Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2022 – 01:07 pm BST

PDB ID	:	7R2F
Title	:	Structure of tabun inhibited acetylcholinesterase in complex with 2-((hydroxyimino)methyl)-1-(5-(4-methyl-3-nitrobenzamido)pentyl)pyridinium
Authors	:	Forsgren, N.; Lindgren, C.; Edvinsson, L.; Linusson, A.; Ekstrom, F.
Deposited on	:	2022-02-04
Resolution	:	2.30 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 following versions of software and data (see references (i)) were used in the production of this report:

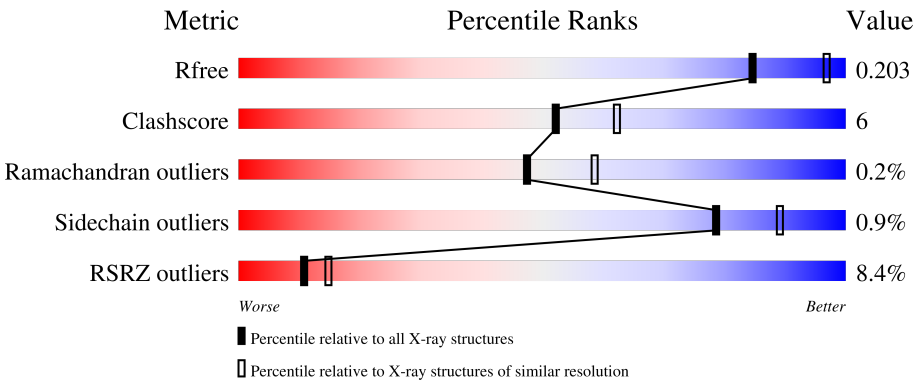
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	543	4% 84% 14% •
1	B	543	12% 83% 14% • •

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
2	NAG	A	601	-	-	-	X
2	NAG	A	602	-	-	-	X

2 Entry composition (i)

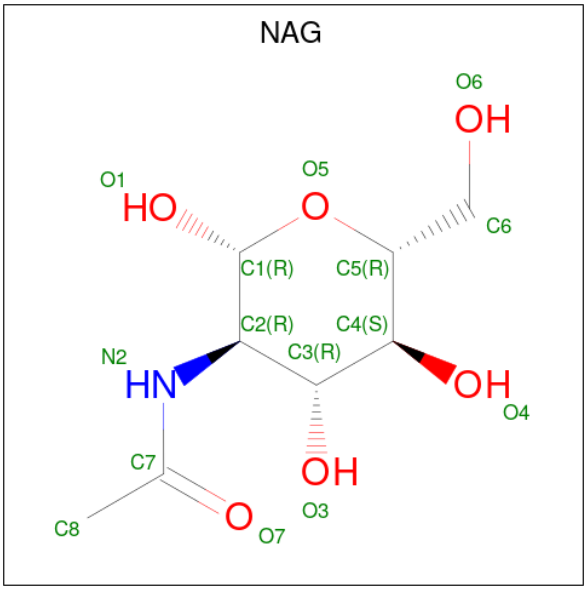
There are 6 unique types of molecules in this entry. The entry contains 9476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

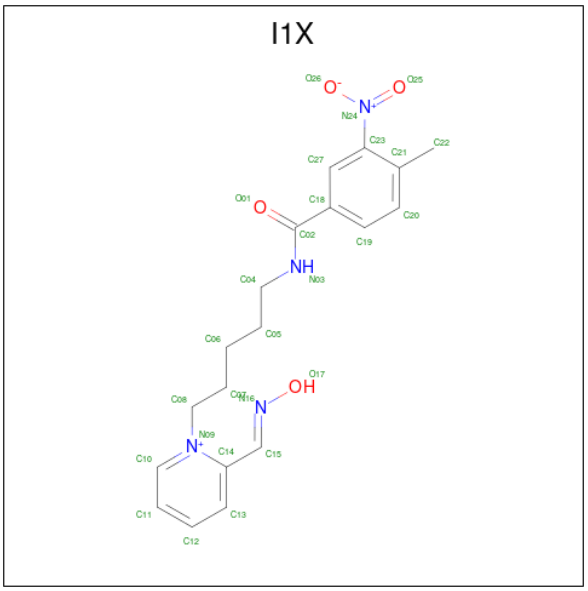
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	536	4528	2931	781	800	1	15	0	42	0
1	B	533	4502	2914	771	799	1	17	0	42	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



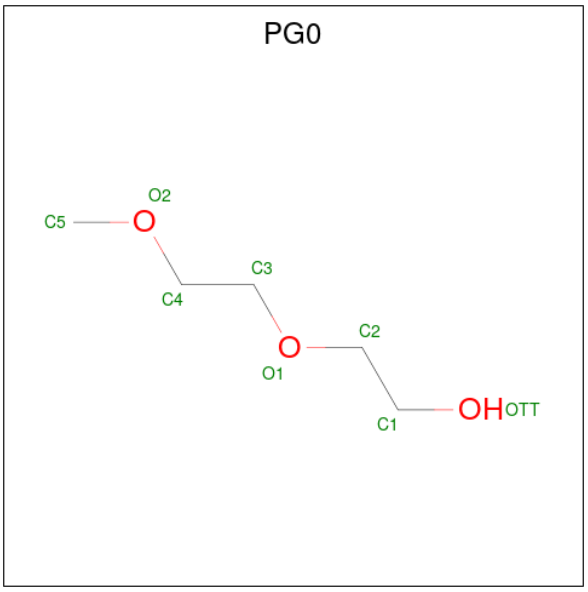
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is 4-methyl-3-nitro- {N}-[(2 {E},4 {E})-5-[2-[(oxidanylamino)methyl]pyridin-1 -yl]penta-2,4-dienyl]benzamide (three-letter code: I1X) (formula: $C_{19}H_{23}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	16	11	2	3	0	0
			Total	C	N	O		
3	B	1	18	13	2	3	0	0

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	8	5	3		0	0

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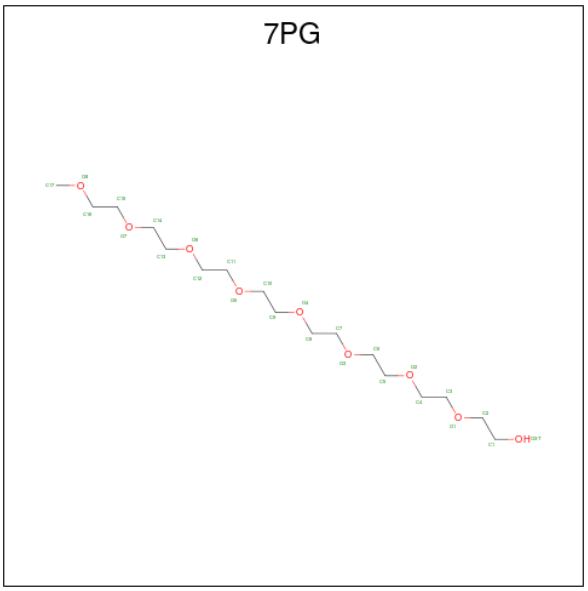
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	7	5	2		0	0
			Total	C	O			
4	A	1	8	5	3		0	0
			Total	C	O			
4	A	1	6	4	2		0	0
			Total	C	O			
4	A	1	8	5	3		0	0
			Total	C	O			
4	A	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0
			Total	C	O			
4	B	1	8	5	3		0	0

- Molecule 5 is 2,5,8,11,14,17,20,23-OCTAOXAPENTACOSAN-25-OL (three-letter code: 7PG) (formula: $C_{17}H_{36}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	23	15	8	0	0

- Molecule 6 is water.

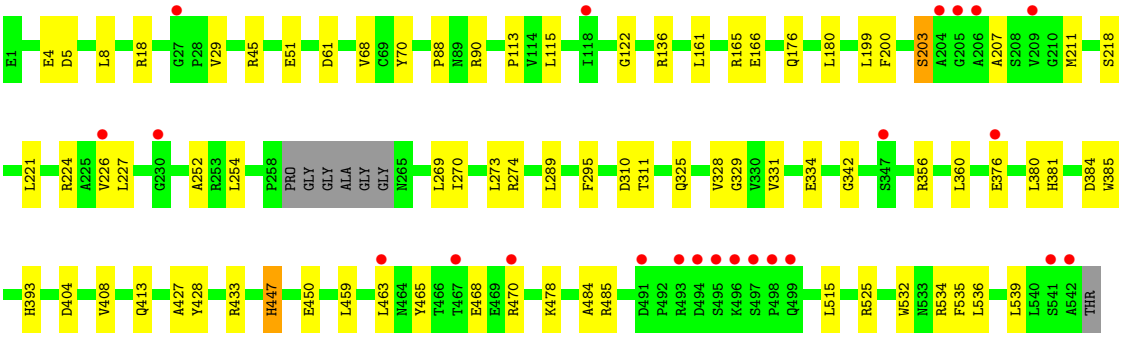
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	151	151	151	0	0
			Total	O		
6	B	101	101	101	0	0

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.

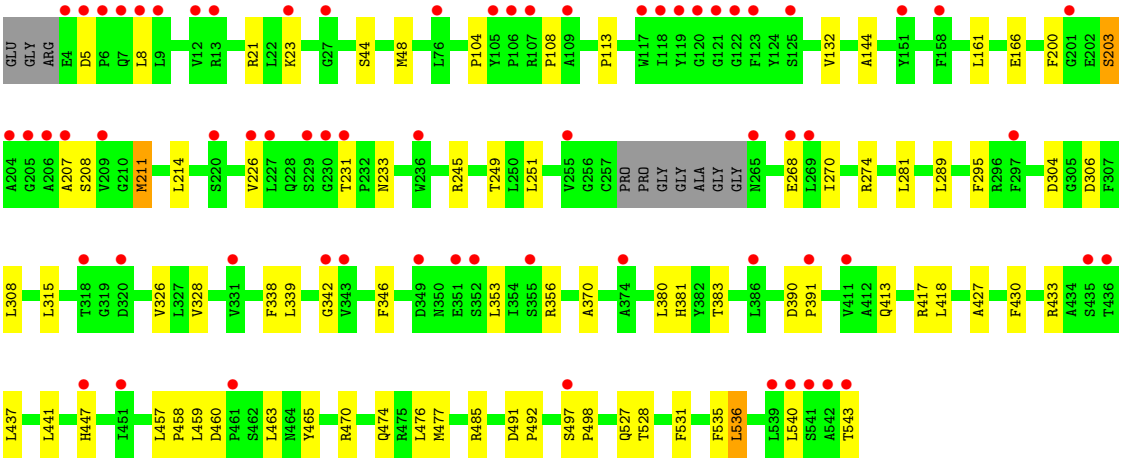
- Molecule 1: Acetylcholinesterase

Chain A:



- Molecule 1: Acetylcholinesterase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.83Å 110.75Å 227.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 2.30 46.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (46.14-2.30) 95.6 (46.13-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.172 , 0.205 0.174 , 0.203	Depositor DCC
R_{free} test set	1691 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	9476	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: NAG, 7PG, PG0, SUN, I1X

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	0.39	0/4642	0.53	0/6343
1	B	0.36	0/4614	0.53	0/6305
All	All	0.37	0/9256	0.53	0/12648

There are no bond length outliers.

There are no bond angle outliers.

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	4528	0	4481	52	0
1	B	4502	0	4458	52	0
2	A	28	0	26	0	0
3	A	16	0	0	0	0
3	B	18	0	0	0	0
4	A	45	0	64	4	0
4	B	64	0	96	4	0
5	B	23	0	29	4	0
6	A	151	0	0	0	0
6	B	101	0	0	2	0
All	All	9476	0	9154	101	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 6.

All (101) 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:B:113:PRO:HG2	4:B:605:PG0:H52	1.58	0.85
1:A:413:GLN:HG3	4:A:605:PG0:H31	1.66	0.77
1:B:214:LEU:HB3	1:B:315[B]:LEU:HD23	1.71	0.71
1:B:268:GLU:N	1:B:268:GLU:OE1	2.27	0.68
1:B:211[A]:MET:HE2	1:B:308:LEU:HD21	1.77	0.65
1:B:132[B]:VAL:HA	1:B:457[B]:LEU:HD11	1.79	0.64
1:B:356[A]:ARG:NH1	1:B:383:THR:OG1	2.32	0.63
1:A:68[B]:VAL:HG21	1:A:88:PRO:HB3	1.82	0.61
1:A:404:ASP:OD1	1:A:525:ARG:NH1	2.34	0.61
1:B:380[B]:LEU:HB3	5:B:610:7PG:H91	1.82	0.61
1:B:207:ALA:O	1:B:211[A]:MET:HG2	2.02	0.59
1:B:459[B]:LEU:HD11	1:B:477[B]:MET:HE1	1.85	0.59
1:A:45:ARG:NE	1:A:51:GLU:OE2	2.36	0.58
1:A:227[B]:LEU:HB2	1:A:328[B]:VAL:HG13	1.84	0.58
1:B:326[B]:VAL:HG11	1:B:418[B]:LEU:HD23	1.88	0.56
1:B:353[A]:LEU:HB3	1:B:391:PRO:HB2	1.88	0.56
1:B:338:PHE:HE1	1:B:447[B]:HIS:NE2	2.04	0.56
1:B:381:HIS:CE1	5:B:610:7PG:H132	2.41	0.55
1:A:463[B]:LEU:HD23	1:A:465:TYR:HE2	1.73	0.54
1:B:23:LYS:NZ	6:B:702:HOH:O	2.27	0.54
1:B:200:PHE:CB	1:B:226:VAL:HB	2.38	0.54
1:A:207:ALA:O	1:A:211:MET:HG2	2.08	0.53
1:B:245:ARG:O	1:B:249:THR:HG23	2.09	0.53
1:A:218:SER:HA	1:A:221[B]:LEU:HD23	1.90	0.53
1:A:115[A]:LEU:HD21	1:A:484:ALA:HB2	1.91	0.52
1:A:433[B]:ARG:H	4:A:607:PG0:H51	1.74	0.52
1:A:270[A]:ILE:HG22	1:A:274[A]:ARG:HH11	1.75	0.51
1:B:144:ALA:HA	4:B:605:PG0:H53	1.92	0.51
1:A:4:GLU:OE2	1:A:18[B]:ARG:NE	2.44	0.51
1:A:534[B]:ARG:HB3	1:B:380[B]:LEU:HD21	1.92	0.50
1:A:180[B]:LEU:HD21	1:A:199[B]:LEU:HD21	1.93	0.50
1:B:161[B]:LEU:HD12	1:B:270:ILE:HD11	1.93	0.50
1:B:459[B]:LEU:HD23	1:B:470:ARG:HG2	1.92	0.49
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.94	0.49
1:A:165:ARG:HH21	1:A:166:GLU:HG3	1.78	0.49
1:B:413:GLN:HG3	4:B:603:PG0:H12	1.95	0.49
1:B:430:PHE:HE2	1:B:476[B]:LEU:HD21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLY:HA2	1:A:203:SUN:H1C3	1.95	0.48
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.96	0.48
1:B:328:VAL:O	1:B:427:ALA:HA	2.14	0.48
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.96	0.47
1:B:370:ALA:HA	1:B:540:LEU:HD21	1.96	0.47
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.50	0.47
1:B:433:ARG:CZ	1:B:437[A]:LEU:HD23	2.44	0.47
1:A:328[B]:VAL:O	1:A:427:ALA:HA	2.15	0.47
1:A:18[A]:ARG:NH2	1:A:61:ASP:OD2	2.39	0.46
1:A:532:TRP:CE3	1:A:536[B]:LEU:HD12	2.51	0.46
1:B:485:ARG:HG2	4:B:605:PG0:H12	1.98	0.46
1:A:376:GLU:O	1:A:380[A]:LEU:HG	2.16	0.46
1:B:251[B]:LEU:HD11	1:B:281[B]:LEU:HG	1.98	0.45
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.96	0.45
1:A:450:GLU:OE1	1:A:450:GLU:N	2.42	0.45
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.16	0.45
1:B:339[B]:LEU:HD23	1:B:346:PHE:CE2	2.52	0.45
1:A:270[A]:ILE:HD13	1:A:273[A]:LEU:HD12	1.99	0.45
1:B:540:LEU:O	1:B:543:THR:HG22	2.16	0.45
1:A:200:PHE:CB	1:A:226:VAL:HB	2.47	0.45
1:B:417:ARG:HD3	1:B:417:ARG:HA	1.72	0.44
1:B:531:PHE:CZ	1:B:536:LEU:HD11	2.52	0.44
1:A:468:GLU:OE1	1:A:468:GLU:N	2.50	0.44
1:B:48:MET:SD	1:B:166:GLU:HA	2.57	0.44
1:B:497:SER:HB2	1:B:498:PRO:HA	2.00	0.44
1:A:534[B]:ARG:NH2	4:A:605:PG0:H41	2.33	0.44
1:B:459[B]:LEU:HD21	1:B:474:GLN:HG3	2.00	0.44
1:A:535:PHE:CE2	1:A:539:LEU:HD22	2.53	0.44
1:A:165:ARG:NH2	1:A:166:GLU:HG3	2.33	0.43
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.83	0.43
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.99	0.43
1:A:331:VAL:HG22	1:A:334:GLU:OE2	2.19	0.43
1:A:408:VAL:HG11	1:A:525:ARG:HG3	2.00	0.43
1:A:536[B]:LEU:HA	1:A:536[B]:LEU:HD23	1.66	0.42
1:B:5:ASP:HB3	1:B:8[B]:LEU:HD22	2.00	0.42
1:B:208:SER:HA	1:B:211[A]:MET:HG3	2.02	0.42
1:B:231:THR:HB	1:B:233:ASN:OD1	2.19	0.42
1:A:459[B]:LEU:HD23	1:A:470:ARG:HG3	2.02	0.42
1:A:381:HIS:ND1	5:B:610:7PG:H12	2.35	0.42
1:A:356:ARG:O	1:A:360[A]:LEU:HG	2.19	0.42
1:A:200:PHE:HB2	1:A:226:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASP:OD1	1:A:311:THR:N	2.44	0.42
1:A:515[A]:LEU:HG	4:A:607:PG0:H31	2.02	0.42
1:B:289[B]:LEU:HD12	1:B:289[B]:LEU:HA	1.81	0.41
1:A:176:GLN:O	1:A:180[A]:LEU:HG	2.19	0.41
1:B:21:ARG:NH1	6:B:702:HOH:O	2.53	0.41
1:B:528:THR:O	1:B:531:PHE:HB3	2.20	0.41
1:A:5:ASP:HB3	1:A:8:LEU:HD12	2.02	0.41
1:A:176:GLN:O	1:A:180[B]:LEU:HD13	2.20	0.41
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.55	0.41
1:A:252:ALA:HA	1:A:273[A]:LEU:HD21	2.01	0.41
1:A:289[B]:LEU:HD12	1:A:289[B]:LEU:HA	1.89	0.41
1:B:203:SUN:H2C2	1:B:338:PHE:CZ	2.56	0.41
1:B:104:PRO:HG2	1:B:108:PRO:HG3	2.02	0.41
1:B:460:ASP:HB3	1:B:463[B]:LEU:HD22	2.03	0.41
1:A:254[B]:LEU:HD12	1:A:254[B]:LEU:HA	1.90	0.41
1:A:384:ASP:HB2	1:A:393:HIS:CE1	2.56	0.41
1:B:527:GLN:HB3	5:B:610:7PG:H22	2.02	0.41
1:A:203:SUN:OG	1:A:447[B]:HIS:NE2	2.54	0.40
1:A:68[A]:VAL:HG23	1:A:90:ARG:HB2	2.02	0.40
1:A:380[A]:LEU:HD12	1:B:535:PHE:HB2	2.02	0.40
1:B:44:SER:HA	1:B:274:ARG:HD2	2.03	0.40
1:A:385:TRP:HD1	1:B:527:GLN:OE1	2.04	0.40
1:B:390:ASP:HA	1:B:391:PRO:HD2	1.78	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	573/543 (106%)	553 (96%)	19 (3%)	1 (0%)	47 58
1	B	570/543 (105%)	554 (97%)	15 (3%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1143/1086 (105%)	1107 (97%)	34 (3%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	GLY
1	A	342	GLY

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	478/442 (108%)	473 (99%)	5 (1%)	76 87
1	B	477/442 (108%)	472 (99%)	5 (1%)	76 87
All	All	955/884 (108%)	945 (99%)	10 (1%)	78 87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TYR
1	A	295	PHE
1	A	447[A]	HIS
1	A	447[B]	HIS
1	A	478	LYS
1	B	211[A]	MET
1	B	211[B]	MET
1	B	295	PHE
1	B	441	LEU
1	B	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SUN	B	203	1	11,13,14	1.45	1 (9%)	11,17,19	2.46	3 (27%)
1	SUN	A	203	1	11,13,14	1.55	2 (18%)	11,17,19	2.15	3 (27%)

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
1	SUN	B	203	1	-	2/15/18/20	-
1	SUN	A	203	1	-	2/15/18/20	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SUN	OG-CB	-2.77	1.34	1.44
1	A	203	SUN	P1-O1	2.76	1.50	1.46
1	B	203	SUN	P1-OG	2.58	1.68	1.57

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	203	SUN	OG-CB-CA	6.60	114.57	108.14
1	A	203	SUN	OG-CB-CA	5.78	113.77	108.14
1	B	203	SUN	OG-P1-O1	-2.78	106.50	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	203	SUN	O2-P1-OG	2.45	108.64	100.53
1	A	203	SUN	O2-P1-OG	2.24	107.94	100.53
1	A	203	SUN	OG-P1-O1	-2.13	108.63	115.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	SUN	N-CA-CB-OG
1	B	203	SUN	N-CA-CB-OG
1	A	203	SUN	C1-N1-P1-OG
1	B	203	SUN	C3-O2-P1-N1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	203	SUN	1	0
1	A	203	SUN	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	PG0	A	605	-	6,6,7	0.52	0	5,5,6	1.10	1 (20%)
4	PG0	B	604	-	7,7,7	0.60	0	6,6,6	0.87	0
4	PG0	A	609	-	7,7,7	0.60	0	6,6,6	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	602	1	14,14,15	0.38	0	17,19,21	0.53	0
4	PG0	A	606	-	7,7,7	0.60	0	6,6,6	0.79	0
4	PG0	B	605	-	7,7,7	0.61	0	6,6,6	1.02	1 (16%)
4	PG0	A	604	-	7,7,7	0.59	0	6,6,6	0.74	0
4	PG0	B	603	-	7,7,7	0.56	0	6,6,6	0.80	0
4	PG0	A	607	-	5,5,7	0.49	0	4,4,6	0.88	0
4	PG0	B	606	-	7,7,7	0.58	0	6,6,6	0.86	0
3	I1X	A	603	-	15,16,28	2.19	2 (13%)	17,21,36	1.09	1 (5%)
4	PG0	B	608	-	7,7,7	0.60	0	6,6,6	0.72	0
4	PG0	B	602	-	7,7,7	0.57	0	6,6,6	0.79	0
4	PG0	A	608	-	7,7,7	0.55	0	6,6,6	0.84	0
2	NAG	A	601	1	14,14,15	0.50	0	17,19,21	0.62	0
5	7PG	B	610	-	22,22,25	0.64	0	21,21,24	0.95	0
3	I1X	B	601	-	17,18,28	2.09	2 (11%)	19,23,36	1.01	0
4	PG0	B	609	-	7,7,7	0.55	0	6,6,6	0.89	0
4	PG0	B	607	-	7,7,7	0.58	0	6,6,6	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG0	A	605	-	-	2/4/4/5	-
4	PG0	B	604	-	-	4/5/5/5	-
4	PG0	A	609	-	-	2/5/5/5	-
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
4	PG0	A	606	-	-	5/5/5/5	-
4	PG0	B	605	-	-	3/5/5/5	-
4	PG0	A	604	-	-	2/5/5/5	-
4	PG0	B	603	-	-	2/5/5/5	-
4	PG0	A	607	-	-	2/3/3/5	-
4	PG0	B	606	-	-	3/5/5/5	-
3	I1X	A	603	-	-	1/10/12/20	0/1/1/2
4	PG0	B	608	-	-	4/5/5/5	-
4	PG0	B	602	-	-	4/5/5/5	-
4	PG0	A	608	-	-	3/5/5/5	-
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	7PG	B	610	-	-	14/20/20/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I1X	B	601	-	-	5/12/14/20	0/1/1/2
4	PG0	B	609	-	-	1/5/5/5	-
4	PG0	B	607	-	-	3/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	I1X	C02-N03	6.89	1.48	1.33
3	A	603	I1X	C02-N03	6.64	1.48	1.33
3	A	603	I1X	O25-N24	4.69	1.30	1.22
3	B	601	I1X	O25-N24	4.65	1.30	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	I1X	O25-N24-C23	2.38	123.10	119.03
4	A	605	PG0	C2-O1-C3	2.08	120.34	112.90
4	B	605	PG0	C2-O1-C3	2.04	122.14	113.29

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	I1X	C21-C23-N24-O25
3	B	601	I1X	C27-C23-N24-O25
2	A	601	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
4	A	607	PG0	O1-C3-C4-O2
4	A	604	PG0	O1-C3-C4-O2
4	A	606	PG0	O1-C3-C4-O2
3	B	601	I1X	N03-C04-C05-C06
4	A	608	PG0	O1-C3-C4-O2
4	B	607	PG0	OTT-C1-C2-O1
2	A	602	NAG	O5-C5-C6-O6
5	B	610	7PG	O5-C10-C9-O4
5	B	610	7PG	O3-C7-C8-O4
4	B	607	PG0	O1-C3-C4-O2
4	B	606	PG0	OTT-C1-C2-O1
4	B	608	PG0	OTT-C1-C2-O1
4	A	609	PG0	O1-C3-C4-O2
4	B	606	PG0	O1-C3-C4-O2

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Mol	Chain	Res	Type	Atoms
4	B	604	PG0	O1-C3-C4-O2
4	B	605	PG0	OTT-C1-C2-O1
4	A	606	PG0	OTT-C1-C2-O1
4	A	608	PG0	OTT-C1-C2-O1
4	B	602	PG0	OTT-C1-C2-O1
4	B	604	PG0	OTT-C1-C2-O1
5	B	610	7PG	OXT-C1-C2-O1
5	B	610	7PG	O5-C11-C12-O6
3	A	603	I1X	C27-C23-N24-O25
5	B	610	7PG	O1-C3-C4-O2
4	B	605	PG0	O1-C3-C4-O2
3	B	601	I1X	C04-C05-C06-C07
5	B	610	7PG	C4-C3-O1-C2
5	B	610	7PG	C12-C11-O5-C10
4	B	604	PG0	C4-C3-O1-C2
4	A	606	PG0	C1-C2-O1-C3
4	B	605	PG0	C3-C4-O2-C5
4	A	604	PG0	C4-C3-O1-C2
4	B	602	PG0	C1-C2-O1-C3
5	B	610	7PG	C10-C9-O4-C8
4	B	602	PG0	C4-C3-O1-C2
4	B	608	PG0	C3-C4-O2-C5
4	B	608	PG0	O1-C3-C4-O2
5	B	610	7PG	C9-C10-O5-C11
4	B	603	PG0	C3-C4-O2-C5
4	B	604	PG0	C1-C2-O1-C3
4	A	606	PG0	C3-C4-O2-C5
4	A	607	PG0	C4-C3-O1-C2
4	A	606	PG0	C4-C3-O1-C2
5	B	610	7PG	C3-C4-O2-C5
3	B	601	I1X	C05-C06-C07-C08
5	B	610	7PG	O2-C5-C6-O3
4	B	602	PG0	O1-C3-C4-O2
4	B	608	PG0	C4-C3-O1-C2
4	A	608	PG0	C3-C4-O2-C5
4	B	607	PG0	C1-C2-O1-C3
4	A	609	PG0	C1-C2-O1-C3
4	A	605	PG0	C4-C3-O1-C2
2	A	602	NAG	C4-C5-C6-O6
5	B	610	7PG	C1-C2-O1-C3
4	A	605	PG0	O1-C3-C4-O2
4	B	609	PG0	O1-C3-C4-O2

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Mol	Chain	Res	Type	Atoms
4	B	603	PG0	O1-C3-C4-O2
4	B	606	PG0	C1-C2-O1-C3
5	B	610	7PG	O6-C13-C14-O7
5	B	610	7PG	C14-C13-O6-C12

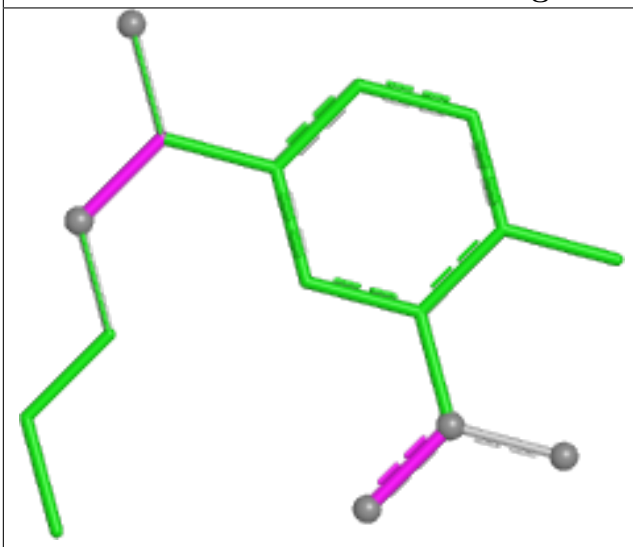
There are no ring outliers.

5 monomers are involved in 12 short contacts:

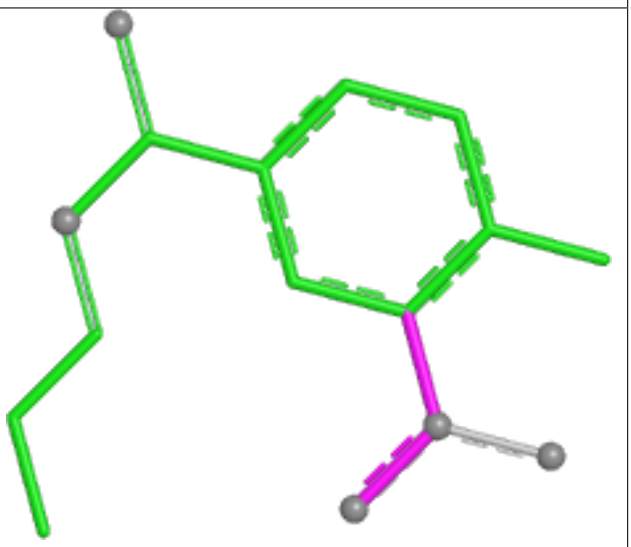
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	PG0	2	0
4	B	605	PG0	3	0
4	B	603	PG0	1	0
4	A	607	PG0	2	0
5	B	610	7PG	4	0

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.

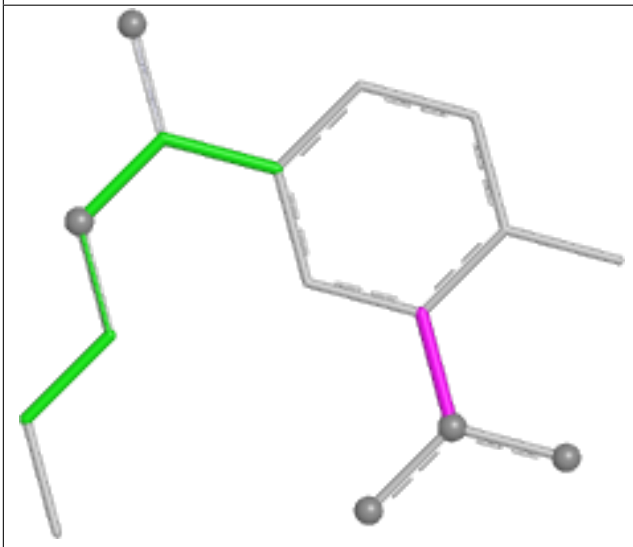
Ligand I1X A 603



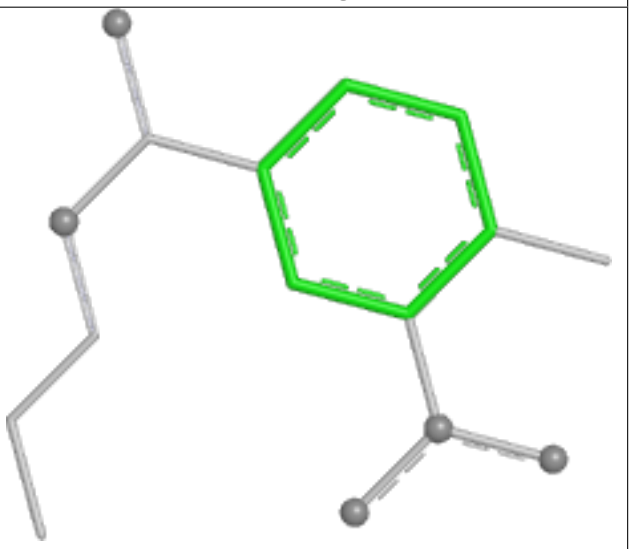
Bond lengths



Bond angles

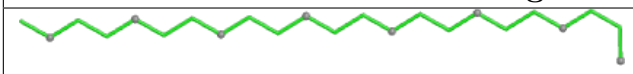


Torsions



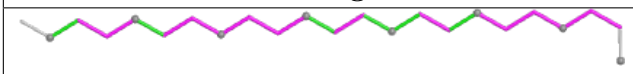
Rings

Ligand 7PG B 610



Bond lengths

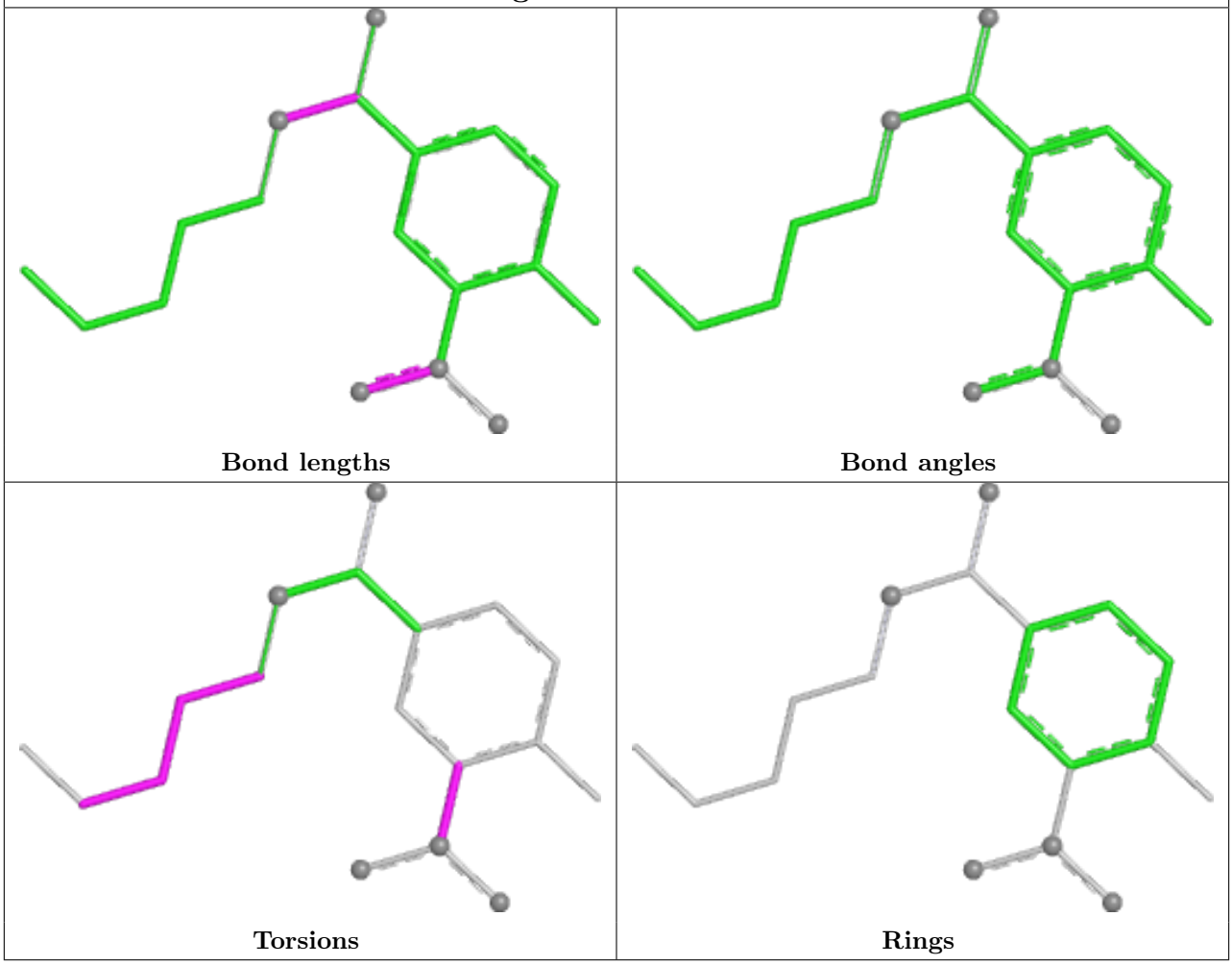
Bond angles



Torsions

Rings

Ligand I1X B 601



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	535/543 (98%)	0.49	23 (4%) 35 42	34, 50, 84, 135	0
1	B	532/543 (97%)	0.79	67 (12%) 3 5	37, 56, 88, 143	0
All	All	1067/1086 (98%)	0.64	90 (8%) 11 15	34, 53, 85, 143	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	SER	7.4
1	B	543	THR	7.1
1	A	495	SER	6.6
1	B	542	ALA	5.9
1	A	542	ALA	5.1
1	B	540	LEU	4.9
1	A	497	SER	4.5
1	A	496	LYS	4.2
1	B	9[A]	LEU	4.0
1	B	349	ASP	3.9
1	B	13	ARG	3.8
1	B	6	PRO	3.7
1	A	491	ASP	3.6
1	B	204	ALA	3.6
1	A	494	ASP	3.5
1	A	541	SER	3.4
1	B	27	GLY	3.3
1	B	76	LEU	3.3
1	B	451	ILE	3.2
1	B	265	ASN	3.1
1	B	342	GLY	3.1
1	A	206	ALA	3.1
1	A	347	SER	3.0
1	B	209	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	386	LEU	2.9
1	B	268	GLU	2.9
1	B	121	GLY	2.9
1	B	236	TRP	2.8
1	B	118	ILE	2.8
1	A	499	GLN	2.8
1	A	493	ARG	2.8
1	B	23	LYS	2.8
1	B	158	PHE	2.8
1	B	230	GLY	2.8
1	B	105	TYR	2.8
1	B	461	PRO	2.7
1	B	8[A]	LEU	2.7
1	A	376	GLU	2.7
1	B	318	THR	2.7
1	B	541	SER	2.7
1	B	201	GLY	2.7
1	B	106	PRO	2.7
1	B	206	ALA	2.7
1	B	207	ALA	2.7
1	A	470	ARG	2.6
1	B	7	GLN	2.6
1	A	463[A]	LEU	2.6
1	A	230	GLY	2.6
1	A	467	THR	2.6
1	B	117	TRP	2.5
1	A	498	PRO	2.5
1	B	226	VAL	2.5
1	B	436	THR	2.5
1	B	227	LEU	2.5
1	B	297	PHE	2.4
1	B	5	ASP	2.4
1	B	125	SER	2.4
1	B	355	SER	2.4
1	B	109	ALA	2.4
1	B	151	TYR	2.4
1	B	447[A]	HIS	2.4
1	B	391	PRO	2.4
1	B	411	VAL	2.4
1	B	4	GLU	2.4
1	B	119	TYR	2.3
1	B	120	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	122	GLY	2.2
1	B	351	GLU	2.2
1	A	27	GLY	2.2
1	B	205	GLY	2.2
1	B	229	SER	2.2
1	B	320	ASP	2.2
1	B	269[A]	LEU	2.2
1	B	352	SER	2.2
1	B	107	ARG	2.2
1	B	12	VAL	2.1
1	B	123	PHE	2.1
1	A	204	ALA	2.1
1	A	209	VAL	2.1
1	B	255[A]	VAL	2.1
1	B	435	SER	2.1
1	A	118	ILE	2.1
1	B	539	LEU	2.1
1	B	231	THR	2.1
1	A	205	GLY	2.1
1	B	331	VAL	2.0
1	B	220	SER	2.0
1	B	374	ALA	2.0
1	A	226	VAL	2.0
1	B	343	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SUN	A	203	14/15	0.96	0.17	34,44,68,76	0
1	SUN	B	203	14/15	0.96	0.22	37,46,74,84	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

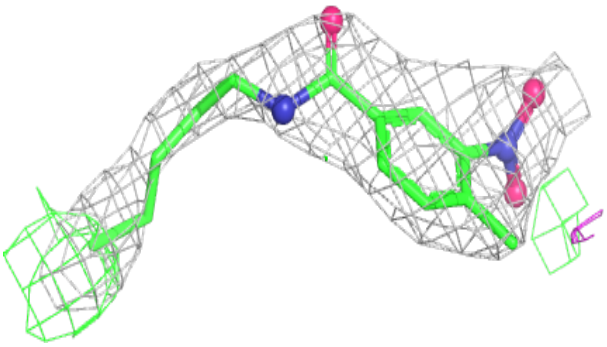
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

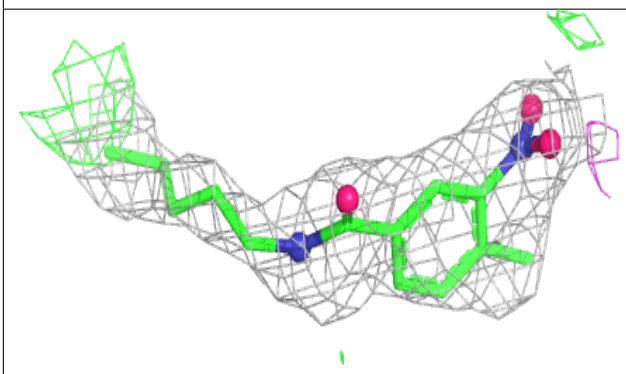
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG0	B	607	8/8	0.41	0.35	83,88,95,96	0
4	PG0	B	609	8/8	0.55	0.22	94,100,104,104	0
2	NAG	A	602	14/15	0.57	0.43	100,111,120,120	0
2	NAG	A	601	14/15	0.64	0.47	83,96,111,112	0
4	PG0	A	608	8/8	0.71	0.18	77,86,90,91	0
4	PG0	B	605	8/8	0.73	0.22	86,94,97,100	0
4	PG0	B	606	8/8	0.73	0.33	86,88,91,93	0
3	I1X	B	601	18/27	0.75	0.32	68,103,114,122	0
4	PG0	B	608	8/8	0.78	0.22	82,89,101,102	0
4	PG0	A	607	6/8	0.78	0.33	80,89,92,94	0
4	PG0	A	606	8/8	0.80	0.21	85,88,95,97	0
4	PG0	A	605	7/8	0.81	0.23	61,69,86,86	0
4	PG0	B	603	8/8	0.82	0.19	60,78,99,101	0
4	PG0	A	604	8/8	0.82	0.22	69,76,88,90	0
4	PG0	A	609	8/8	0.83	0.35	85,91,109,111	0
4	PG0	B	602	8/8	0.83	0.17	74,80,86,92	0
4	PG0	B	604	8/8	0.85	0.18	79,84,91,93	0
5	7PG	B	610	23/26	0.86	0.18	46,75,90,91	0
3	I1X	A	603	16/27	0.90	0.21	69,76,85,95	0

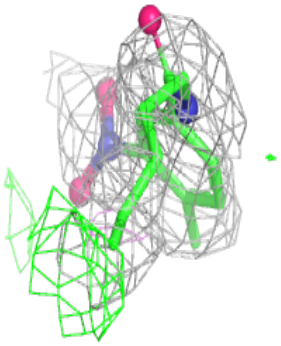
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around I1X B 601:

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

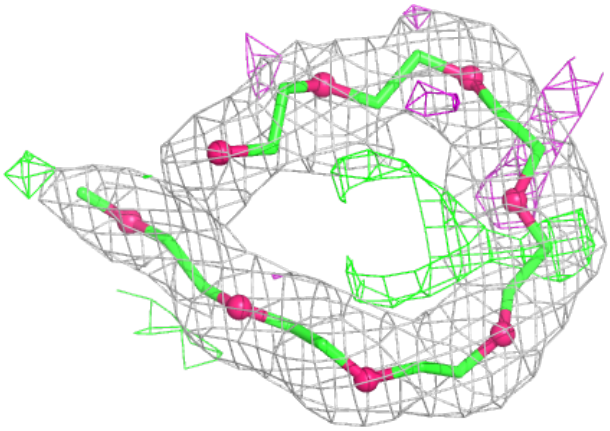


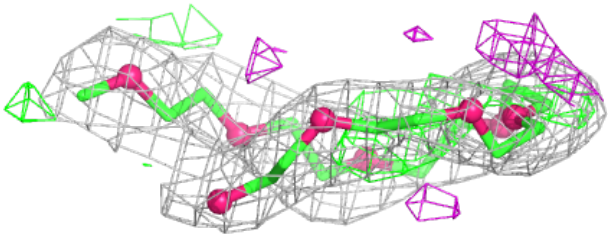


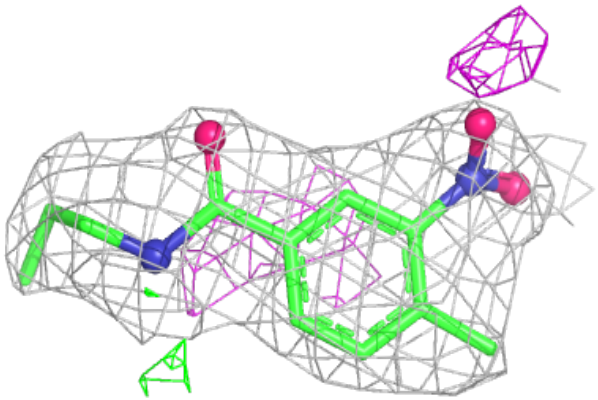
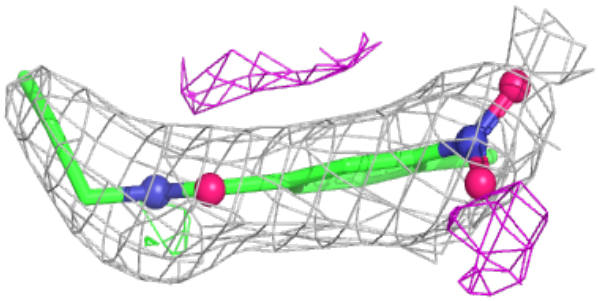
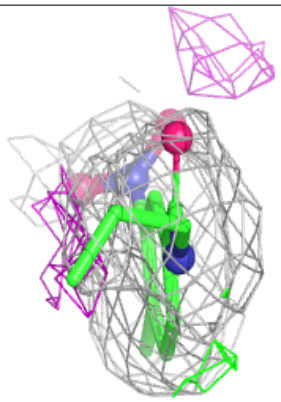


Electron density around 7PG B 610:

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





Electron density around I1X A 603: 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.