Full wwPDB X-ray Structure Validation Report (i)

May 22, 2023 – 01:29 pm BST

PDB ID	:	7ZXA
Title	:	Crystal structure of human cathepsin L with covalently bound aloxistatin (E-64D)
Authors	:	Falke, S.; Lieske, J.; Guenther, S.; Reinke, P.Y.A.; Ewert, W.; Loboda, J.; Karnicar, K.; Usenik, A.; Lindic, N.; Sekirnik, A.; Chapman, H.N.; Hinrichs, W.; Turk, D.; Meents, A.
Deposited on	:	2022-05-20
Resolution	:	1.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

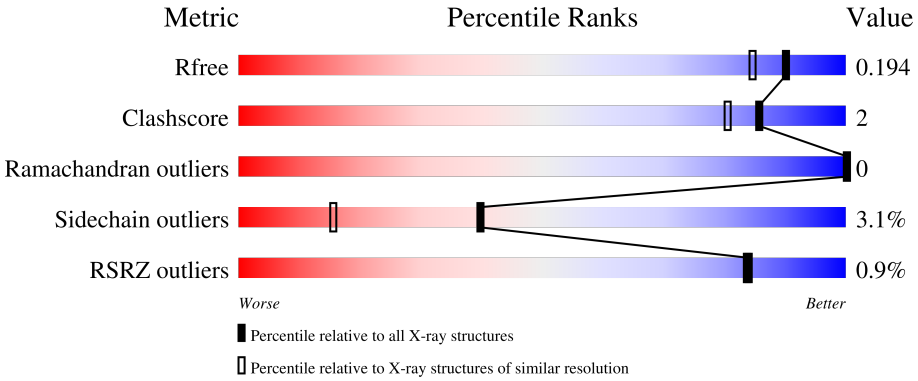
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	94% 6%
1	B	220	2% 90% 10%
1	C	220	2% 91% 6%
1	D	220	97%

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
5	DMS	A	304	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14830 atoms, of which 6895 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.

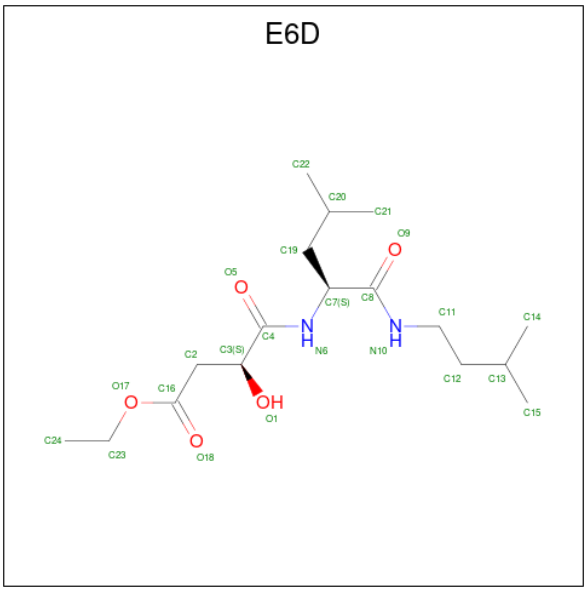
- Molecule 1 is a protein called Cathepsin L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	220	Total	C	H	N	O	S	0	8	0
			3407	1099	1642	299	351	16			
1	B	220	Total	C	H	N	O	S	0	5	0
			3344	1084	1608	288	349	15			
1	C	216	Total	C	H	N	O	S	0	6	0
			3307	1073	1588	288	343	15			
1	D	220	Total	C	H	N	O	S	0	10	0
			3428	1106	1653	298	355	16			

There are 4 discrepancies between the modelled and reference sequences:

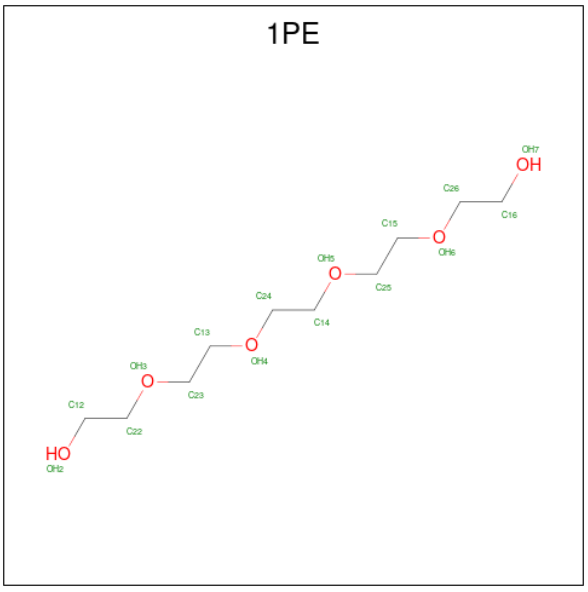
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	THR	engineered mutation	UNP P07711
B	110	ALA	THR	engineered mutation	UNP P07711
C	110	ALA	THR	engineered mutation	UNP P07711
D	110	ALA	THR	engineered mutation	UNP P07711

- Molecule 2 is ethyl (3S)-3-hydroxy-4-({(2S)-4-methyl-1-[(3-methylbutyl)amino]-1-oxopentan-2-yl}amino)-4-oxobutanoate (three-letter code: E6D) (formula: $C_{17}H_{32}N_2O_5$) (labeled as "Ligand of Interest" by depositor).



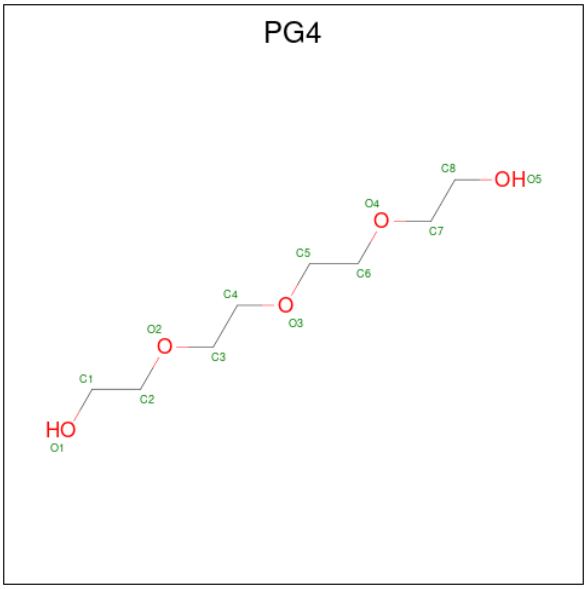
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			55	17	31	2	5		
2	B	1	Total	C	H	N	O	0	0
			55	17	31	2	5		
2	C	1	Total	C	H	N	O	0	0
			55	17	31	2	5		
2	D	1	Total	C	H	N	O	0	0
			55	17	31	2	5		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



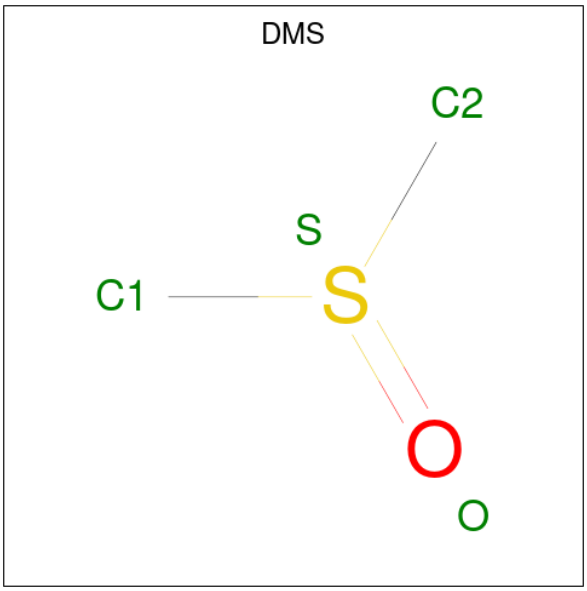
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



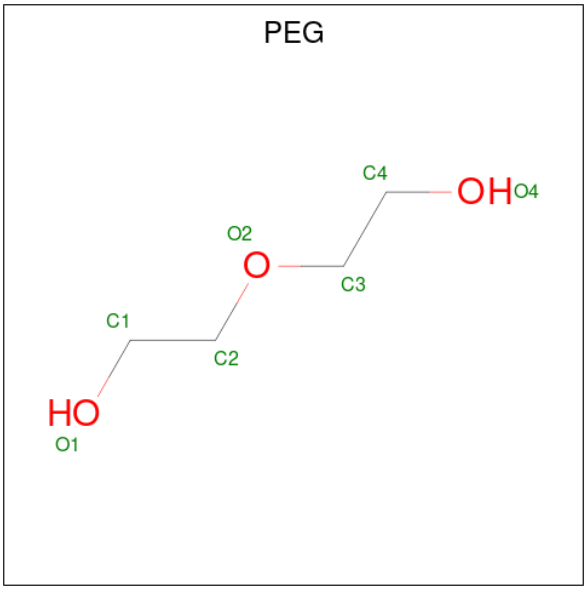
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			31	8	18	5		
4	D	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	C	1	Total	C	H	O	0	0
			17	4	10	3		
6	C	1	Total	C	H	O	0	0
			17	4	10	3		
6	C	1	Total	C	H	O	0	0
			17	4	10	3		

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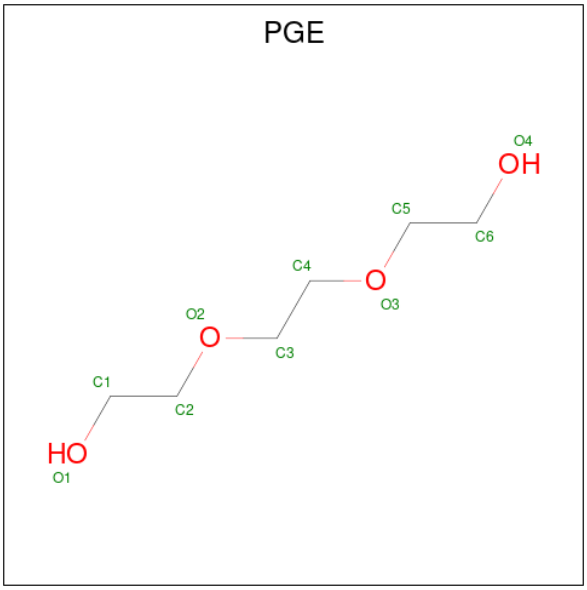
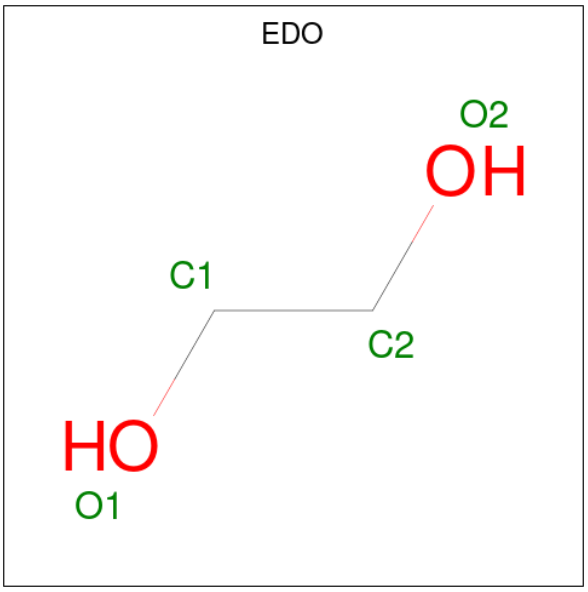
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C H O 17 4 10 3	0	0

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



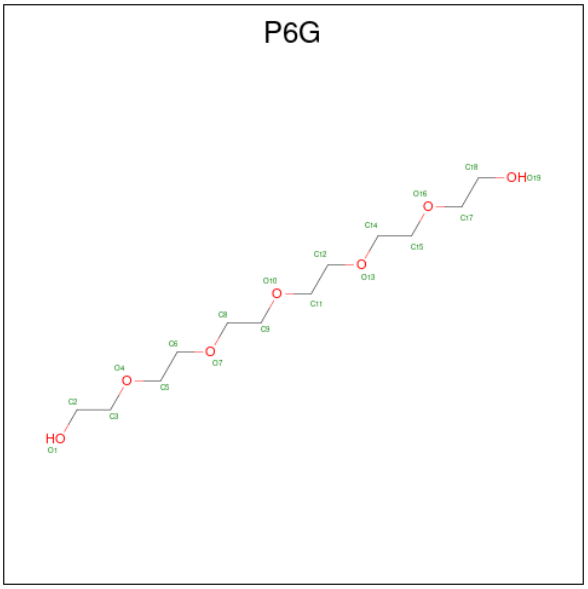
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 24 6 14 4	0	0
7	A	1	Total C H O 24 6 14 4	0	0
7	C	1	Total C H O 24 6 14 4	0	0
7	D	1	Total C H O 24 6 14 4	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 10 2 6 2	0	0
8	B	1	Total C H O 10 2 6 2	0	0
8	C	1	Total C H O 10 2 6 2	0	0
8	C	1	Total C H O 10 2 6 2	0	0
8	D	1	Total C H O 10 2 6 2	0	0

- Molecule 9 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	H	O	0	0
			45	12	26	7		

- Molecule 10 is water.

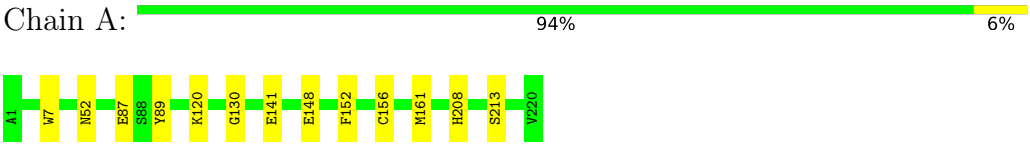
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	144	Total	O	0	0
			144	144		
10	B	171	Total	O	0	0
			171	171		
10	C	128	Total	O	0	0
			128	128		
10	D	204	Total	O	0	0
			204	204		

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.

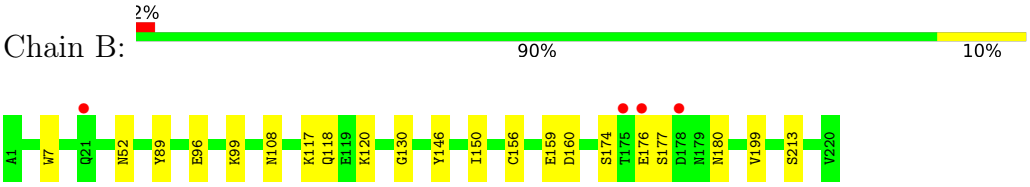
• Molecule 1: Cathepsin L

Chain A:



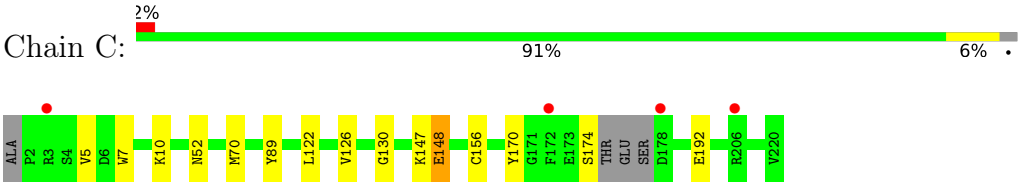
• Molecule 1: Cathepsin L

Chain B:



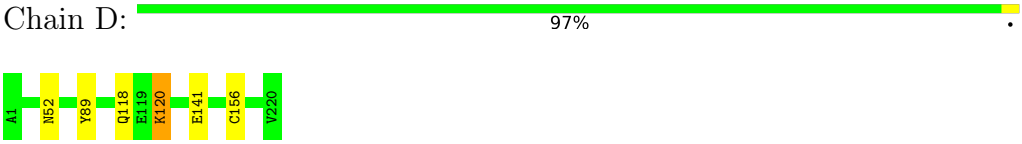
• Molecule 1: Cathepsin L

Chain C:



• Molecule 1: Cathepsin L

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.07Å 62.26Å 67.42Å 105.27° 93.74° 115.78°	Depositor
Resolution (Å)	49.38 – 1.60 49.38 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.38-1.60) 84.0 (49.38-1.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.91 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.18-3855_9999	Depositor
R, R_{free}	0.164 , 0.194 0.164 , 0.194	Depositor DCC
R_{free} test set	1998 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14830	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E6D, 1PE, DMS, PEG, P6G, PGE, EDO, PG4

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	0.33	0/1807	0.52	0/2438
1	B	0.35	0/1778	0.53	0/2401
1	C	0.31	0/1760	0.51	0/2374
1	D	0.35	0/1817	0.55	0/2451
All	All	0.33	0/7162	0.53	0/9664

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

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	1765	1642	1635	8	0
1	B	1736	1608	1604	11	0
1	C	1719	1588	1583	9	0
1	D	1775	1653	1644	1	0
2	A	24	31	0	0	0
2	B	24	31	0	0	0
2	C	24	31	0	0	0
2	D	24	31	0	0	0
3	A	16	22	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	18	18	0	0
4	D	13	18	18	0	0
5	A	4	6	6	4	0
5	B	8	12	12	0	0
5	D	8	12	12	0	0
6	A	7	10	10	0	0
6	B	21	30	30	2	0
6	C	21	30	30	0	0
6	D	7	10	10	0	0
7	A	20	28	28	5	0
7	C	10	14	14	0	0
7	D	10	14	14	0	0
8	A	4	6	6	0	0
8	B	4	6	6	0	0
8	C	8	12	12	2	0
8	D	4	6	6	0	0
9	D	19	26	26	0	0
10	A	144	0	0	2	0
10	B	171	0	0	3	0
10	C	128	0	0	0	0
10	D	204	0	0	0	0
All	All	7935	6895	6746	31	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 2.

All (31) 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:120:LYS:HE2	10:B:467:HOH:O	2.02	0.60
1:B:108:ASN:HD21	6:B:306:PEG:H32	1.69	0.57
1:C:70:MET:HB2	8:C:306:EDO:H12	1.89	0.55
1:B:117:LYS:HG3	1:B:213:SER:HA	1.89	0.55
7:A:307:PGE:H42	1:C:192:GLU:HB2	1.91	0.52
1:C:5:VAL:HG23	1:C:170:TYR:CZ	2.46	0.51
1:A:161:MET:CE	1:A:213:SER:HB2	2.41	0.51
1:B:99:LYS:NZ	10:B:401:HOH:O	2.39	0.49
1:A:7:TRP:CE2	1:A:130:GLY:HA2	2.48	0.48
1:B:96:GLU:HB3	1:B:99:LYS:HZ1	1.79	0.47
1:A:161:MET:HE3	1:A:213:SER:HB2	1.98	0.46
1:A:141:GLU:OE2	10:A:401:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HD21	6:B:306:PEG:C3	2.28	0.45
1:C:70:MET:HB2	8:C:306:EDO:C1	2.47	0.45
1:B:150:ILE:CD1	1:B:180:ASN:HB3	2.47	0.44
1:B:180:ASN:ND2	10:B:406:HOH:O	2.51	0.44
1:B:7:TRP:CE2	1:B:130:GLY:HA2	2.52	0.44
5:A:304:DMS:C1	7:A:307:PGE:H6	2.48	0.44
1:B:117:LYS:NZ	1:B:159:GLU:OE2	2.51	0.44
1:B:146:TYR:CZ	1:B:199:VAL:HG23	2.53	0.43
1:A:152:PHE:HA	1:A:208:HIS:CE1	2.53	0.43
1:C:7:TRP:CE2	1:C:130:GLY:HA2	2.53	0.43
5:A:304:DMS:H13	7:A:307:PGE:C6	2.49	0.43
1:A:120:LYS:HG3	10:A:519:HOH:O	2.19	0.42
1:C:147:LYS:C	1:C:148[B]:GLU:HG2	2.39	0.42
5:A:304:DMS:H13	7:A:307:PGE:H6	2.02	0.42
1:A:87:GLU:OE2	1:C:10:LYS:NZ	2.46	0.41
1:C:122:LEU:O	1:C:126:VAL:HG23	2.20	0.41
1:D:120:LYS:HD2	1:D:120:LYS:HA	1.96	0.40
1:A:148:GLU:OE1	1:C:192:GLU:OE2	2.39	0.40
5:A:304:DMS:C1	7:A:307:PGE:C6	2.99	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	226/220 (103%)	223 (99%)	3 (1%)	0	100	100
1	B	223/220 (101%)	218 (98%)	5 (2%)	0	100	100
1	C	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
1	D	228/220 (104%)	223 (98%)	5 (2%)	0	100	100
All	All	895/880 (102%)	874 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	186/178 (104%)	183 (98%)	3 (2%)	62 41
1	B	183/178 (103%)	175 (96%)	8 (4%)	28 8
1	C	181/178 (102%)	175 (97%)	6 (3%)	38 14
1	D	188/178 (106%)	182 (97%)	6 (3%)	39 15
All	All	738/712 (104%)	715 (97%)	23 (3%)	40 15

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	89	TYR
1	A	156	CYS
1	B	52	ASN
1	B	89	TYR
1	B	118	GLN
1	B	156	CYS
1	B	160	ASP
1	B	174	SER
1	B	176	GLU
1	B	177	SER
1	C	52	ASN
1	C	89	TYR
1	C	148[A]	GLU
1	C	148[B]	GLU
1	C	156	CYS
1	C	174	SER
1	D	52	ASN
1	D	89	TYR
1	D	118	GLN
1	D	120	LYS
1	D	141	GLU

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Mol	Chain	Res	Type
1	D	156	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	118	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

30 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	E6D	A	301	1	23,23,23	0.23	0	27,29,29	0.45	0
6	PEG	D	506	-	6,6,6	0.24	0	5,5,5	0.12	0
7	PGE	A	306	-	9,9,9	0.38	0	8,8,8	0.42	0
8	EDO	D	508	-	3,3,3	0.53	0	2,2,2	0.18	0
5	DMS	D	501	-	3,3,3	0.65	0	3,3,3	0.41	0
8	EDO	C	307	-	3,3,3	0.51	0	2,2,2	0.22	0
6	PEG	C	304	-	6,6,6	0.24	0	5,5,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	A	304	-	3,3,3	0.61	0	3,3,3	0.51	0
3	1PE	A	302	-	15,15,15	0.20	0	14,14,14	0.18	0
2	E6D	B	301	1	23,23,23	0.22	0	27,29,29	0.63	1 (3%)
8	EDO	B	307	-	3,3,3	0.43	0	2,2,2	0.40	0
8	EDO	C	306	-	3,3,3	0.38	0	2,2,2	0.85	0
5	DMS	B	302	-	3,3,3	0.67	0	3,3,3	0.75	0
6	PEG	C	303	-	6,6,6	0.23	0	5,5,5	0.26	0
4	PG4	D	505	-	12,12,12	0.19	0	11,11,11	0.35	0
7	PGE	A	307	-	9,9,9	0.28	0	8,8,8	0.48	0
6	PEG	A	305	-	6,6,6	0.26	0	5,5,5	0.06	0
2	E6D	C	301	1	23,23,23	0.21	0	27,29,29	0.58	1 (3%)
7	PGE	D	507	-	9,9,9	0.31	0	8,8,8	0.35	0
7	PGE	C	305	-	9,9,9	0.31	0	8,8,8	0.48	0
6	PEG	B	305	-	6,6,6	0.27	0	5,5,5	0.31	0
6	PEG	C	302	-	6,6,6	0.28	0	5,5,5	0.18	0
9	P6G	D	504	-	18,18,18	0.23	0	17,17,17	0.17	0
6	PEG	B	306	-	6,6,6	0.29	0	5,5,5	0.14	0
8	EDO	A	308	-	3,3,3	0.54	0	2,2,2	0.35	0
4	PG4	A	303	-	12,12,12	0.20	0	11,11,11	0.19	0
6	PEG	B	304	-	6,6,6	0.22	0	5,5,5	0.25	0
2	E6D	D	502	1	23,23,23	0.24	0	27,29,29	0.55	1 (3%)
5	DMS	B	303	-	3,3,3	0.65	0	3,3,3	0.62	0
5	DMS	D	503	-	3,3,3	0.67	0	3,3,3	0.57	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
2	E6D	A	301	1	-	4/29/29/29	-
6	PEG	D	506	-	-	2/4/4/4	-
7	PGE	A	306	-	-	3/7/7/7	-
8	EDO	D	508	-	-	0/1/1/1	-
8	EDO	C	307	-	-	0/1/1/1	-
6	PEG	C	304	-	-	3/4/4/4	-
3	1PE	A	302	-	-	8/13/13/13	-
2	E6D	B	301	1	-	4/29/29/29	-
8	EDO	B	307	-	-	1/1/1/1	-
8	EDO	C	306	-	-	0/1/1/1	-
6	PEG	C	303	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	D	505	-	-	2/10/10/10	-
7	PGE	A	307	-	-	5/7/7/7	-
6	PEG	A	305	-	-	2/4/4/4	-
2	E6D	C	301	1	-	4/29/29/29	-
7	PGE	D	507	-	-	2/7/7/7	-
7	PGE	C	305	-	-	4/7/7/7	-
6	PEG	B	305	-	-	2/4/4/4	-
6	PEG	C	302	-	-	1/4/4/4	-
9	P6G	D	504	-	-	4/16/16/16	-
6	PEG	B	306	-	-	1/4/4/4	-
8	EDO	A	308	-	-	1/1/1/1	-
4	PG4	A	303	-	-	3/10/10/10	-
6	PEG	B	304	-	-	2/4/4/4	-
2	E6D	D	502	1	-	4/29/29/29	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	E6D	C3-C2-C16	-2.76	107.49	113.22
2	C	301	E6D	C3-C2-C16	-2.45	108.13	113.22
2	D	502	E6D	C3-C2-C16	-2.06	108.95	113.22

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	E6D	O1-C3-C4-N6
2	B	301	E6D	O1-C3-C4-N6
2	C	301	E6D	O1-C3-C4-N6
2	D	502	E6D	O1-C3-C4-N6
6	D	506	PEG	O2-C3-C4-O4
9	D	504	P6G	O16-C17-C18-O19
3	A	302	1PE	OH4-C13-C23-OH3
7	A	306	PGE	O2-C3-C4-O3
9	D	504	P6G	O7-C8-C9-O10
6	B	304	PEG	O1-C1-C2-O2
6	B	305	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
7	D	507	PGE	O1-C1-C2-O2
7	A	307	PGE	O2-C3-C4-O3
4	D	505	PG4	O1-C1-C2-O2
6	D	506	PEG	O1-C1-C2-O2
7	C	305	PGE	O3-C5-C6-O4
6	B	305	PEG	O1-C1-C2-O2
6	C	304	PEG	O2-C3-C4-O4
2	A	301	E6D	O1-C3-C4-O5
2	C	301	E6D	O1-C3-C4-O5
2	D	502	E6D	O1-C3-C4-O5
2	B	301	E6D	C2-C3-C4-N6
2	B	301	E6D	O1-C3-C4-O5
7	D	507	PGE	C4-C3-O2-C2
6	C	304	PEG	C1-C2-O2-C3
7	A	307	PGE	C6-C5-O3-C4
4	A	303	PG4	C5-C6-O4-C7
4	A	303	PG4	C1-C2-O2-C3
3	A	302	1PE	C23-C13-OH4-C24
4	D	505	PG4	C8-C7-O4-C6
4	A	303	PG4	C3-C4-O3-C5
6	A	305	PEG	O2-C3-C4-O4
9	D	504	P6G	C12-C11-O10-C9
6	C	302	PEG	C1-C2-O2-C3
3	A	302	1PE	C13-C23-OH3-C22
6	B	304	PEG	C4-C3-O2-C2
3	A	302	1PE	C14-C24-OH4-C13
7	C	305	PGE	C1-C2-O2-C3
7	C	305	PGE	C4-C3-O2-C2
7	A	306	PGE	C3-C4-O3-C5
6	A	305	PEG	O1-C1-C2-O2
6	B	306	PEG	O1-C1-C2-O2
7	A	306	PGE	C1-C2-O2-C3
8	B	307	EDO	O1-C1-C2-O2
7	A	307	PGE	C4-C3-O2-C2
9	D	504	P6G	O1-C2-C3-O4
7	A	307	PGE	O1-C1-C2-O2
8	A	308	EDO	O1-C1-C2-O2
3	A	302	1PE	OH6-C15-C25-OH5
3	A	302	1PE	C16-C26-OH6-C15
7	A	307	PGE	C1-C2-O2-C3
7	C	305	PGE	O2-C3-C4-O3
3	A	302	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
3	A	302	1PE	OH5-C14-C24-OH4
6	C	304	PEG	O1-C1-C2-O2
2	A	301	E6D	C2-C3-C4-O5
2	B	301	E6D	C2-C3-C4-O5
2	C	301	E6D	C2-C3-C4-O5
2	D	502	E6D	C2-C3-C4-O5
2	A	301	E6D	C2-C3-C4-N6
2	C	301	E6D	C2-C3-C4-N6
2	D	502	E6D	C2-C3-C4-N6

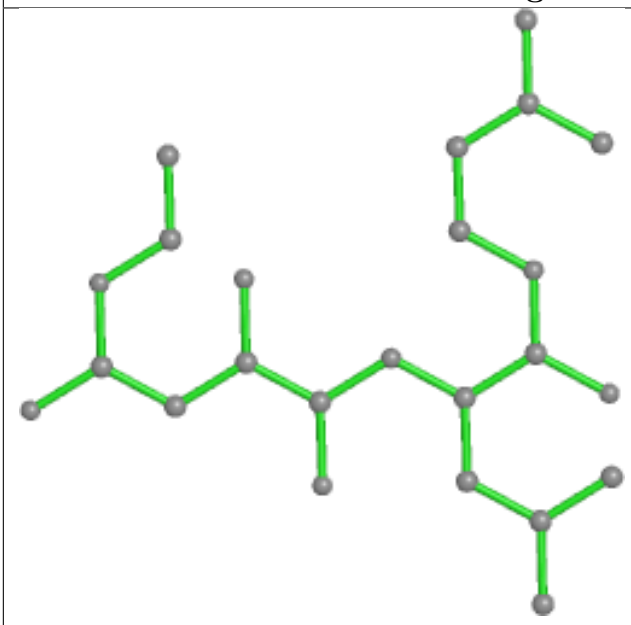
There are no ring outliers.

4 monomers are involved in 9 short contacts:

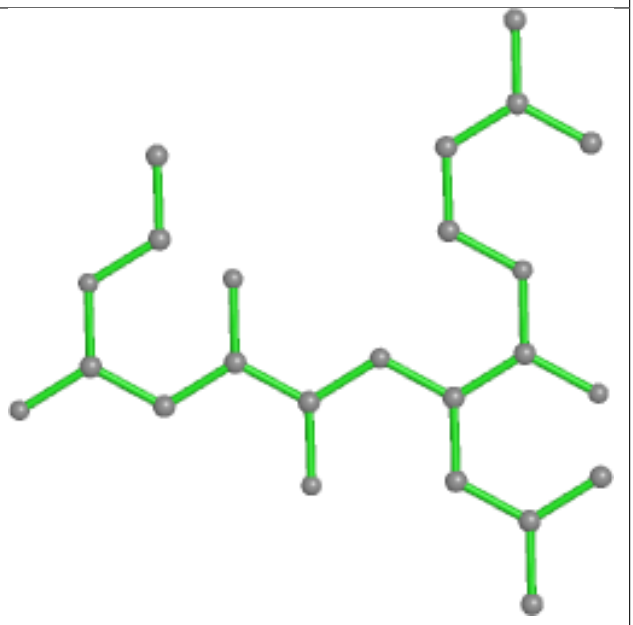
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	DMS	4	0
8	C	306	EDO	2	0
7	A	307	PGE	5	0
6	B	306	PEG	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

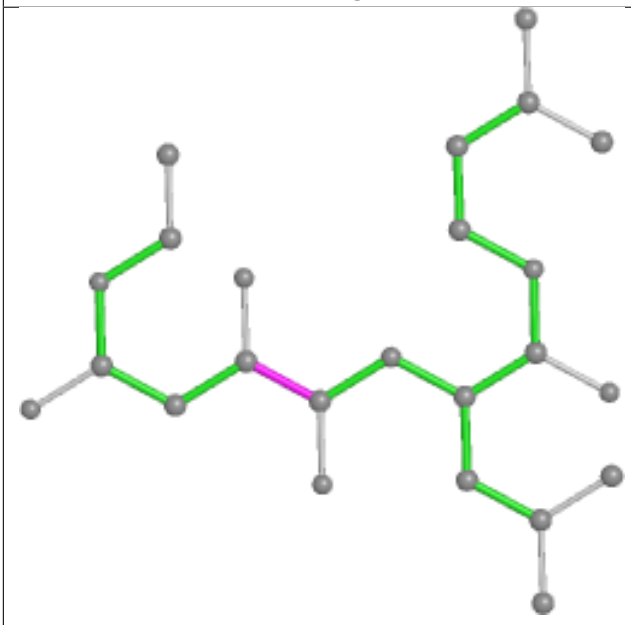
Ligand E6D A 301



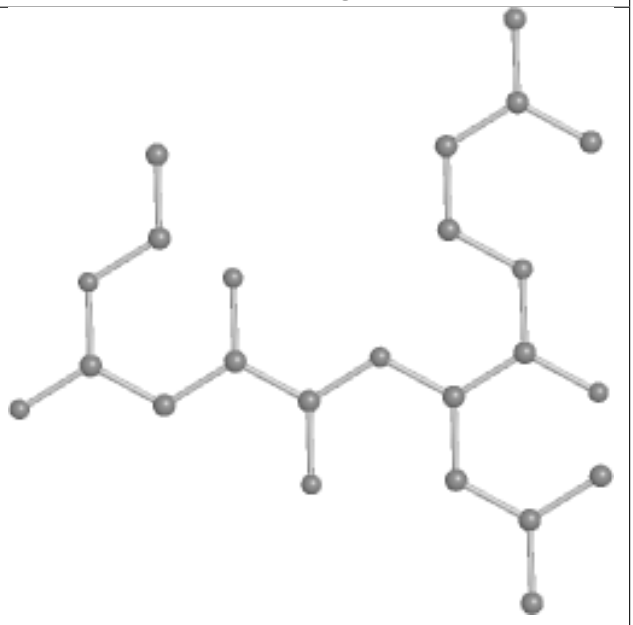
Bond lengths



Bond angles

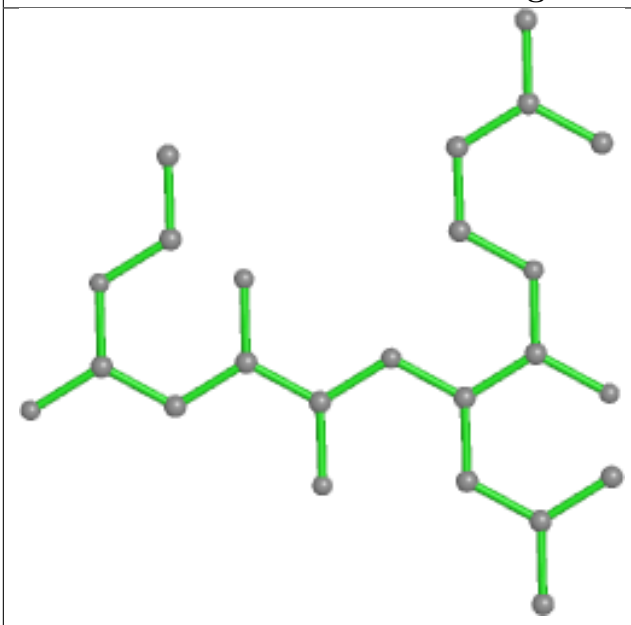


Torsions

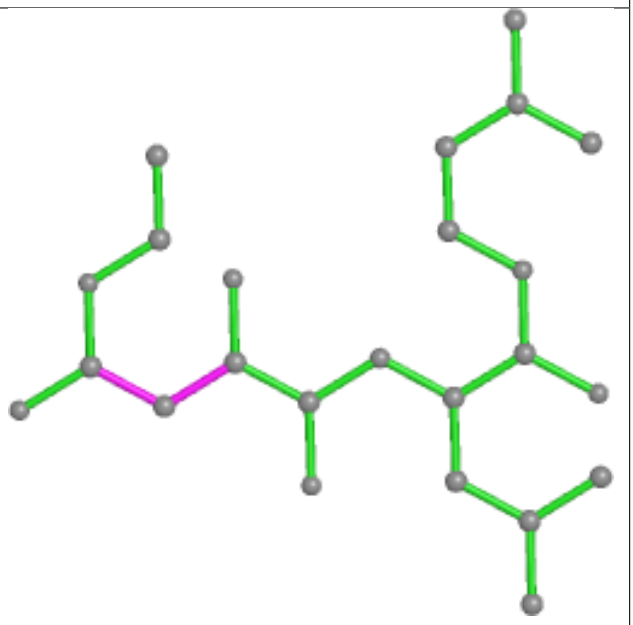


Rings

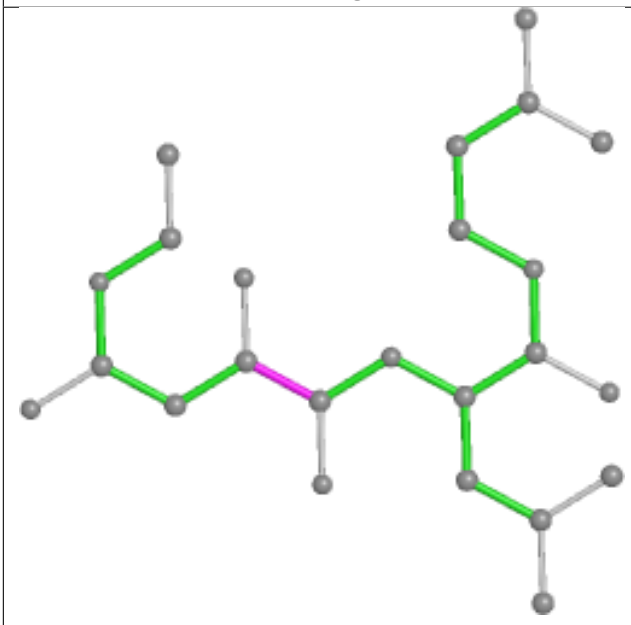
Ligand E6D B 301



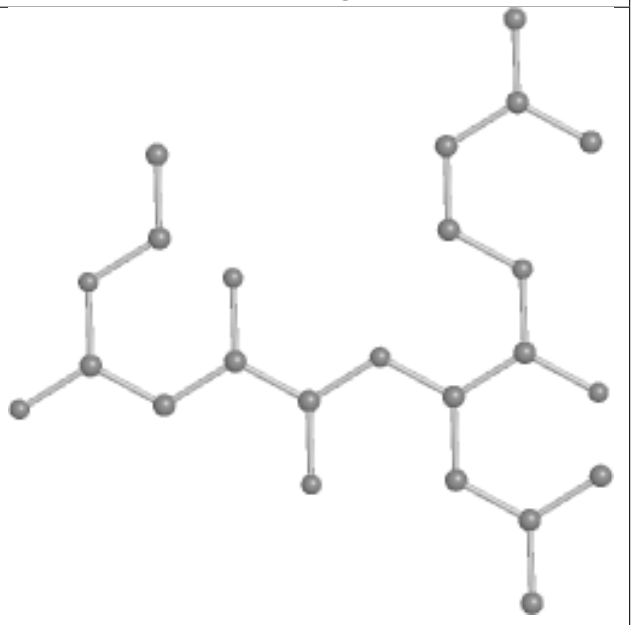
Bond lengths



Bond angles

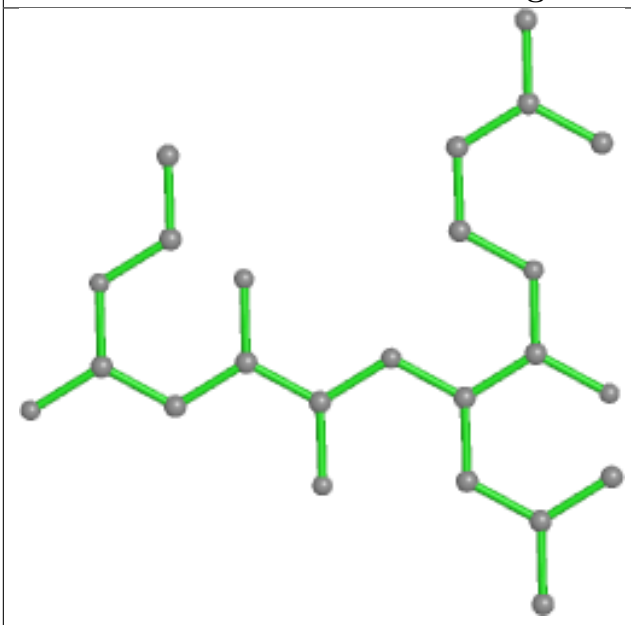


Torsions

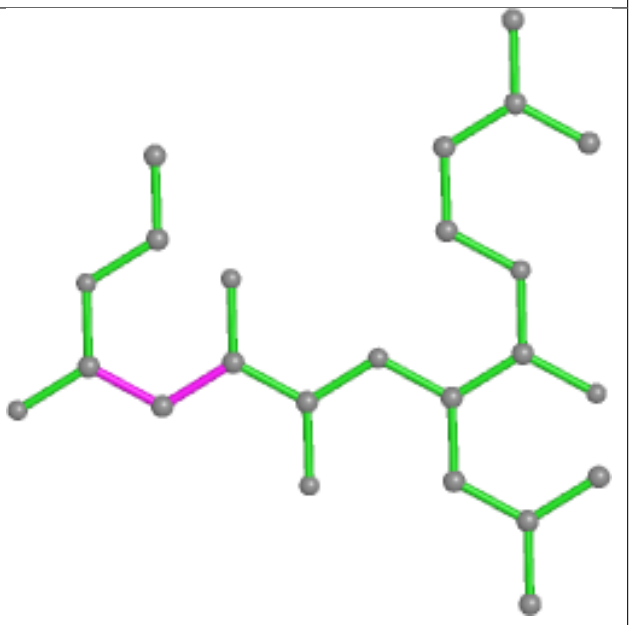


Rings

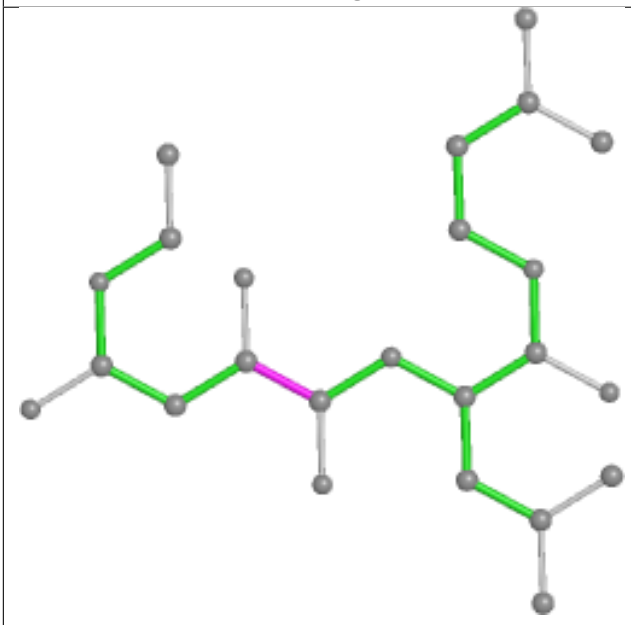
Ligand E6D C 301



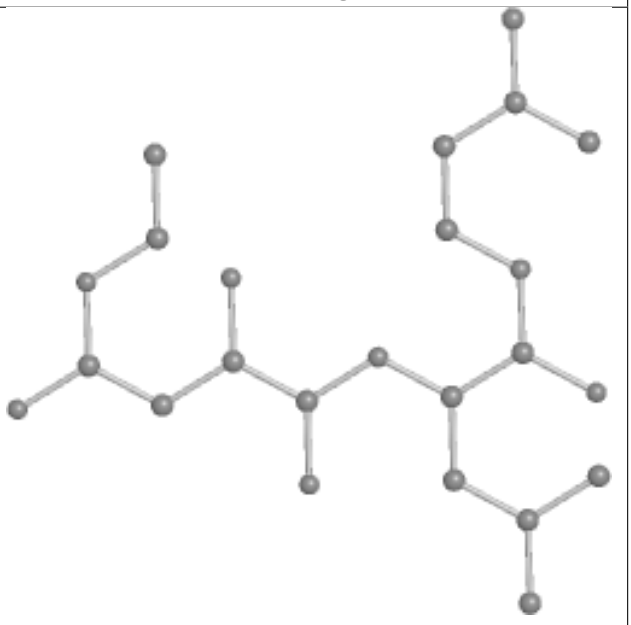
Bond lengths



Bond angles

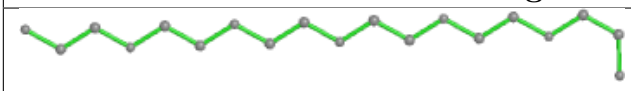


Torsions

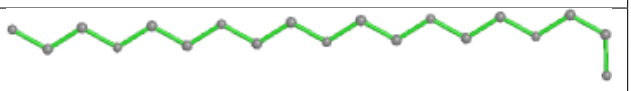


Rings

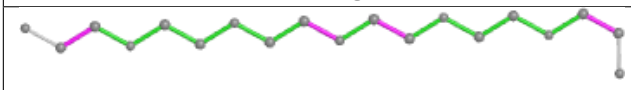
Ligand P6G D 504



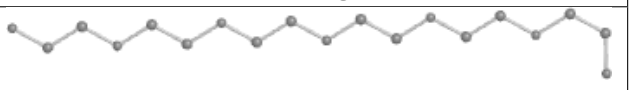
Bond lengths



Bond angles

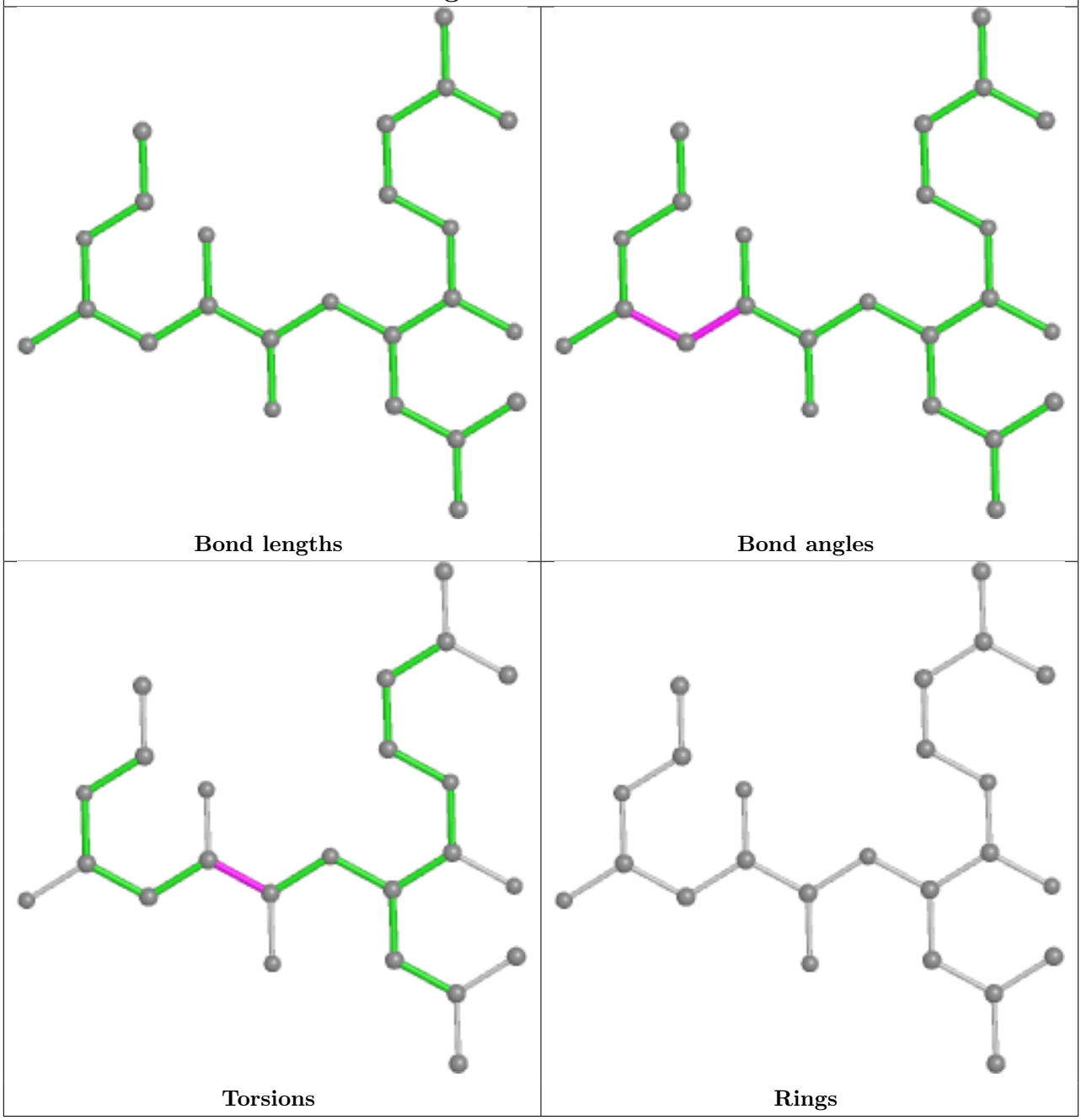


Torsions



Rings

Ligand E6D D 502



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

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, 95^{th} 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	220/220 (100%)	-0.41	0 100 100	19, 28, 41, 63	0
1	B	220/220 (100%)	-0.25	4 (1%) 68 67	17, 25, 51, 95	0
1	C	216/220 (98%)	-0.13	4 (1%) 66 65	21, 32, 59, 88	0
1	D	220/220 (100%)	-0.41	0 100 100	17, 24, 40, 53	0
All	All	876/880 (99%)	-0.30	8 (0%) 84 84	17, 27, 51, 95	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	THR	6.4
1	C	172	PHE	3.7
1	B	178	ASP	3.1
1	B	176	GLU	2.7
1	C	206[A]	ARG	2.6
1	C	178	ASP	2.3
1	C	3	ARG	2.1
1	B	21[A]	GLN	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 (i)

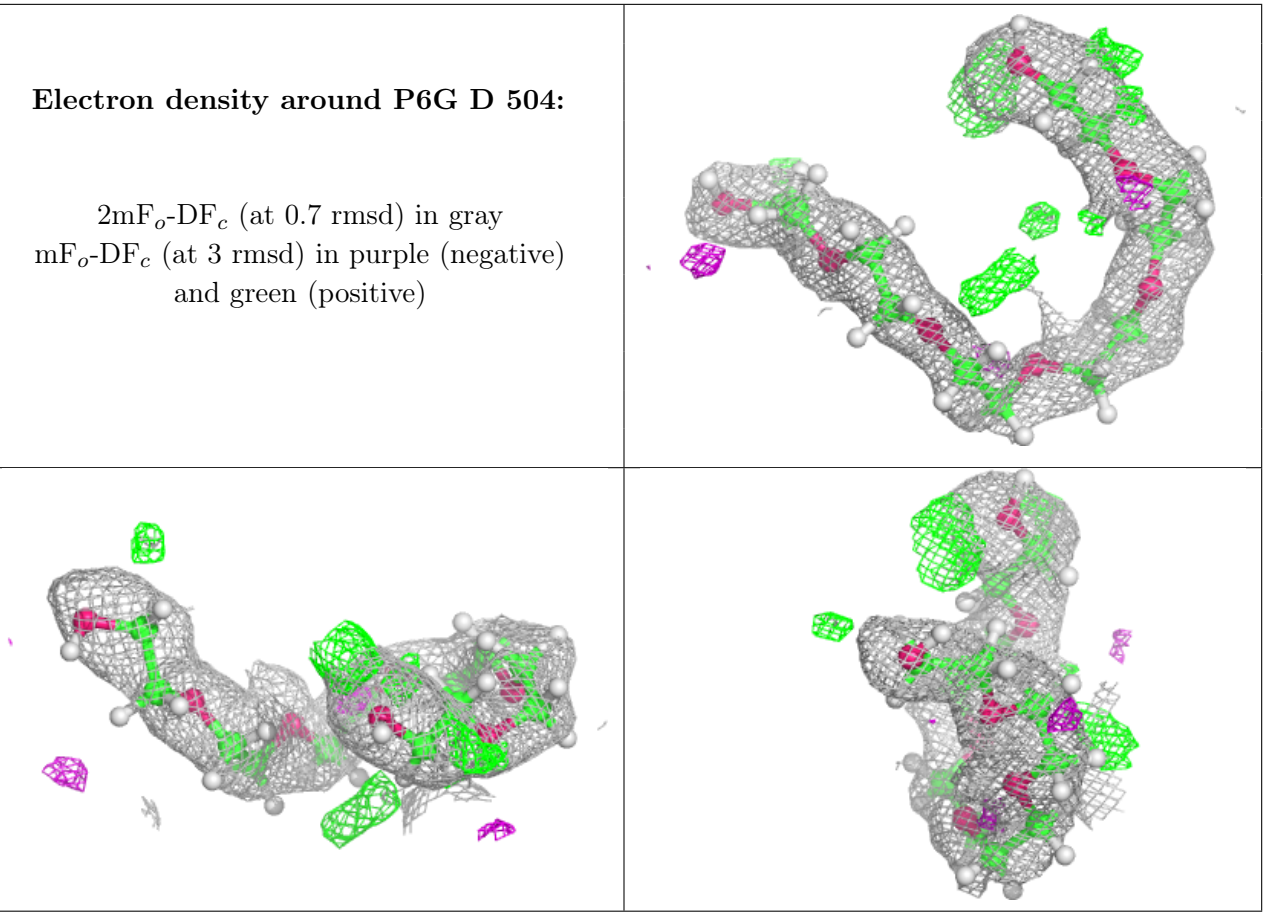
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	EDO	C	307	4/4	0.71	0.19	39,47,52,53	0
8	EDO	B	307	4/4	0.73	0.19	39,48,55,66	0
8	EDO	A	308	4/4	0.78	0.19	32,39,42,47	0
6	PEG	C	303	7/7	0.79	0.14	45,59,66,74	0
8	EDO	D	508	4/4	0.80	0.16	33,40,41,43	0
7	PGE	A	307	10/10	0.81	0.17	34,54,61,61	0
9	P6G	D	504	19/19	0.81	0.14	38,50,63,64	0
7	PGE	D	507	10/10	0.82	0.18	42,55,64,67	0
6	PEG	B	305	7/7	0.82	0.21	41,50,60,60	0
7	PGE	A	306	10/10	0.83	0.14	40,51,68,68	0
6	PEG	C	304	7/7	0.84	0.11	42,50,57,65	0
3	1PE	A	302	16/16	0.84	0.25	41,53,70,71	0
4	PG4	A	303	13/13	0.84	0.21	39,48,57,57	0
8	EDO	C	306	4/4	0.85	0.17	28,35,42,42	0
4	PG4	D	505	13/13	0.85	0.17	35,47,73,79	0
6	PEG	D	506	7/7	0.85	0.10	38,46,49,57	0
7	PGE	C	305	10/10	0.85	0.17	39,51,61,65	0
6	PEG	B	306	7/7	0.86	0.18	32,52,63,69	0
6	PEG	A	305	7/7	0.86	0.30	38,53,70,70	0
6	PEG	B	304	7/7	0.87	0.11	42,50,55,56	0
6	PEG	C	302	7/7	0.89	0.10	43,52,62,63	0
5	DMS	B	303	4/4	0.90	0.13	31,50,69,69	0
5	DMS	A	304	4/4	0.93	0.12	32,39,46,47	0
2	E6D	A	301	24/24	0.93	0.15	28,37,46,47	0
2	E6D	B	301	24/24	0.93	0.15	25,35,47,48	0
2	E6D	D	502	24/24	0.93	0.15	23,32,47,48	0
2	E6D	C	301	24/24	0.94	0.13	26,37,47,47	0
5	DMS	B	302	4/4	0.97	0.09	33,40,47,48	0
5	DMS	D	503	4/4	0.97	0.09	29,52,55,55	0
5	DMS	D	501	4/4	0.98	0.10	32,39,46,46	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.

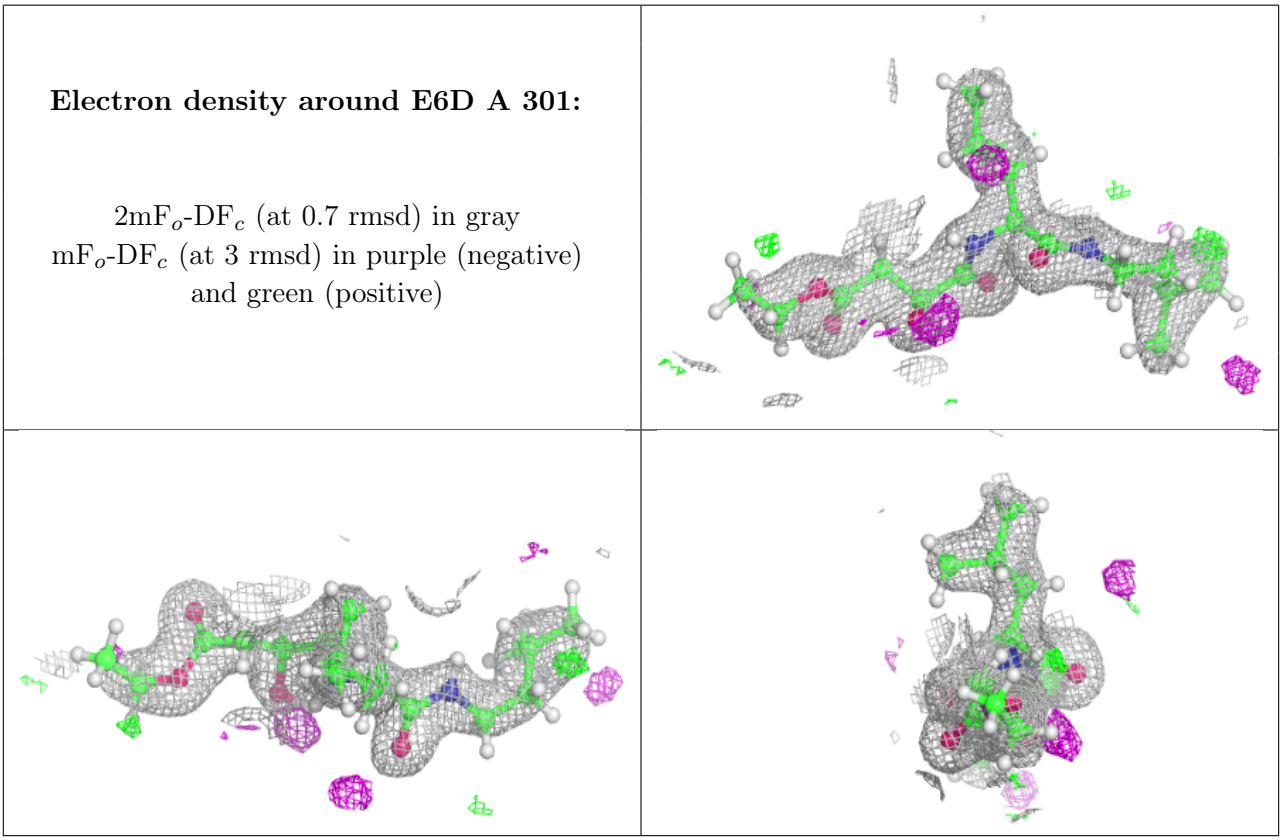
Electron density around P6G D 504:

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



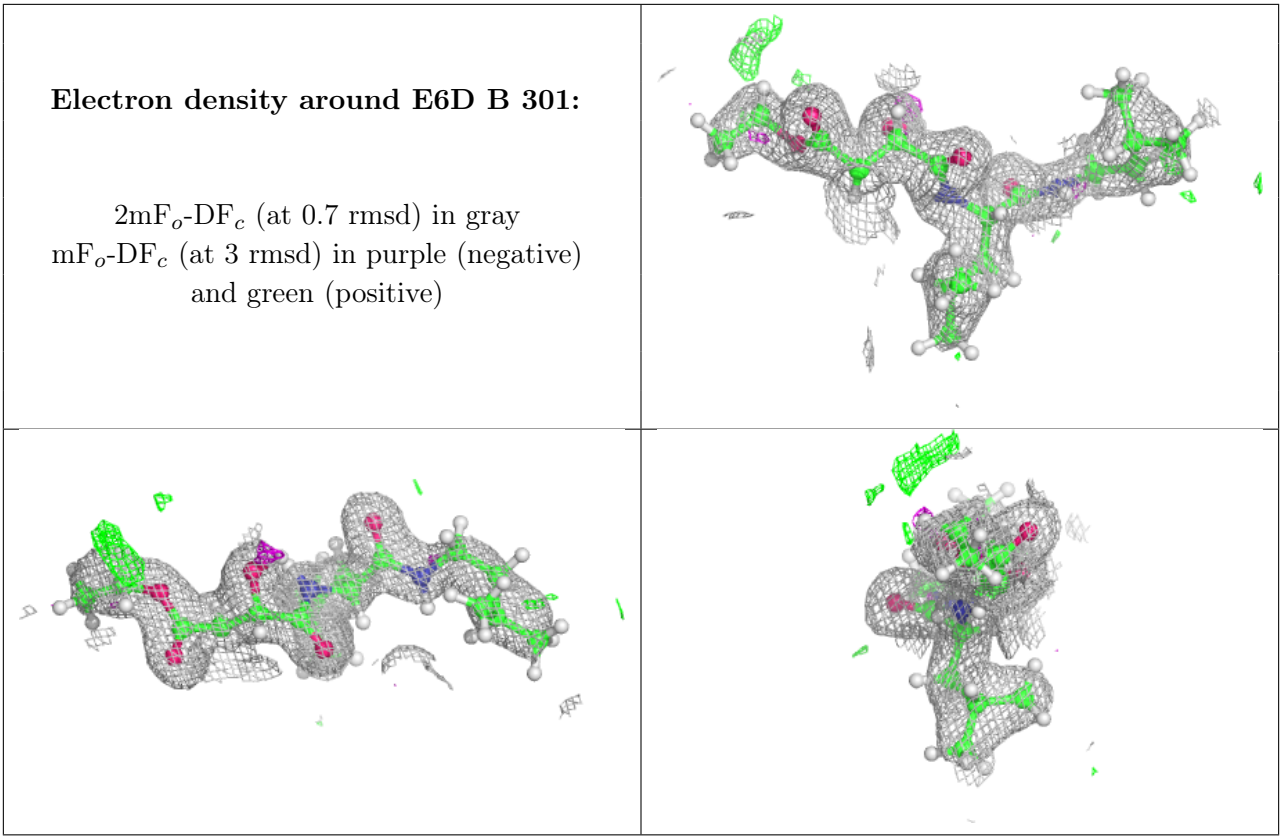
Electron density around E6D A 301:

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



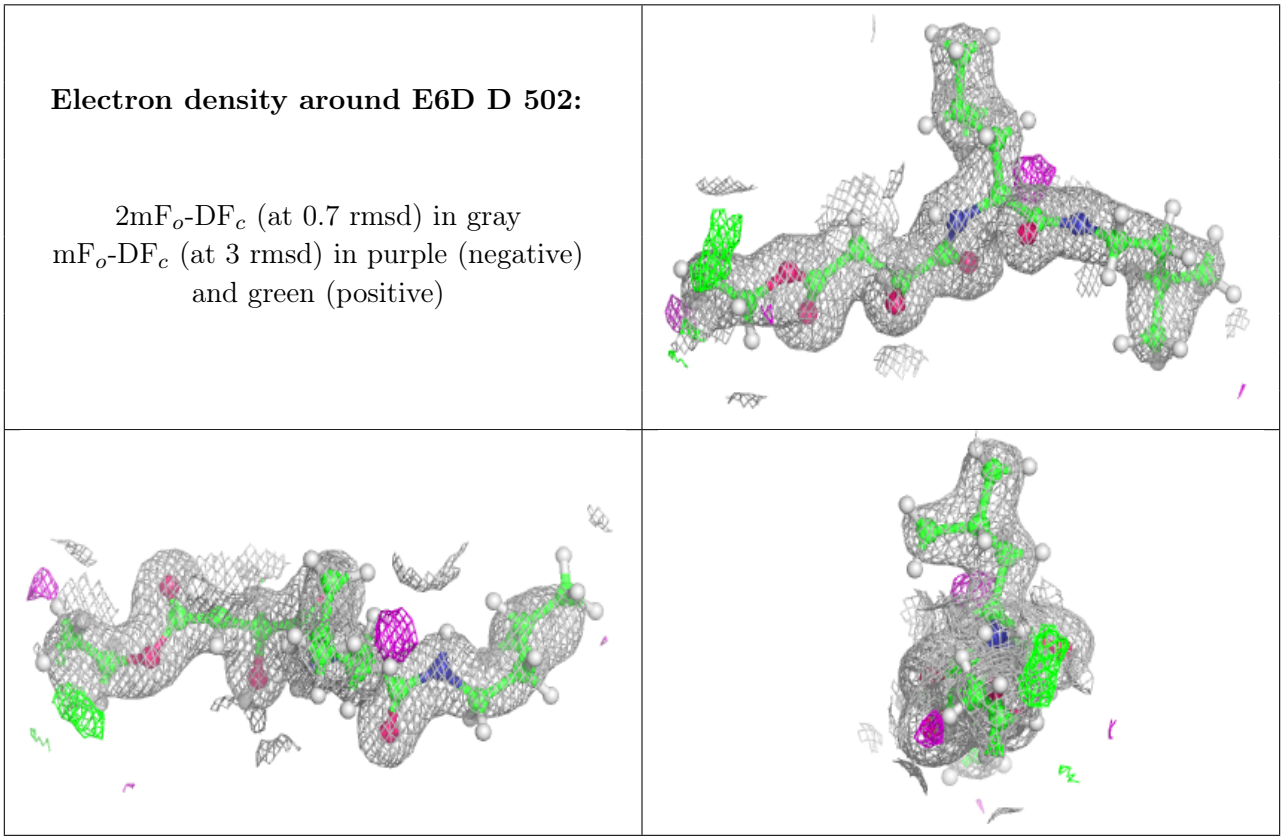
Electron density around E6D B 301:

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



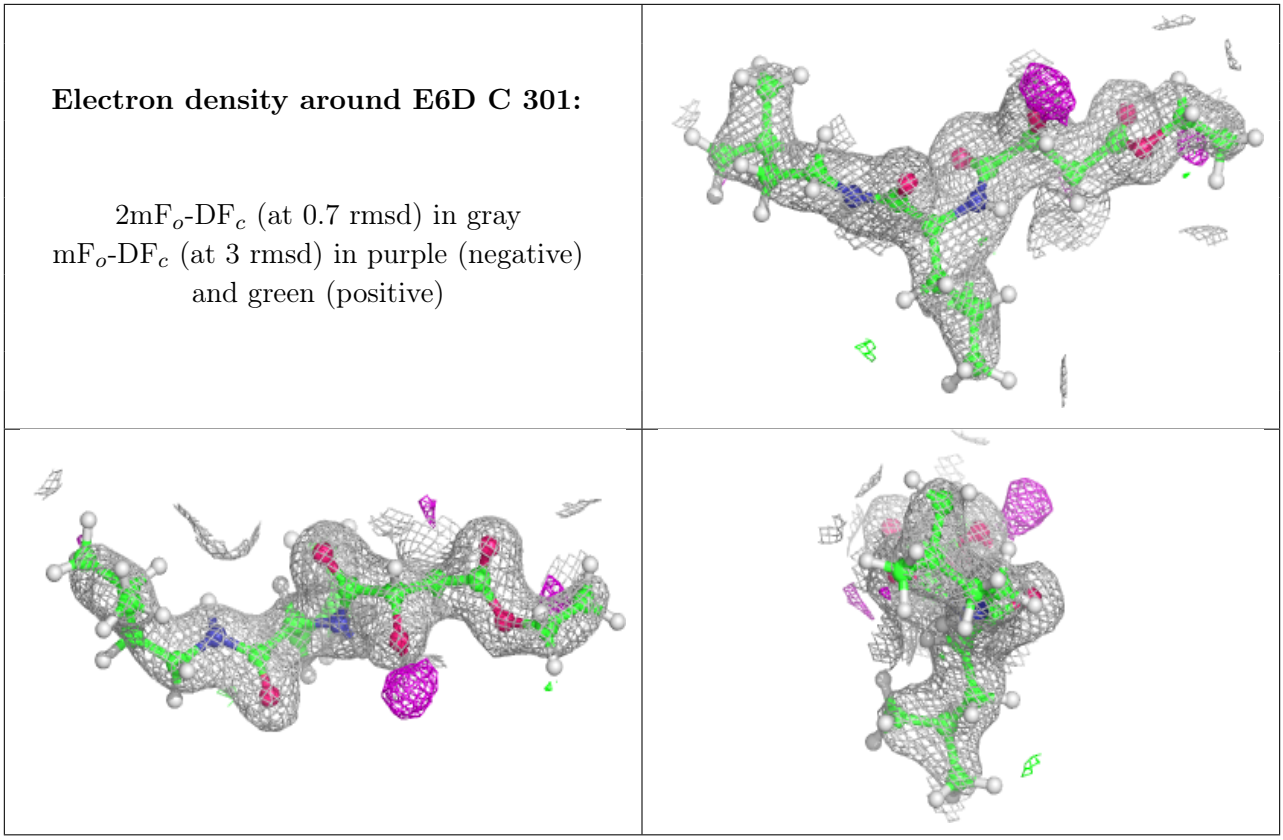
Electron density around E6D D 502:

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



Electron density around E6D C 301:

$2mF_o$-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.