



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 10:19 am BST

PDB ID : 8BB0
Title : The surface-exposed lipo-protein of BtuG2 in complex with hydroxycobalamin.
Authors : Whittaker, J.; Felices Martinez, J.M.; Guskov, A.; Slotboom, D.J.
Deposited on : 2022-10-12
Resolution : 1.50 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

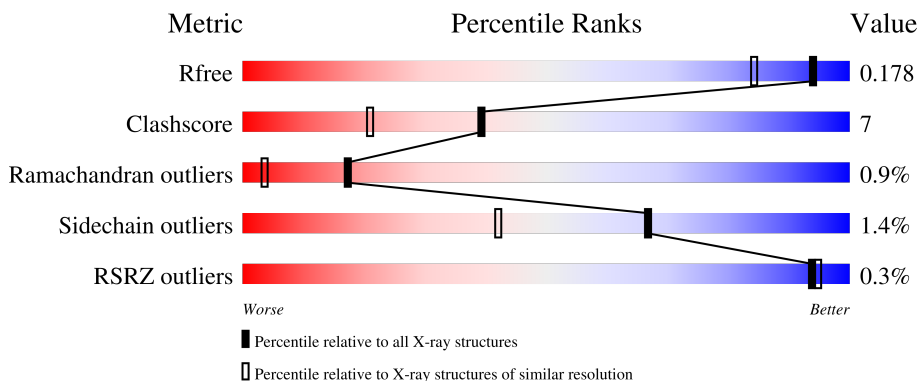
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	327	 % 86% 11% ..
1	B	327	 87% 10% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SCN	A	413	-	-	X	-
5	ACT	A	424	-	X	X	X
5	ACT	B	417	-	-	X	-
6	I2A	A	426	X	-	-	-
6	I2A	B	418	X	-	-	-

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 6137 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 Surface layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	Total 2643	C 1711	N 417	O 504	S 11	0	4	0
1	B	321	Total 2626	C 1696	N 418	O 501	S 11	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8A6D0
A	322	LEU	-	expression tag	UNP Q8A6D0
A	323	GLU	-	expression tag	UNP Q8A6D0
A	324	VAL	-	expression tag	UNP Q8A6D0
A	325	LEU	-	expression tag	UNP Q8A6D0
A	326	PHE	-	expression tag	UNP Q8A6D0
A	327	GLN	-	expression tag	UNP Q8A6D0
B	1	MET	-	initiating methionine	UNP Q8A6D0
B	322	LEU	-	expression tag	UNP Q8A6D0
B	323	GLU	-	expression tag	UNP Q8A6D0
B	324	VAL	-	expression tag	UNP Q8A6D0
B	325	LEU	-	expression tag	UNP Q8A6D0
B	326	PHE	-	expression tag	UNP Q8A6D0
B	327	GLN	-	expression tag	UNP Q8A6D0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total 9	Na 9	0	0
2	B	1	Total 1	Na 1	0	0

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



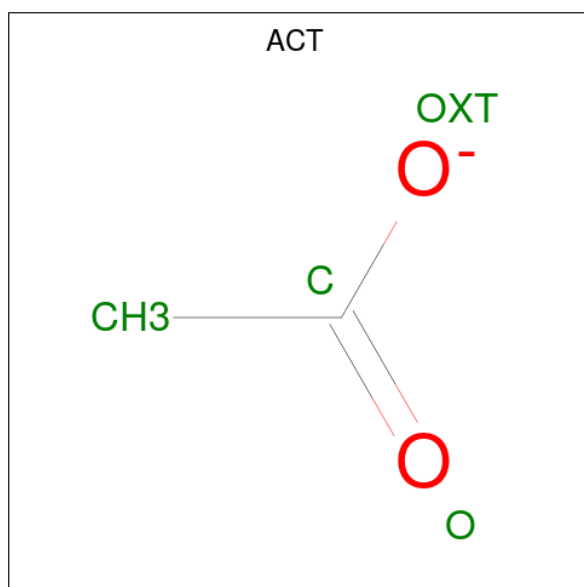
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0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

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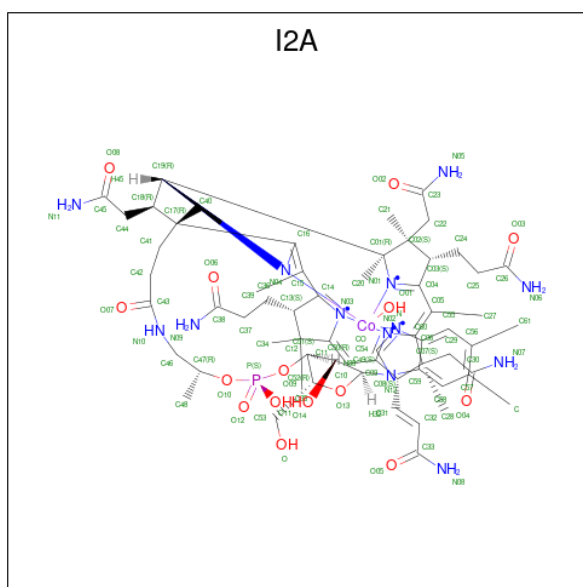
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



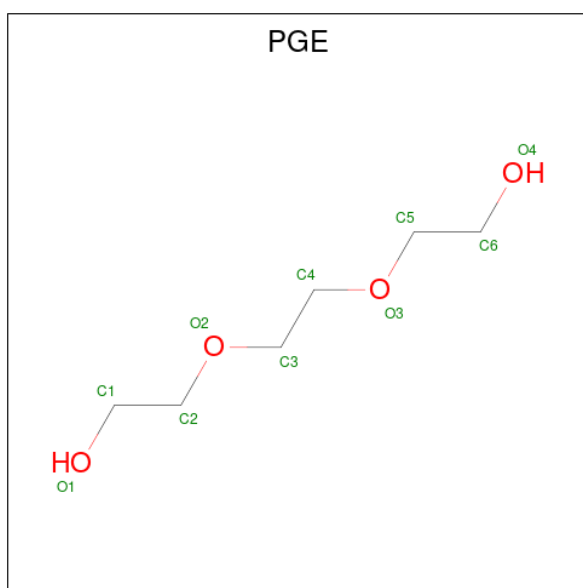
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is Hydroxocobalamin (three-letter code: I2A) (formula: C₆₂H₈₈CoN₁₃O₁₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
6	A	1	92	62	1	13	15	1	0	0
6	B	1	92	62	1	13	15	1	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
7	B	1	10	6 4	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0

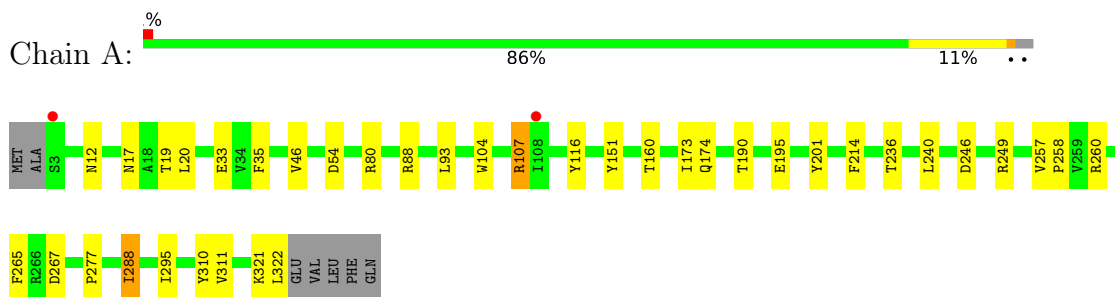
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	263	Total O 263 263	0	0
9	B	245	Total O 245 245	0	0

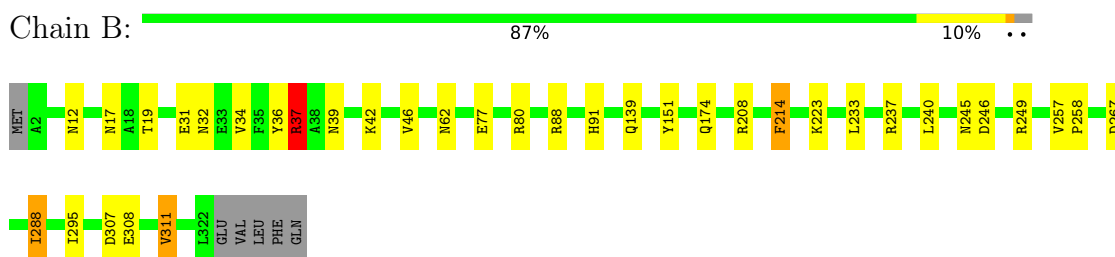
3 Residue-property plots [i](#)

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: Surface layer protein



- Molecule 1: Surface layer protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.11Å 101.10Å 79.89Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	62.40 – 1.50 62.32 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (62.40-1.50) 96.1 (62.32-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.143 , 0.174 0.149 , 0.178	Depositor DCC
R_{free} test set	5900 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtrriage
Anisotropy	0.264	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6137	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: I2A, GOL, SCN, PGE, PEG, NA, ACT

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	0.49	0/2728	0.84	0/3713
1	B	0.52	0/2699	0.83	0/3674
All	All	0.50	0/5427	0.83	0/7387

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
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	B	208	ARG	Sidechain
1	B	37	ARG	Sidechain

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	2643	0	2535	27	0
1	B	2626	0	2506	38	0
2	A	9	0	0	0	0
2	B	1	0	0	0	0
3	A	21	0	0	2	0
3	B	3	0	0	0	0
4	A	42	0	56	2	0
4	B	60	0	80	4	0
5	A	8	0	6	9	0
5	B	8	0	6	7	0
6	A	92	0	85	11	0
6	B	92	0	85	11	0
7	B	10	0	14	3	0
8	B	14	0	20	5	0
9	A	263	0	0	1	0
9	B	245	0	0	2	0
All	All	6137	0	5393	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (82) 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)
5:A:424:ACT:C	5:A:424:ACT:CH3	1.74	1.65
5:A:424:ACT:C	5:A:424:ACT:O	1.68	1.42
1:B:42:LYS:CD	5:B:417:ACT:H1	1.85	1.04
1:B:42:LYS:HD2	5:B:417:ACT:CH3	1.89	1.01
1:B:42:LYS:HD2	5:B:417:ACT:H1	1.00	0.97
1:A:20:LEU:H	5:A:424:ACT:H3	1.31	0.95
1:B:307:ASP:OD1	8:B:405:PEG:H12	1.68	0.94
6:A:426:I2A:H73	6:A:426:I2A:H6	1.48	0.93
1:B:62:ASN:HD21	6:B:418:I2A:H48	1.23	0.87
6:B:418:I2A:H6	6:B:418:I2A:H73	1.57	0.86
1:B:19:THR:HG22	5:B:417:ACT:H3	1.58	0.85
1:B:39:ASN:HD21	1:B:77:GLU:H	1.30	0.80
1:A:88:ARG:HH22	6:A:426:I2A:H47	1.30	0.79
1:B:307:ASP:OD1	8:B:405:PEG:C1	2.31	0.78
1:A:33:GLU:HA	5:A:424:ACT:H1	1.66	0.76
6:B:418:I2A:H80	6:B:418:I2A:H18	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:426:I2A:H80	6:A:426:I2A:H18	1.71	0.72
1:B:88:ARG:HH22	6:B:418:I2A:H47	1.40	0.70
1:A:19:THR:HG22	5:A:424:ACT:OXT	1.96	0.66
1:A:260:ARG:HH12	1:B:80:ARG:HH22	1.45	0.63
6:A:426:I2A:H6	6:A:426:I2A:C28	2.27	0.63
1:A:19:THR:HA	5:A:424:ACT:C	2.29	0.63
1:B:42:LYS:CD	5:B:417:ACT:CH3	2.64	0.63
1:B:91:HIS:HE1	1:B:139:GLN:OE1	1.83	0.61
4:B:412:GOL:H12	9:B:676:HOH:O	2.01	0.60
1:B:288:ILE:HD11	1:B:295:ILE:HG22	1.85	0.59
6:A:426:I2A:H80	6:A:426:I2A:C41	2.31	0.59
1:A:260:ARG:NH1	1:B:80:ARG:HH22	2.01	0.58
1:B:249:ARG:HG3	7:B:401:PGE:H42	1.86	0.58
6:B:418:I2A:H46	6:B:418:I2A:H59	1.69	0.57
1:B:37:ARG:HH11	1:B:37:ARG:HB2	1.68	0.57
1:B:12:ASN:HD22	1:B:17:ASN:HD21	1.52	0.57
1:B:42:LYS:HE3	9:B:548:HOH:O	2.05	0.57
6:B:418:I2A:H80	6:B:418:I2A:C41	2.35	0.56
1:A:288:ILE:HD11	1:A:295[B]:ILE:HG22	1.89	0.55
6:A:426:I2A:H59	6:A:426:I2A:H46	1.71	0.54
6:B:418:I2A:H6	6:B:418:I2A:C28	2.34	0.54
1:A:12:ASN:HD22	1:A:17:ASN:HD21	1.55	0.53
1:A:321:LYS:NZ	9:A:504:HOH:O	2.43	0.52
1:A:20:LEU:N	5:A:424:ACT:H3	2.14	0.52
1:A:88:ARG:NH2	6:A:426:I2A:H47	2.04	0.50
6:B:418:I2A:H82	6:B:418:I2A:H14	1.95	0.49
1:A:295[A]:ILE:HG12	1:A:310:TYR:CD1	2.48	0.49
1:B:249:ARG:O	7:B:401:PGE:H4	2.12	0.48
1:B:91:HIS:HD2	4:B:406:GOL:O2	1.95	0.48
6:B:418:I2A:H59	6:B:418:I2A:N05	2.28	0.48
1:A:93[B]:LEU:CD2	1:A:160:THR:HB	2.43	0.48
1:B:214:PHE:O	5:B:416:ACT:H2	2.13	0.48
1:B:31:GLU:HG2	1:B:34:VAL:HG12	1.95	0.48
6:A:426:I2A:N	6:A:426:I2A:H3	2.29	0.48
1:A:236:THR:HG23	4:A:421:GOL:H32	1.96	0.47
6:A:426:I2A:H59	6:A:426:I2A:N05	2.26	0.47
1:A:240:LEU:O	1:A:249:ARG:HA	2.15	0.46
1:B:245:ASN:HD22	4:B:411:GOL:C1	2.28	0.46
1:A:80:ARG:O	3:A:413:SCN:S	2.73	0.46
1:A:35:PHE:HB3	5:A:424:ACT:H2	1.97	0.46
1:A:151:TYR:H	1:A:174:GLN:NE2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:TYR:HB2	5:B:417:ACT:H2	1.99	0.45
1:A:277:PRO:O	4:A:421:GOL:H12	2.17	0.44
6:A:426:I2A:H73	6:A:426:I2A:C27	2.34	0.44
1:A:116:TYR:O	3:A:413:SCN:N	2.51	0.44
1:B:237:ARG:HG2	8:B:404:PEG:H22	1.99	0.44
5:A:424:ACT:CH3	5:A:424:ACT:OXT	2.54	0.44
1:B:223:LYS:HD3	4:B:411:GOL:C3	2.47	0.44
1:A:265:PHE:CZ	1:A:267:ASP:HA	2.53	0.43
1:A:195:GLU:HG2	1:A:201:TYR:CE2	2.53	0.43
1:B:249:ARG:O	7:B:401:PGE:C4	2.67	0.43
1:B:151:TYR:H	1:B:174:GLN:NE2	2.15	0.43
1:B:31:GLU:CG	1:B:34:VAL:HG12	2.49	0.43
1:B:39:ASN:ND2	1:B:77:GLU:H	2.07	0.42
1:B:37:ARG:HB2	1:B:37:ARG:NH1	2.31	0.42
1:A:104:TRP:HE1	6:A:426:I2A:H49	1.68	0.42
1:B:62:ASN:ND2	6:B:418:I2A:H48	2.04	0.42
1:B:240:LEU:O	1:B:249:ARG:HA	2.19	0.42
1:B:32:ASN:HD21	1:B:311:VAL:HA	1.85	0.41
1:B:233:LEU:HB2	8:B:404:PEG:H41	2.01	0.41
1:B:257:VAL:HB	1:B:258:PRO:HD2	2.02	0.41
1:B:88:ARG:NH2	6:B:418:I2A:H47	2.13	0.41
1:A:257:VAL:HB	1:A:258:PRO:HD2	2.02	0.41
1:A:277:PRO:HG2	1:A:322:LEU:HD11	2.02	0.40
1:A:173:ILE:O	1:A:190:THR:HB	2.22	0.40
1:B:308:GLU:HG3	8:B:405:PEG:H42	2.04	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	322/327 (98%)	301 (94%)	18 (6%)	3 (1%)	17 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	319/327 (98%)	301 (94%)	15 (5%)	3 (1%)	17	3
All	All	641/654 (98%)	602 (94%)	33 (5%)	6 (1%)	17	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	VAL
1	B	311	VAL
1	B	288	ILE
1	A	46	VAL
1	A	288	ILE
1	B	46	VAL

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	288/290 (99%)	284 (99%)	4 (1%)	67	42
1	B	284/290 (98%)	280 (99%)	4 (1%)	67	42
All	All	572/580 (99%)	564 (99%)	8 (1%)	67	42

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	107	ARG
1	A	214	PHE
1	A	246	ASP
1	B	37	ARG
1	B	214	PHE
1	B	246	ASP
1	B	267	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	32	ASN
1	A	48	GLN
1	A	174	GLN
1	A	245	ASN
1	B	12	ASN
1	B	32	ASN
1	B	39	ASN
1	B	48	GLN
1	B	62	ASN
1	B	91	HIS
1	B	174	GLN
1	B	184	ASN
1	B	232	GLN
1	B	302	GLN

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](#)

Of 44 ligands modelled in this entry, 10 are monoatomic - leaving 34 for Mogul analysis.

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	GOL	B	410	-	5,5,5	0.14	0	5,5,5	0.35	0
3	SCN	A	415	-	1,2,2	1.30	0	0,1,1	-	-
4	GOL	A	421	-	5,5,5	0.15	0	5,5,5	0.60	0
3	SCN	A	412	-	1,2,2	0.89	0	0,1,1	-	-
4	GOL	B	407	-	5,5,5	0.53	0	5,5,5	1.01	0
4	GOL	B	409	-	5,5,5	0.12	0	5,5,5	0.53	0
4	GOL	B	411	-	5,5,5	0.12	0	5,5,5	0.37	0
3	SCN	A	411	-	1,2,2	0.85	0	0,1,1	-	-
4	GOL	B	412	-	5,5,5	0.14	0	5,5,5	0.53	0
4	GOL	A	423	-	5,5,5	0.12	0	5,5,5	0.33	0
4	GOL	A	422	-	5,5,5	0.16	0	5,5,5	0.35	0
4	GOL	B	415	-	5,5,5	0.17	0	5,5,5	0.35	0
7	PGE	B	401	-	9,9,9	0.49	0	8,8,8	0.45	0
3	SCN	B	403	-	1,2,2	2.07	1 (100%)	0,1,1	-	-
4	GOL	A	420	-	5,5,5	0.15	0	5,5,5	0.42	0
6	I2A	B	418	-	93,103,103	1.66	15 (16%)	133,177,177	1.75	23 (17%)
3	SCN	A	413	-	1,2,2	1.63	0	0,1,1	-	-
8	PEG	B	405	-	6,6,6	0.38	0	5,5,5	0.30	0
4	GOL	B	414	-	5,5,5	0.14	0	5,5,5	0.52	0
8	PEG	B	404	-	6,6,6	0.19	0	5,5,5	0.22	0
5	ACT	B	417	-	3,3,3	0.71	0	3,3,3	1.19	0
3	SCN	A	410	-	1,2,2	2.37	1 (100%)	0,1,1	-	-
5	ACT	B	416	-	3,3,3	0.98	0	3,3,3	0.91	0
4	GOL	A	418	-	5,5,5	0.12	0	5,5,5	0.24	0
3	SCN	A	416	-	1,2,2	0.63	0	0,1,1	-	-
3	SCN	A	414	-	1,2,2	0.08	0	0,1,1	-	-
4	GOL	B	408	-	5,5,5	0.14	0	5,5,5	0.78	0
4	GOL	B	413	-	5,5,5	0.12	0	5,5,5	0.24	0
4	GOL	A	419	-	5,5,5	0.16	0	5,5,5	0.70	0
5	ACT	A	424	-	3,3,3	7.06	3 (100%)	3,3,3	2.32	2 (66%)
4	GOL	B	406	-	5,5,5	0.18	0	5,5,5	0.39	0
5	ACT	A	425	-	3,3,3	1.16	0	3,3,3	0.64	0
4	GOL	A	417	-	5,5,5	0.21	0	5,5,5	0.46	0
6	I2A	A	426	2	93,103,103	1.72	17 (18%)	133,177,177	1.86	22 (16%)

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	GOL	B	410	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	421	-	-	4/4/4/4	-
4	GOL	B	407	-	-	0/4/4/4	-
4	GOL	B	409	-	-	2/4/4/4	-
4	GOL	B	411	-	-	4/4/4/4	-
4	GOL	B	412	-	-	4/4/4/4	-
4	GOL	A	423	-	-	4/4/4/4	-
4	GOL	A	422	-	-	4/4/4/4	-
4	GOL	B	415	-	-	2/4/4/4	-
7	PGE	B	401	-	-	4/7/7/7	-
4	GOL	A	420	-	-	2/4/4/4	-
6	I2A	B	418	-	1/1/42/49	9/52/277/277	-
8	PEG	B	405	-	-	3/4/4/4	-
4	GOL	B	414	-	-	2/4/4/4	-
8	PEG	B	404	-	-	2/4/4/4	-
4	GOL	A	418	-	-	1/4/4/4	-
4	GOL	B	408	-	-	3/4/4/4	-
4	GOL	B	413	-	-	2/4/4/4	-
4	GOL	A	419	-	-	2/4/4/4	-
4	GOL	B	406	-	-	1/4/4/4	-
4	GOL	A	417	-	-	1/4/4/4	-
6	I2A	A	426	2	1/1/42/49	11/52/277/277	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	426	I2A	C32-C31	10.14	1.56	1.32
5	A	424	ACT	O-C	10.12	1.68	1.22
6	B	418	I2A	C32-C31	9.43	1.54	1.32
5	A	424	ACT	CH3-C	6.08	1.74	1.49
6	A	426	I2A	C57-C56	3.81	1.50	1.40
6	B	418	I2A	C08-C09	-3.43	1.46	1.51
6	B	418	I2A	C08-C31	3.40	1.55	1.50
6	A	426	I2A	C09-N02	3.25	1.42	1.34
6	B	418	I2A	C18-C19	-3.23	1.47	1.54
5	A	424	ACT	OXT-C	3.19	1.46	1.30
6	B	418	I2A	C35-C12	-2.89	1.47	1.54
6	A	426	I2A	C54-N12	2.89	1.38	1.33
6	A	426	I2A	C19-N04	-2.88	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	418	I2A	C01-C02	-2.87	1.52	1.58
6	B	418	I2A	C50-C49	2.82	1.58	1.53
6	B	418	I2A	C16-N04	2.81	1.37	1.30
6	B	418	I2A	C59-C60	2.80	1.47	1.39
6	A	426	I2A	C08-C09	-2.78	1.47	1.51
6	A	426	I2A	C18-C19	-2.74	1.48	1.54
6	B	418	I2A	C09-N02	2.66	1.40	1.34
6	A	426	I2A	C14-N03	-2.57	1.29	1.38
6	A	426	I2A	C08-C31	2.56	1.54	1.50
6	A	426	I2A	O13-C52	-2.46	1.39	1.45
6	A	426	I2A	C16-N04	2.41	1.36	1.30
6	B	418	I2A	C14-N03	-2.40	1.29	1.38
6	A	426	I2A	O02-C23	2.38	1.31	1.24
3	A	410	SCN	C-N	2.37	1.23	1.15
6	A	426	I2A	C01-C02	-2.37	1.53	1.58
6	A	426	I2A	C12-C11	-2.36	1.43	1.51
6	B	418	I2A	C12-C11	-2.30	1.44	1.51
6	A	426	I2A	C34-C12	-2.27	1.49	1.54
6	B	418	I2A	O02-C23	2.23	1.30	1.24
6	B	418	I2A	C54-N12	2.23	1.37	1.33
6	A	426	I2A	C04-N01	-2.22	1.25	1.30
6	A	426	I2A	C59-C60	2.17	1.45	1.39
6	B	418	I2A	O13-C49	2.11	1.44	1.41
3	B	403	SCN	C-N	-2.07	1.08	1.15

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	426	I2A	C12-C11-C10	-10.92	113.57	123.54
6	B	418	I2A	C12-C11-C10	-8.42	115.85	123.54
6	B	418	I2A	C01-C19-C18	6.30	131.12	121.81
6	B	418	I2A	C12-C11-N03	6.06	118.14	111.50
6	B	418	I2A	C01-C19-N04	5.68	115.33	106.33
6	A	426	I2A	C01-C19-C18	5.52	129.97	121.81
6	A	426	I2A	C12-C11-N03	5.25	117.25	111.50
6	A	426	I2A	C01-C19-N04	4.99	114.23	106.33
6	A	426	I2A	C20-C01-C19	-3.92	102.38	110.23
6	B	418	I2A	C02-C01-C19	3.79	125.23	118.72
6	A	426	I2A	C10-C11-N03	3.78	128.84	124.72
6	A	426	I2A	C02-C01-C19	3.31	124.41	118.72
6	A	426	I2A	O08-C45-C44	3.26	127.72	120.87
6	A	426	I2A	C18-C19-N04	3.25	107.05	101.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	424	ACT	OXT-C-O	3.18	133.77	122.05
6	B	418	I2A	C18-C19-N04	3.11	106.83	101.88
6	A	426	I2A	C15-C16-N04	-3.03	119.31	122.38
6	A	426	I2A	C17-C18-C19	2.99	106.26	102.66
6	B	418	I2A	C03-C04-C05	-2.91	118.91	123.81
6	A	426	I2A	C35-C12-C11	2.90	120.32	110.29
6	B	418	I2A	C20-C01-C19	-2.85	104.51	110.23
6	A	426	I2A	C36-C37-C38	-2.82	103.01	112.59
6	B	418	I2A	C14-N03-C11	-2.82	106.42	110.10
6	B	418	I2A	C17-C16-N04	-2.77	106.21	110.87
6	A	426	I2A	O05-C33-N08	-2.67	116.88	122.58
6	A	426	I2A	O13-C49-C50	-2.62	103.09	106.93
6	B	418	I2A	C05-C04-N01	2.61	128.45	124.18
6	A	426	I2A	C28-C07-C29	2.58	115.06	110.80
6	A	426	I2A	C10-C09-N02	-2.56	122.78	125.73
6	B	418	I2A	C10-C09-N02	-2.55	122.79	125.73
6	B	418	I2A	C39-C15-C14	2.54	121.98	116.79
6	B	418	I2A	C40-C17-C18	-2.50	109.29	112.98
6	B	418	I2A	C35-C12-C11	2.48	118.85	110.29
5	A	424	ACT	OXT-C-CH3	-2.45	105.07	115.18
6	A	426	I2A	C08-C09-C10	2.38	128.46	123.32
6	B	418	I2A	C08-C09-C10	2.29	128.26	123.32
6	B	418	I2A	C17-C18-C19	2.23	105.34	102.66
6	A	426	I2A	C19-C01-N01	2.22	104.49	101.67
6	B	418	I2A	C13-C12-C11	-2.17	97.94	100.90
6	B	418	I2A	O04-C30-C29	-2.16	115.17	121.99
6	B	418	I2A	C01-C02-C03	2.15	104.34	101.60
6	A	426	I2A	C39-C15-C14	2.10	121.07	116.79
6	A	426	I2A	O04-C30-N07	2.10	128.23	122.50
6	B	418	I2A	O07-C43-N10	2.09	126.97	123.01
6	B	418	I2A	O08-C45-C44	2.09	125.27	120.87
6	B	418	I2A	C28-C07-C29	2.06	114.19	110.80
6	A	426	I2A	C14-N03-C11	-2.02	107.47	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	426	I2A	N04
6	B	418	I2A	N04

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	420	GOL	O1-C1-C2-C3
4	A	421	GOL	O1-C1-C2-C3
4	A	422	GOL	O1-C1-C2-C3
4	A	423	GOL	O1-C1-C2-O2
4	A	423	GOL	O1-C1-C2-C3
4	B	408	GOL	O1-C1-C2-C3
4	B	411	GOL	O1-C1-C2-C3
4	B	411	GOL	C1-C2-C3-O3
4	B	412	GOL	O1-C1-C2-O2
4	B	412	GOL	O1-C1-C2-C3
4	B	412	GOL	C1-C2-C3-O3
4	B	412	GOL	O2-C2-C3-O3
4	B	413	GOL	O1-C1-C2-C3
4	B	414	GOL	O1-C1-C2-C3
4	B	415	GOL	O1-C1-C2-C3
6	A	426	I2A	C07-C08-C31-C32
6	A	426	I2A	C09-C08-C31-C32
6	A	426	I2A	C31-C32-C33-N08
6	A	426	I2A	C31-C32-C33-O05
6	B	418	I2A	C07-C08-C31-C32
6	B	418	I2A	C09-C08-C31-C32
6	B	418	I2A	C31-C32-C33-O05
6	B	418	I2A	C13-C36-C37-C38
4	A	421	GOL	O2-C2-C3-O3
4	B	411	GOL	O1-C1-C2-O2
4	B	413	GOL	O1-C1-C2-O2
7	B	401	PGE	O2-C3-C4-O3
7	B	401	PGE	O3-C5-C6-O4
8	B	404	PEG	O1-C1-C2-O2
8	B	404	PEG	O2-C3-C4-O4
8	B	405	PEG	O2-C3-C4-O4
4	A	418	GOL	C1-C2-C3-O3
4	A	419	GOL	O1-C1-C2-C3
4	A	421	GOL	C1-C2-C3-O3
4	A	422	GOL	C1-C2-C3-O3
4	A	423	GOL	C1-C2-C3-O3
4	B	406	GOL	C1-C2-C3-O3
4	B	409	GOL	C1-C2-C3-O3
4	A	420	GOL	O1-C1-C2-O2
4	A	421	GOL	O1-C1-C2-O2
4	A	423	GOL	O2-C2-C3-O3
4	B	408	GOL	O1-C1-C2-O2
4	B	411	GOL	O2-C2-C3-O3

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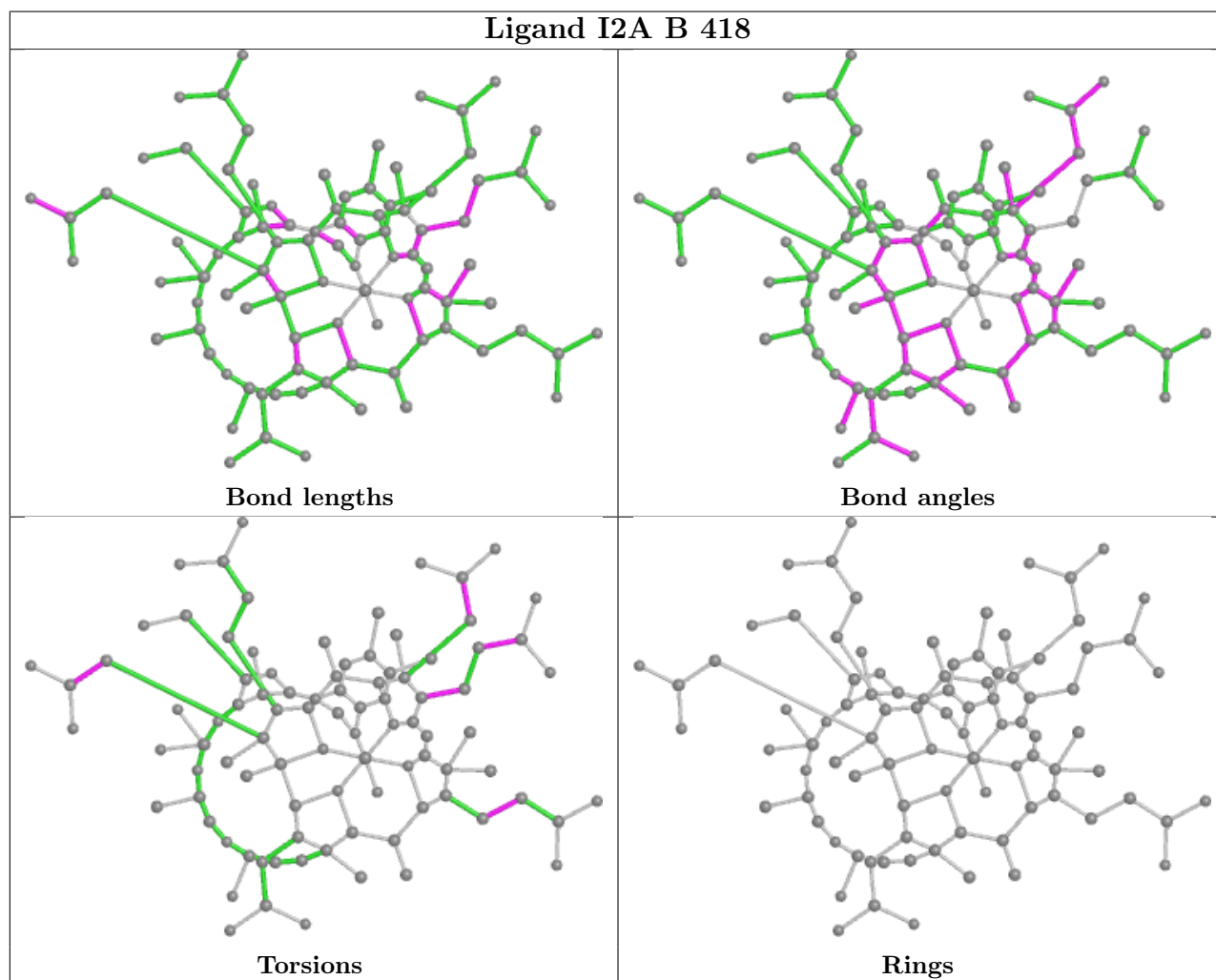
Mol	Chain	Res	Type	Atoms
4	B	414	GOL	O1-C1-C2-O2
6	A	426	I2A	C13-C36-C37-C38
8	B	405	PEG	O1-C1-C2-O2
4	A	422	GOL	O1-C1-C2-O2
6	A	426	I2A	C02-C22-C23-N05
6	A	426	I2A	C02-C22-C23-O02
6	B	418	I2A	C02-C22-C23-N05
6	B	418	I2A	C31-C32-C33-N08
6	A	426	I2A	C24-C25-C26-O03
6	A	426	I2A	C07-C29-C30-O04
4	B	409	GOL	O2-C2-C3-O3
4	B	415	GOL	O1-C1-C2-O2
4	A	417	GOL	O1-C1-C2-C3
8	B	405	PEG	C4-C3-O2-C2
6	A	426	I2A	C24-C25-C26-N06
6	B	418	I2A	C07-C29-C30-N07
7	B	401	PGE	C6-C5-O3-C4
7	B	401	PGE	O1-C1-C2-O2
6	B	418	I2A	C07-C29-C30-O04
6	B	418	I2A	C02-C22-C23-O02
6	A	426	I2A	C07-C29-C30-N07
4	A	419	GOL	O1-C1-C2-O2
4	A	422	GOL	O2-C2-C3-O3
4	B	408	GOL	O2-C2-C3-O3

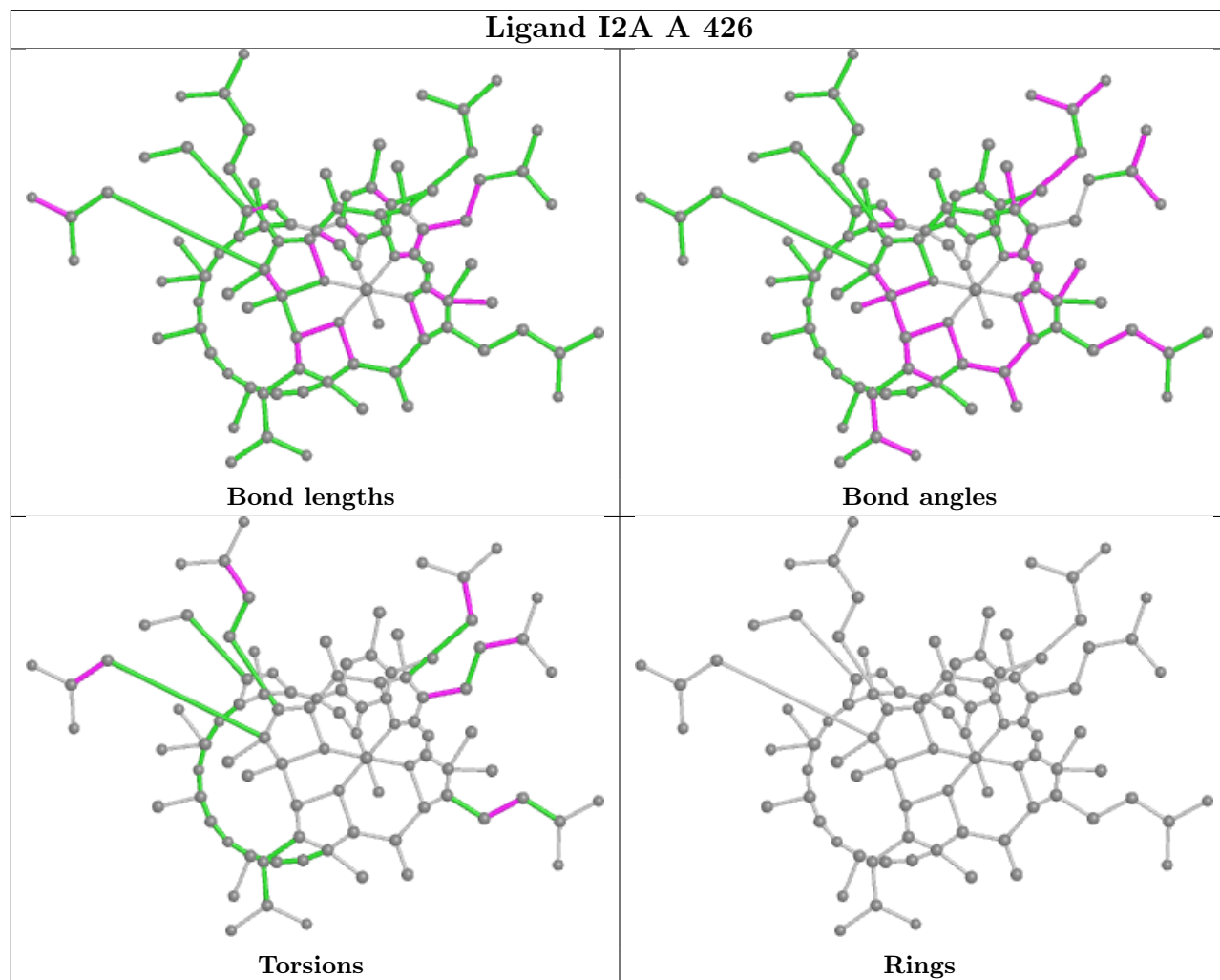
There are no ring outliers.

13 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	421	GOL	2	0
4	B	411	GOL	2	0
4	B	412	GOL	1	0
7	B	401	PGE	3	0
6	B	418	I2A	11	0
3	A	413	SCN	2	0
8	B	405	PEG	3	0
8	B	404	PEG	2	0
5	B	417	ACT	6	0
5	B	416	ACT	1	0
5	A	424	ACT	9	0
4	B	406	GOL	1	0
6	A	426	I2A	11	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	320/327 (97%)	0.00	2 (0%) 89 91	11, 15, 24, 38	0
1	B	321/327 (98%)	0.02	0 100 100	12, 15, 23, 31	0
All	All	641/654 (98%)	0.01	2 (0%) 94 95	11, 15, 24, 38	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ILE	3.0
1	A	3	SER	2.5

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	ACT	A	424	4/4	0.49	0.78	69,125,147,685	0
5	ACT	B	416	4/4	0.76	0.12	48,49,49,50	0
4	GOL	B	412	6/6	0.82	0.17	27,33,39,42	0

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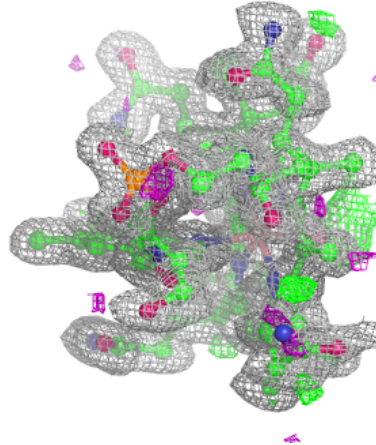
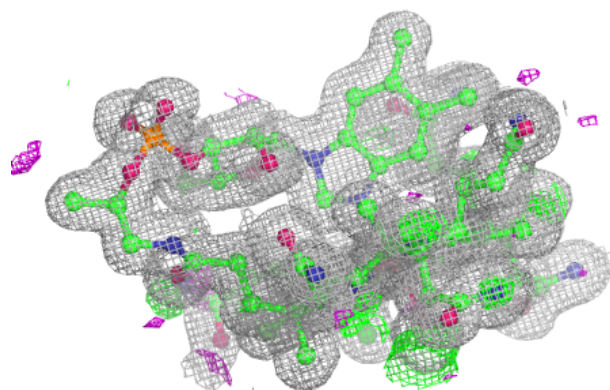
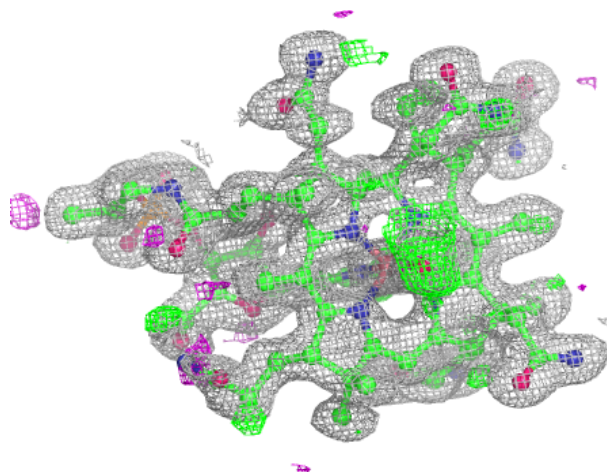
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ACT	A	425	4/4	0.83	0.17	45,53,55,55	0
4	GOL	B	411	6/6	0.83	0.15	39,41,43,48	0
8	PEG	B	405	7/7	0.83	0.16	23,29,39,41	0
3	SCN	A	410	3/3	0.87	0.16	17,17,35,48	0
7	PGE	B	401	10/10	0.87	0.16	24,30,34,41	0
4	GOL	A	419	6/6	0.87	0.17	25,34,38,38	0
4	GOL	B	413	6/6	0.88	0.15	33,42,45,52	0
4	GOL	A	418	6/6	0.88	0.34	46,57,62,64	0
4	GOL	B	415	6/6	0.89	0.19	35,42,44,44	0
4	GOL	A	423	6/6	0.89	0.17	23,39,43,51	0
3	SCN	A	415	3/3	0.89	0.16	29,29,40,60	0
4	GOL	A	422	6/6	0.90	0.14	34,40,43,47	0
3	SCN	A	414	3/3	0.90	0.18	48,48,50,52	0
5	ACT	B	417	4/4	0.90	0.19	18,26,27,30	0
4	GOL	B	409	6/6	0.90	0.11	27,34,38,39	0
3	SCN	A	412	3/3	0.90	0.09	42,42,53,68	0
4	GOL	A	421	6/6	0.91	0.19	18,28,39,49	0
8	PEG	B	404	7/7	0.91	0.19	20,34,44,45	0
3	SCN	A	416	3/3	0.91	0.10	48,48,57,66	0
4	GOL	B	410	6/6	0.93	0.16	19,32,41,43	0
3	SCN	B	403	3/3	0.93	0.09	20,20,23,41	0
3	SCN	A	411	3/3	0.94	0.08	23,23,28,29	0
4	GOL	B	414	6/6	0.94	0.14	17,23,28,36	0
4	GOL	A	417	6/6	0.95	0.12	17,20,24,26	0
3	SCN	A	413	3/3	0.95	0.15	25,25,28,32	0
6	I2A	A	426	92/92	0.96	0.10	10,13,21,36	0
6	I2A	B	418	92/92	0.96	0.10	12,14,21,36	0
4	GOL	B	408	6/6	0.96	0.10	26,28,29,30	0
4	GOL	A	420	6/6	0.96	0.14	21,30,34,40	0
4	GOL	B	407	6/6	0.96	0.10	15,16,20,20	0
2	NA	A	409	1/1	0.97	0.15	16,16,16,16	0
4	GOL	B	406	6/6	0.97	0.10	16,18,21,25	0
2	NA	B	402	1/1	0.98	0.11	17,17,17,17	0
2	NA	A	403	1/1	0.99	0.06	17,17,17,17	0
2	NA	A	406	1/1	0.99	0.05	20,20,20,20	0
2	NA	A	407	1/1	0.99	0.11	24,24,24,24	0
2	NA	A	408	1/1	0.99	0.06	23,23,23,23	0
2	NA	A	405	1/1	1.00	0.07	20,20,20,20	0
2	NA	A	402	1/1	1.00	0.07	20,20,20,20	0
2	NA	A	401	1/1	1.00	0.20	12,12,12,12	0
2	NA	A	404	1/1	1.00	0.06	19,19,19,19	0

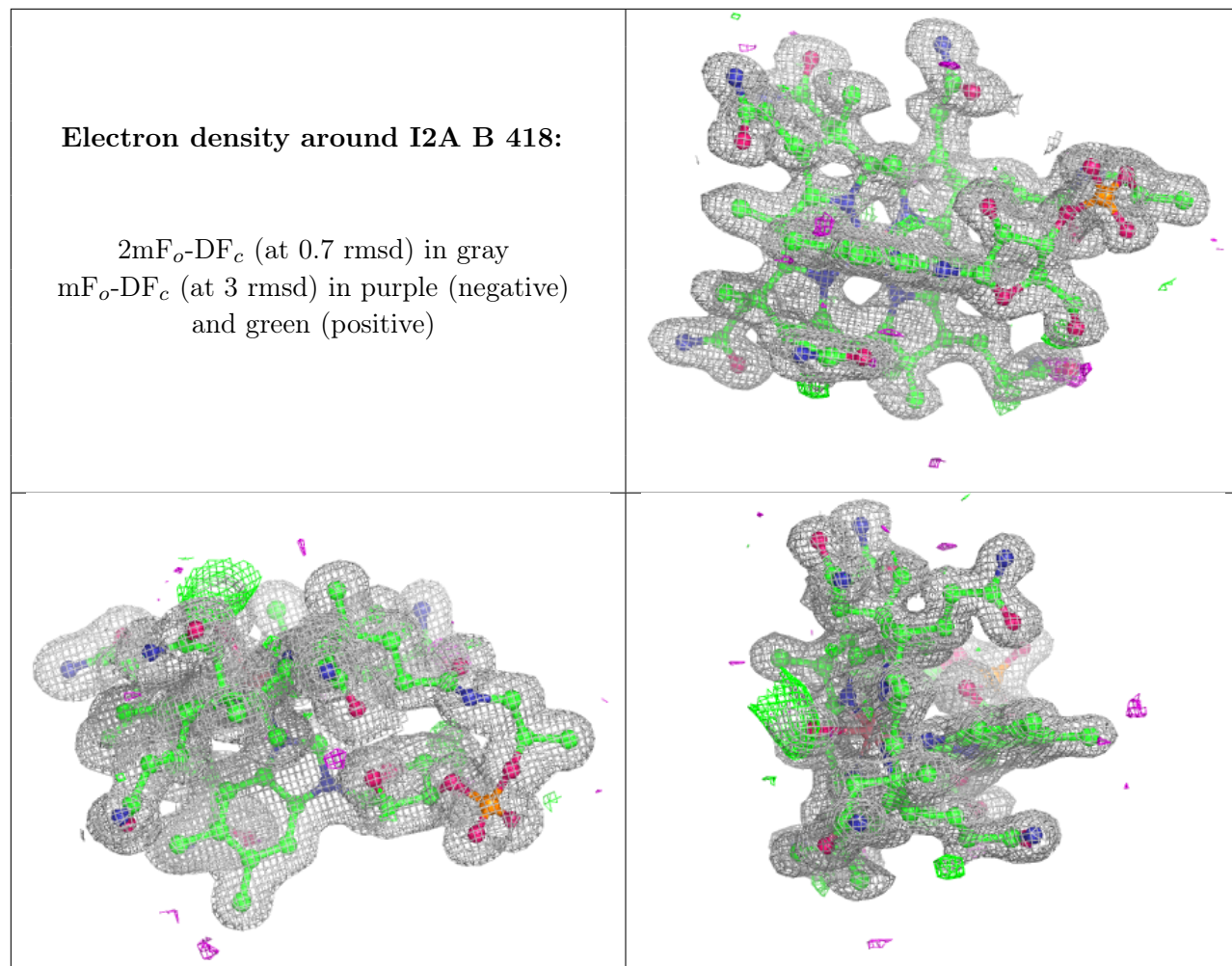
The following is a graphical depiction of the model fit to experimental electron density of all

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 I2A A 426:

$2mF_o-DF_c$ (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.