89	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	635/645 (98%)	589 (93%)	43 (7%)	3 (0%)	24	34
2	B	312/350 (89%)	285 (91%)	23 (7%)	4 (1%)	9	12
All	All	947/995 (95%)	874 (92%)	66 (7%)	7 (1%)	18	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	A	398	VAL
2	B	209	SER
2	B	295	ALA
1	A	627	ASN
2	B	257	CYS
1	A	292	PRO

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	568/570 (100%)	532 (94%)	36 (6%)	16	26
2	B	266/298 (89%)	252 (95%)	14 (5%)	20	33
All	All	834/868 (96%)	784 (94%)	50 (6%)	18	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	52	ARG
1	A	62	ARG
1	A	97	GLU
1	A	136	ARG
1	A	147	HIS
1	A	169	GLU
1	A	176	THR
1	A	182	GLU
1	A	193	ARG
1	A	214	SER
1	A	217[A]	VAL
1	A	217[B]	VAL
1	A	222[A]	LEU
1	A	222[B]	LEU
1	A	231	LEU
1	A	235	ILE
1	A	256	ARG
1	A	288	SER
1	A	302	LYS
1	A	312[A]	LEU
1	A	312[B]	LEU
1	A	358	VAL
1	A	393	LYS
1	A	400	THR
1	A	405	GLN
1	A	421	ARG

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Mol	Chain	Res	Type
1	A	435	GLU
1	A	439	SER
1	A	475	ILE
1	A	497	GLN
1	A	504	VAL
1	A	525	ASN
1	A	536	CYS
1	A	565	LEU
1	A	633	TYR
2	B	17	TRP
2	B	28	GLU
2	B	110	GLU
2	B	111	ASN
2	B	131	VAL
2	B	141	VAL
2	B	162	SER
2	B	180	ASP
2	B	206	ILE
2	B	208	CYS
2	B	247	CYS
2	B	274	LEU
2	B	290	LEU
2	B	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	79	ASN
1	A	175	HIS
1	A	215	ASN
1	A	251	GLN
1	A	263	GLN
1	A	289	GLN
1	A	309	GLN
1	A	508	ASN
1	A	511	GLN
1	A	525	ASN
1	A	545	ASN
2	B	78	GLN
2	B	139	GLN
2	B	169	GLN

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Mol	Chain	Res	Type
2	B	178	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	1.44	5 (17%)	34,42,42	2.05	7 (20%)
5	GOL	A	703	-	5,5,5	0.27	0	5,5,5	0.50	0
5	GOL	A	704	-	5,5,5	0.31	0	5,5,5	0.21	0
4	5QL	A	702	-	33,33,33	1.91	5 (15%)	42,44,44	1.39	5 (11%)

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	703	-	-	4/4/4/4	-
5	GOL	A	704	-	-	4/4/4/4	-
4	5QL	A	702	-	-	3/17/34/34	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	5QL	CAW-CAX	-7.00	1.39	1.51
4	A	702	5QL	CAZ-CAY	-5.04	1.40	1.51
3	A	701	SFG	C5-C4	4.44	1.47	1.39
4	A	702	5QL	CAG-CAE	-4.27	1.40	1.50
3	A	701	SFG	C5-N7	-2.61	1.34	1.39
3	A	701	SFG	C5-C6	2.54	1.48	1.41
4	A	702	5QL	CAI-NAJ	-2.45	1.35	1.39
3	A	701	SFG	C8-N7	2.37	1.36	1.31
4	A	702	5QL	CAT-CAB	2.30	1.58	1.52
3	A	701	SFG	C8-N9	-2.24	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	SFG	C5-C4-N3	-6.42	117.88	126.72
3	A	701	SFG	N3-C4-N9	5.02	135.70	127.17
4	A	702	5QL	CAI-NAJ-CAK	4.23	131.10	122.67
3	A	701	SFG	C2-N3-C4	3.86	121.26	111.83
4	A	702	5QL	CAP-CAK-NAJ	3.73	116.79	110.77
3	A	701	SFG	C4-C5-N7	-3.69	106.37	110.58
3	A	701	SFG	N3-C2-N1	-3.32	123.56	128.58
4	A	702	5QL	CAB-CAC-NAD	-3.21	102.36	111.42
3	A	701	SFG	C5-N7-C8	2.67	107.64	103.45
4	A	702	5QL	CAW-CAV-NAU	-2.57	108.30	111.03
3	A	701	SFG	C4-N9-C8	2.43	108.29	105.74
4	A	702	5QL	CAZ-NAU-CAT	-2.14	107.93	111.26

There are no chirality outliers.

All (14) 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

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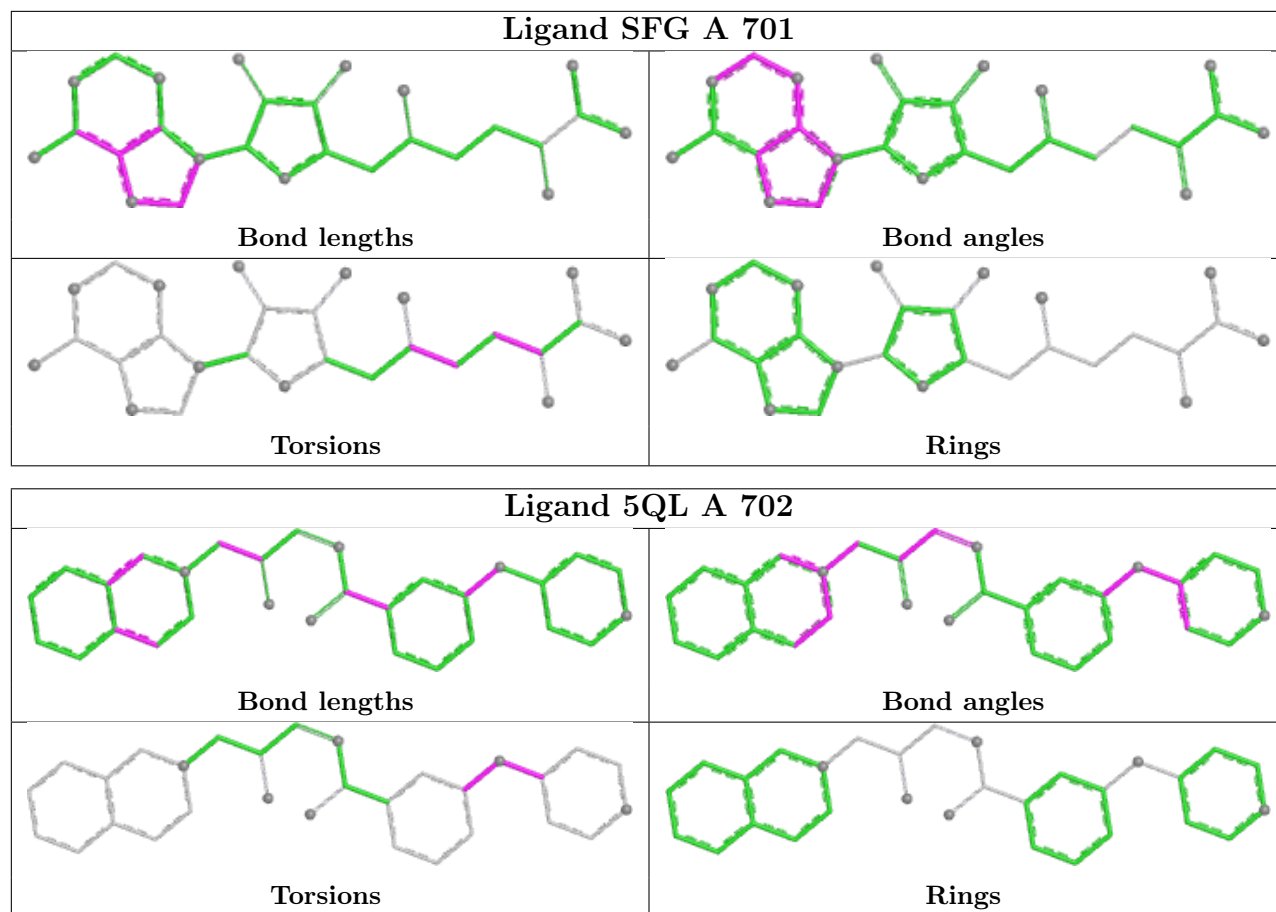
Mol	Chain	Res	Type	Atoms
4	A	702	5QL	CAP-CAK-NAJ-CAI
5	A	703	GOL	C1-C2-C3-O3
5	A	704	GOL	O1-C1-C2-C3
5	A	703	GOL	O1-C1-C2-C3
5	A	704	GOL	C1-C2-C3-O3
5	A	703	GOL	O2-C2-C3-O3
5	A	704	GOL	O1-C1-C2-O2
5	A	703	GOL	O1-C1-C2-O2
4	A	702	5QL	CAQ-CAI-NAJ-CAK
5	A	704	GOL	O2-C2-C3-O3
4	A	702	5QL	CAH-CAI-NAJ-CAK
3	A	701	SFG	N-CA-CB-CG

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

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%)	0.31	34 (5%) 31 31	13, 52, 107, 141	12 (1%)
2	B	313/350 (89%)	0.72	21 (6%) 24 22	38, 67, 119, 149	1 (0%)
All	All	938/995 (94%)	0.45	55 (5%) 28 27	13, 59, 111, 149	13 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312[A]	LEU	6.9
2	B	225	SER	5.6
1	A	311[A]	PRO	5.4
2	B	21	PRO	5.4
1	A	179	TYR	4.9
1	A	294	PRO	4.8
2	B	19	LEU	4.6
1	A	243	PHE	3.9
1	A	299	LEU	3.9
1	A	176	THR	3.6
2	B	206	ILE	3.5
2	B	268	VAL	3.5
2	B	328	PRO	3.4
1	A	296	ALA	3.3
2	B	17	TRP	3.3
1	A	217[A]	VAL	3.2
1	A	297	TYR	3.2
1	A	277	PHE	3.1
1	A	300	PHE	3.1
1	A	529	MET	3.1
1	A	431	ILE	3.1
2	B	246	SER	3.1
1	A	301	ALA	3.0
2	B	248	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	544	VAL	2.9
1	A	175	HIS	2.9
1	A	361	LEU	2.8
1	A	242	GLY	2.8
2	B	249	LEU	2.8
2	B	245	THR	2.8
1	A	293	PRO	2.7
1	A	528	PRO	2.7
2	B	247	CYS	2.7
2	B	25	ALA	2.6
1	A	292	PRO	2.6
1	A	216[A]	HIS	2.6
2	B	312	LEU	2.5
2	B	23	ALA	2.5
2	B	211	PRO	2.5
2	B	22	ASN	2.5
1	A	214	SER	2.4
1	A	218[A]	ILE	2.3
2	B	208	CYS	2.3
1	A	404	TRP	2.3
1	A	181	GLY	2.2
1	A	303	GLY	2.2
2	B	72	PHE	2.2
1	A	180	SER	2.2
1	A	146	HIS	2.1
1	A	14	VAL	2.1
1	A	147	HIS	2.1
1	A	633	TYR	2.1
2	B	24	PRO	2.0
2	B	218	LEU	2.0
1	A	213	PRO	2.0

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 [i](#)

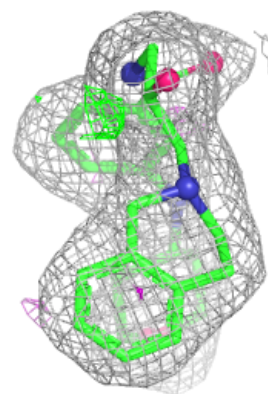
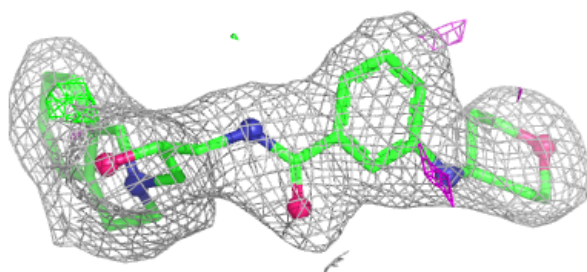
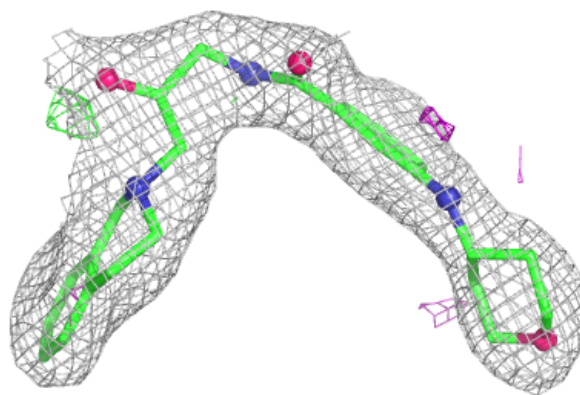
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.80	0.13	63,70,71,73	0
5	GOL	A	703	6/6	0.90	0.13	67,70,75,78	0
4	5QL	A	702	30/30	0.95	0.08	32,41,59,60	0
3	SFG	A	701	27/27	0.96	0.07	40,43,49,53	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.

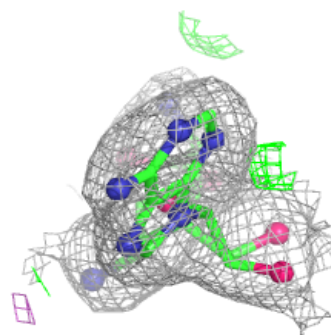
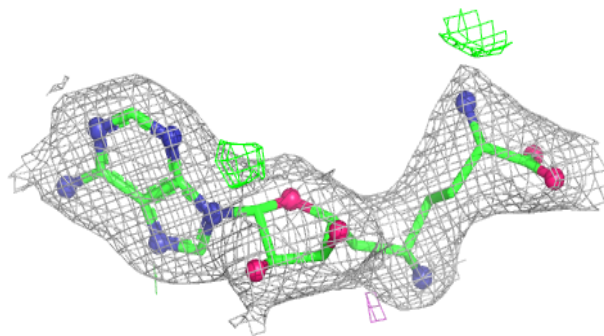
Electron density around 5QL A 702:

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.