Worldwide PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 01:20 am BST

PDB ID	:	4X60
Title	:	Crystal structure of PRMT5:MEP50 with EPZ015666 and sinefungin
Authors	:	Boriack-Sjodin, P.A.
Deposited on	:	2014-12-06
Resolution	:	2.35 Å(reported)

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	:	2.11
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)	:	2.11

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 2.35 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.
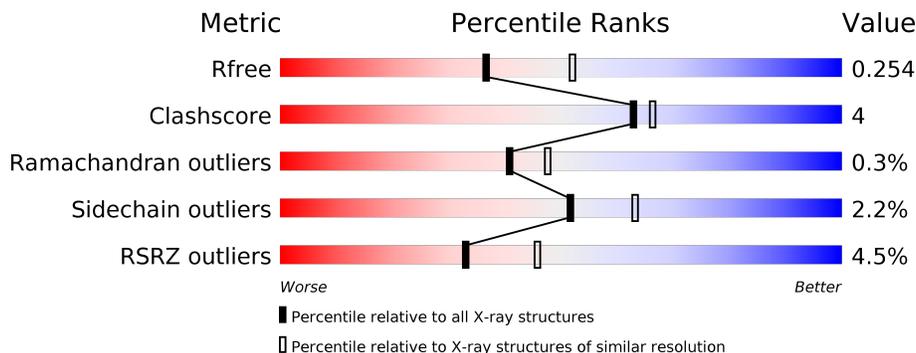
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	4% / 86% / 11% / •
2	B	350	5% / 75% / 13% / 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7623 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
1	A	625	Total 5070	C 3244	N 870	O 931	S 25	0	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	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
2	B	310	Total 2342	C 1470	N 400	O 457	S 15	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	expression tag	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

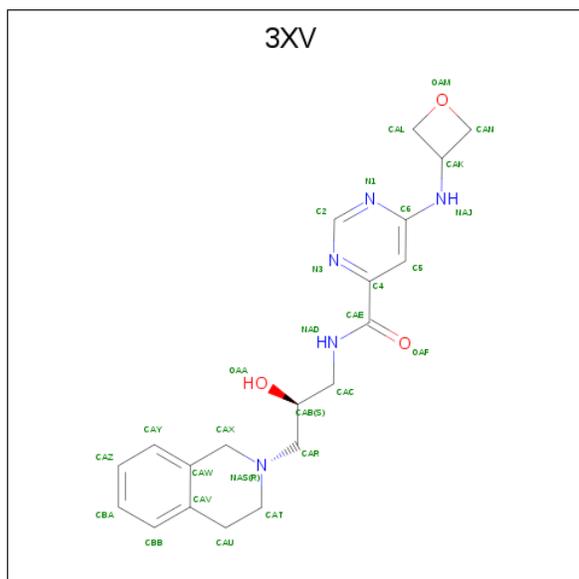*Continued on next page...*

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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: $C_{15}H_{23}N_7O_5$).
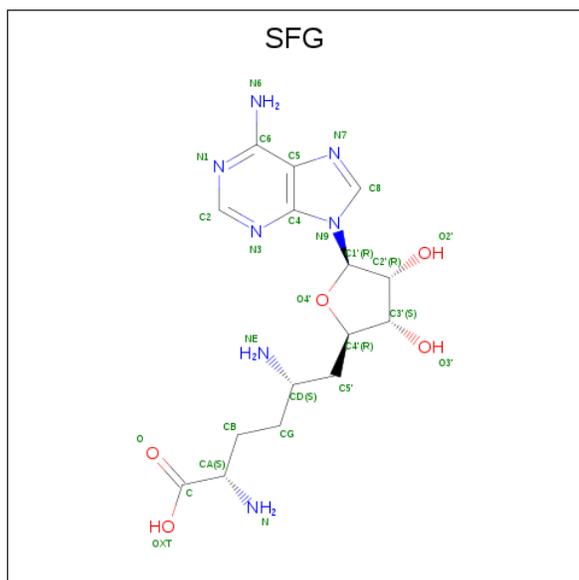
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	15	7	5	0	0

- Molecule 4 is N-[(2S)-3-(3,4-dihydroisoquinolin-2(1H)-yl)-2-hydroxypropyl]-6-(oxetan-3-ylamino)pyrimidine-4-carboxamide (three-letter code: 3XV) (formula: $C_{20}H_{25}N_5O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 28	C 20	N 5	O 3	0	0

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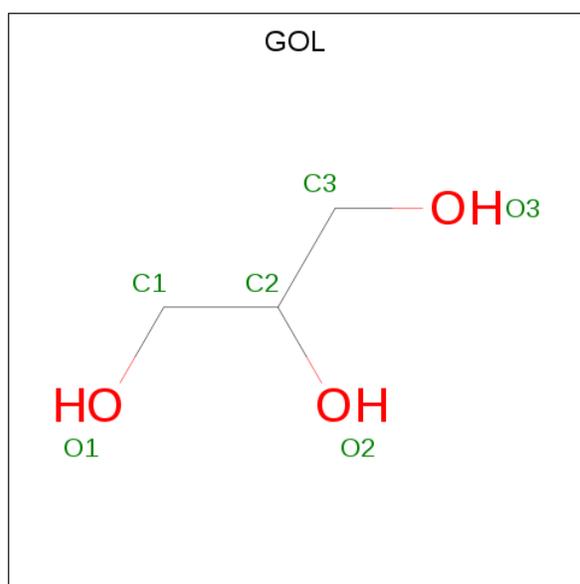
GOL

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total 111	O 111	0	0
6	B	27	Total 27	O 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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
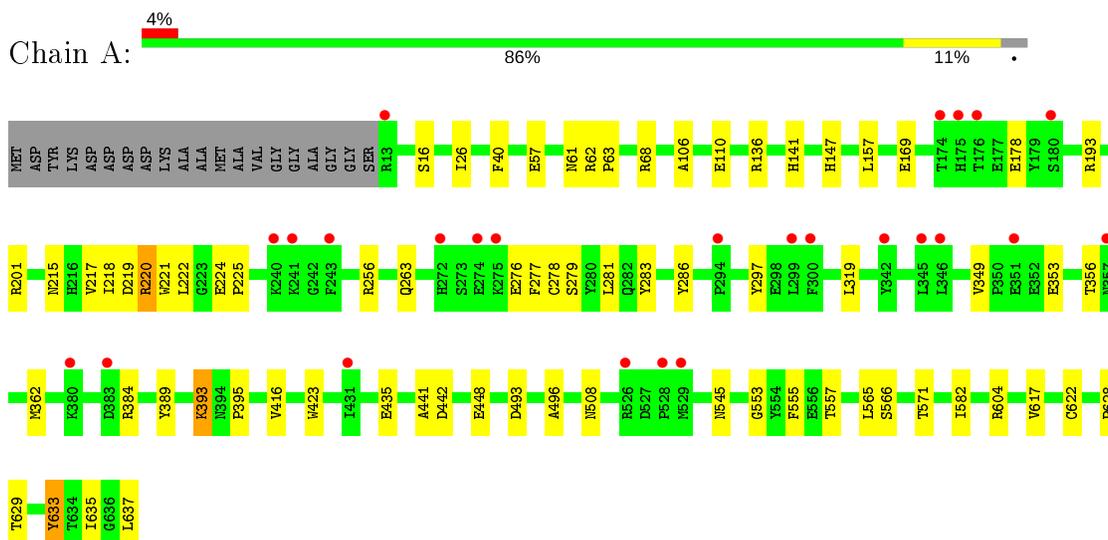
- Molecule 2: Methylosome protein 50
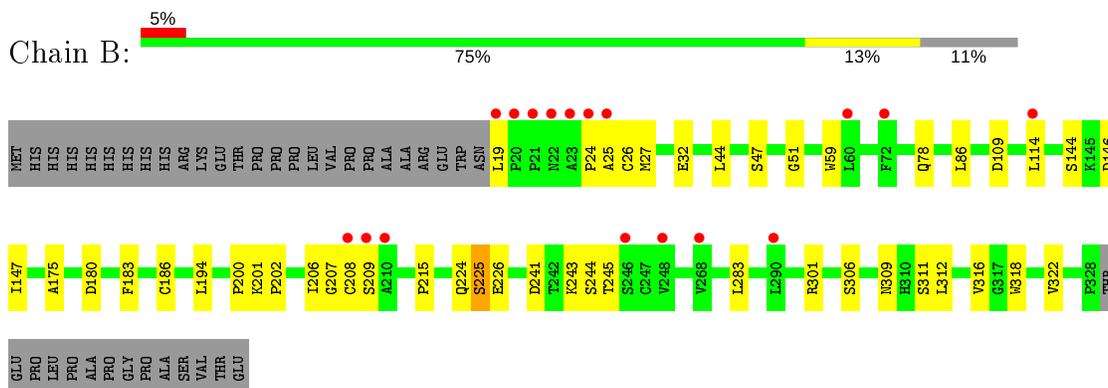
4   Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	103.67Å 137.96Å 179.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.75 – 2.35 44.75 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.9 (44.75-2.35) 95.0 (44.75-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.202 , 0.254 0.203 , 0.254	Depositor DCC
R_{free} test set	2569 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	56.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.4	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	7623	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 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, 3XV, 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	0.43	0/5215	0.59	0/7095
2	B	0.46	1/2402 (0.0%)	0.63	1/3283 (0.0%)
All	All	0.44	1/7617 (0.0%)	0.60	1/10378 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	209	SER	CB-OG	7.72	1.52	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	209	SER	CA-CB-OG	-6.84	92.74	111.20

There are no chirality outliers.

There are no planarity outliers.

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	5070	0	4962	39	0
2	B	2342	0	2263	27	0
3	A	27	0	22	0	0
4	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	24	3	0
6	A	111	0	0	0	0
6	B	27	0	0	2	0
All	All	7623	0	7296	64	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 4.

All (64) 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:194:LEU:HB2	2:B:206:ILE:HD11	1.16	1.10
2:B:194:LEU:CB	2:B:206:ILE:HD11	2.06	0.82
2:B:206:ILE:HG22	2:B:207:GLY:N	1.99	0.77
1:A:217:VAL:O	1:A:220:ARG:HG3	1.85	0.76
2:B:194:LEU:HB2	2:B:206:ILE:CD1	2.08	0.72
1:A:218:ILE:HG22	1:A:256:ARG:HH21	1.55	0.70
1:A:26:ILE:HG22	6:B:403:HOH:O	2.02	0.60
1:A:217:VAL:O	1:A:220:ARG:CG	2.51	0.58
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.88	0.56
2:B:206:ILE:CG2	2:B:207:GLY:N	2.68	0.54
1:A:628:PRO:O	1:A:629:THR:HB	2.09	0.53
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.23	0.52
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.09	0.52
2:B:24:PRO:HG3	2:B:78:GLN:HG2	1.92	0.52
2:B:207:GLY:O	2:B:208:CYS:C	2.48	0.52
1:A:220:ARG:HG3	1:A:221:TRP:H	1.75	0.50
2:B:224:GLN:O	2:B:226:GLU:N	2.45	0.50
1:A:553:GLY:HA3	1:A:582:ILE:HG22	1.94	0.49
2:B:47:SER:HB2	6:B:419:HOH:O	2.12	0.49
1:A:557:THR:HG22	1:A:565:LEU:HB2	1.95	0.49
1:A:283:TYR:O	1:A:286:TYR:HB3	2.13	0.48
2:B:27:MET:HG3	2:B:59:TRP:NE1	2.29	0.48
1:A:16:SER:OG	1:A:281:LEU:HD11	2.14	0.48
2:B:316:VAL:HG12	2:B:322:VAL:HG22	1.97	0.47
2:B:19:LEU:HD11	2:B:25:ALA:HA	1.96	0.47
1:A:393:LYS:O	1:A:395:PRO:HD3	2.14	0.47
1:A:629:THR:O	1:A:629:THR:CG2	2.63	0.47
2:B:224:GLN:C	2:B:226:GLU:H	2.18	0.47
2:B:109:ASP:HB2	2:B:114:LEU:H	1.80	0.47
1:A:220:ARG:HH22	1:A:545:ASN:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HB3	2:B:51:GLY:O	2.15	0.46
2:B:241:ASP:OD1	2:B:243:LYS:HG2	2.16	0.46
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.96	0.46
1:A:297:TYR:CG	5:A:705:GOL:H11	2.50	0.46
1:A:633:TYR:OH	1:A:635:ILE:HD11	2.15	0.46
1:A:263:GLN:HE22	5:A:703:GOL:H31	1.81	0.46
2:B:32:GLU:OE2	2:B:301:ARG:HD3	2.16	0.46
2:B:200:PRO:O	2:B:202:PRO:HD3	2.16	0.46
1:A:141:HIS:NE2	1:A:147:HIS:HE1	2.15	0.45
2:B:44:LEU:HB2	2:B:59:TRP:HB2	1.99	0.45
1:A:40:PHE:CD1	5:A:703:GOL:H32	2.51	0.45
1:A:169:GLU:HA	2:B:201:LYS:HD3	1.98	0.45
1:A:617:VAL:O	1:A:622:CYS:HA	2.17	0.44
1:A:441:ALA:HB2	1:A:555:PHE:HB2	2.00	0.44
1:A:353:GLU:HA	1:A:356:THR:HG22	2.00	0.43
1:A:349:VAL:HG23	1:A:384:ARG:HE	1.84	0.43
1:A:448:GLU:HG2	1:A:637:LEU:HD21	2.02	0.42
2:B:175:ALA:HA	2:B:183:PHE:HB3	2.00	0.42
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.94	0.42
1:A:416:VAL:HG21	1:A:423:TRP:CZ2	2.55	0.42
2:B:306:SER:HB3	2:B:309:ASN:O	2.20	0.41
1:A:222:LEU:O	1:A:508:ASN:ND2	2.52	0.41
2:B:241:ASP:HB3	2:B:244:SER:HB3	2.02	0.41
1:A:147:HIS:CE1	1:A:201:ARG:HH22	2.38	0.41
1:A:277:PHE:C	1:A:279:SER:H	2.23	0.41
1:A:442:ASP:OD2	1:A:604:ARG:NE	2.52	0.41
1:A:493:ASP:HB3	1:A:496:ALA:HB2	2.01	0.41
1:A:106:ALA:O	1:A:110:GLU:HG3	2.21	0.41
1:A:276:GLU:HG3	1:A:277:PHE:N	2.35	0.40
2:B:186:CYS:HB2	2:B:215:PRO:HG2	2.03	0.40
2:B:301:ARG:HD2	2:B:318:TRP:CE2	2.57	0.40
1:A:566:SER:HB3	1:A:571:THR:O	2.21	0.40
1:A:57:GLU:HG2	1:A:61:ASN:ND2	2.35	0.40
1:A:62:ARG:HA	1:A:63:PRO:HD2	1.99	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	625/645 (97%)	591 (95%)	33 (5%)	1 (0%)	47	56
2	B	309/350 (88%)	293 (95%)	14 (4%)	2 (1%)	25	27
All	All	934/995 (94%)	884 (95%)	47 (5%)	3 (0%)	41	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
2	B	225	SER
1	A	278	CYS

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	559/570 (98%)	549 (98%)	10 (2%)	59	70
2	B	264/298 (89%)	256 (97%)	8 (3%)	41	50
All	All	823/868 (95%)	805 (98%)	18 (2%)	52	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ARG
1	A	178	GLU
1	A	193	ARG

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Mol	Chain	Res	Type
1	A	215	ASN
1	A	219	ASP
1	A	220	ARG
1	A	319	LEU
1	A	393	LYS
1	A	435	GLU
1	A	633	TYR
2	B	26	CYS
2	B	86	LEU
2	B	180	ASP
2	B	225	SER
2	B	245	THR
2	B	283	LEU
2	B	311	SER
2	B	312	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	61	ASN
1	A	147	HIS
1	A	215	ASN
1	A	263	GLN
1	A	508	ASN
2	B	169	GLN
2	B	310	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	#$|Z| > 2$
5	GOL	A	705	-	5,5,5	0.28	0	5,5,5	0.25	0
5	GOL	A	703	-	5,5,5	0.32	0	5,5,5	0.63	0
5	GOL	A	704	-	5,5,5	0.30	0	5,5,5	0.28	0
3	SFG	A	701	-	22,29,29	1.03	2 (9%)	18,42,42	1.41	3 (16%)
4	3XV	A	702	-	29,31,31	1.93	5 (17%)	34,42,42	2.22	5 (14%)

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
5	GOL	A	705	-	-	2/4/4/4	-
5	GOL	A	703	-	-	2/4/4/4	-
5	GOL	A	704	-	-	0/4/4/4	-
3	SFG	A	701	-	-	3/9/33/33	0/3/3/3
4	3XV	A	702	-	-	4/17/32/32	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	3XV	CAU-CAV	-5.98	1.40	1.51
4	A	702	3XV	CAX-CAW	-4.84	1.40	1.51
4	A	702	3XV	C4-CAE	-3.96	1.41	1.50
4	A	702	3XV	C2-N1	3.45	1.40	1.33
4	A	702	3XV	C2-N3	3.18	1.39	1.33
3	A	701	SFG	C5-C4	2.21	1.46	1.40
3	A	701	SFG	C2-N3	2.16	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	702	3XV	C2-N3-C4	9.71	120.95	115.74
4	A	702	3XV	N1-C2-N3	-6.32	118.71	128.60
3	A	701	SFG	N3-C2-N1	-3.38	123.39	128.68
3	A	701	SFG	C4-C5-N7	-2.43	106.86	109.40
3	A	701	SFG	O4'-C1'-C2'	-2.39	103.44	106.93
4	A	702	3XV	C5-C4-N3	-2.33	120.25	123.19
4	A	702	3XV	CAX-NAS-CAT	2.31	112.86	109.91
4	A	702	3XV	C5-C6-N1	-2.06	119.88	122.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	GOL	C1-C2-C3-O3
5	A	703	GOL	C1-C2-C3-O3
3	A	701	SFG	NE-CD-CG-CB
3	A	701	SFG	C5'-CD-CG-CB
4	A	702	3XV	C5-C4-CAE-NAD
4	A	702	3XV	N3-C4-CAE-NAD
4	A	702	3XV	C5-C4-CAE-OAF
4	A	702	3XV	N3-C4-CAE-OAF
5	A	705	GOL	O2-C2-C3-O3
5	A	703	GOL	O2-C2-C3-O3
3	A	701	SFG	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	GOL	1	0
5	A	703	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Ligand SFG A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand 3XV A 702

Bond lengths

Bond angles

Torsions

Rings
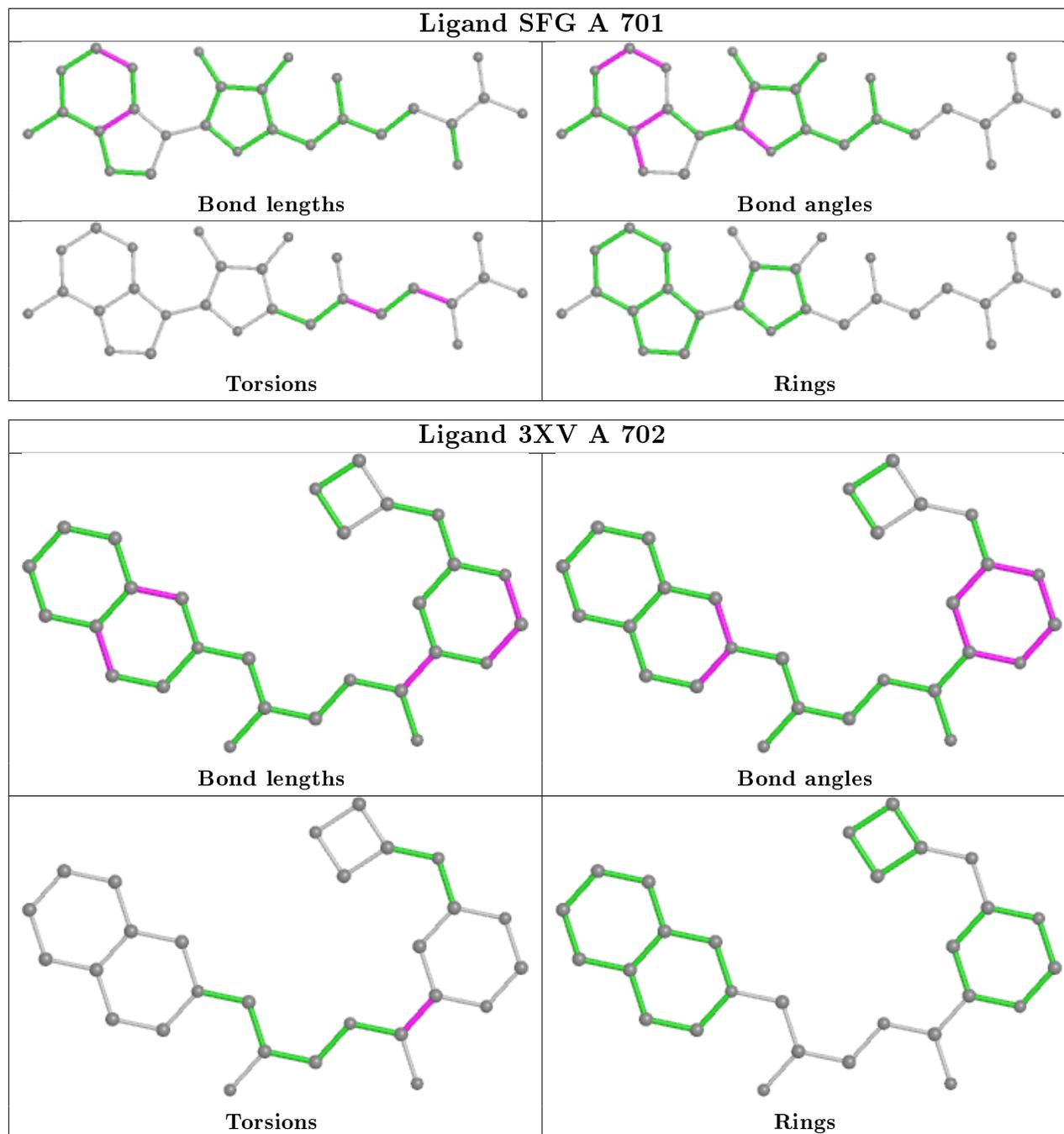
5.7 Other polymers (i)

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%)	0.09	25 (4%)	38	51	36, 53, 96, 142	0
2	B	310/350 (88%)	0.32	17 (5%)	25	36	48, 67, 114, 152	0
All	All	935/995 (93%)	0.16	42 (4%)	33	46	36, 59, 100, 152	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	21	PRO	7.4
1	A	176	THR	6.8
2	B	208	CYS	5.5
2	B	19	LEU	5.0
2	B	22	ASN	4.9
2	B	210	ALA	4.9
2	B	25	ALA	4.4
1	A	174	THR	4.3
2	B	23	ALA	4.1
2	B	20	PRO	4.1
1	A	175	HIS	4.0
1	A	529	MET	3.7
2	B	248	VAL	3.7
1	A	243	PHE	3.7
2	B	246	SER	3.4
1	A	528	PRO	3.4
1	A	240	LYS	3.4
1	A	345	LEU	3.3
1	A	13	ARG	3.2
1	A	294	PRO	3.2
1	A	380	LYS	3.1
1	A	274	GLU	3.1
1	A	180	SER	2.9
1	A	299	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	268	VAL	2.9
2	B	290	LEU	2.9
1	A	342	TYR	2.9
2	B	24	PRO	2.8
1	A	275	LYS	2.7
1	A	383	ASP	2.6
2	B	60	LEU	2.6
2	B	209	SER	2.5
2	B	72	PHE	2.5
1	A	300	PHE	2.4
1	A	241	LYS	2.3
1	A	346	LEU	2.3
1	A	357	ASN	2.3
1	A	351	GLU	2.2
1	A	431	ILE	2.1
2	B	114	LEU	2.1
1	A	272	HIS	2.1
1	A	526	ARG	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.
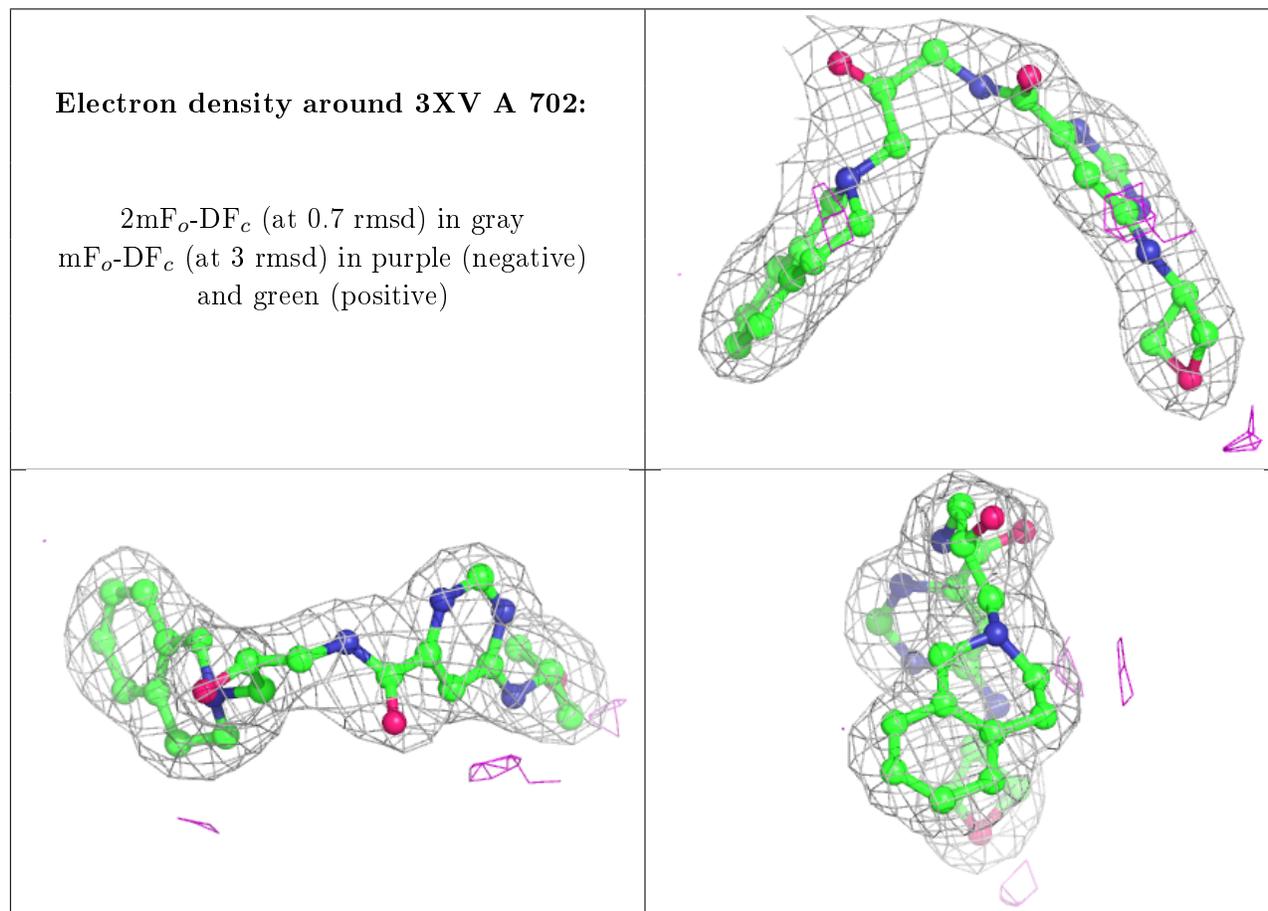
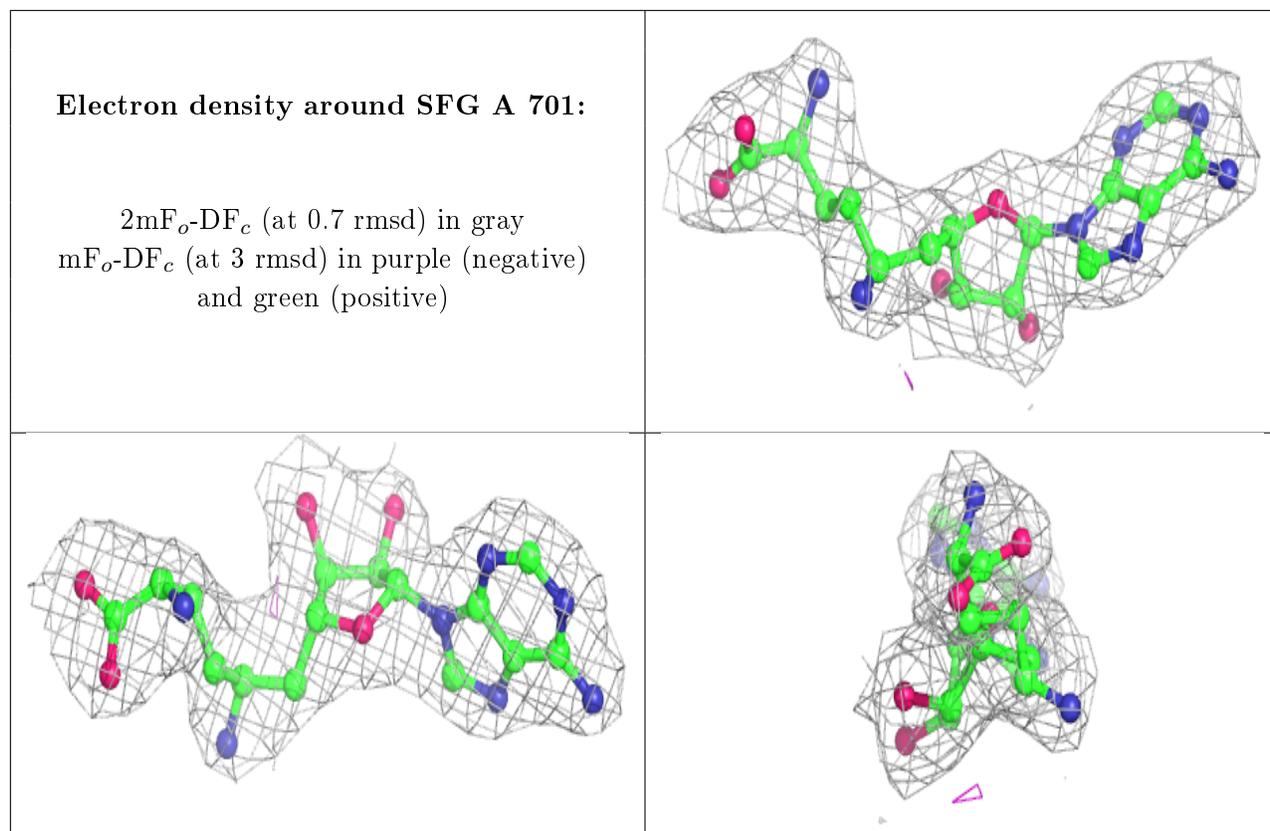## 6.3 Carbohydrates (i)

There are no carbohydrates 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	705	6/6	0.89	0.15	75,77,81,82	0
5	GOL	A	703	6/6	0.89	0.12	66,71,74,76	0
5	GOL	A	704	6/6	0.91	0.19	71,75,83,90	0
4	3XV	A	702	28/28	0.97	0.12	40,45,51,53	0
3	SFG	A	701	27/27	0.98	0.13	36,42,47,51	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 3XV 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:

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

6.5 Other polymers (i)

There are no such residues in this entry.