



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2021 – 10:09 pm BST

PDB ID : 5FPP
Title : Structure of a pre-reaction ternary complex between sarin- acetylcholinesterase and HI-6
Authors : Allgardsson, A.; Berg, L.; Akfur, C.; Hornberg, A.; Worek, F.; Linusson, A.; Ekstrom, F.
Deposited on : 2015-12-02
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.18
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) : 2.18

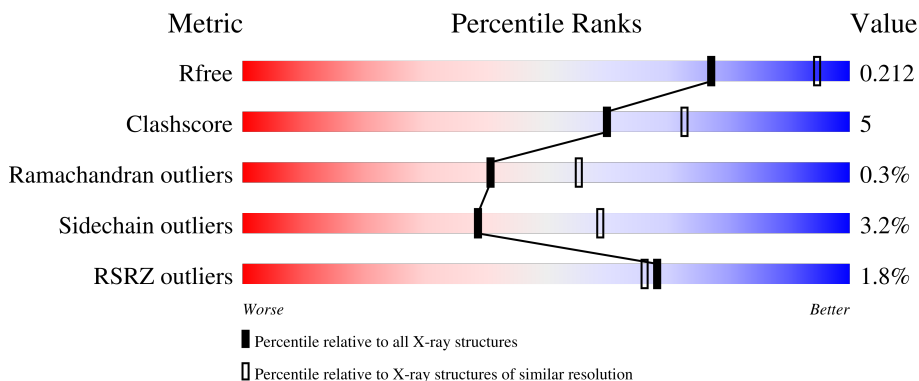
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


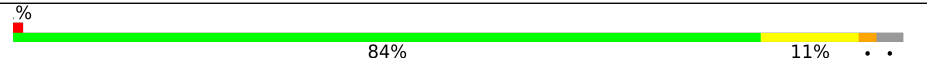
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	548	
1	B	548	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9061 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	541	Total	C	N	O	P	S	0	7	0
			4277	2737	748	777	1	14			
1	B	533	Total	C	N	O	P	S	0	2	0
			4190	2688	724	763	1	14			

There are 10 discrepancies between the modelled and reference sequences:

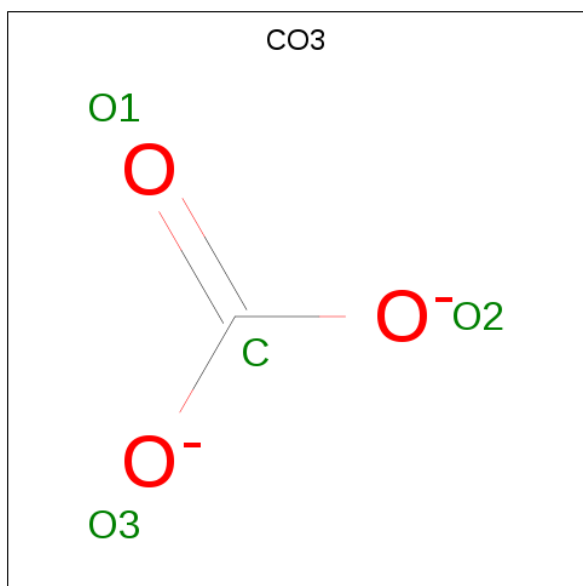
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ALA	-	expression tag	UNP P21836
A	545	THR	-	expression tag	UNP P21836
A	546	GLU	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	expression tag	UNP P21836
B	544	ALA	-	expression tag	UNP P21836
B	545	THR	-	expression tag	UNP P21836
B	546	GLU	-	expression tag	UNP P21836
B	547	ALA	-	expression tag	UNP P21836
B	548	PRO	-	expression tag	UNP P21836

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



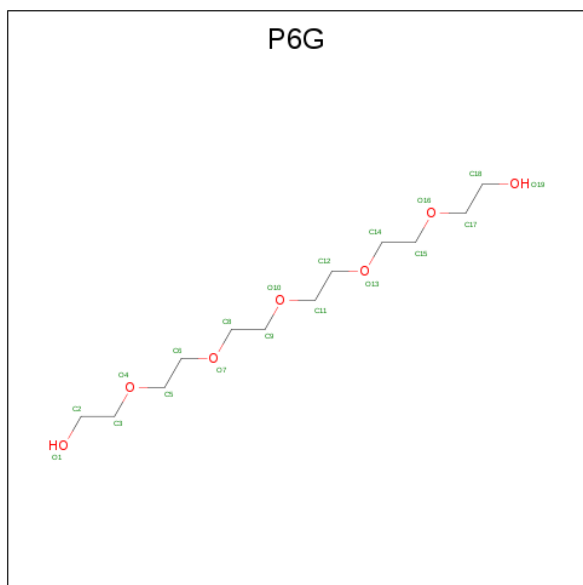
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	14	8	1	5	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



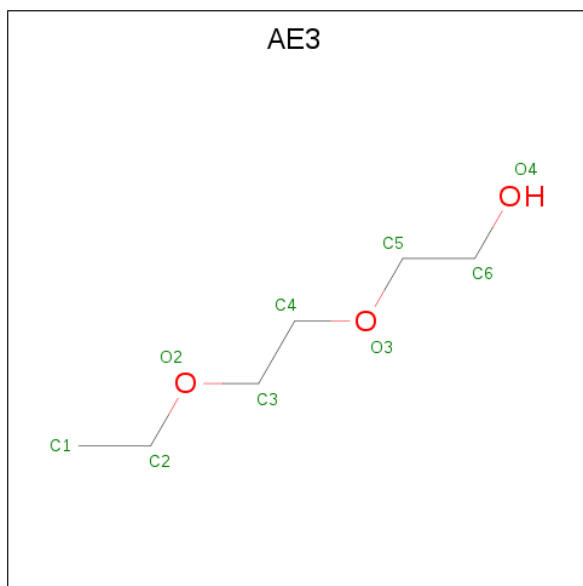
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	1	3	0	0
3	B	1	4	1	3	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



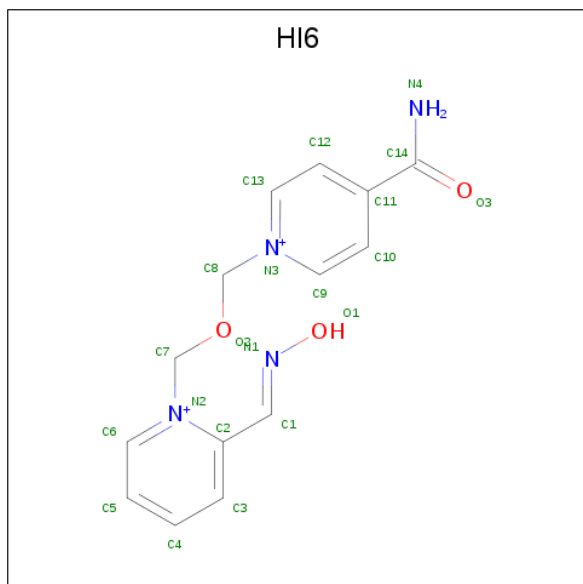
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: $C_6H_{14}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	6	3		
5	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 6 is 4-(AMINOCARBONYL)-1-[(2-[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL)METHOXY]METHYL]PYRIDINIUM (three-letter code: HI6) (formula: $C_{14}H_{16}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	Total	C	N	O	0	1
			42	28	8	6		
6	B	1	Total	C	N	O	0	1
			36	26	6	4		

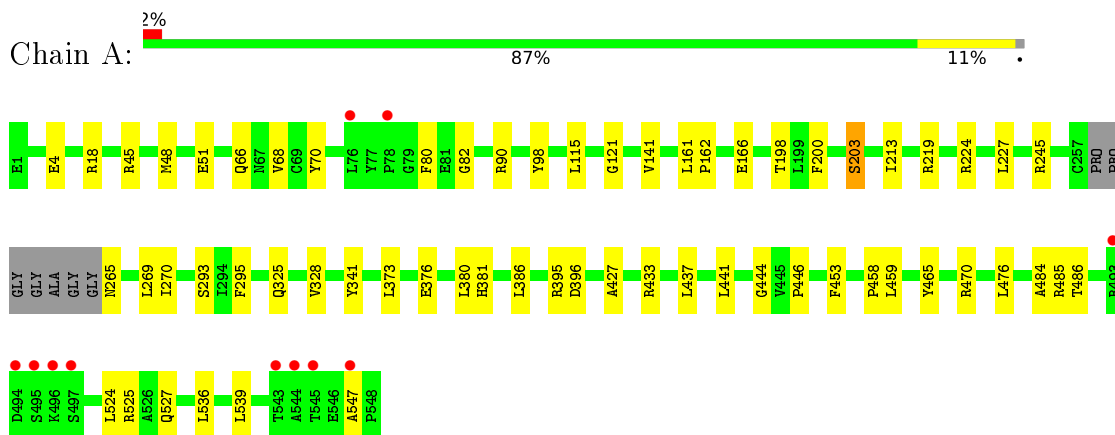
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	263	Total	O	0	0
			263	263		
7	B	194	Total	O	0	0
			194	194		

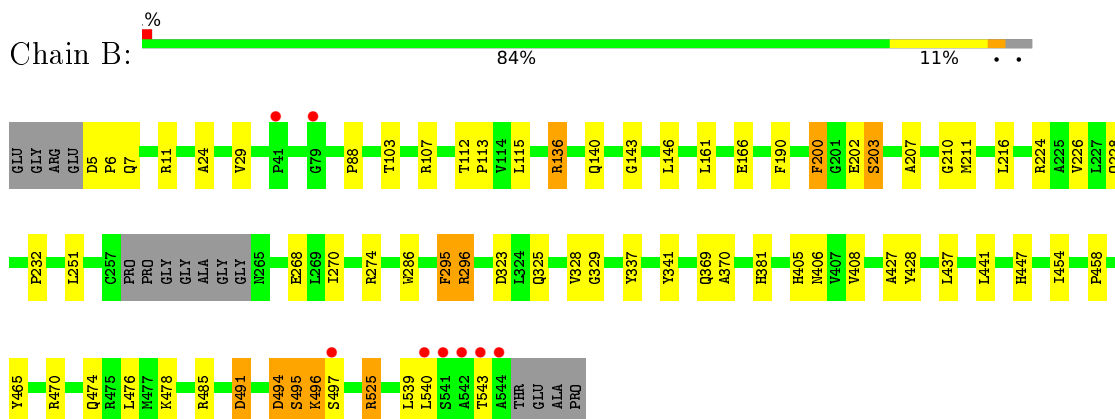
3 Residue-property plots [i](#)

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



- Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.83Å 111.55Å 227.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.95 – 2.40 28.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.95-2.40) 98.0 (28.95-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.176 , 0.213 0.178 , 0.212	Depositor DCC
R_{free} test set	1542 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9061	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: NAG, HI6, SGB, AE3, CO3, P6G

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	0.40	0/4390	0.56	0/5994
1	B	0.38	0/4299	0.54	0/5874
All	All	0.39	0/8689	0.55	0/11868

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	4277	0	4143	36	0
1	B	4190	0	4078	39	0
2	A	14	0	13	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	19	0	24	5	0
5	A	9	0	14	0	0
5	B	9	0	14	0	0
6	A	42	0	32	5	0
6	B	36	0	28	9	0
7	A	263	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	194	0	0	3	0
All	All	9061	0	8346	78	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 5.

All (78) 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:203:SGB:H4C1	6:B:1545[A]:HI6:H13	1.49	0.94
1:A:121:GLY:HA2	1:A:203:SGB:H3C3	1.60	0.84
1:B:203:SGB:H3C1	6:B:1545[B]:HI6:H3	1.73	0.69
6:B:1545[A]:HI6:O3	7:B:2194:HOH:O	2.12	0.68
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.77	0.66
1:B:495:SER:OG	1:B:496:LYS:N	2.29	0.66
1:B:203:SGB:H3C3	1:B:447:HIS:CD2	2.32	0.65
1:B:203:SGB:H3C3	1:B:447:HIS:HD2	1.63	0.63
1:A:341:TYR:CZ	6:A:1552[B]:HI6:H5	2.32	0.63
1:B:295:PHE:H	6:B:1545[A]:HI6:HN41	1.45	0.62
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.81	0.62
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.85	0.59
1:A:381:HIS:HA	4:A:1550:P6G:H31	1.84	0.58
1:B:203:SGB:C3	6:B:1545[B]:HI6:H3	2.33	0.58
1:B:7:GLN:O	1:B:107[B]:ARG:NH2	2.35	0.58
1:A:341:TYR:CZ	6:A:1552[A]:HI6:H5	2.38	0.58
6:A:1552[B]:HI6:O1	6:A:1552[B]:HI6:H3	2.04	0.57
1:B:341:TYR:CD1	6:B:1545[B]:HI6:H72	2.39	0.57
6:A:1552[B]:HI6:O1	6:A:1552[B]:HI6:C3	2.53	0.56
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.87	0.55
1:A:527:GLN:HG3	4:A:1550:P6G:H182	1.87	0.55
1:A:328:VAL:O	1:A:427:ALA:HA	2.06	0.55
1:A:485:ARG:HB3	1:A:486:THR:HG23	1.89	0.54
1:A:45:ARG:NH1	1:A:51:GLU:OE1	2.31	0.53
1:B:328:VAL:O	1:B:427:ALA:HA	2.11	0.51
1:B:112:THR:HG21	1:B:143:GLY:O	2.12	0.50
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.94	0.50
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.94	0.50
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.45	0.49
1:B:539:LEU:O	1:B:543:THR:HG22	2.13	0.49
1:B:286:TRP:CH2	6:B:1545[B]:HI6:H82	2.48	0.49
1:A:376[A]:GLU:O	1:A:380:LEU:HG	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ALA:O	1:B:211:MET:HG2	2.12	0.49
1:A:381:HIS:ND1	4:A:1550:P6G:H22	2.28	0.49
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.93	0.49
1:A:45:ARG:HA	1:A:48:MET:HG3	1.94	0.48
1:A:4:GLU:OE1	1:A:18:ARG:HD3	2.13	0.48
1:B:369:GLN:HE22	1:B:405:HIS:CE1	2.32	0.48
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.95	0.47
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.96	0.47
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.96	0.47
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.96	0.47
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.96	0.47
1:B:203:SGB:H4C1	6:B:1545[A]:HI6:C13	2.34	0.45
1:A:458:PRO:O	1:A:470[B]:ARG:HG2	2.17	0.45
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.52	0.44
4:A:1550:P6G:H172	1:B:381:HIS:ND1	2.32	0.44
1:B:370:ALA:HA	1:B:540:LEU:HD21	1.99	0.44
1:B:103:THR:HG21	1:B:190:PHE:HB3	2.00	0.44
1:B:200:PHE:CB	1:B:226:VAL:HB	2.48	0.43
1:B:202:GLU:HA	1:B:228:GLN:O	2.18	0.43
1:A:376[B]:GLU:O	1:A:380:LEU:HG	2.16	0.43
1:A:381:HIS:HD1	4:A:1550:P6G:H22	1.83	0.43
1:A:48:MET:HE1	1:A:166:GLU:HA	2.00	0.43
1:A:373:LEU:HD23	1:A:539:LEU:HD11	1.99	0.43
1:B:5:ASP:HA	1:B:6:PRO:HD2	1.91	0.43
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.54	0.43
1:B:88:PRO:HD3	7:B:2039:HOH:O	2.17	0.43
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.53	0.43
1:A:166:GLU:HB2	1:A:270:ILE:HD13	2.01	0.42
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.54	0.42
1:B:454:ILE:HD13	1:B:476:LEU:HB3	2.01	0.42
1:A:162:PRO:HB2	1:A:245[B]:ARG:HH21	1.85	0.41
1:A:265:ASN:ND2	7:A:2168:HOH:O	2.35	0.41
1:A:433[B]:ARG:CZ	1:A:437:LEU:HD23	2.50	0.41
1:A:115:LEU:HD23	1:A:198:THR:HB	2.03	0.41
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.01	0.41
1:B:337:TYR:OH	6:B:1545[A]:HI6:H71	2.20	0.41
1:A:213:ILE:O	1:A:219:ARG:HD3	2.21	0.41
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.21	0.41
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.56	0.40
1:A:444:GLY:O	1:A:446:PRO:HD3	2.20	0.40
1:B:29:VAL:HG21	1:B:136:ARG:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.52	0.40
1:A:341:TYR:CZ	6:A:1552[A]:HI6:C5	3.02	0.40
1:B:274:ARG:NH1	7:B:2022:HOH:O	2.44	0.40
1:B:470:ARG:O	1:B:474:GLN:HG3	2.22	0.40
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.57	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	543/548 (99%)	524 (96%)	18 (3%)	1 (0%)	47 62
1	B	531/548 (97%)	512 (96%)	17 (3%)	2 (0%)	34 48
All	All	1074/1096 (98%)	1036 (96%)	35 (3%)	3 (0%)	41 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	ALA
1	B	496	LYS
1	B	495	SER

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	444/445 (100%)	435 (98%)	9 (2%)	55	74
1	B	439/445 (99%)	420 (96%)	19 (4%)	29	46
All	All	883/890 (99%)	855 (97%)	28 (3%)	39	59

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TYR
1	A	200	PHE
1	A	293	SER
1	A	295	PHE
1	A	386	LEU
1	A	441	LEU
1	A	524	LEU
1	A	525	ARG
1	A	536	LEU
1	B	11	ARG
1	B	115	LEU
1	B	136	ARG
1	B	146	LEU
1	B	161	LEU
1	B	200	PHE
1	B	216	LEU
1	B	251	LEU
1	B	268	GLU
1	B	295	PHE
1	B	296	ARG
1	B	323	ASP
1	B	437	LEU
1	B	441	LEU
1	B	478	LYS
1	B	491	ASP
1	B	494	ASP
1	B	497	SER
1	B	525	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	SGB	B	203	1	10,12,13	1.29	1 (10%)	9,16,18	0.65	0
1	SGB	A	203	1	10,12,13	1.28	1 (10%)	9,16,18	0.65	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
1	SGB	B	203	1	-	3/10/13/15	-
1	SGB	A	203	1	-	1/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	SGB	P1-OG	2.95	1.62	1.58
1	A	203	SGB	P1-OG	2.93	1.62	1.58

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	203	SGB	C2-O2-P1-O1
1	B	203	SGB	C2-O2-P1-C1
1	A	203	SGB	N-CA-CB-OG
1	B	203	SGB	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	203	SGB	6	0
1	A	203	SGB	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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$
6	HI6	A	1552[B]	-	18,22,22	2.56	7 (38%)	19,28,28	1.61	4 (21%)
2	NAG	A	601	1	14,14,15	0.78	1 (7%)	17,19,21	0.80	1 (5%)
5	AE3	A	1551	-	8,8,8	0.60	0	7,7,7	1.53	1 (14%)
3	CO3	A	1549	-	0,3,3	0.00	-	0,3,3	0.00	-
6	HI6	B	1545[B]	-	15,19,22	2.00	6 (40%)	17,24,28	1.37	3 (17%)
6	HI6	A	1552[A]	-	18,22,22	2.56	7 (38%)	19,28,28	1.62	4 (21%)
4	P6G	A	1550	-	18,18,18	1.76	5 (27%)	17,17,17	2.02	9 (52%)
3	CO3	B	1547	-	0,3,3	0.00	-	0,3,3	0.00	-
5	AE3	B	1546	-	8,8,8	0.56	0	7,7,7	1.63	1 (14%)
6	HI6	B	1545[A]	-	15,19,22	2.04	6 (40%)	17,24,28	1.22	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HI6	A	1552[B]	-	-	1/12/13/13	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	AE3	A	1551	-	-	4/6/6/6	-
6	HI6	B	1545[B]	-	-	5/10/10/13	0/2/2/2
6	HI6	A	1552[A]	-	-	0/12/13/13	0/2/2/2
4	P6G	A	1550	-	-	6/16/16/16	-
5	AE3	B	1546	-	-	5/6/6/6	-
6	HI6	B	1545[A]	-	-	1/10/10/13	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1552[A]	HI6	O1-N1	-6.54	1.26	1.40
6	A	1552[B]	HI6	O1-N1	-6.50	1.26	1.40
6	A	1552[B]	HI6	C14-N4	4.53	1.41	1.33
6	A	1552[A]	HI6	C14-N4	4.47	1.41	1.33
6	B	1545[B]	HI6	C14-N4	4.20	1.41	1.33
6	A	1552[B]	HI6	C2-N2	4.19	1.41	1.37
6	A	1552[A]	HI6	C2-N2	4.17	1.41	1.37
6	B	1545[A]	HI6	C14-N4	3.81	1.40	1.33
6	A	1552[A]	HI6	C11-C14	3.16	1.55	1.50
6	B	1545[A]	HI6	O3-C14	-3.14	1.18	1.24
6	A	1552[B]	HI6	C11-C14	3.06	1.55	1.50
6	B	1545[A]	HI6	C11-C14	3.01	1.55	1.50
4	A	1550	P6G	C17-C18	-3.01	1.33	1.49
6	B	1545[B]	HI6	O3-C14	-3.00	1.18	1.24
6	B	1545[A]	HI6	C2-N2	2.94	1.41	1.34
6	A	1552[A]	HI6	O3-C14	-2.94	1.18	1.24
4	A	1550	P6G	C9-C8	-2.92	1.33	1.49
6	A	1552[B]	HI6	O3-C14	-2.92	1.18	1.24
4	A	1550	P6G	C15-C14	-2.88	1.34	1.49
4	A	1550	P6G	C3-C2	-2.86	1.34	1.49
4	A	1550	P6G	C6-C5	-2.81	1.34	1.49
6	B	1545[B]	HI6	C2-N2	2.70	1.41	1.34
2	A	601	NAG	O5-C1	2.62	1.47	1.43
6	B	1545[A]	HI6	C9-N3	2.51	1.40	1.34
6	A	1552[B]	HI6	C9-N3	2.49	1.40	1.34
6	B	1545[B]	HI6	C9-N3	2.49	1.40	1.34
6	A	1552[A]	HI6	C9-N3	2.46	1.40	1.34
6	B	1545[B]	HI6	C11-C14	2.45	1.54	1.50
6	B	1545[B]	HI6	C12-C11	2.31	1.43	1.39
6	A	1552[B]	HI6	C12-C11	2.21	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1552[A]	HI6	C12-C11	2.19	1.43	1.39
6	B	1545[A]	HI6	C12-C11	2.09	1.42	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1552[A]	HI6	O1-N1-C1	4.55	119.89	111.86
6	A	1552[B]	HI6	O1-N1-C1	4.49	119.78	111.86
6	B	1545[B]	HI6	C11-C14-N4	3.54	122.00	117.75
6	B	1545[A]	HI6	C11-C14-N4	3.09	121.46	117.75
4	A	1550	P6G	O7-C8-C9	3.08	124.28	110.39
6	B	1545[A]	HI6	O3-C14-N4	-2.96	118.37	122.58
6	A	1552[B]	HI6	C11-C14-N4	2.91	121.24	117.75
4	A	1550	P6G	O10-C9-C8	2.89	123.44	110.39
6	A	1552[A]	HI6	C11-C14-N4	2.88	121.21	117.75
2	A	601	NAG	C1-O5-C5	2.77	115.94	112.19
4	A	1550	P6G	O16-C17-C18	2.44	120.81	110.07
4	A	1550	P6G	O7-C6-C5	2.37	121.08	110.39
4	A	1550	P6G	O16-C15-C14	2.34	120.93	110.39
6	A	1552[B]	HI6	O3-C14-N4	-2.34	119.26	122.58
6	B	1545[B]	HI6	C2-C3-C4	2.34	122.34	118.85
5	B	1546	AE3	C2-O2-C3	2.33	121.24	112.90
6	A	1552[A]	HI6	O3-C14-N4	-2.30	119.31	122.58
6	A	1552[B]	HI6	C3-C2-N2	2.28	120.31	117.52
4	A	1550	P6G	C5-O4-C3	2.25	123.03	113.29
6	A	1552[A]	HI6	C3-C2-N2	2.25	120.27	117.52
6	B	1545[B]	HI6	O3-C14-N4	-2.22	119.42	122.58
4	A	1550	P6G	O13-C14-C15	2.19	120.27	110.39
4	A	1550	P6G	O4-C3-C2	2.18	119.66	110.07
4	A	1550	P6G	O4-C5-C6	2.15	120.11	110.39
5	A	1551	AE3	C2-O2-C3	2.01	120.12	112.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1545[A]	HI6	O2-C7-N2-C6
6	B	1545[B]	HI6	O2-C8-N3-C9
6	B	1545[B]	HI6	O2-C8-N3-C13
6	B	1545[B]	HI6	O2-C7-N2-C6
5	B	1546	AE3	O2-C3-C4-O3
2	A	601	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

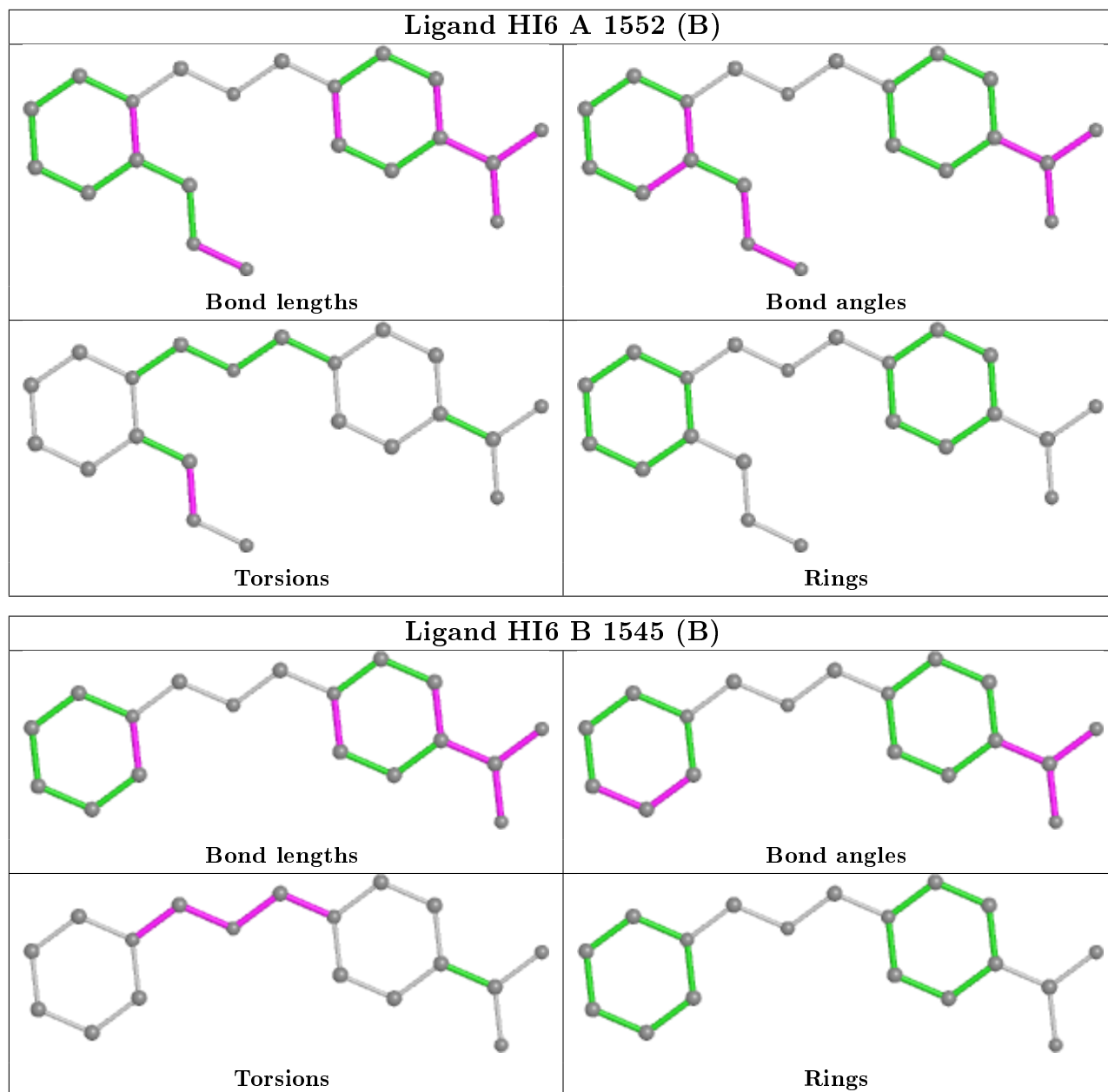
Mol	Chain	Res	Type	Atoms
6	B	1545[B]	HI6	N2-C7-O2-C8
2	A	601	NAG	C4-C5-C6-O6
4	A	1550	P6G	O13-C14-C15-O16
4	A	1550	P6G	O4-C5-C6-O7
4	A	1550	P6G	O7-C8-C9-O10
5	B	1546	AE3	C4-C3-O2-C2
4	A	1550	P6G	C18-C17-O16-C15
5	A	1551	AE3	C1-C2-O2-C3
5	A	1551	AE3	C4-C3-O2-C2
6	B	1545[B]	HI6	N3-C8-O2-C7
6	A	1552[B]	HI6	C2-C1-N1-O1
4	A	1550	P6G	C14-C15-O16-C17
5	B	1546	AE3	O3-C5-C6-O4
5	B	1546	AE3	C1-C2-O2-C3
4	A	1550	P6G	C6-C5-O4-C3
5	B	1546	AE3	C6-C5-O3-C4
5	A	1551	AE3	O2-C3-C4-O3
5	A	1551	AE3	C3-C4-O3-C5

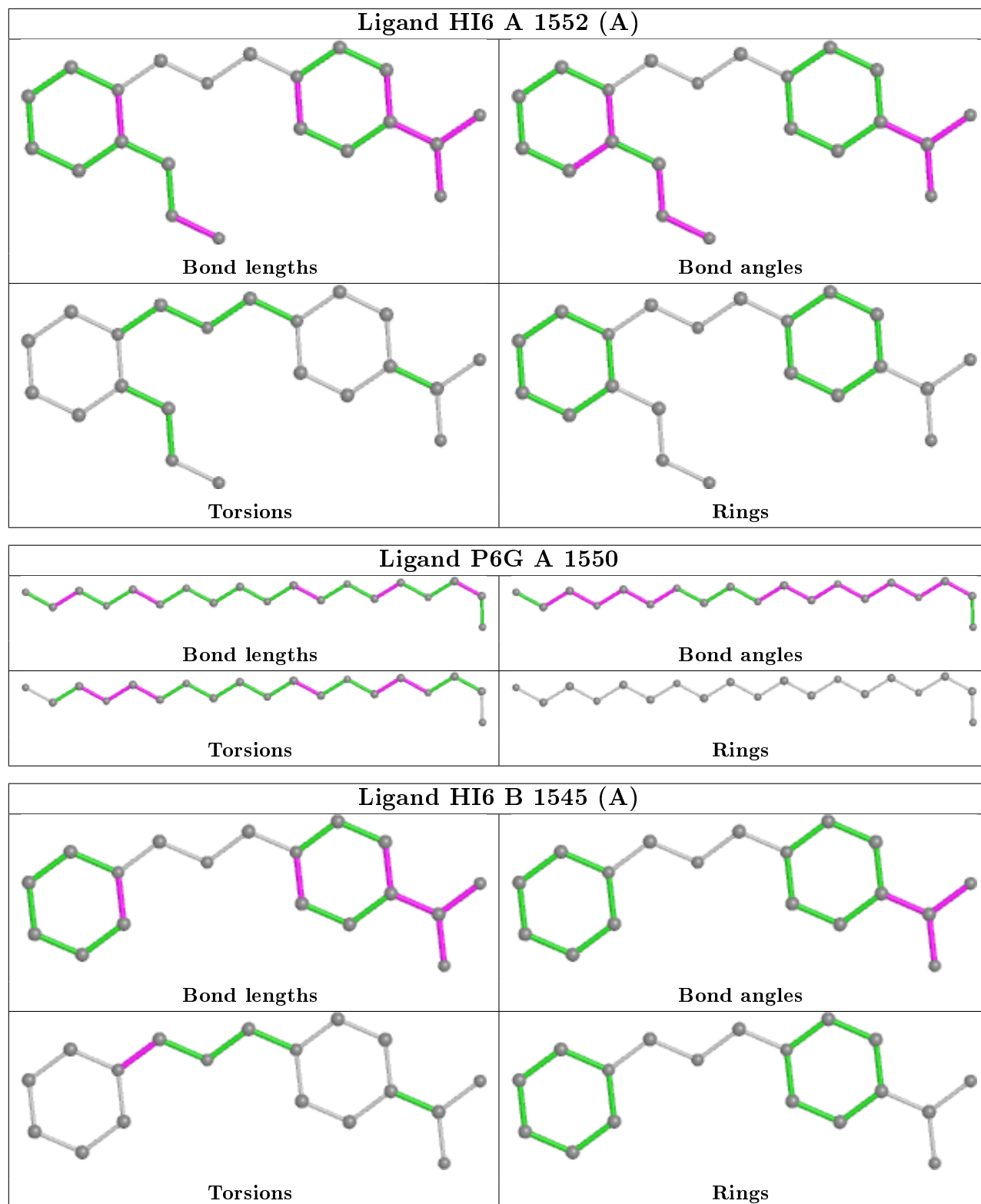
There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1552[B]	HI6	3	0
6	B	1545[B]	HI6	4	0
6	A	1552[A]	HI6	2	0
4	A	1550	P6G	5	0
6	B	1545[A]	HI6	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	540/548 (98%)	-0.54	11 (2%) 65 63	22, 36, 71, 126	0
1	B	532/548 (97%)	-0.45	8 (1%) 73 72	24, 42, 70, 135	0
All	All	1072/1096 (97%)	-0.49	19 (1%) 68 66	22, 39, 71, 135	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	4.8
1	B	497	SER	4.4
1	A	544	ALA	4.0
1	B	542	ALA	3.5
1	B	544	ALA	3.2
1	A	494	ASP	3.0
1	B	543	THR	3.0
1	A	547	ALA	3.0
1	A	497	SER	3.0
1	A	76	LEU	3.0
1	A	545	THR	2.9
1	A	493	ARG	2.9
1	B	540	LEU	2.8
1	A	78	PRO	2.7
1	A	543	THR	2.5
1	B	541	SER	2.4
1	A	496	LYS	2.3
1	B	79	GLY	2.2
1	B	41	PRO	2.2

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	SGB	A	203	13/14	0.93	0.36	20,28,48,50	7
1	SGB	B	203	13/14	0.96	0.27	24,28,36,37	7

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

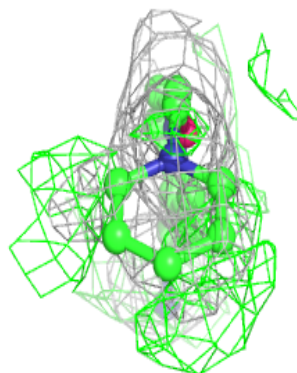
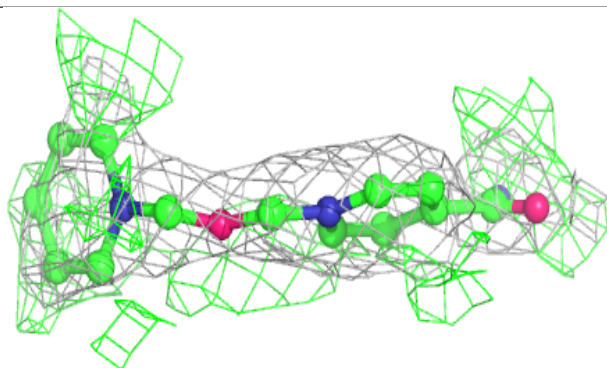
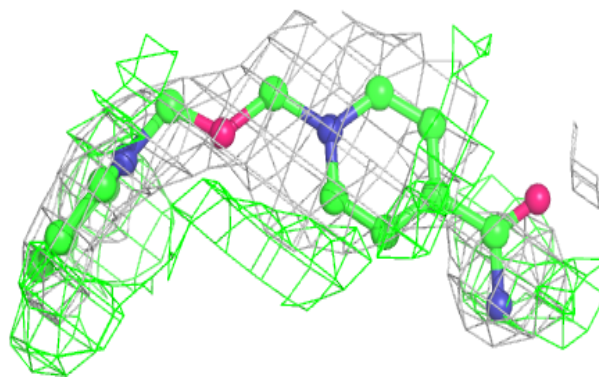
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	HI6	B	1545[A]	18/21	0.83	0.36	12,40,60,61	18
6	HI6	B	1545[B]	18/21	0.83	0.36	12,26,60,62	18
2	NAG	A	601	14/15	0.84	0.34	69,85,90,91	0
5	AE3	B	1546	9/9	0.87	0.16	47,57,74,76	0
5	AE3	A	1551	9/9	0.88	0.17	57,72,81,83	0
3	CO3	A	1549	4/4	0.88	0.20	64,65,70,74	0
4	P6G	A	1550	19/19	0.91	0.23	40,63,83,85	0
6	HI6	A	1552[B]	21/21	0.92	0.18	43,61,75,75	21
3	CO3	B	1547	4/4	0.92	0.24	89,90,91,92	0
6	HI6	A	1552[A]	21/21	0.92	0.18	43,62,74,75	21

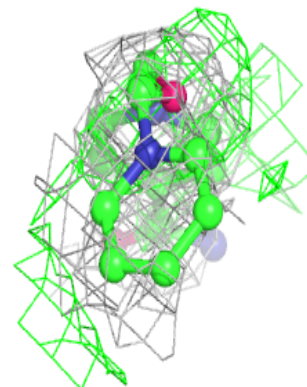
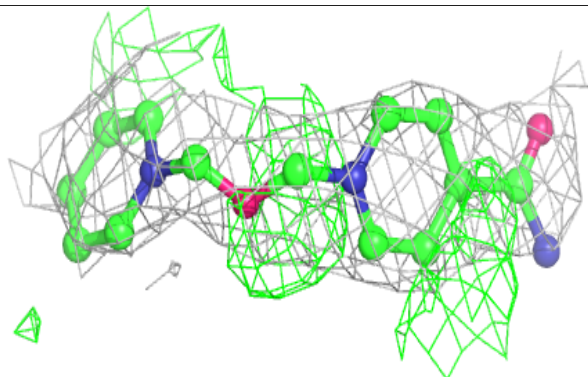
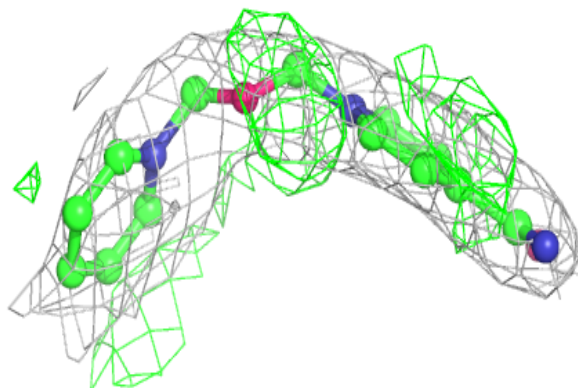
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HI6 B 1545 (A):

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

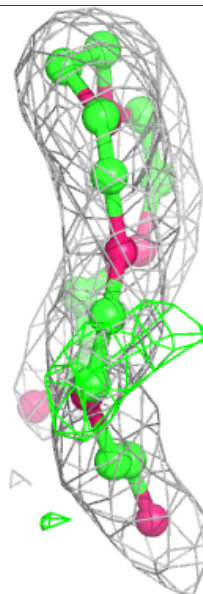
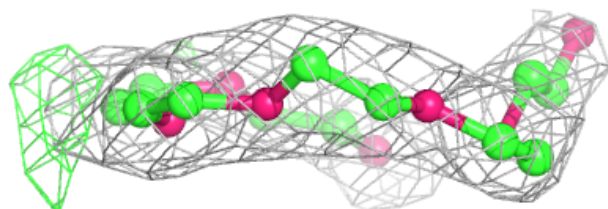
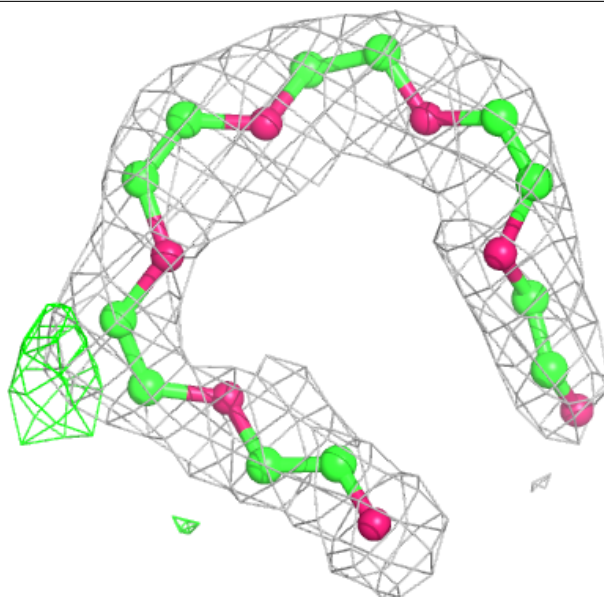
**Electron density around HI6 B 1545 (B):**

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



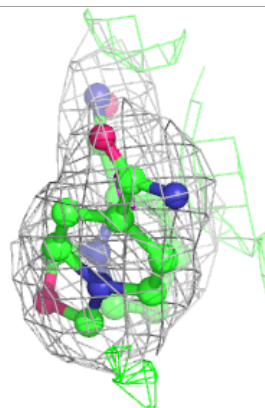
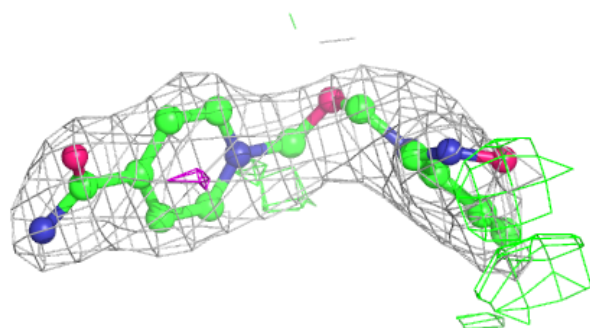
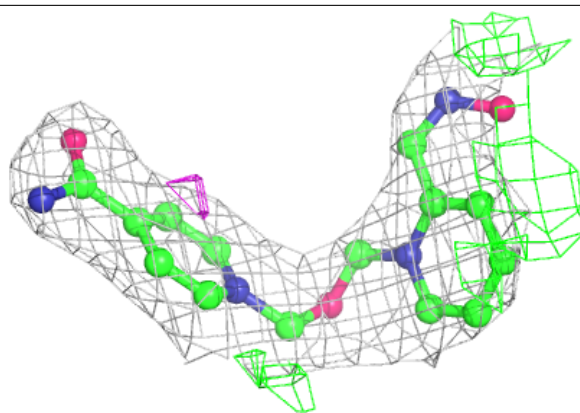
Electron density around P6G A 1550:

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

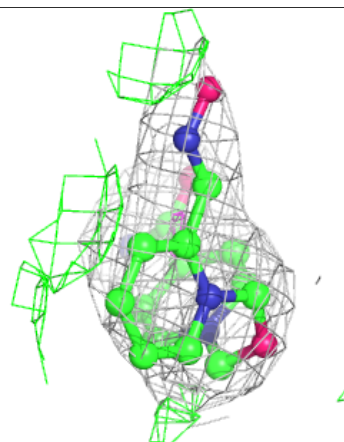
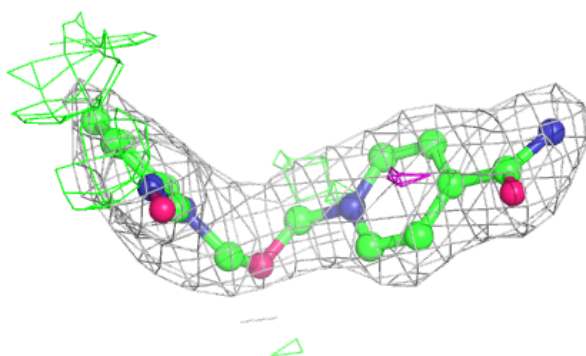
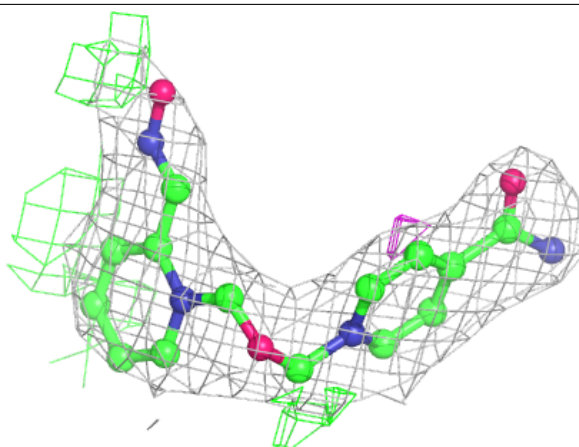


Electron density around HI6 A 1552 (B):

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

**Electron density around HI6 A 1552 (A):**

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



6.5 Other polymers

There are no such residues in this entry.