



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2021 – 10:12 pm BST

PDB ID : 5OV9
Title : Crystal structure of Acetylcholinesterase in complex with Crystal Violet
Authors : Allgardsson, A.; Andersson, C.D.; Akfur, C.; Worek, F.; Linusson, A.; Ekstrom, F.
Deposited on : 2017-08-28
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

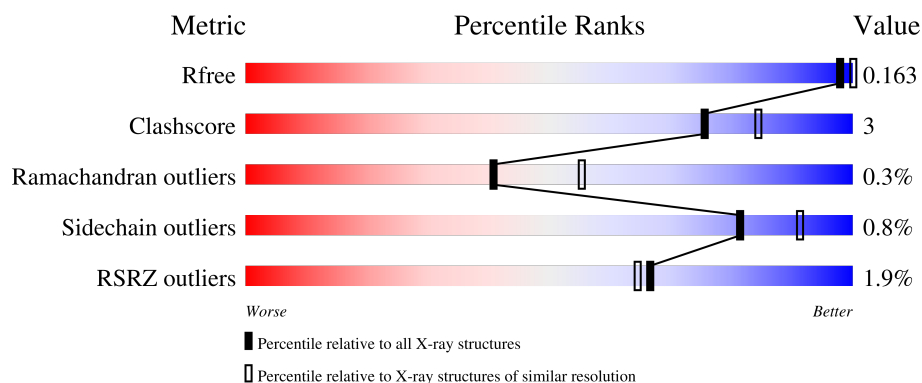
1 Overall quality at a glance

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	<div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div>
1	B	548	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div></div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9130 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.

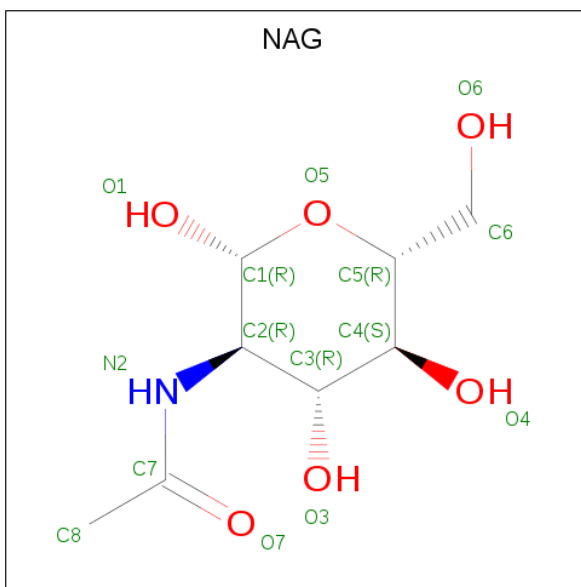
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	3	0
			4184	2683	733	754	14			
1	B	531	Total	C	N	O	S	0	3	0
			4164	2672	727	751	14			

There are 10 discrepancies between the modelled and reference sequences:

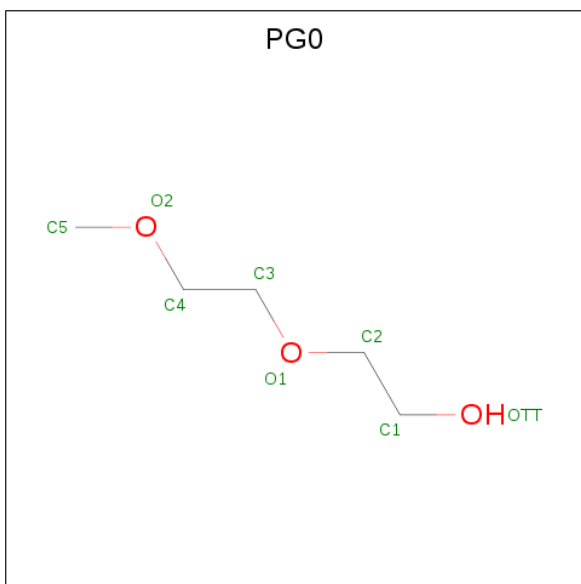
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ALA	-	expression tag	UNP P21836
A	545	THR	-	expression tag	UNP P21836
A	546	GLU	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	expression tag	UNP P21836
B	544	ALA	-	expression tag	UNP P21836
B	545	THR	-	expression tag	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
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	1	0
			14	8	1	5		

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



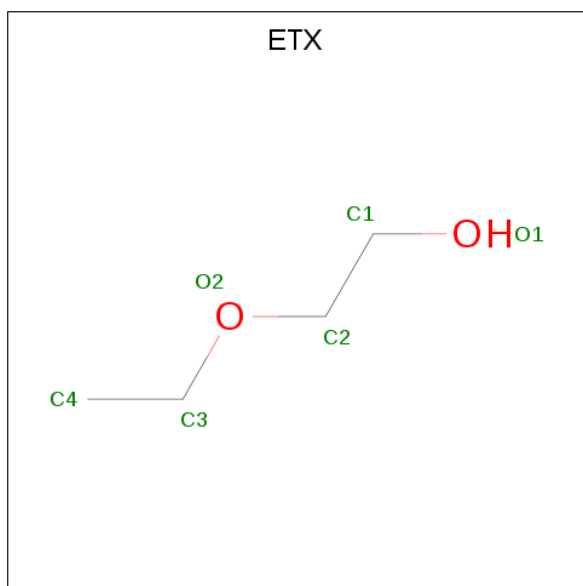
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		

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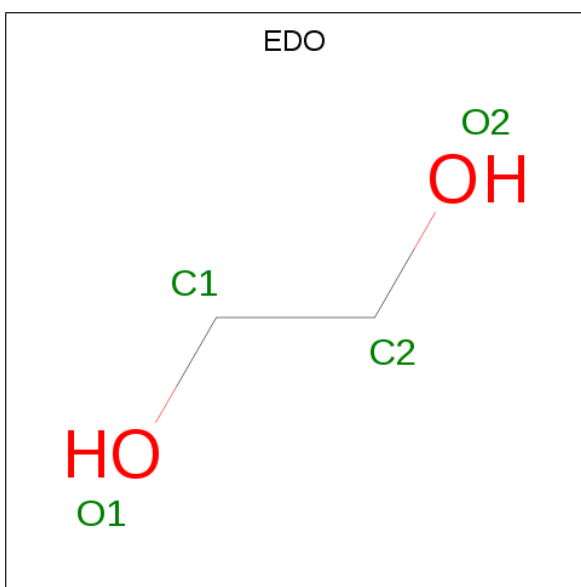
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		

- Molecule 4 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: $C_4H_{10}O_2$).



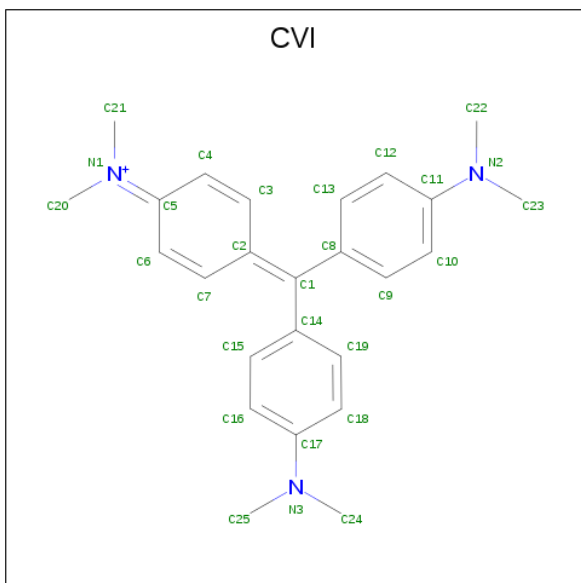
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



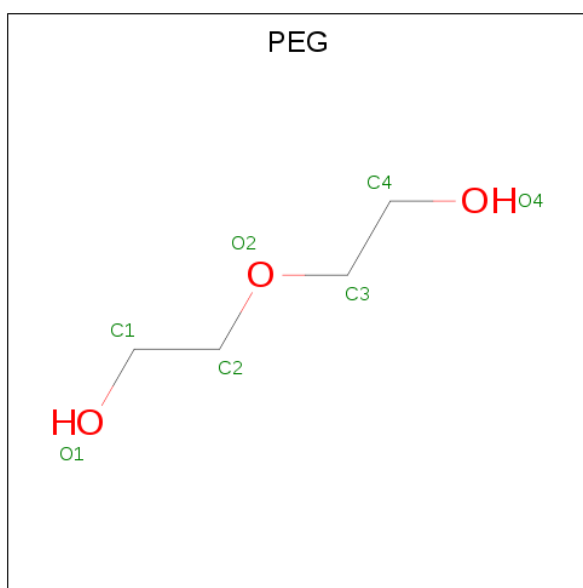
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CRYSTAL VIOLET (three-letter code: CVI) (formula: $C_{25}H_{30}N_3$).



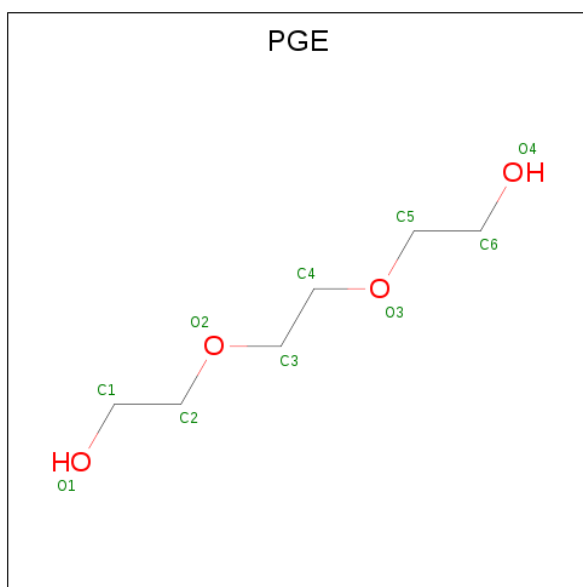
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			28	25	3		
6	A	1	Total	C	N	0	0
			28	25	3		
6	B	1	Total	C	N	0	0
			28	25	3		
6	B	1	Total	C	N	0	0
			28	25	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



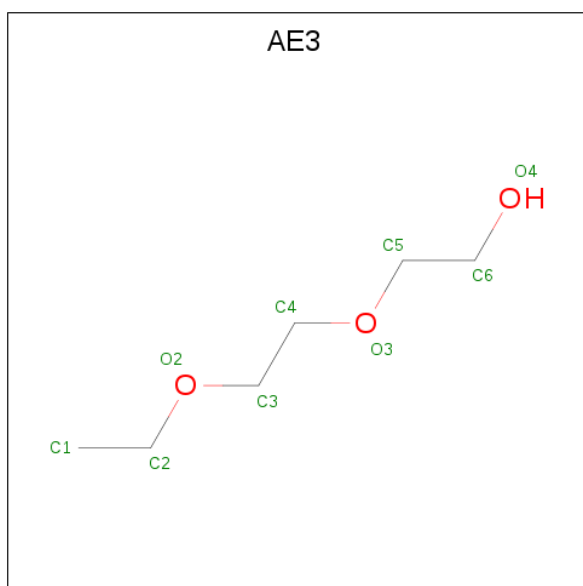
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



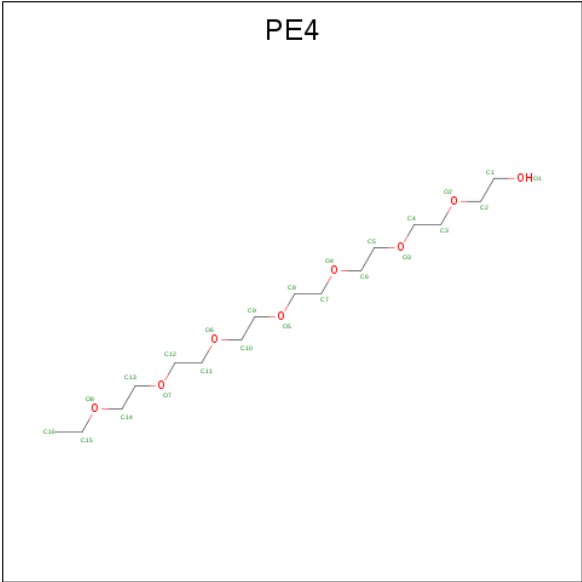
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: $C_6H_{14}O_3$).



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

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



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

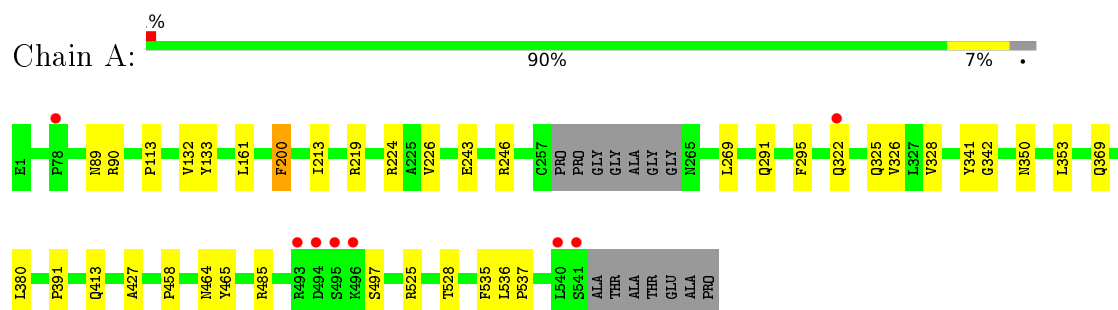
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	311	Total	O	0	0
			311	311		
11	B	232	Total	O	0	0
			232	232		

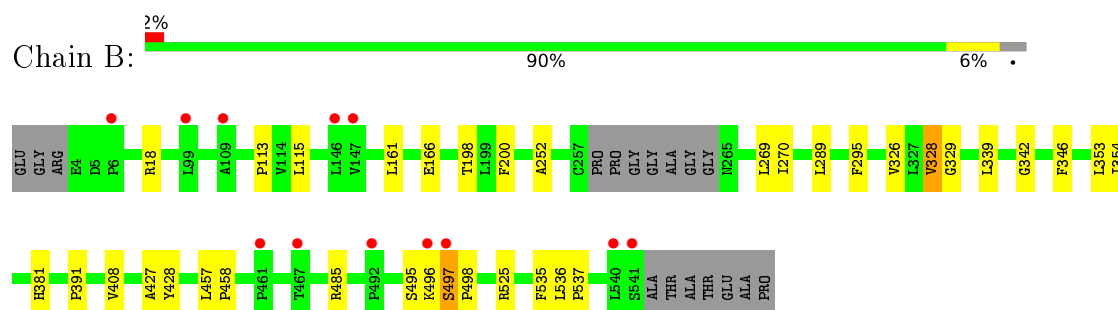
3 Residue-property plots [i](#)

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	79.63Å 113.89Å 226.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.11 – 2.40 29.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.11-2.40) 98.4 (29.11-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.159 , 0.195 0.166 , 0.163	Depositor DCC
R_{free} test set	1610 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9130	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: CVI, NAG, AE3, PEG, EDO, PE4, PGE, ETX, PG0

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	0.57	0/4307	0.65	0/5885
1	B	0.54	1/4287 (0.0%)	0.66	0/5858
All	All	0.56	1/8594 (0.0%)	0.65	0/11743

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	VAL	CB-CG1	-5.25	1.41	1.52

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	4184	0	4063	21	0
1	B	4164	0	4041	21	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	16	0	24	2	0
4	A	12	0	20	0	0
4	B	6	0	10	0	0
5	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	8	0	12	0	0
6	A	56	0	60	11	0
6	B	56	0	60	0	0
7	B	7	0	10	0	0
8	B	10	0	13	1	0
9	B	9	0	14	0	0
10	B	23	0	29	2	0
11	A	311	0	0	3	0
11	B	232	0	0	0	0
All	All	9130	0	8394	52	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 3.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.32	0.62
6:A:609:CVI:H71	6:A:609:CVI:C15	2.32	0.60
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.84	0.60
1:B:381:HIS:HA	10:B:607:PE4:H111	1.85	0.58
1:A:291:GLN:OE1	1:A:369:GLN:NE2	2.36	0.58
1:B:289:LEU:HD12	8:B:605:PGE:H1	1.86	0.56
1:B:495:SER:HA	1:B:496:LYS:CB	2.36	0.56
1:B:497:SER:CB	1:B:498:PRO:HA	2.37	0.54
3:A:602:PG0:H12	11:A:969:HOH:O	2.06	0.54
1:A:89:ASN:O	1:A:90:ARG:NH1	2.41	0.54
1:A:161:LEU:HD21	1:A:269:LEU:HD22	1.90	0.54
6:A:609:CVI:C15	6:A:609:CVI:C7	2.85	0.53
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.90	0.53
1:A:536:LEU:N	1:A:537:PRO:CD	2.73	0.51
1:A:380:LEU:HD12	1:B:535:PHE:HB2	1.93	0.50
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.94	0.49
1:B:497:SER:HB3	1:B:498:PRO:HA	1.94	0.49
6:A:608:CVI:C7	6:A:608:CVI:C15	2.90	0.49
1:A:341:TYR:CE2	6:A:608:CVI:H243	2.48	0.49
1:A:464:ASN:ND2	11:A:703:HOH:O	2.46	0.48
6:A:609:CVI:C7	6:A:609:CVI:H151	2.45	0.47
1:A:413:GLN:NE2	11:A:705:HOH:O	2.48	0.46
1:A:350:ASN:ND2	2:A:601:NAG:H83	2.31	0.46
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:CB	1:A:226:VAL:HB	2.45	0.46
1:B:497:SER:CB	1:B:498:PRO:CA	2.94	0.45
1:B:326:VAL:HG12	1:B:328:VAL:HG13	1.99	0.45
6:A:609:CVI:C13	6:A:609:CVI:C3	2.94	0.44
1:A:132:VAL:HG13	1:A:133:TYR:CD1	2.52	0.44
1:A:535:PHE:CD2	10:B:607:PE4:H71	2.53	0.44
6:A:609:CVI:C13	6:A:609:CVI:H31	2.47	0.44
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.99	0.44
6:A:608:CVI:H222	6:A:609:CVI:H232	2.00	0.44
1:A:224:ARG:HG2	1:A:325:GLN:HB2	2.00	0.43
6:A:608:CVI:C15	6:A:608:CVI:H71	2.48	0.43
1:A:328:VAL:O	1:A:427:ALA:HA	2.17	0.43
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.48	0.43
1:B:166:GLU:HG2	1:B:270:ILE:HD13	2.01	0.42
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.54	0.42
3:A:602:PG0:H42	6:A:609:CVI:H233	2.02	0.42
1:A:213:ILE:O	1:A:219:ARG:HD3	2.19	0.42
1:A:525:ARG:HG2	1:A:528:THR:HB	2.00	0.42
1:B:457:LEU:N	1:B:458:PRO:CD	2.83	0.41
1:B:328:VAL:O	1:B:427:ALA:HA	2.19	0.41
1:B:353:LEU:HB3	1:B:391:PRO:HB2	2.01	0.41
1:B:115:LEU:HD23	1:B:198:THR:HB	2.01	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.56	0.40
1:B:536:LEU:N	1:B:537:PRO:CD	2.84	0.40
6:A:609:CVI:C3	6:A:609:CVI:H131	2.51	0.40
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.56	0.40
1:B:252:ALA:HB2	1:B:269:LEU:HD21	2.02	0.40
1:B:346:PHE:CE1	1:B:354:ILE:HG21	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	533/548 (97%)	514 (96%)	18 (3%)	1 (0%)	47 62
1	B	530/548 (97%)	510 (96%)	18 (3%)	2 (0%)	34 48
All	All	1063/1096 (97%)	1024 (96%)	36 (3%)	3 (0%)	41 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER
1	B	342	GLY
1	A	342	GLY

5.3.2 Protein sidechains ⓘ

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	436/446 (98%)	432 (99%)	4 (1%)	78 90
1	B	435/446 (98%)	432 (99%)	3 (1%)	84 92
All	All	871/892 (98%)	864 (99%)	7 (1%)	81 91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	PHE
1	A	295	PHE
1	A	322	GLN
1	A	497	SER
1	B	18	ARG
1	B	200	PHE
1	B	295	PHE

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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	NAG	A	601	1	14,14,15	1.36	1 (7%)	17,19,21	1.82	1 (5%)
8	PGE	B	605	-	9,9,9	1.73	2 (22%)	8,8,8	1.59	2 (25%)
4	ETX	B	608	-	5,5,5	0.56	0	4,4,4	0.38	0
7	PEG	B	604	-	6,6,6	0.51	0	5,5,5	0.32	0
5	EDO	B	610	-	3,3,3	0.42	0	2,2,2	0.39	0
6	CVI	B	603	-	30,30,30	1.42	2 (6%)	42,42,42	1.21	5 (11%)
5	EDO	A	607	-	3,3,3	0.34	0	2,2,2	0.40	0
4	ETX	A	605	-	5,5,5	0.53	0	4,4,4	0.25	0
5	EDO	A	606	-	3,3,3	0.34	0	2,2,2	0.36	0
2	NAG	B	601	1	14,14,15	0.91	1 (7%)	17,19,21	0.69	0
9	AE3	B	606	-	8,8,8	1.30	1 (12%)	7,7,7	1.86	3 (42%)
6	CVI	A	608	-	30,30,30	1.44	6 (20%)	42,42,42	1.55	10 (23%)
5	EDO	B	609	-	3,3,3	0.68	0	2,2,2	0.45	0
3	PG0	A	602	-	7,7,7	1.30	1 (14%)	6,6,6	1.72	2 (33%)
3	PG0	A	603	-	7,7,7	1.33	1 (14%)	6,6,6	1.67	1 (16%)
4	ETX	A	604	-	5,5,5	0.71	0	4,4,4	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CVI	A	609	-	30,30,30	1.49	6 (20%)	42,42,42	1.26	4 (9%)
6	CVI	B	602	-	30,30,30	1.52	2 (6%)	42,42,42	0.96	1 (2%)
10	PE4	B	607	-	22,22,23	0.61	0	21,21,22	3.72	9 (42%)

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
2	NAG	A	601	1	-	4/6/23/26	0/1/1/1
8	PGE	B	605	-	-	3/7/7/7	-
4	ETX	B	608	-	-	2/3/3/3	-
7	PEG	B	604	-	-	1/4/4/4	-
5	EDO	B	610	-	-	0/1/1/1	-
6	CVI	B	603	-	-	1/24/34/34	0/3/3/3
5	EDO	A	607	-	-	0/1/1/1	-
4	ETX	A	605	-	-	2/3/3/3	-
5	EDO	A	606	-	-	1/1/1/1	-
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
9	AE3	B	606	-	-	4/6/6/6	-
6	CVI	A	608	-	-	2/24/34/34	0/3/3/3
5	EDO	B	609	-	-	0/1/1/1	-
3	PG0	A	602	-	-	2/5/5/5	-
3	PG0	A	603	-	-	3/5/5/5	-
4	ETX	A	604	-	-	1/3/3/3	-
6	CVI	A	609	-	-	0/24/34/34	0/3/3/3
6	CVI	B	602	-	-	3/24/34/34	0/3/3/3
10	PE4	B	607	-	-	12/20/20/21	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	602	CVI	C5-N1	5.41	1.41	1.34
2	A	601	NAG	O5-C1	4.97	1.51	1.43
6	A	609	CVI	C5-N1	4.26	1.40	1.34
6	B	602	CVI	C1-C2	4.17	1.52	1.39
6	B	603	CVI	C5-N1	4.16	1.40	1.34
6	B	603	CVI	C1-C2	3.87	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	605	PGE	C2-C1	-3.31	1.31	1.49
8	B	605	PGE	C4-C3	-3.28	1.32	1.49
6	A	608	CVI	C5-N1	3.23	1.38	1.34
2	B	601	NAG	O5-C1	3.14	1.48	1.43
6	A	609	CVI	C1-C2	3.11	1.49	1.39
3	A	603	PG0	C2-C1	-2.96	1.33	1.49
6	A	608	CVI	C7-C2	-2.86	1.37	1.43
3	A	602	PG0	C2-C1	-2.85	1.34	1.49
6	A	608	CVI	C6-C5	-2.80	1.37	1.42
9	B	606	AE3	C4-C3	-2.80	1.34	1.49
6	A	608	CVI	C3-C2	-2.75	1.37	1.43
6	A	608	CVI	C1-C2	2.70	1.47	1.39
6	A	609	CVI	C7-C2	-2.67	1.37	1.43
6	A	609	CVI	C3-C2	-2.38	1.38	1.43
6	A	608	CVI	C4-C5	-2.29	1.38	1.42
6	A	609	CVI	C6-C5	-2.27	1.38	1.42
6	A	609	CVI	C4-C5	-2.07	1.38	1.42

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	607	PE4	O7-C13-C14	12.85	168.34	110.39
2	A	601	NAG	C1-O5-C5	6.88	121.52	112.19
10	B	607	PE4	C15-O8-C14	6.42	152.91	112.96
10	B	607	PE4	O8-C14-C13	4.72	147.03	111.07
6	A	608	CVI	C14-C1-C2	-3.27	116.12	121.71
3	A	603	PG0	O1-C2-C1	3.20	124.11	110.07
9	B	606	AE3	C2-O2-C3	3.18	124.31	112.90
6	B	603	CVI	C21-N1-C20	3.06	121.39	115.29
6	A	609	CVI	C10-C11-N2	-2.95	117.63	121.63
6	B	603	CVI	C14-C1-C8	2.94	121.28	115.43
10	B	607	PE4	O6-C10-C9	2.75	122.78	110.39
3	A	602	PG0	O1-C2-C1	2.73	122.06	110.07
6	A	609	CVI	C14-C1-C8	2.73	120.85	115.43
6	A	608	CVI	C7-C2-C1	-2.70	118.00	122.16
6	A	608	CVI	C16-C17-N3	-2.66	118.03	121.63
10	B	607	PE4	O5-C9-C10	2.64	122.32	110.39
6	A	608	CVI	C7-C2-C3	2.50	121.12	117.22
6	A	608	CVI	C4-C5-N1	-2.50	119.57	121.77
6	A	608	CVI	C4-C3-C2	-2.49	118.53	121.34
9	B	606	AE3	O3-C4-C3	2.42	121.33	110.39
6	A	608	CVI	C6-C5-C4	2.39	120.67	116.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	608	CVI	C20-N1-C5	-2.37	118.39	121.53
6	A	608	CVI	C21-N1-C20	2.29	119.85	115.29
6	A	608	CVI	C6-C5-N1	-2.29	119.75	121.77
6	B	603	CVI	C6-C5-N1	-2.29	119.75	121.77
10	B	607	PE4	O6-C11-C12	2.24	120.50	110.39
8	B	605	PGE	O2-C2-C1	2.22	119.83	110.07
3	A	602	PG0	C2-O1-C3	2.21	122.85	113.29
6	B	603	CVI	C6-C5-C4	2.20	120.33	116.55
9	B	606	AE3	O2-C3-C4	2.14	120.06	110.39
10	B	607	PE4	C3-O2-C2	2.13	122.52	113.29
10	B	607	PE4	C5-O3-C4	2.11	122.43	113.29
6	B	603	CVI	C4-C5-N1	-2.11	119.91	121.77
6	A	609	CVI	C7-C2-C1	-2.08	118.96	122.16
8	B	605	PGE	O3-C4-C3	2.05	119.64	110.39
6	B	602	CVI	C6-C5-N1	-2.05	119.97	121.77
10	B	607	PE4	O5-C8-C7	2.03	119.54	110.39
6	A	609	CVI	C21-N1-C20	2.01	119.30	115.29

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAG	O5-C5-C6-O6
3	A	602	PG0	OTT-C1-C2-O1
2	B	601	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
3	A	602	PG0	O1-C3-C4-O2
10	B	607	PE4	O7-C13-C14-O8
10	B	607	PE4	O6-C11-C12-O7
10	B	607	PE4	O1-C1-C2-O2
10	B	607	PE4	C13-C14-O8-C15
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	B	601	NAG	C4-C5-C6-O6
3	A	603	PG0	OTT-C1-C2-O1
4	B	608	ETX	O1-C1-C2-O2
9	B	606	AE3	O2-C3-C4-O3
4	A	604	ETX	C4-C3-O2-C2
10	B	607	PE4	O2-C3-C4-O3
10	B	607	PE4	O4-C7-C8-O5
4	A	605	ETX	C4-C3-O2-C2
3	A	603	PG0	C3-C4-O2-C5

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Mol	Chain	Res	Type	Atoms
4	A	605	ETX	O1-C1-C2-O2
6	A	608	CVI	C8-C1-C2-C3
6	B	602	CVI	C8-C1-C2-C3
4	B	608	ETX	C4-C3-O2-C2
9	B	606	AE3	C1-C2-O2-C3
7	B	604	PEG	C1-C2-O2-C3
8	B	605	PGE	C3-C4-O3-C5
6	B	602	CVI	C8-C1-C2-C7
10	B	607	PE4	O3-C5-C6-O4
9	B	606	AE3	C6-C5-O3-C4
10	B	607	PE4	C6-C5-O3-C4
5	A	606	EDO	O1-C1-C2-O2
10	B	607	PE4	C12-C11-O6-C10
3	A	603	PG0	C1-C2-O1-C3
6	A	608	CVI	C8-C1-C2-C7
8	B	605	PGE	O2-C3-C4-O3
10	B	607	PE4	C7-C8-O5-C9
10	B	607	PE4	O6-C10-C9-O5
10	B	607	PE4	C1-C2-O2-C3
8	B	605	PGE	C6-C5-O3-C4
9	B	606	AE3	O3-C5-C6-O4
6	B	603	CVI	C8-C1-C14-C15
6	B	602	CVI	C8-C1-C14-C15

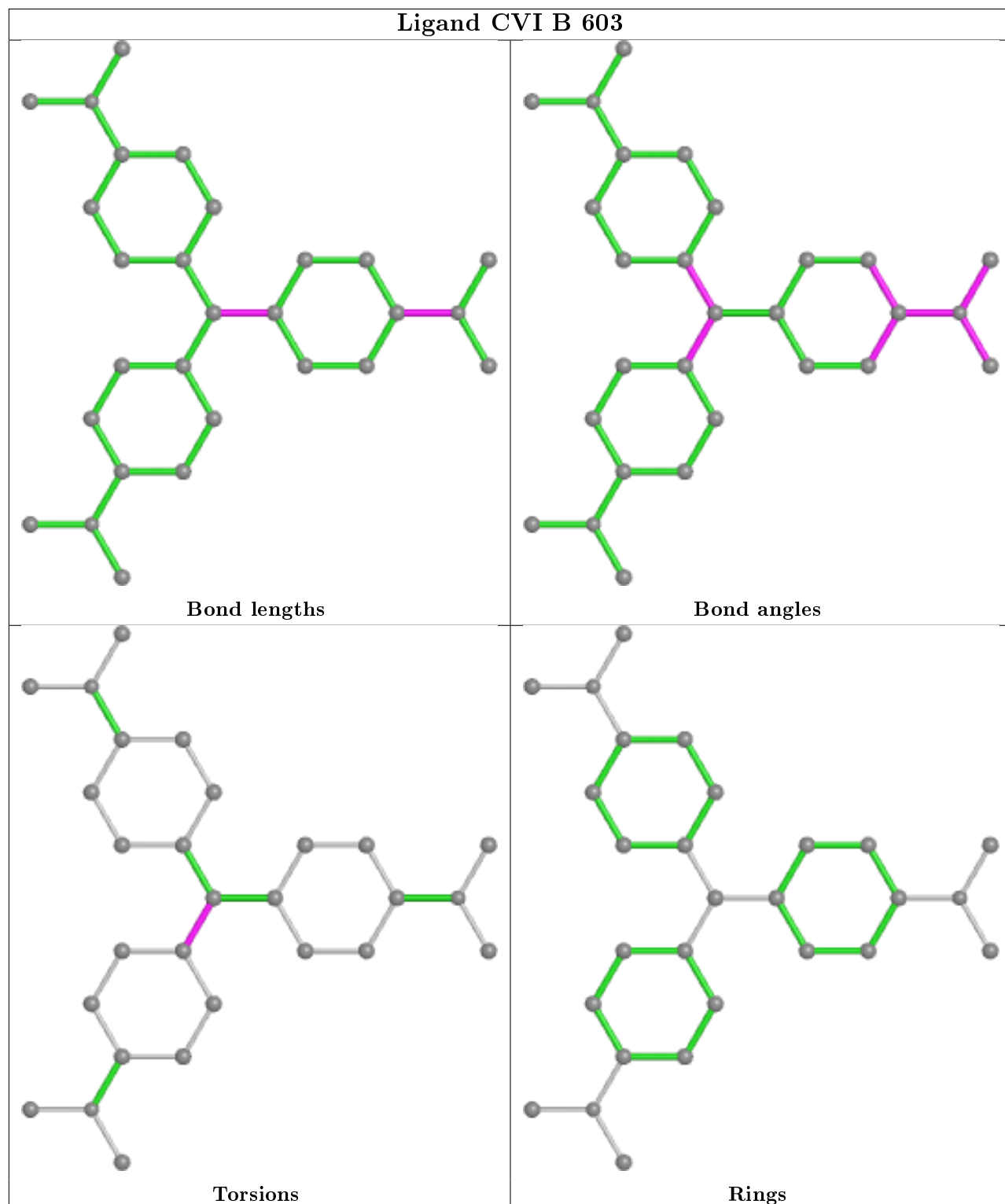
There are no ring outliers.

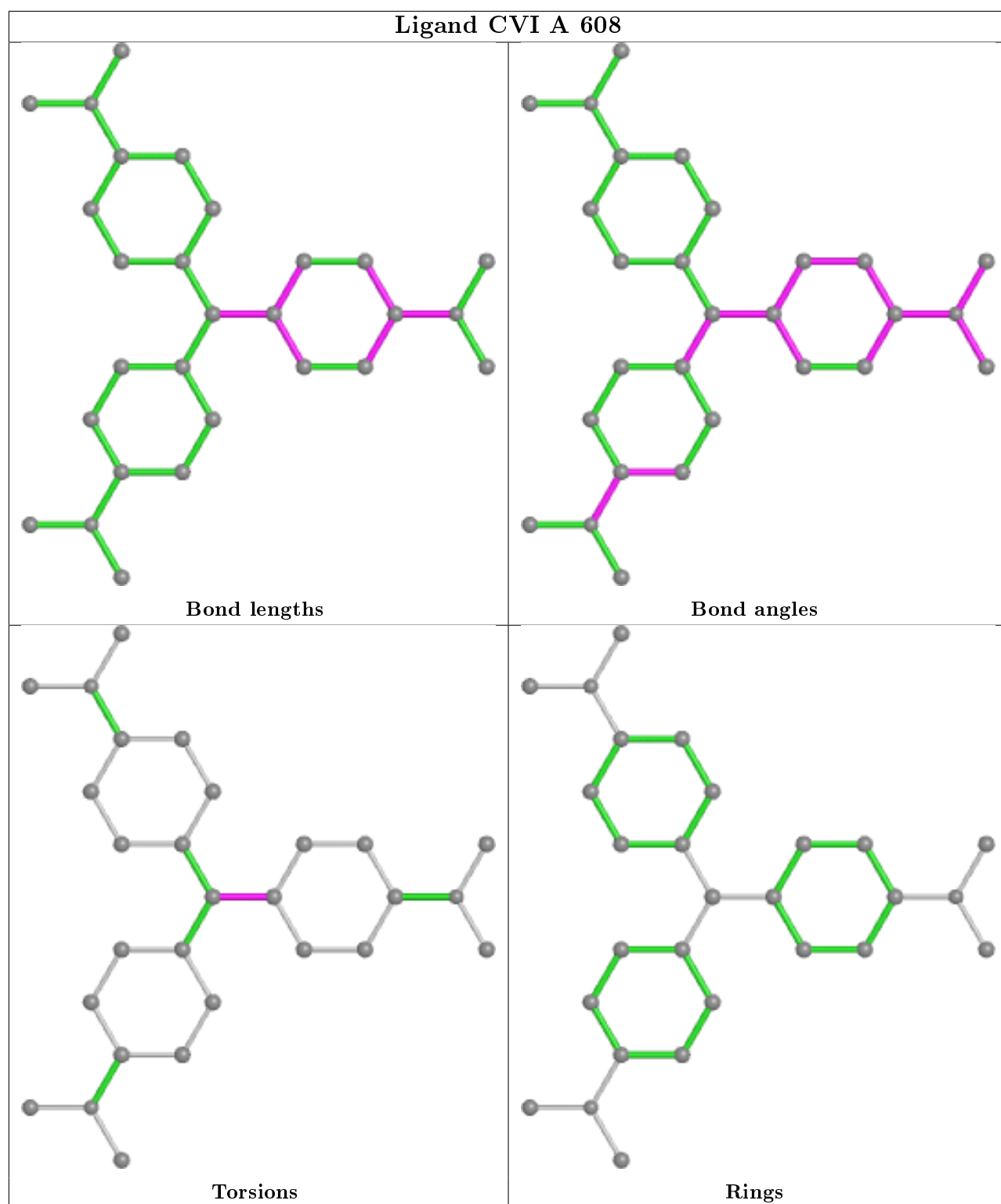
6 monomers are involved in 16 short contacts:

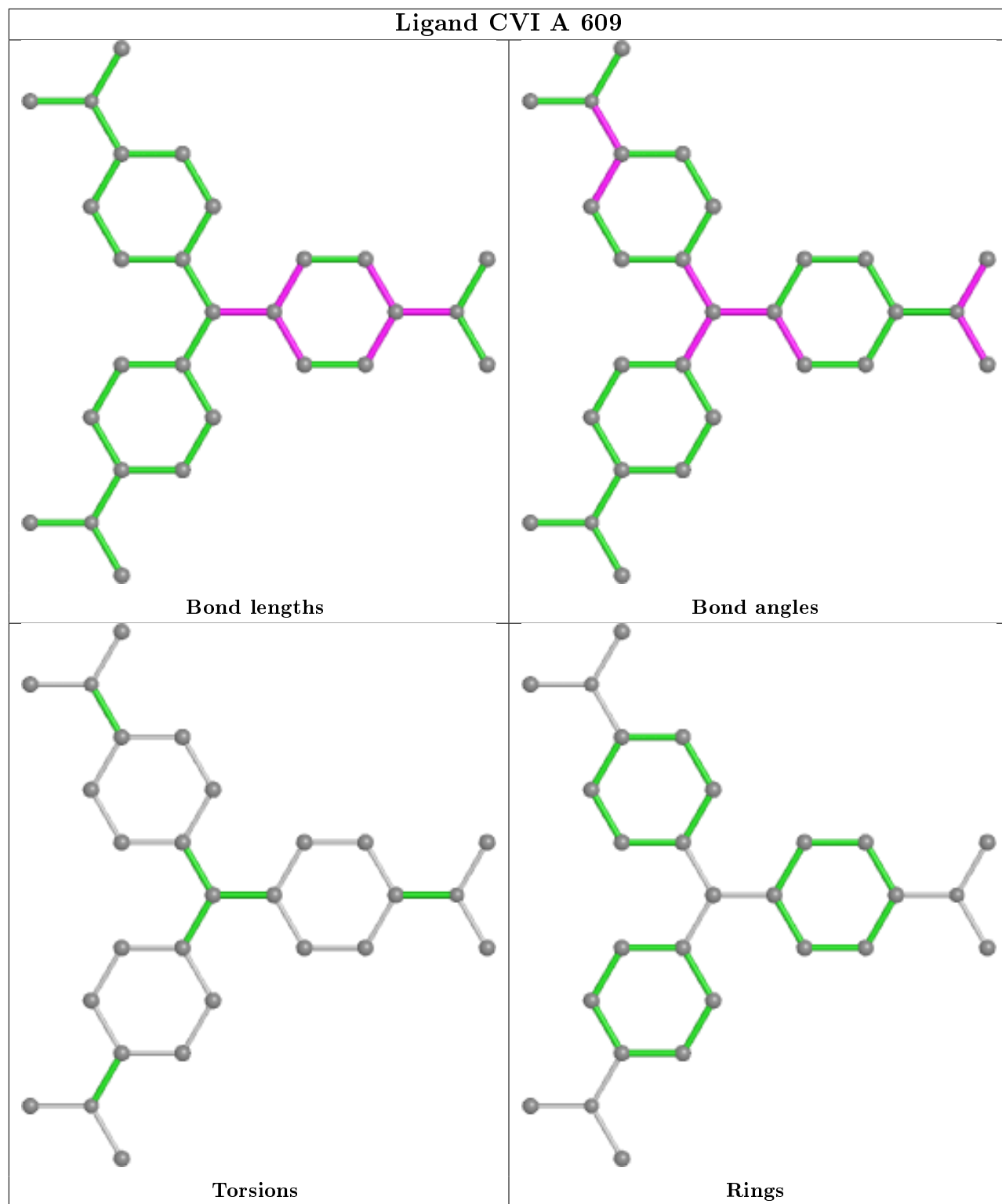
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0
8	B	605	PGE	1	0
6	A	608	CVI	4	0
3	A	602	PG0	2	0
6	A	609	CVI	8	0
10	B	607	PE4	2	0

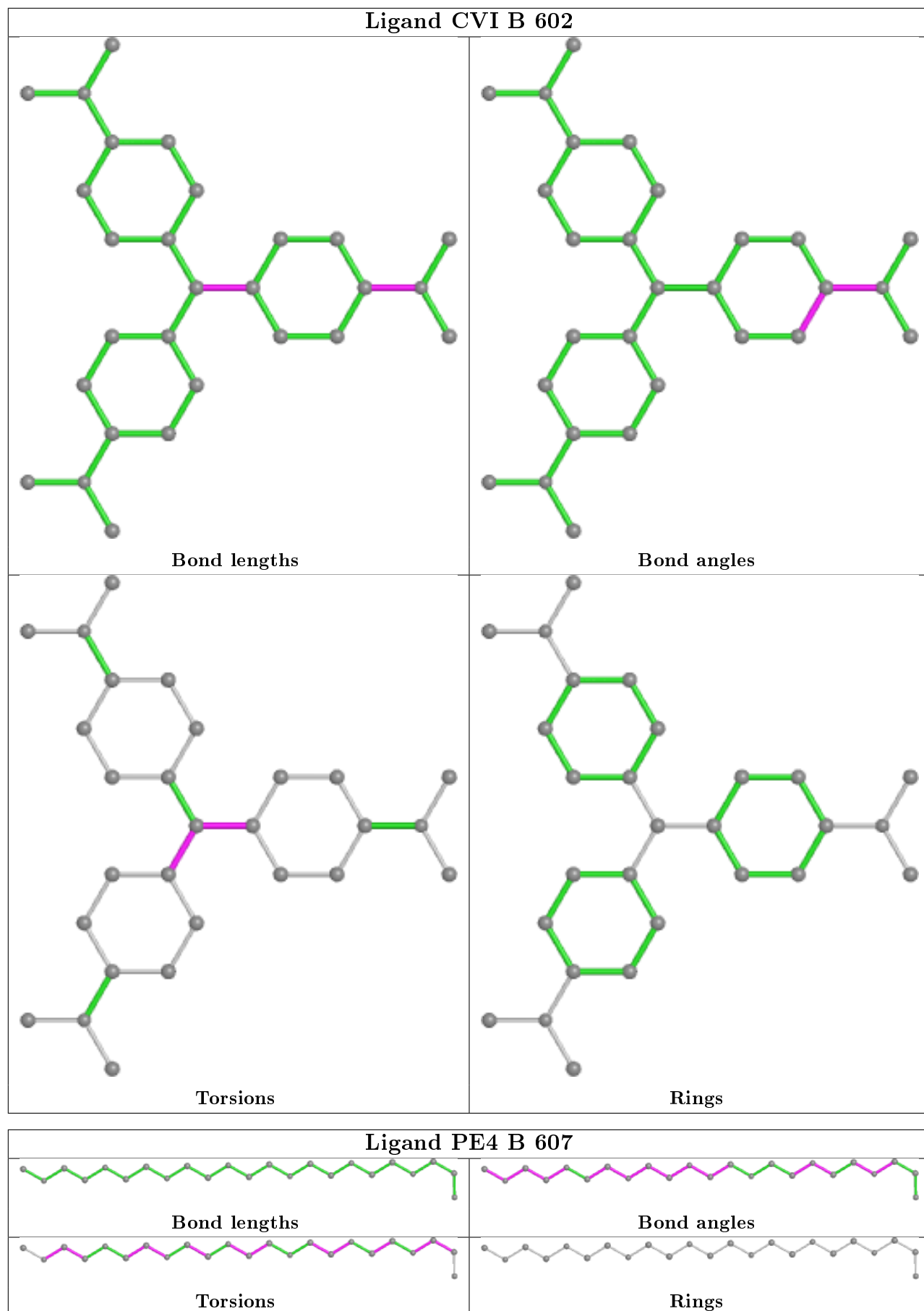
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

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	534/548 (97%)	-0.27	8 (1%) 73 72	35, 48, 80, 151	0
1	B	531/548 (96%)	-0.17	12 (2%) 60 58	39, 52, 83, 203	0
All	All	1065/1096 (97%)	-0.22	20 (1%) 66 64	35, 50, 81, 203	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	541	SER	4.0
1	A	496	LYS	3.5
1	B	497	SER	3.3
1	B	492	PRO	3.3
1	B	6	PRO	3.2
1	A	495	SER	3.1
1	A	540	LEU	3.1
1	B	496	LYS	3.1
1	B	146	LEU	2.9
1	B	147	VAL	2.8
1	A	493	ARG	2.7
1	B	540	LEU	2.7
1	A	494	ASP	2.6
1	A	541	SER	2.5
1	B	461	PRO	2.4
1	B	109	ALA	2.4
1	B	99	LEU	2.2
1	A	322	GLN	2.1
1	A	78	PRO	2.1
1	B	467	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

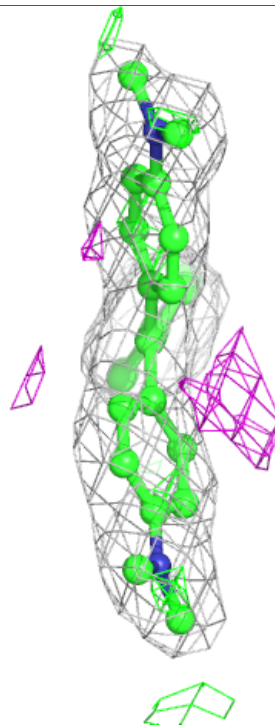
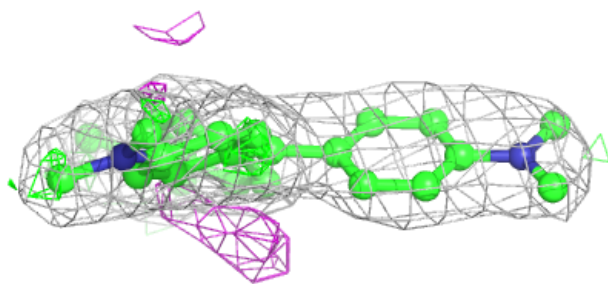
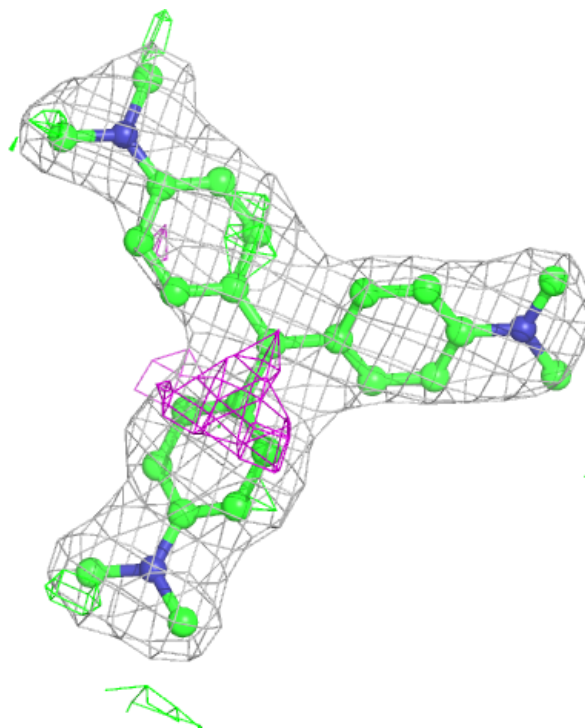
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	609	4/4	0.65	0.18	91,91,92,92	0
2	NAG	A	601	14/15	0.72	0.33	81,92,106,117	0
5	EDO	B	610	4/4	0.77	0.19	79,80,83,84	0
6	CVI	A	609	28/28	0.81	0.21	57,96,120,134	0
5	EDO	A	607	4/4	0.82	0.11	68,68,69,71	0
2	NAG	B	601	14/15	0.83	0.33	83,108,114,115	3
4	ETX	B	608	6/6	0.83	0.15	71,75,79,81	0
6	CVI	A	608	28/28	0.85	0.27	63,81,107,112	0
3	PG0	A	602	8/8	0.85	0.17	61,70,83,84	0
7	PEG	B	604	7/7	0.86	0.16	62,73,79,83	0
4	ETX	A	605	6/6	0.87	0.17	64,72,75,78	0
3	PG0	A	603	8/8	0.87	0.18	66,78,88,91	0
5	EDO	A	606	4/4	0.88	0.22	81,83,84,84	0
4	ETX	A	604	6/6	0.90	0.18	60,65,67,76	0
6	CVI	B	603	28/28	0.91	0.17	58,69,79,80	0
6	CVI	B	602	28/28	0.91	0.19	52,72,81,86	0
8	PGE	B	605	10/10	0.91	0.17	58,72,87,88	0
10	PE4	B	607	23/24	0.91	0.23	44,77,84,87	0
9	AE3	B	606	9/9	0.92	0.13	63,69,79,80	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.

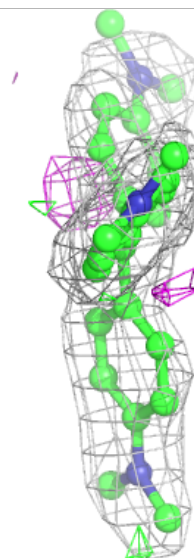
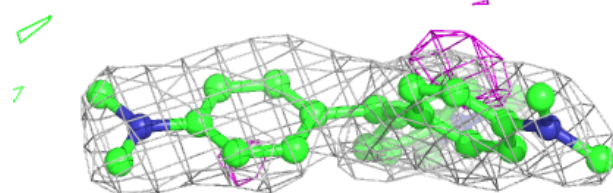
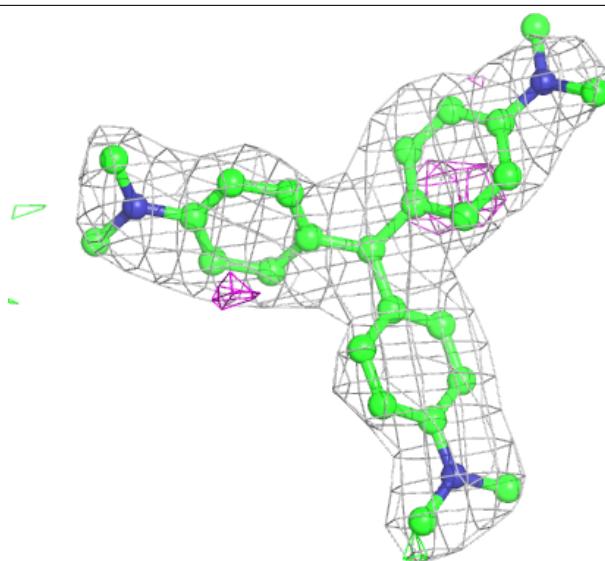
Electron density around CVI A 609:

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



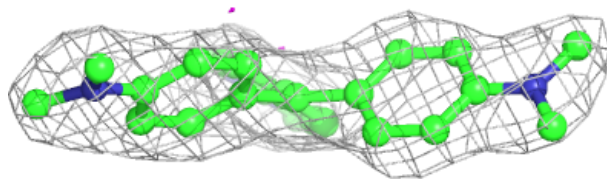
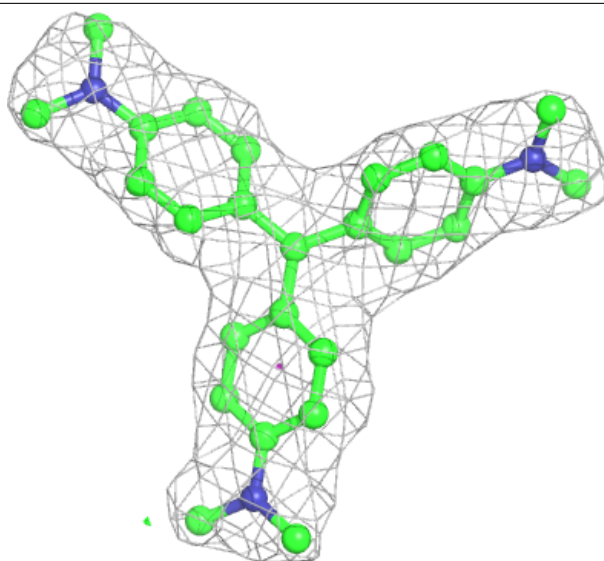
Electron density around CVI A 608:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



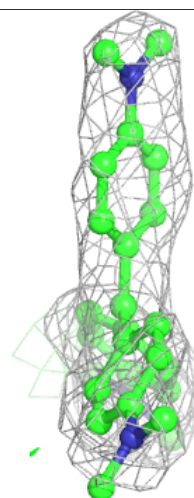
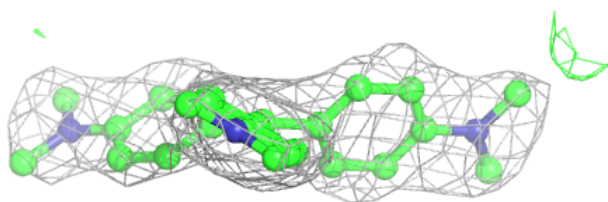
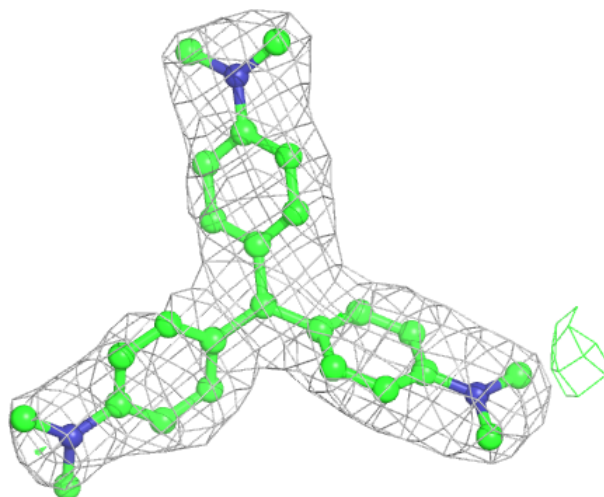
Electron density around CVI B 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



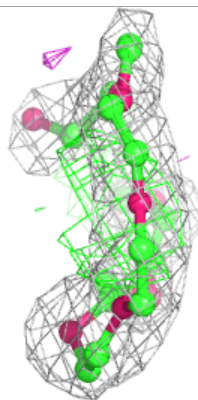
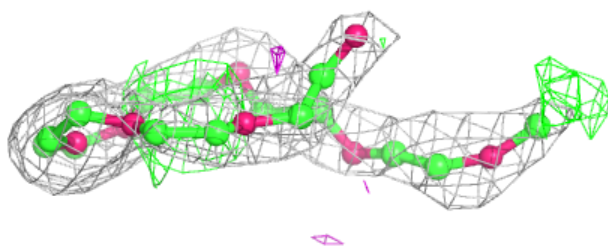
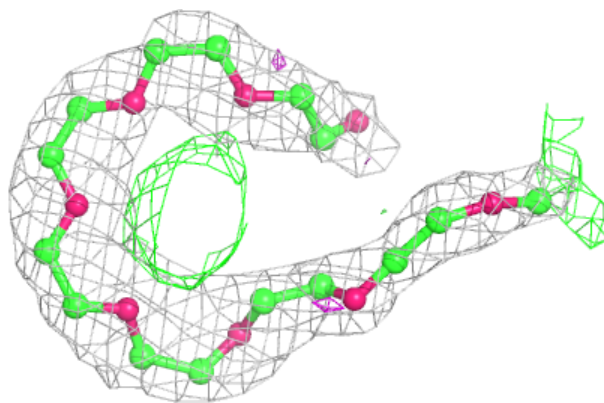
Electron density around CVI B 602:

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



Electron density around PE4 B 607:

$2mF_o-DF_c$ (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.