



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:27 AM UTC

PDB ID : 6I9A / pdb_00006i9a
Title : Porphyromonas gingivalis gingipain K (Kgp) in complex with inhibitor KYT-36
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Deposited on : 2018-11-22
Resolution : 1.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

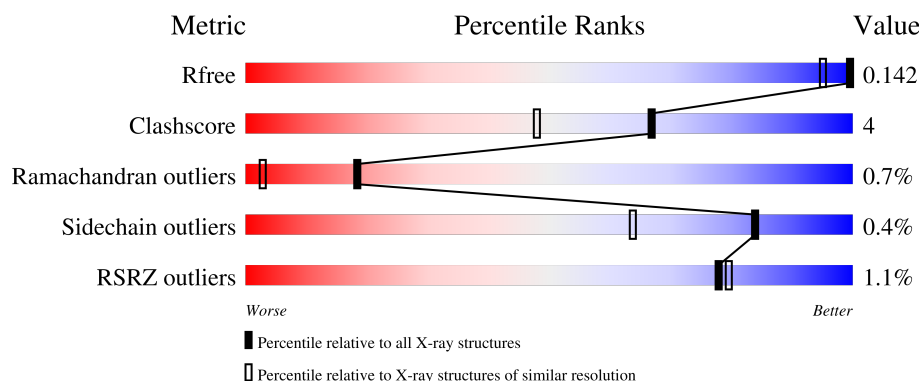
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	461	% 91% 7% .
1	B	461	2% 92% 6% .

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	UNX	A	701	-	-	X	-
2	UNX	B	701	-	-	X	-
6	EPE	B	708[B]	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9311 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 Lys-gingipain W83.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	22	0
			3639	2348	575	699	17			
1	B	453	Total	C	N	O	S	0	23	0
			3640	2350	574	698	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	684	HIS	-	expression tag	UNP Q51817
A	685	HIS	-	expression tag	UNP Q51817
A	686	HIS	-	expression tag	UNP Q51817
A	687	HIS	-	expression tag	UNP Q51817
A	688	HIS	-	expression tag	UNP Q51817
A	689	HIS	-	expression tag	UNP Q51817
B	684	HIS	-	expression tag	UNP Q51817
B	685	HIS	-	expression tag	UNP Q51817
B	686	HIS	-	expression tag	UNP Q51817
B	687	HIS	-	expression tag	UNP Q51817
B	688	HIS	-	expression tag	UNP Q51817
B	689	HIS	-	expression tag	UNP Q51817

- Molecule 2 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	X	0	0
			2	2		
2	B	2	Total	X	0	0
			2	2		

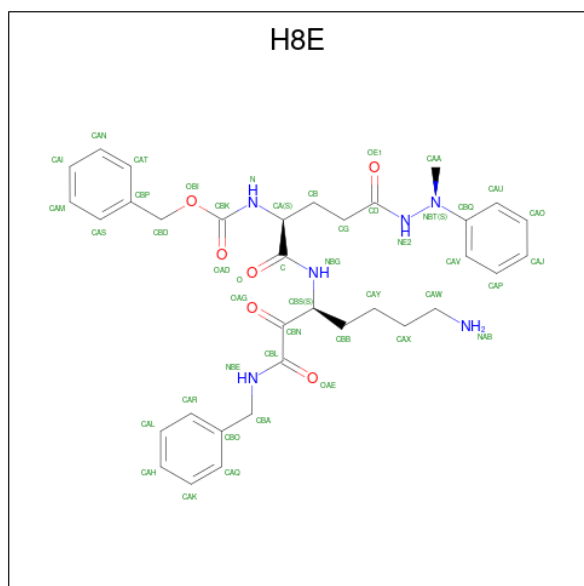
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

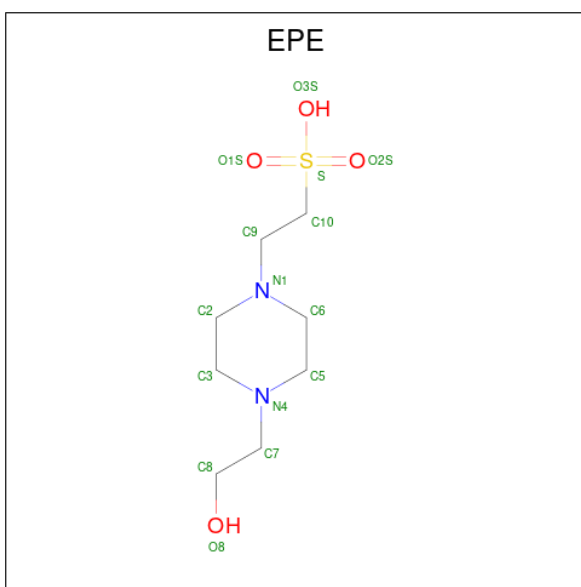
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		

- Molecule 5 is benzyl-N-[(2S)-1-[[[(3S)-7-amino-1-(benzylamino)-1,2-dioxoheptan-3-yl]amino]-5-(2-methyl-2-phenylhydrazinyl)-1,5-dioxopentan-2-yl]carbamate (CCD ID: H8E) (formula: C₃₄H₄₂N₆O₆).



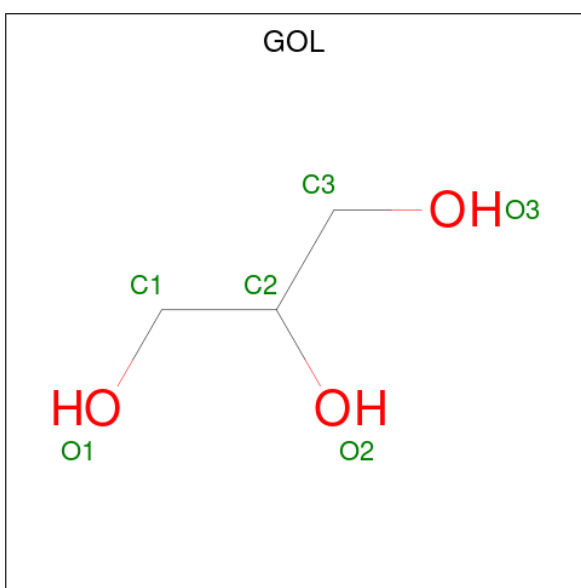
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			55	41	8	6		
5	B	1	Total	C	N	O	0	0
			46	34	6	6		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	1
			30	16	4	8	2		
6	B	1	Total	C	N	O	S	0	1
			30	16	4	8	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



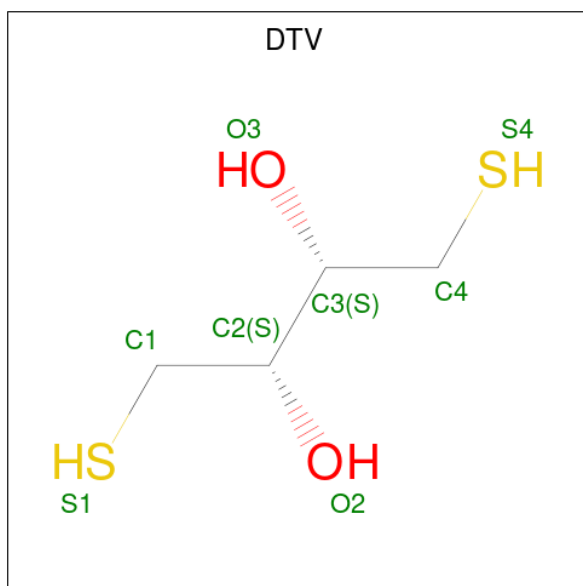
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	1
			12	6	6		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (CCD ID: DTV) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	S	0	0
			8	4	2	2		

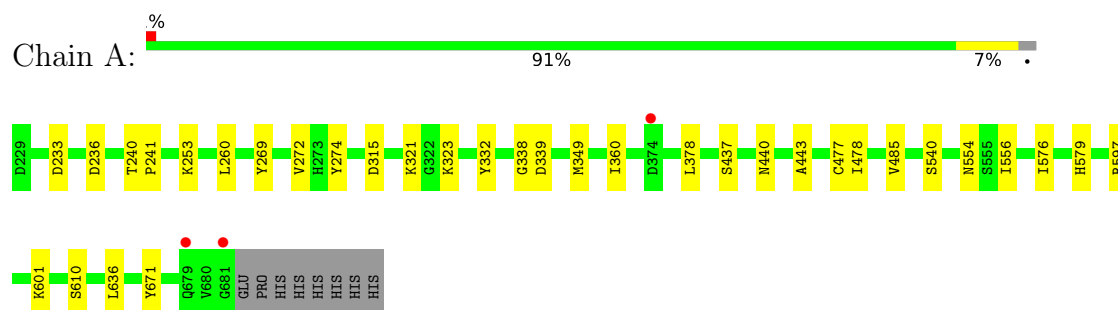
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	790	Total	O	0	120
			913	913		
9	B	790	Total	O	0	103
			896	896		

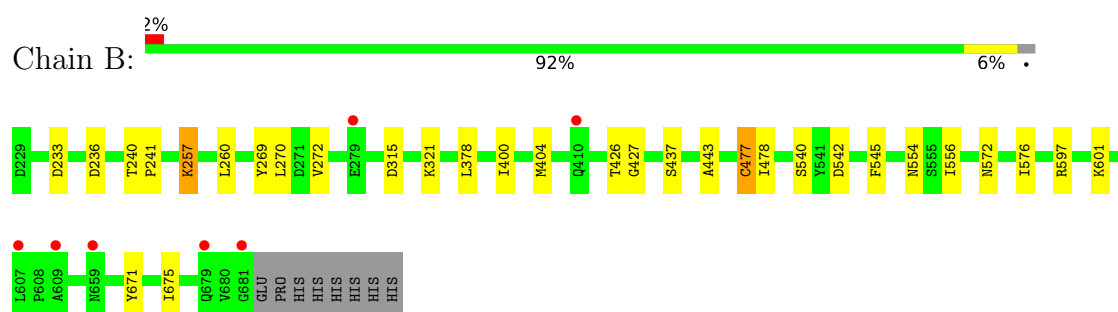
3 Residue-property plots

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: Lys-gingipain W83



• Molecule 1: Lys-gingipain W83



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.67Å 87.05Å 129.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.19 – 1.20 72.19 – 1.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (72.19-1.20) 95.8 (72.19-1.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.146 , 0.148 0.140 , 0.142	Depositor DCC
R_{free} test set	1120 reflections (0.37%)	wwPDB-VP
Wilson B-factor (Å ²)	10.5	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9311	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, EPE, UNX, DTV, CA, H8E

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	0.81	0/3801	0.93	7/5172 (0.1%)
1	B	0.79	0/3802	0.92	8/5173 (0.2%)
All	All	0.80	0/7603	0.92	15/10345 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	CA-CB-CG	7.40	120.00	112.60
1	B	236	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	315	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	440	ASN	CA-CB-CG	5.90	118.50	112.60
1	B	477	CYS	CA-C-N	5.87	132.53	121.97
1	B	477	CYS	C-N-CA	5.87	132.53	121.97
1	A	477	CYS	CA-C-N	5.86	132.51	121.97
1	A	477	CYS	C-N-CA	5.86	132.51	121.97
1	B	233	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	236	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	572	ASN	CA-CB-CG	5.30	117.91	112.60
1	A	338	GLY	N-CA-C	5.29	120.57	114.16
1	B	545	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	542	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	315	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3639	0	3567	23	0
1	B	3640	0	3575	25	0
2	A	2	0	0	2	0
2	B	2	0	0	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	55	0	0	0	0
5	B	46	0	0	4	0
6	A	30	0	34	8	0
6	B	30	0	34	9	0
7	A	24	0	32	0	0
7	B	18	0	24	1	0
8	B	8	0	10	2	0
9	A	913	0	0	5	0
9	B	896	0	0	5	0
All	All	9311	0	7276	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (54) 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:477:CYS:SG	5:B:707:H8E:CBN	2.03	1.45
1:A:597:ARG:HH22	2:A:701:UNX:UNK	1.08	0.97
9:A:1064[B]:HOH:O	1:B:675:ILE:HD12	1.64	0.97
1:A:597:ARG:NH2	2:A:701:UNX:UNK	1.63	0.94
1:B:597:ARG:HH22	2:B:701:UNX:UNK	1.16	0.90
1:B:270:LEU:HB2	6:B:708[B]:EPE:H91	1.54	0.90
1:B:260:LEU:HD13	6:B:708[B]:EPE:H72	1.58	0.85
1:B:597:ARG:NH2	2:B:701:UNX:UNK	1.75	0.82
1:A:260:LEU:HD13	6:A:708[B]:EPE:H72	1.61	0.81
1:A:323[B]:LYS:HE2	1:A:332:TYR:OH	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:708[B]:EPE:H22	9:B:988:HOH:O	1.82	0.78
1:B:426:THR:HA	8:B:709:DTV:H4C1	1.65	0.78
1:B:477:CYS:SG	5:B:707:H8E:CBL	2.74	0.75
6:B:708[B]:EPE:H71	9:B:1351:HOH:O	1.94	0.67
1:B:477:CYS:SG	5:B:707:H8E:CBS	2.83	0.64
6:A:708[A]:EPE:H22	6:A:708[A]:EPE:O1S	2.01	0.59
1:A:323[B]:LYS:HE3	1:A:579:HIS:CE1	2.40	0.56
1:B:257[B]:LYS:HB2	1:B:257[B]:LYS:NZ	2.22	0.54
1:B:240:THR:HA	1:B:241:PRO:C	2.32	0.53
1:A:601:LYS:HE2	1:A:671:TYR:CE1	2.44	0.53
1:A:485[B]:VAL:HG13	9:A:1316:HOH:O	2.07	0.52
1:B:260:LEU:HD13	6:B:708[B]:EPE:C7	2.36	0.52
1:A:636:LEU:O	6:A:708[A]:EPE:H101	2.10	0.52
1:B:272:VAL:CG2	6:B:708[B]:EPE:H52	2.40	0.51
1:A:323[B]:LYS:HE2	1:A:332:TYR:CZ	2.45	0.51
1:A:269:TYR:CD1	6:A:708[A]:EPE:H21	2.46	0.51
6:A:708[B]:EPE:H22	9:A:1123:HOH:O	2.11	0.50
1:B:257[A]:LYS:HG2	9:B:955[A]:HOH:O	2.11	0.50
1:A:240:THR:HA	1:A:241:PRO:C	2.35	0.49
1:A:272:VAL:CG2	6:A:708[B]:EPE:H52	2.43	0.48
1:A:540[B]:SER:OG	1:A:556:ILE:HG23	2.14	0.48
1:A:253[B]:LYS:HG2	1:A:274:TYR:CE1	2.49	0.48
7:B:711:GOL:H31	9:B:1121[A]:HOH:O	2.14	0.47
1:B:477:CYS:SG	5:B:707:H8E:NBG	2.88	0.47
1:A:339:ASP:HB2	9:A:1298:HOH:O	2.16	0.45
1:A:349[B]:MET:HE3	1:A:360:ILE:CG2	2.47	0.45
1:B:321[A]:LYS:HA	1:B:321[A]:LYS:HD3	1.87	0.44
1:A:349[B]:MET:HE3	1:A:360:ILE:HG21	2.00	0.43
1:A:378:LEU:HA	1:A:437:SER:HB3	2.01	0.43
1:B:601[B]:LYS:HE3	1:B:671:TYR:CE1	2.53	0.43
1:A:321[B]:LYS:HD3	1:A:321[B]:LYS:HA	1.81	0.42
1:A:269:TYR:HD1	6:A:708[A]:EPE:H21	1.85	0.42
1:B:540[B]:SER:OG	1:B:556:ILE:HG23	2.18	0.42
1:A:323[B]:LYS:HE3	1:A:579:HIS:HE1	1.84	0.41
1:B:257[A]:LYS:HB3	1:B:257[A]:LYS:HE3	1.48	0.41
1:A:260:LEU:CD1	6:A:708[B]:EPE:H72	2.40	0.41
1:B:269:TYR:HB3	6:B:708[A]:EPE:H81	2.02	0.41
1:B:427:GLY:H	8:B:709:DTV:H4	1.68	0.41
1:A:610:SER:HB2	9:A:898:HOH:O	2.20	0.41
1:B:269:TYR:HD1	6:B:708[A]:EPE:H62	1.86	0.41
1:B:400:ILE:HG22	1:B:404:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HA	1:B:437:SER:HB3	2.02	0.41
1:B:257[B]:LYS:NZ	1:B:257[B]:LYS:CB	2.84	0.40
6:B:708[B]:EPE:H81	9:B:1520[B]:HOH:O	2.21	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	473/461 (103%)	457 (97%)	13 (3%)	3 (1%)	21	4
1	B	474/461 (103%)	458 (97%)	13 (3%)	3 (1%)	21	4
All	All	947/922 (103%)	915 (97%)	26 (3%)	6 (1%)	18	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	ALA
1	B	443	ALA
1	A	478	ILE
1	B	478	ILE
1	B	576	ILE
1	A	576	ILE

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	392/378 (104%)	391 (100%)	1 (0%)	86	67
1	B	392/378 (104%)	389 (99%)	3 (1%)	73	44
All	All	784/756 (104%)	780 (100%)	4 (0%)	84	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	ASN
1	B	257[A]	LYS
1	B	257[B]	LYS
1	B	554	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	613	GLN
1	B	419	ASN
1	B	510	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 4 are unknown and 8 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EPE	A	708[B]	-	15,15,15	1.70	1 (6%)	19,20,20	0.88	0
6	EPE	B	708[A]	-	15,15,15	1.03	1 (6%)	19,20,20	0.93	1 (5%)
6	EPE	B	708[B]	-	15,15,15	1.52	1 (6%)	19,20,20	1.83	3 (15%)
7	GOL	A	709	-	5,5,5	0.20	0	5,5,5	0.08	0
7	GOL	B	711	-	5,5,5	0.55	0	5,5,5	0.59	0
7	GOL	B	710	-	5,5,5	0.13	0	5,5,5	0.35	0
6	EPE	A	708[A]	-	15,15,15	1.26	1 (6%)	19,20,20	1.07	1 (5%)
7	GOL	A	711[A]	-	5,5,5	0.16	0	5,5,5	0.11	0
7	GOL	A	711[B]	-	5,5,5	0.09	0	5,5,5	0.12	0
7	GOL	A	710	-	5,5,5	0.15	0	5,5,5	0.18	0
8	DTV	B	709	-	7,7,7	0.63	0	4,8,8	0.96	0
5	H8E	A	707[A]	-	45,48,48	1.26	4 (8%)	50,61,61	1.22	6 (12%)
7	GOL	B	712	-	5,5,5	0.15	0	5,5,5	0.31	0
5	H8E	B	707	-	45,48,48	1.42	7 (15%)	50,61,61	1.08	2 (4%)
5	H8E	A	707[B]	-	45,48,48	1.23	4 (8%)	50,61,61	1.25	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	A	708[B]	-	-	5/9/19/19	0/1/1/1
6	EPE	B	708[A]	-	-	5/9/19/19	0/1/1/1
6	EPE	B	708[B]	-	-	3/9/19/19	0/1/1/1
7	GOL	A	709	-	-	0/4/4/4	-
7	GOL	B	711	-	-	0/4/4/4	-
7	GOL	B	710	-	-	0/4/4/4	-
6	EPE	A	708[A]	-	-	4/9/19/19	0/1/1/1
7	GOL	A	711[A]	-	-	0/4/4/4	-
7	GOL	A	711[B]	-	-	0/4/4/4	-
7	GOL	A	710	-	-	0/4/4/4	-
8	DTV	B	709	-	-	3/8/8/8	-
5	H8E	A	707[A]	-	-	2/48/48/48	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	712	-	-	1/4/4/4	-
5	H8E	B	707	-	-	3/48/48/48	0/3/3/3
5	H8E	A	707[B]	-	-	2/48/48/48	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	708[B]	EPE	C10-S	-6.52	1.68	1.77
6	B	708[B]	EPE	C10-S	-5.64	1.69	1.77
5	A	707[A]	H8E	CBA-CBO	-4.49	1.41	1.51
5	A	707[B]	H8E	CBA-CBO	-4.49	1.41	1.51
6	A	708[A]	EPE	C10-S	-4.31	1.71	1.77
5	B	707	H8E	CBA-CBO	-4.01	1.42	1.51
5	B	707	H8E	OBI-CBK	-3.92	1.27	1.35
6	B	708[A]	EPE	C10-S	-3.55	1.72	1.77
5	A	707[A]	H8E	OBI-CBK	-3.40	1.28	1.35
5	A	707[B]	H8E	OBI-CBK	-3.40	1.28	1.35
5	A	707[A]	H8E	OAG-CBN	2.88	1.27	1.22
5	A	707[B]	H8E	OAG-CBN	2.88	1.27	1.22
5	B	707	H8E	OAG-CBN	2.57	1.26	1.22
5	A	707[A]	H8E	CAM-CAS	2.54	1.43	1.38
5	A	707[B]	H8E	CAM-CAS	2.54	1.43	1.38
5	B	707	H8E	CBQ-NBT	-2.51	1.38	1.42
5	B	707	H8E	CBD-CBP	-2.35	1.45	1.50
5	B	707	H8E	CAM-CAS	2.34	1.42	1.38
5	B	707	H8E	OAD-CBK	2.15	1.25	1.21

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	708[B]	EPE	O2S-S-C10	-5.04	99.12	106.73
6	B	708[B]	EPE	C10-C9-N1	3.89	127.08	112.36
5	A	707[A]	H8E	CAI-CAM-CAS	-3.64	115.74	120.24
5	A	707[B]	H8E	CAI-CAM-CAS	-3.64	115.74	120.24
5	A	707[A]	H8E	OAD-CBK-N	-3.21	119.61	124.86
5	A	707[B]	H8E	OAD-CBK-N	-3.21	119.61	124.86
6	A	708[A]	EPE	C6-N1-C2	3.06	115.44	108.84
5	B	707	H8E	OAD-CBK-N	-3.01	119.93	124.86
6	B	708[B]	EPE	C9-N1-C6	3.00	119.23	111.24
5	A	707[B]	H8E	OE1-CD-NE2	2.45	126.52	123.32
6	B	708[A]	EPE	C6-N1-C2	2.36	113.91	108.84
5	A	707[A]	H8E	OBI-CBK-N	2.34	115.45	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	707[B]	H8E	OBI-CBK-N	2.34	115.45	110.45
5	A	707[A]	H8E	CAH-CAL-CAR	-2.26	117.45	120.24
5	A	707[B]	H8E	CAH-CAL-CAR	-2.26	117.45	120.24
5	A	707[A]	H8E	CBS-NBG-C	2.15	126.26	121.65
5	A	707[B]	H8E	CBS-NBG-C	2.15	126.26	121.65
5	B	707	H8E	O-C-NBG	2.06	126.64	122.96
5	A	707[A]	H8E	CAL-CAR-CBO	2.05	123.50	120.61
5	A	707[B]	H8E	CAL-CAR-CBO	2.05	123.50	120.61

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	707[A]	H8E	OAG-CBN-CBS-NBG
5	A	707[B]	H8E	OAG-CBN-CBS-NBG
5	B	707	H8E	OAG-CBN-CBS-NBG
6	A	708[A]	EPE	S-C10-C9-N1
6	A	708[B]	EPE	C8-C7-N4-C5
6	A	708[B]	EPE	C9-C10-S-O2S
6	A	708[B]	EPE	C9-C10-S-O3S
6	B	708[A]	EPE	C10-C9-N1-C6
6	B	708[B]	EPE	C10-C9-N1-C6
6	B	708[B]	EPE	S-C10-C9-N1
8	B	709	DTV	S1-C1-C2-O2
8	B	709	DTV	S1-C1-C2-C3
6	A	708[A]	EPE	N4-C7-C8-O8
6	B	708[A]	EPE	N4-C7-C8-O8
6	A	708[A]	EPE	C10-C9-N1-C2
6	A	708[A]	EPE	C10-C9-N1-C6
6	B	708[A]	EPE	C10-C9-N1-C2
6	B	708[B]	EPE	C10-C9-N1-C2
6	A	708[B]	EPE	C9-C10-S-O1S
6	B	708[A]	EPE	C8-C7-N4-C5
8	B	709	DTV	C2-C3-C4-S4
6	B	708[A]	EPE	C8-C7-N4-C3
5	B	707	H8E	NBE-CBL-CBN-CBS
6	A	708[B]	EPE	C10-C9-N1-C2
7	B	712	GOL	O1-C1-C2-O2
5	A	707[A]	H8E	CBL-CBN-CBS-NBG
5	A	707[B]	H8E	CBL-CBN-CBS-NBG
5	B	707	H8E	CBL-CBN-CBS-NBG

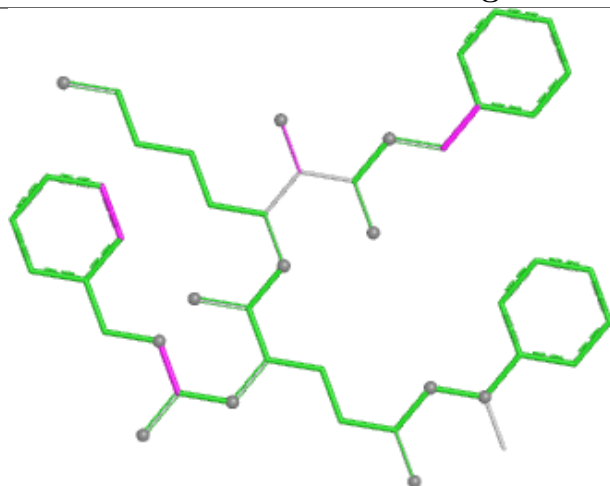
There are no ring outliers.

7 monomers are involved in 24 short contacts:

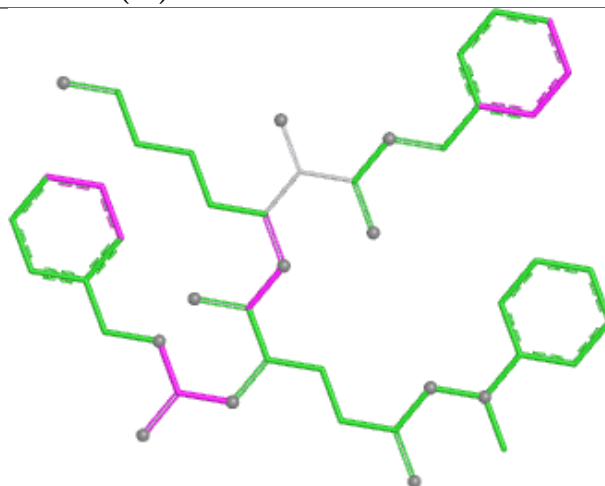
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	708[B]	EPE	4	0
6	B	708[A]	EPE	2	0
6	B	708[B]	EPE	7	0
7	B	711	GOL	1	0
6	A	708[A]	EPE	4	0
8	B	709	DTV	2	0
5	B	707	H8E	4	0

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 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.

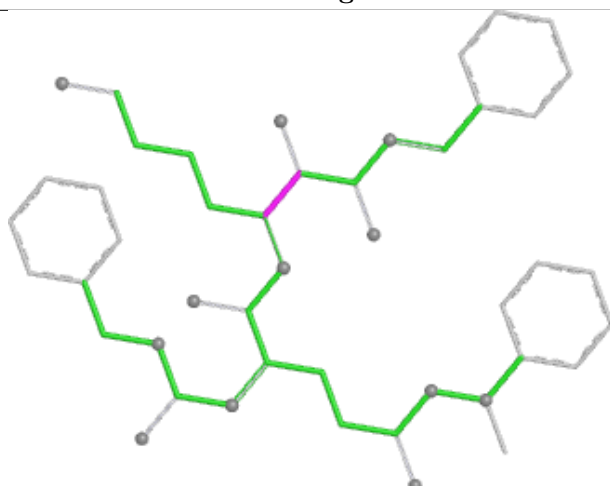
Ligand H8E A 707 (A)



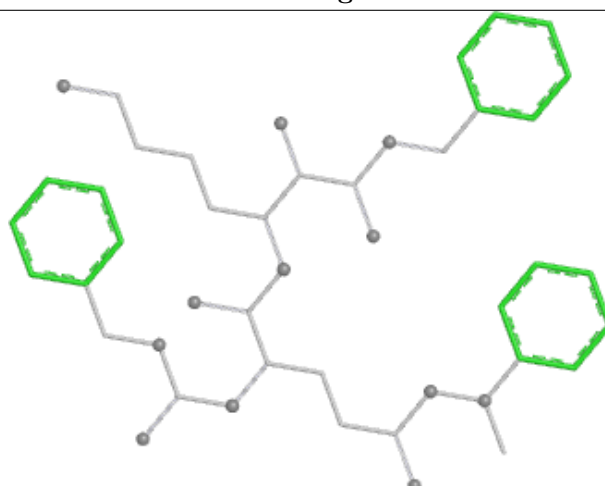
Bond lengths



Bond angles

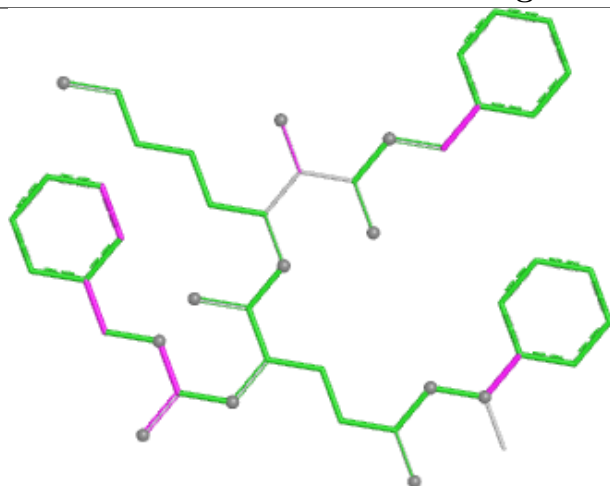


Torsions

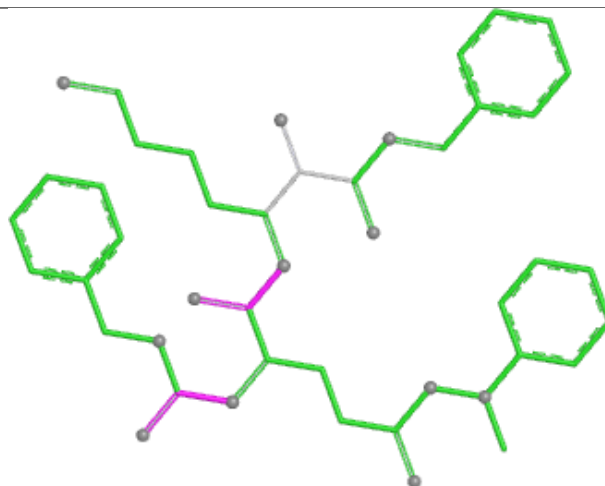


Rings

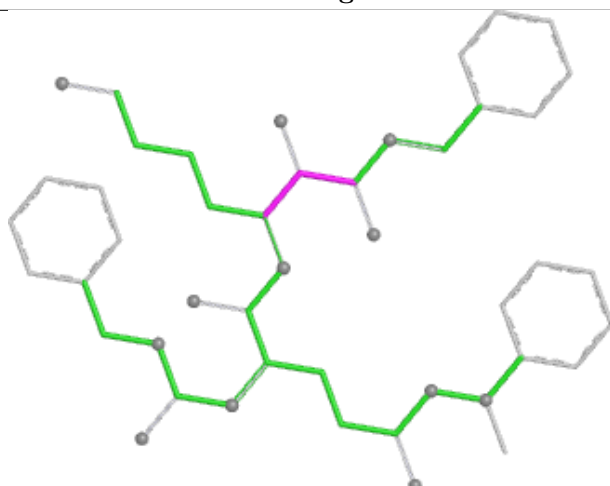
Ligand H8E B 707



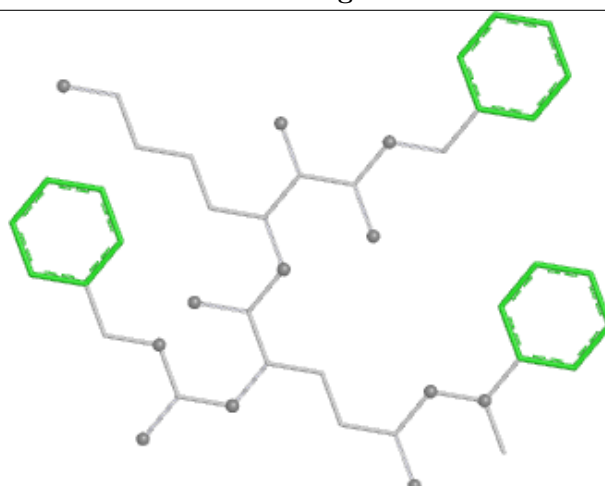
Bond lengths



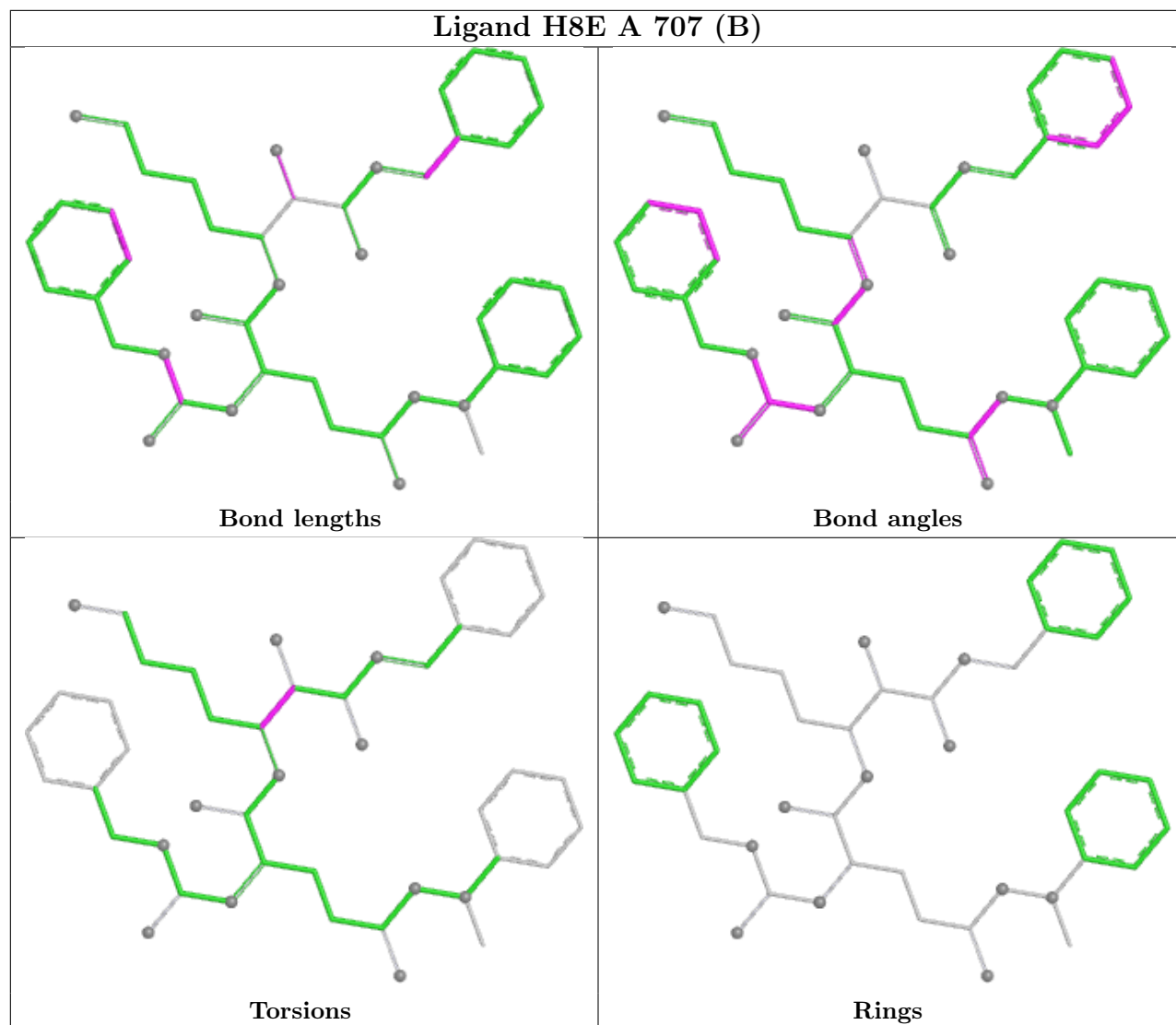
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	453/461 (98%)	-0.40	3 (0%) 84 87	6, 11, 20, 63	22 (4%)
1	B	453/461 (98%)	-0.37	7 (1%) 72 73	6, 12, 21, 63	23 (5%)
All	All	906/922 (98%)	-0.38	10 (1%) 78 79	6, 12, 21, 63	45 (4%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	681	GLY	6.0
1	A	681	GLY	4.9
1	B	609	ALA	4.6
1	A	679[A]	GLN	2.8
1	B	607	LEU	2.7
1	A	374	ASP	2.5
1	B	279	GLU	2.4
1	B	659	ASN	2.4
1	B	679[A]	GLN	2.3
1	B	410	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

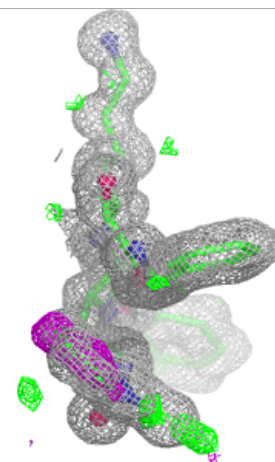
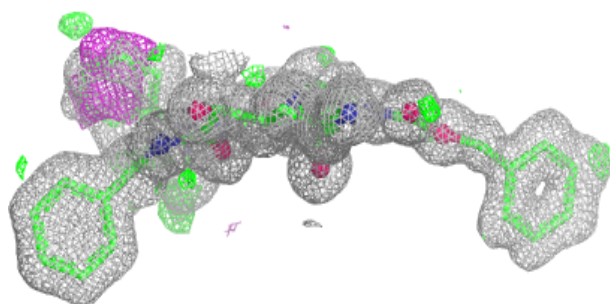
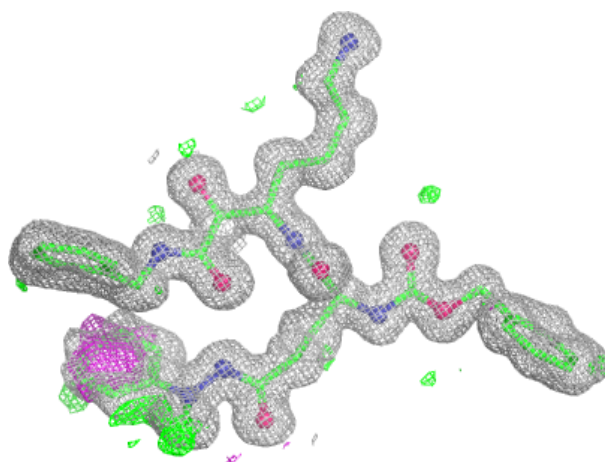
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EPE	A	708[A]	15/15	0.58	0.33	18,26,34,34	15
6	EPE	A	708[B]	15/15	0.58	0.33	17,26,36,38	15
6	EPE	B	708[A]	15/15	0.63	0.30	19,26,33,41	15
6	EPE	B	708[B]	15/15	0.63	0.30	19,26,32,42	15
7	GOL	B	712	6/6	0.76	0.17	38,41,42,42	0
8	DTV	B	709	8/8	0.82	0.16	35,40,42,50	0
2	UNX	A	702	1/1	0.87	0.28	21,21,21,21	0
2	UNX	A	701	1/1	0.90	0.33	25,25,25,25	0
7	GOL	A	709	6/6	0.92	0.10	22,24,25,26	0
7	GOL	A	711[A]	6/6	0.93	0.09	20,22,23,24	6
7	GOL	A	711[B]	6/6	0.93	0.09	23,25,26,26	6
2	UNX	B	701	1/1	0.95	0.48	22,22,22,22	0
7	GOL	B	710	6/6	0.95	0.08	16,18,19,21	0
2	UNX	B	702	1/1	0.96	0.25	20,20,20,20	0
7	GOL	B	711	6/6	0.96	0.07	14,15,16,17	0
5	H8E	B	707	46/46	0.97	0.07	9,13,21,26	0
7	GOL	A	710	6/6	0.97	0.06	15,17,18,21	0
5	H8E	A	707[B]	46/46	0.98	0.06	9,12,19,20	9
5	H8E	A	707[A]	46/46	0.98	0.06	9,12,18,20	9
4	CA	A	705	1/1	0.99	0.03	15,15,15,15	0
3	NA	B	703	1/1	1.00	0.01	9,9,9,9	0
3	NA	B	704	1/1	1.00	0.01	9,9,9,9	0
3	NA	A	703	1/1	1.00	0.01	9,9,9,9	0
4	CA	A	706	1/1	1.00	0.02	10,10,10,10	0
4	CA	B	705	1/1	1.00	0.02	10,10,10,10	0
4	CA	B	706	1/1	1.00	0.02	9,9,9,9	0
3	NA	A	704	1/1	1.00	0.01	8,8,8,8	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.

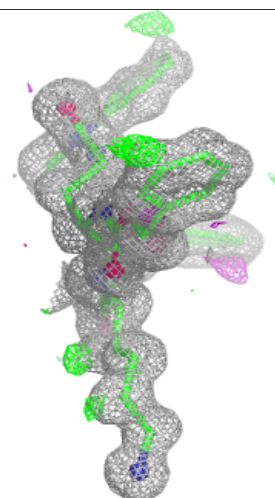
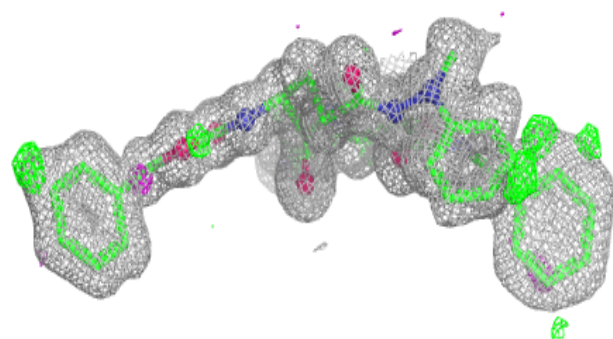
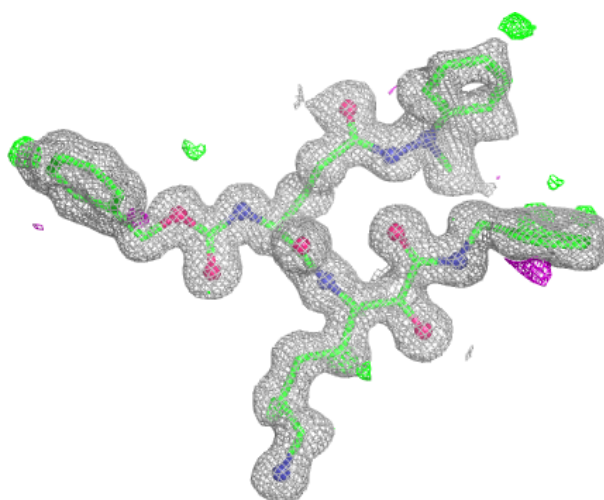
Electron density around H8E B 707:

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



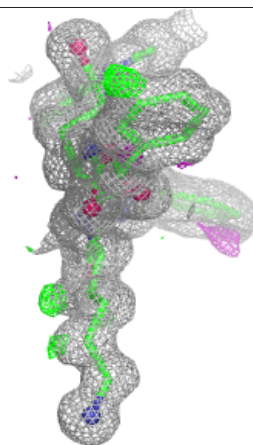
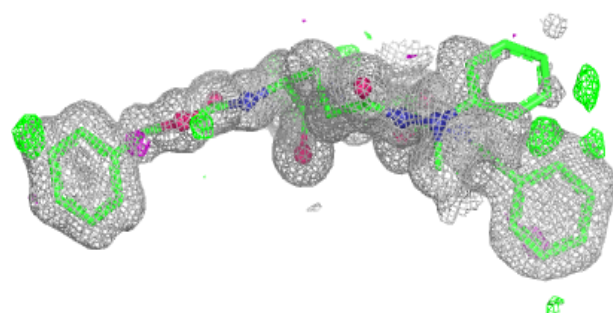
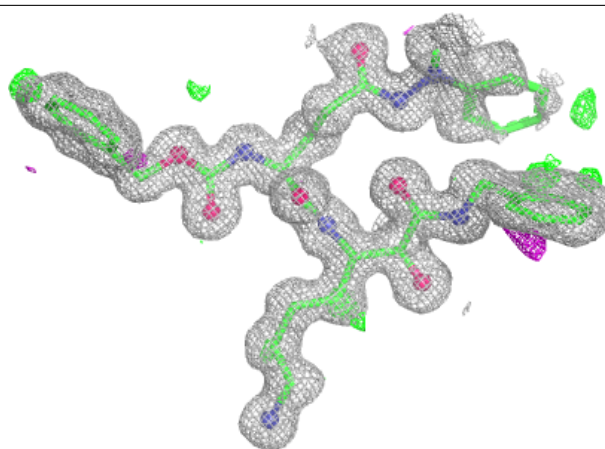
Electron density around H8E A 707 (B):

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



Electron density around H8E A 707 (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 [i](#)

There are no such residues in this entry.