Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 07:07 PM EDT

PDB ID	:	5EMK
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 (i) 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 (i)) were used in the production of this report:

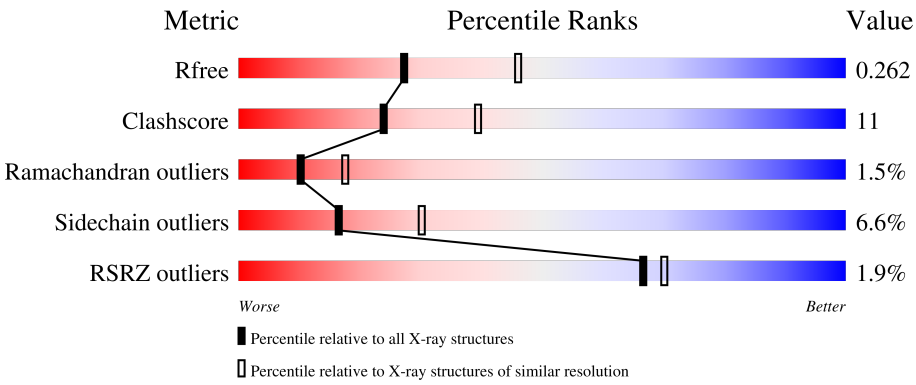
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (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 <=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	% 76% 18% • •
2	B	350	4% 62% 24% • 11%

2 Entry composition (i)

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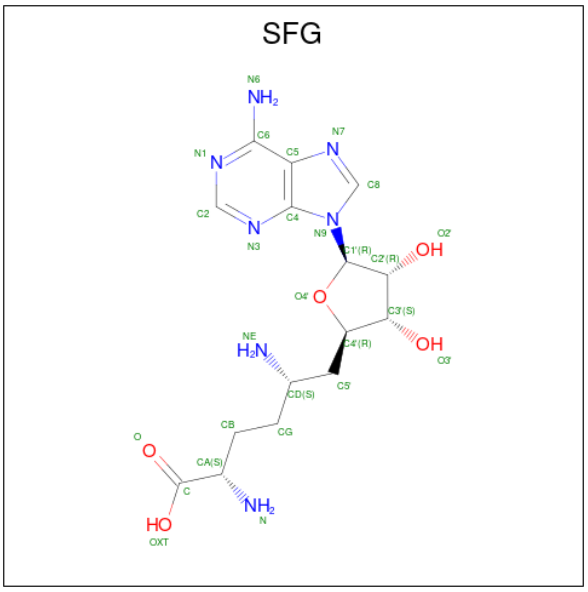
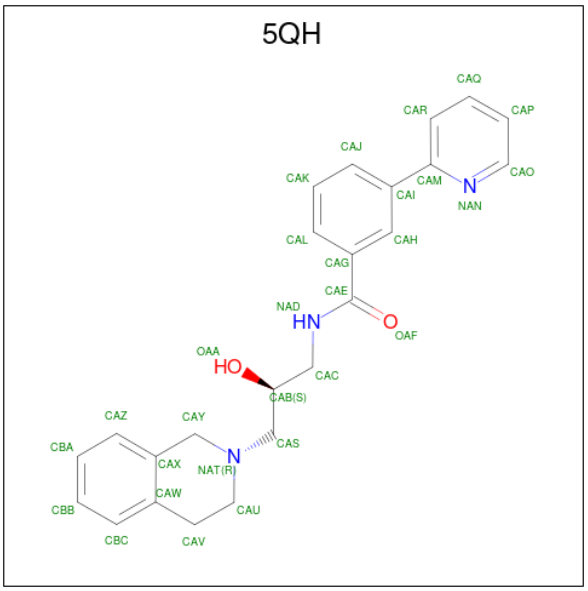
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$).



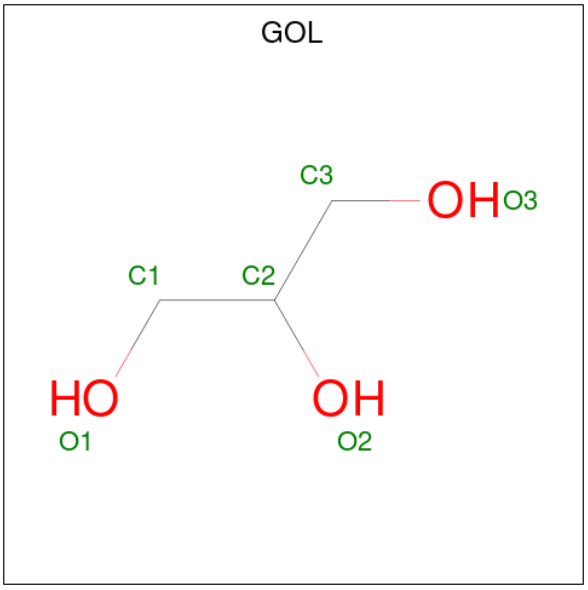
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	15	7	5	0	0

- Molecule 4 is {N}-[(2 {S})-3-(3,4-dihydro-1 {H}-isoquinolin-2-yl)-2-oxidanyl-propyl]-3-pyridin-2-yl-benzamide (three-letter code: 5QH) (formula: $C_{24}H_{25}N_3O_2$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

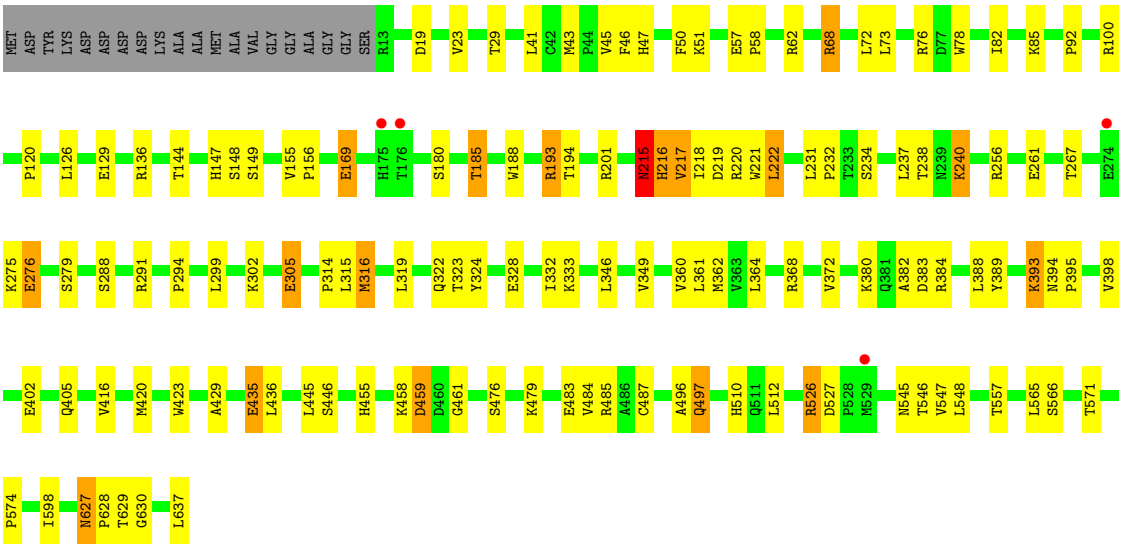
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	65	65	65	0	0
			Total	O		
6	B	13	13	13	0	0

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.

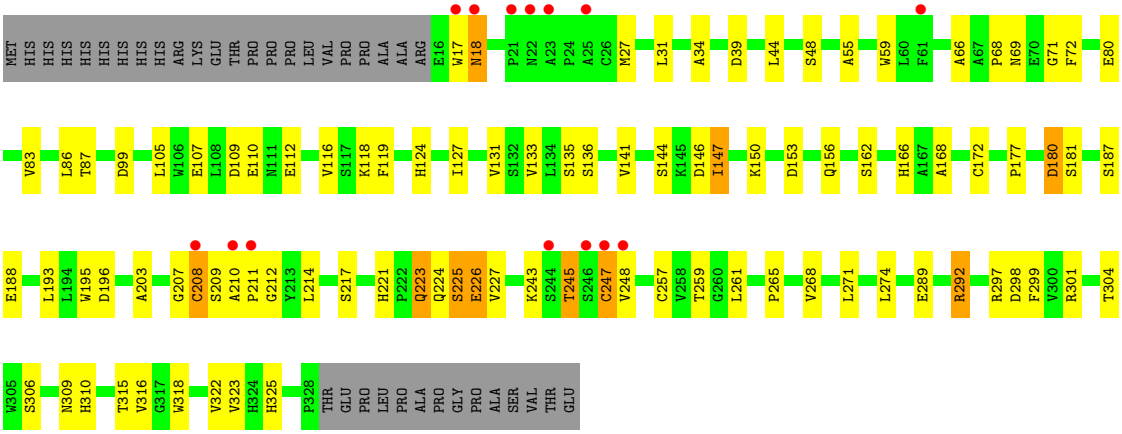
• Molecule 1: Protein arginine N-methyltransferase 5

Chain A:



• Molecule 2: Methylosome protein 50

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.31 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, SFG, 5QH

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	0.53	0/5292	0.72	0/7200
2	B	0.48	0/2438	0.71	0/3333
All	All	0.52	0/7730	0.72	0/10533

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.

There are no bond angle outliers.

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 (i)

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	116	1
2	B	2376	0	2278	51	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	166	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 11.

All (166) 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
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: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:HD12	1:A:218[B]:ILE:C	2.04	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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[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
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:218[A]:ILE:O	1:A:219[A]:ASP:C	2.41	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:217[A]:VAL:HG23	1:A:217[A]:VAL:O	2.06	0.55
1:A:217[A]:VAL:O	1:A:217[A]:VAL:CG2	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:294:PRO:HB2	1:A:299:LEU:HG	1.92	0.51
1:A:215:ASN:C	1:A:217[B]:VAL:H	2.13	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:221[B]:TRP:C	1:A:222[B]:LEU:HD12	2.29	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: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
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
1:A:193:ARG:HD2	1:A:193:ARG:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:496:ALA:O	1:A:497:GLN:C	2.55	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
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
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:224:GLN:C	2:B:226:GLU:H	2.21	0.43
2:B:208:CYS:HB2	2:B:247:CYS:HB3	1.82	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: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:27:MET:HE3	2:B:31:LEU:HD21	2.01	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
2:B:299:PHE:CD2	2:B:318:TRP:CZ3	3.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:445:LEU:HD12	1:A:637:LEU:HD23	2.02	0.41
2:B:27:MET:HE1	2:B:68:PRO:HB2	2.03	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:218[B]:ILE:CD1	1:A:218[B]:ILE:C	2.68	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
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: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%)	12 20
2	B	313/350 (89%)	290 (93%)	16 (5%)	7 (2%)	6 10
All	All	946/995 (95%)	871 (92%)	60 (6%)	15 (2%)	10 16

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
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 (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	567/570 (100%)	532 (94%)	35 (6%)	18 33
2	B	267/298 (90%)	246 (92%)	21 (8%)	12 22
All	All	834/868 (96%)	778 (93%)	56 (7%)	16 29

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	68	ARG
1	A	76	ARG
1	A	136	ARG
1	A	144	THR
1	A	147	HIS
1	A	148	SER
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	180	SER
1	A	185	THR
1	A	193	ARG
1	A	215	ASN
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	237	LEU
1	A	238	THR
1	A	240	LYS
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	380	LYS
1	A	393	LYS
1	A	405	GLN
1	A	435	GLU
1	A	459	ASP
1	A	485	ARG
1	A	497	GLN
1	A	526	ARG
1	A	527	ASP
2	B	18	ASN
2	B	39	ASP
2	B	80	GLU
2	B	83	VAL
2	B	86	LEU
2	B	110	GLU
2	B	116	VAL
2	B	131	VAL
2	B	141	VAL
2	B	162	SER
2	B	180	ASP
2	B	209	SER
2	B	223	GLN
2	B	225	SER
2	B	226	GLU

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Mol	Chain	Res	Type
2	B	245	THR
2	B	248	VAL
2	B	257	CYS
2	B	268	VAL
2	B	274	LEU
2	B	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	511	GLN
1	A	545	ASN
2	B	223	GLN
2	B	254	HIS
2	B	310	HIS
2	B	325	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	5QH	A	702	-	32,32,32	2.08	6 (18%)	42,43,43	1.34	6 (14%)
5	GOL	A	704	-	5,5,5	0.45	0	5,5,5	0.27	0
5	GOL	A	703	-	5,5,5	0.25	0	5,5,5	0.41	0
3	SFG	A	701	-	25,29,29	1.20	3 (12%)	23,42,42	1.28	3 (13%)

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	5QH	A	702	-	-	0/17/26/26	0/4/4/4
5	GOL	A	704	-	-	2/4/4/4	-
5	GOL	A	703	-	-	2/4/4/4	-
3	SFG	A	701	-	-	2/13/33/33	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	5QH	CAI-CAM	-5.90	1.39	1.48
4	A	702	5QH	CAV-CAW	-5.81	1.41	1.51
4	A	702	5QH	CAY-CAX	-4.97	1.40	1.51
4	A	702	5QH	CAG-CAE	-4.29	1.41	1.50
4	A	702	5QH	CAO-NAN	3.19	1.41	1.34
3	A	701	SFG	C5-C4	2.99	1.48	1.40
4	A	702	5QH	CAU-CAV	-2.22	1.47	1.51
3	A	701	SFG	C2-N3	2.19	1.35	1.32
3	A	701	SFG	C2'-C1'	-2.10	1.50	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	702	5QH	CAY-NAT-CAU	4.38	115.50	109.91
3	A	701	SFG	O4'-C1'-C2'	-3.44	101.91	106.93
4	A	702	5QH	CAB-CAC-NAD	-3.36	101.49	111.37
4	A	702	5QH	CAP-CAO-NAN	-2.99	118.54	123.43
3	A	701	SFG	N3-C2-N1	-2.62	124.59	128.68
4	A	702	5QH	CAO-NAN-CAM	2.27	120.41	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	702	5QH	CAJ-CAI-CAM	-2.19	117.83	121.28
3	A	701	SFG	C4-C5-N7	-2.13	107.18	109.40
4	A	702	5QH	CAB-CAS-NAT	-2.03	108.54	112.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

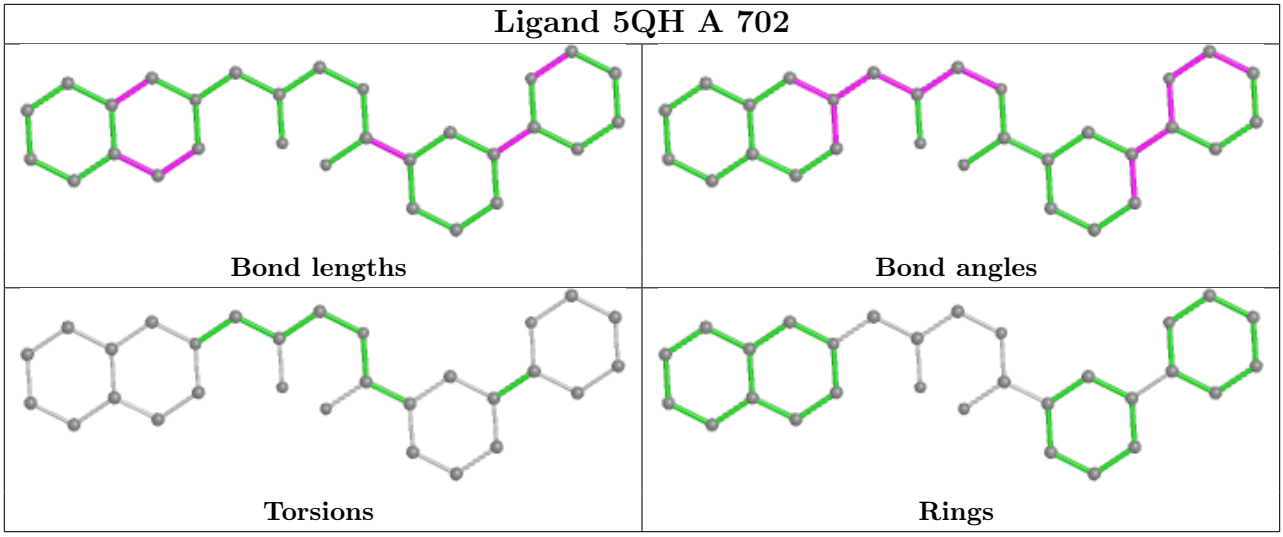
Mol	Chain	Res	Type	Atoms
3	A	701	SFG	NE-CD-CG-CB
3	A	701	SFG	C5'-CD-CG-CB
5	A	704	GOL	O1-C1-C2-C3
5	A	704	GOL	O1-C1-C2-O2
5	A	703	GOL	O1-C1-C2-C3
5	A	703	GOL	O1-C1-C2-O2

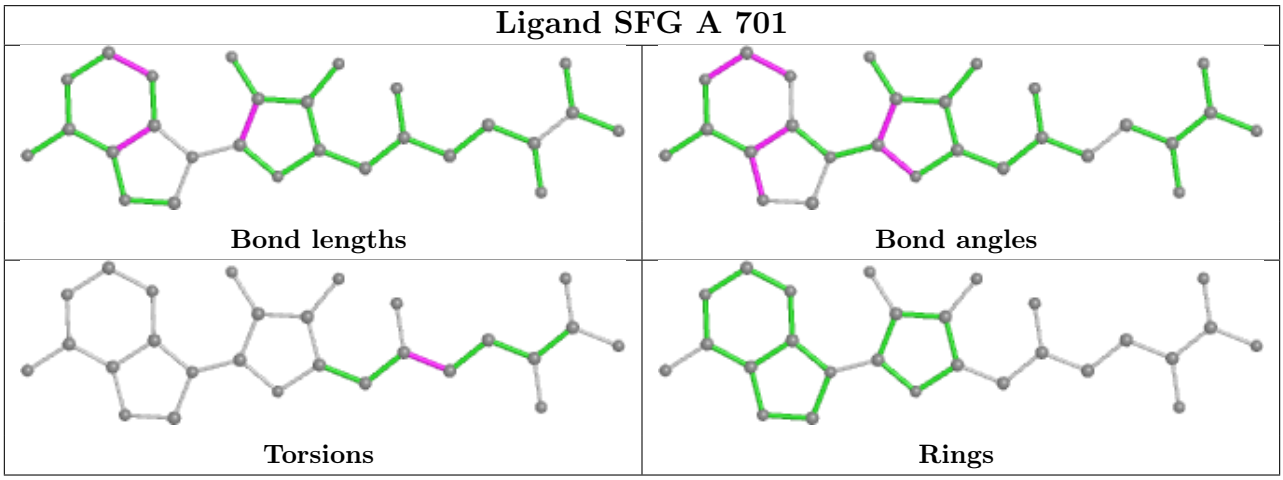
There are no ring outliers.

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 then 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%)	-0.07	4 (0%)	89	90	24, 55, 93, 145	0
2	B	313/350 (89%)	0.07	14 (4%)	33	36	47, 69, 121, 167	0
All	All	938/995 (94%)	-0.02	18 (1%)	66	70	24, 61, 104, 167	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	208	CYS	7.6
2	B	17	TRP	6.1
2	B	248	VAL	4.7
2	B	247	CYS	4.6
1	A	176	THR	4.4
2	B	18	ASN	3.9
2	B	210	ALA	3.7
2	B	246	SER	3.0
1	A	175	HIS	2.9
2	B	25	ALA	2.6
2	B	23	ALA	2.6
2	B	22	ASN	2.4
2	B	21	PRO	2.4
2	B	61	PHE	2.2
2	B	211	PRO	2.2
2	B	244	SER	2.1
1	A	274	GLU	2.1
1	A	529	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

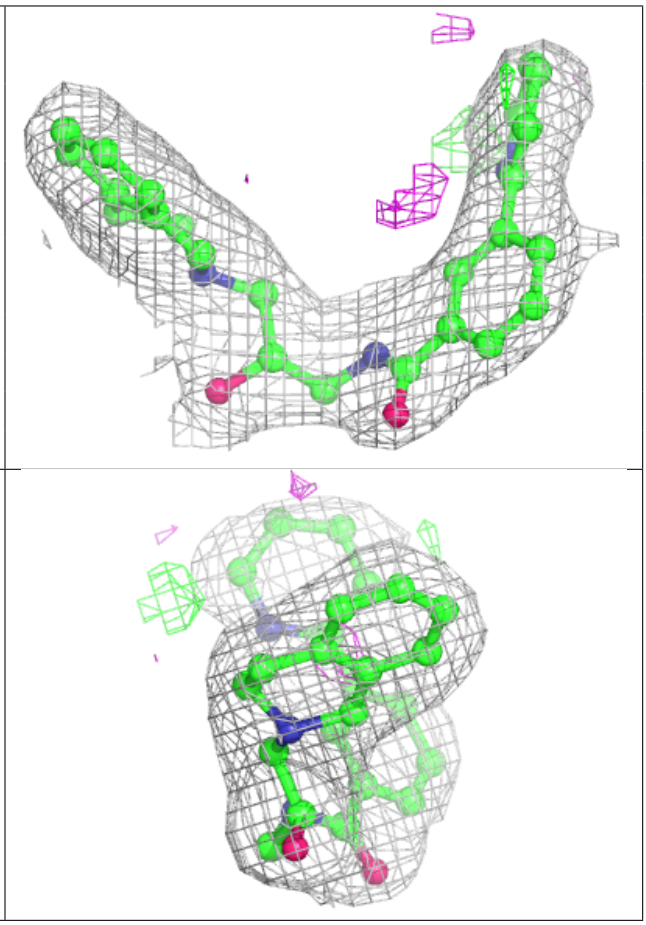
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	703	6/6	0.90	0.17	67,67,72,77	0
5	GOL	A	704	6/6	0.91	0.17	58,65,67,68	0
4	5QH	A	702	29/29	0.97	0.14	39,50,75,79	0
3	SFG	A	701	27/27	0.98	0.14	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.

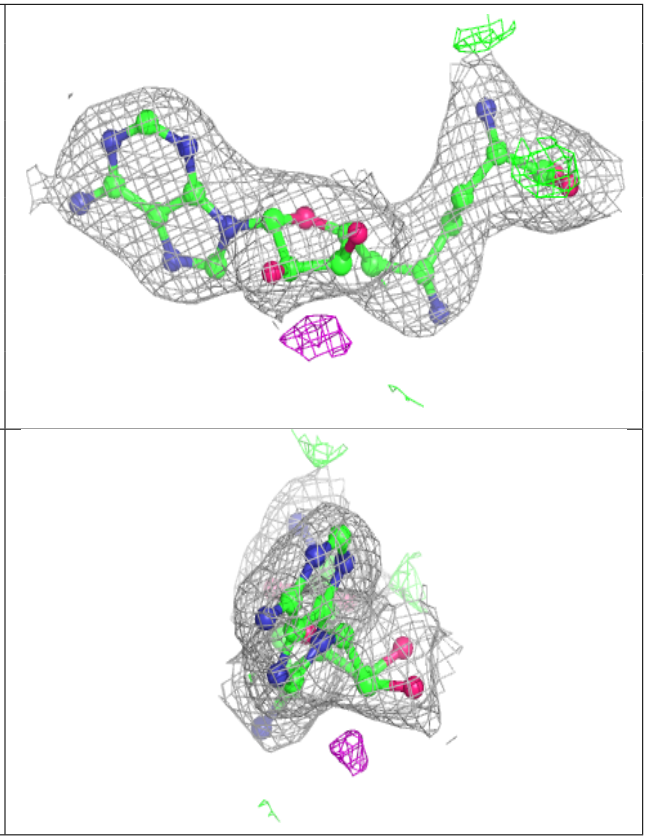
Electron density around 5QH A 702:

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.