



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:51 am BST

PDB ID : 5LBO
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-001
Authors : Singh, A.K.; Brown, D.G.
Deposited on : 2016-06-16
Resolution : 2.25 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 : 2.11
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) : 2.11

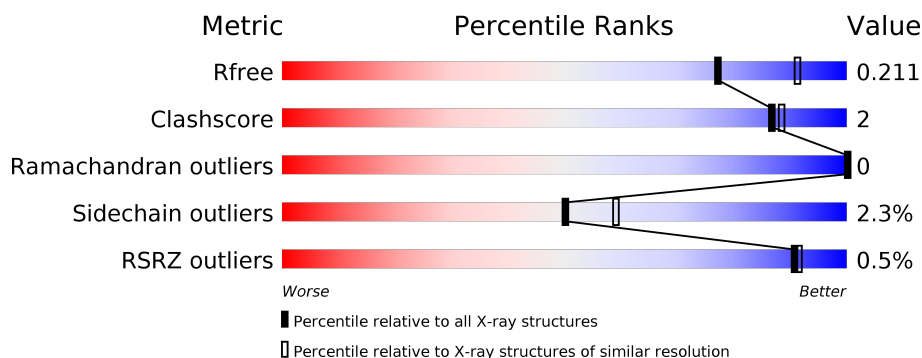
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	364	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 84% 6% • 9% </div> </div>
1	B	364	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 82% 7% • 11% </div> </div>
1	C	364	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 85% • • 11% </div> </div>
1	D	364	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 84% • • 11% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DTT	A	1013	-	-	X	-
5	DTT	D	1014	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11475 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	1	0
			2679	1696	458	511	14			
1	B	324	Total	C	N	O	S	0	2	0
			2638	1668	452	504	14			
1	C	323	Total	C	N	O	S	0	0	0
			2613	1654	446	499	14			
1	D	324	Total	C	N	O	S	0	1	0
			2632	1665	451	502	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	expression tag	UNP Q08499
A	76	SER	-	expression tag	UNP Q08499
A	77	HIS	-	expression tag	UNP Q08499
A	78	MET	-	expression tag	UNP Q08499
B	75	GLY	-	expression tag	UNP Q08499
B	76	SER	-	expression tag	UNP Q08499
B	77	HIS	-	expression tag	UNP Q08499
B	78	MET	-	expression tag	UNP Q08499
C	75	GLY	-	expression tag	UNP Q08499
C	76	SER	-	expression tag	UNP Q08499
C	77	HIS	-	expression tag	UNP Q08499
C	78	MET	-	expression tag	UNP Q08499
D	75	GLY	-	expression tag	UNP Q08499
D	76	SER	-	expression tag	UNP Q08499
D	77	HIS	-	expression tag	UNP Q08499
D	78	MET	-	expression tag	UNP Q08499

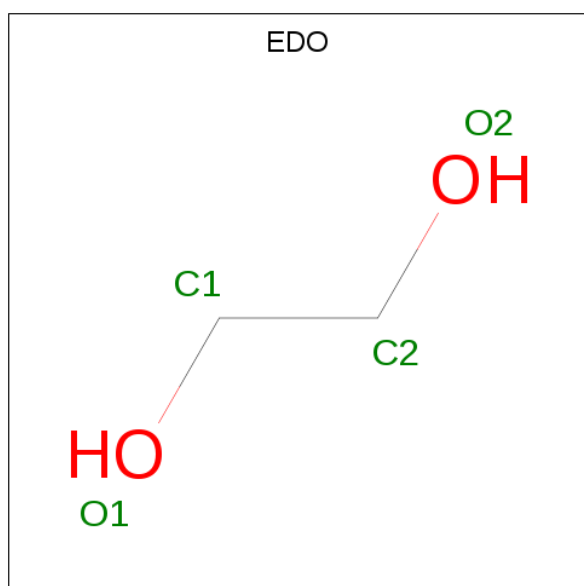
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

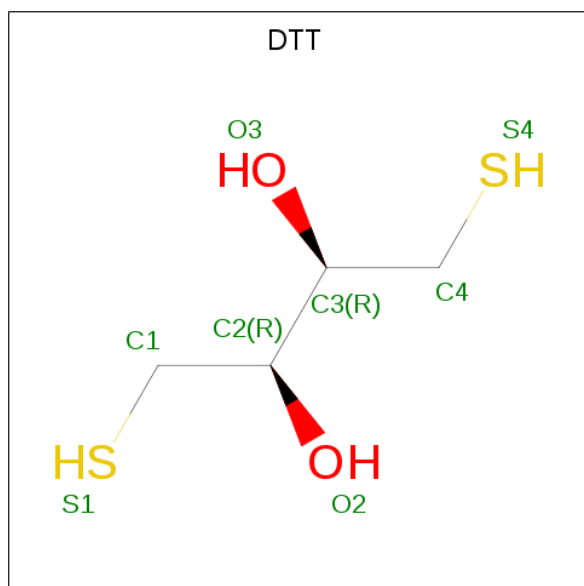
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0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

Continued on next page...

Continued from previous page...

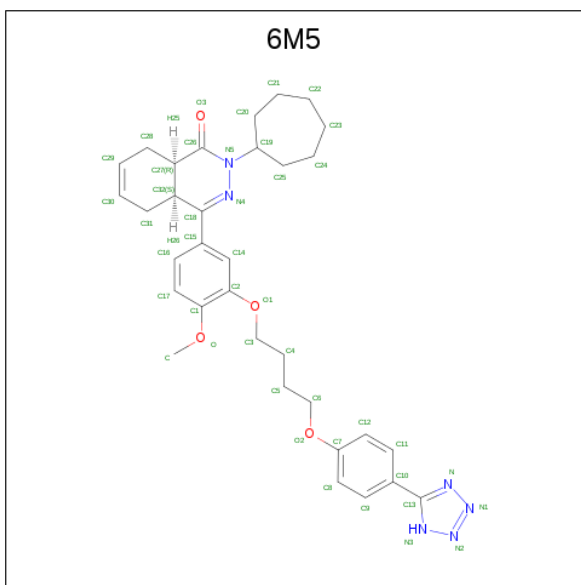
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



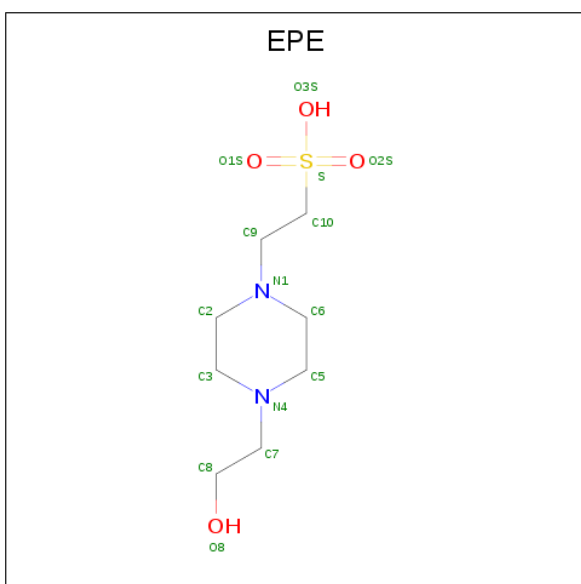
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	4	2	2		
5	A	1	Total	C	O	S	0	0
			8	4	2	2		
5	D	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is (4 {a} {S},8 {a} {R})-2-cycloheptyl-4-[4-methoxy-3-[4-[4-(1 {H})-1,2,3,4-tetrazol-5-yl)phenoxy]butoxy]phenyl]-4 {a},5,8,8 {a}-tetrahydrophthalazin-1-one (three-letter code: 6M5) (formula: $C_{33}H_{40}N_6O_4$).



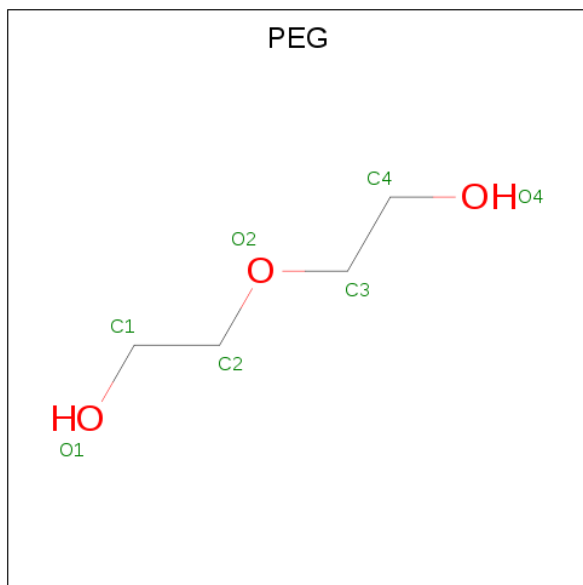
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			43	33	6	4		
6	B	1	Total	C	N	O	0	0
			43	33	6	4		
6	C	1	Total	C	N	O	0	0
			43	33	6	4		
6	D	1	Total	C	N	O	0	0
			43	33	6	4		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

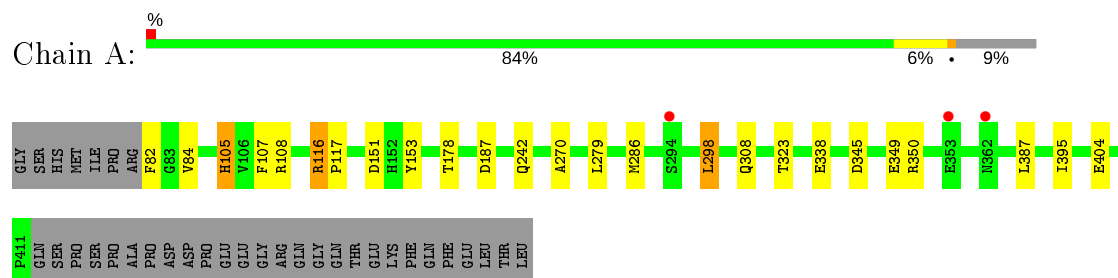
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	152	Total	O	0	0
			152	152		
9	B	124	Total	O	0	0
			124	124		
9	C	113	Total	O	0	0
			113	113		
9	D	164	Total	O	0	0
			164	164		

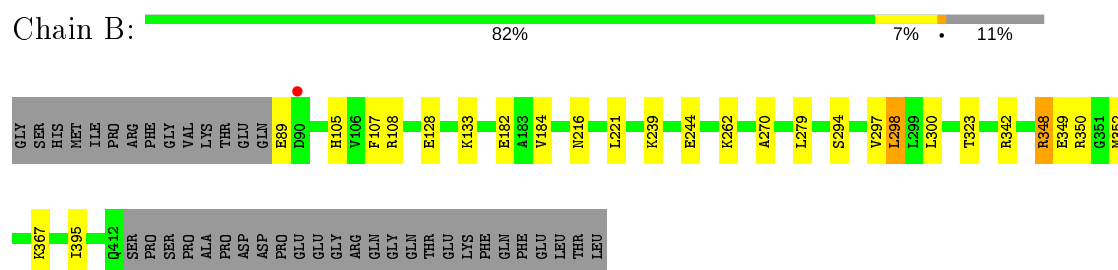
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

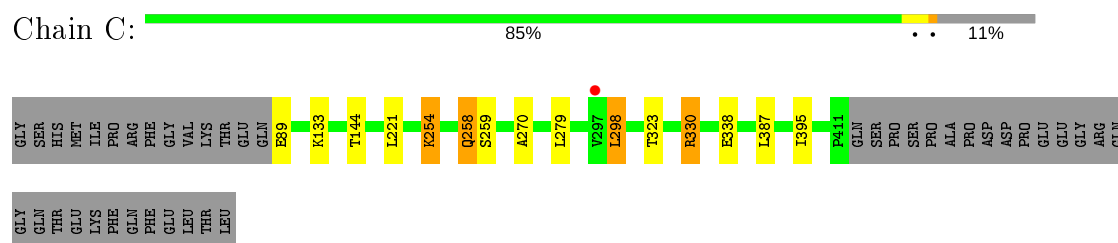
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



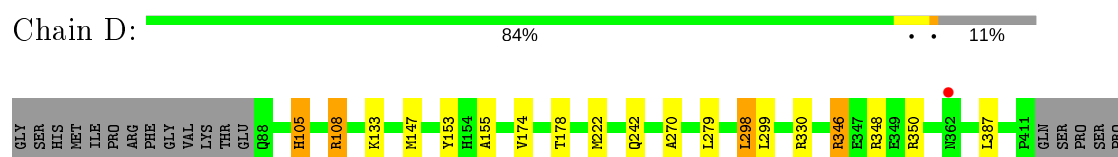
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



ALA
PRO
ASP
ASP
PRO
GLU
GLU
GLY
ARG
GLN
GLY
GLN
THR
GLU
LYS
PHE
GLN
PHE
GLU
LEU
THR
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.22Å 111.09Å 160.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.40 – 2.25 91.40 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.4 (91.40-2.25) 96.4 (91.40-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.174 , 0.210 0.181 , 0.211	Depositor DCC
R_{free} test set	4023 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11475	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: MG, 6M5, ZN, EDO, PEG, EPE, DTT

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	0.79	0/2735	0.84	3/3715 (0.1%)
1	B	0.75	1/2693 (0.0%)	0.84	6/3659 (0.2%)
1	C	0.75	0/2667	0.83	0/3624
1	D	0.83	0/2687	0.88	10/3651 (0.3%)
All	All	0.78	1/10782 (0.0%)	0.85	19/14649 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	GLU	CD-OE1	-5.03	1.20	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105[A]	HIS	N-CA-CB	7.86	124.74	110.60
1	D	105[B]	HIS	N-CA-CB	7.86	124.74	110.60
1	A	105[A]	HIS	N-CA-CB	7.70	124.46	110.60
1	A	105[B]	HIS	N-CA-CB	7.70	124.46	110.60
1	B	348	ARG	CG-CD-NE	7.20	126.91	111.80
1	B	348	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	D	330	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	346	ARG	CG-CD-NE	5.86	124.11	111.80
1	B	221	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	D	222	MET	CG-SD-CE	5.62	109.19	100.20
1	D	147	MET	CG-SD-CE	5.55	109.08	100.20
1	B	348	ARG	CD-NE-CZ	5.25	130.95	123.60
1	B	348	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	350	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	108	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	108	ARG	NE-CZ-NH1	-5.13	117.74	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	D	299	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	216	ASN	N-CA-CB	5.03	119.64	110.60

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	2679	0	2631	16	0
1	B	2638	0	2588	14	1
1	C	2613	0	2570	9	1
1	D	2632	0	2584	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	32	0	48	0	0
4	B	28	0	42	3	0
4	C	16	0	24	0	0
4	D	36	0	54	0	0
5	A	16	0	20	5	0
5	D	8	0	10	2	0
6	A	43	0	0	0	0
6	B	43	0	0	0	0
6	C	43	0	0	0	0
6	D	43	0	0	0	0
7	B	15	0	18	0	0
7	C	15	0	18	0	0
8	D	14	0	20	1	0
9	A	152	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	124	0	0	1	0
9	C	113	0	0	0	0
9	D	164	0	0	2	0
All	All	11475	0	10627	45	1

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 (45) 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)
5:A:1013:DTT:S1	9:A:1156:HOH:O	2.36	0.82
1:A:345:ASP:O	1:A:349:GLU:HG3	1.78	0.82
1:A:153:TYR:O	5:A:1013:DTT:H3	1.90	0.72
1:D:346:ARG:NH2	9:D:1101:HOH:O	2.27	0.66
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.15	0.65
1:D:153:TYR:O	5:D:1014:DTT:H12	1.99	0.63
1:A:350:ARG:HG2	1:C:144:THR:HG23	1.82	0.61
1:A:308:GLN:HB3	9:A:1236:HOH:O	2.00	0.61
1:A:105[A]:HIS:CE1	1:A:107:PHE:HB2	2.38	0.59
1:B:298:LEU:HD23	1:B:300:LEU:HD21	1.86	0.58
1:A:105[A]:HIS:HE1	1:A:107:PHE:HB2	1.69	0.58
1:A:286:MET:HE3	9:A:1236:HOH:O	2.05	0.55
1:A:187:ASP:OD2	5:A:1010:DTT:S1	2.65	0.55
1:D:348:ARG:NH1	9:D:1102:HOH:O	2.41	0.54
1:C:330:ARG:HH11	1:C:330:ARG:HG3	1.73	0.52
1:B:244:GLU:OE2	1:C:254:LYS:CE	2.57	0.52
1:C:330:ARG:HH11	1:C:330:ARG:CG	2.24	0.50
1:A:151:ASP:O	5:A:1013:DTT:C4	2.62	0.48
1:B:350:ARG:HB3	9:B:1111:HOH:O	2.13	0.48
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.96	0.47
1:A:116:ARG:N	1:A:117:PRO:CD	2.77	0.47
1:B:342:ARG:NH2	1:B:342:ARG:HB3	2.30	0.47
1:D:105[A]:HIS:HD2	1:D:108:ARG:H	1.63	0.47
1:A:350:ARG:NH2	9:A:1103:HOH:O	2.49	0.45
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.98	0.45
1:B:352:MET:HE2	4:B:1007:EDO:H21	1.97	0.45
1:B:244:GLU:OE2	1:C:254:LYS:HE2	2.16	0.45
1:C:298:LEU:HD11	1:C:387:LEU:HG	1.98	0.45
1:C:330:ARG:NH1	1:C:330:ARG:CG	2.81	0.44
1:A:298:LEU:HD11	1:A:387:LEU:HG	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:LEU:HD11	1:D:387:LEU:HG	1.99	0.44
1:A:151:ASP:O	5:A:1013:DTT:H41	2.18	0.44
1:B:105[B]:HIS:CE1	1:B:107:PHE:HB2	2.52	0.44
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.00	0.44
1:C:270:ALA:HB1	1:C:279:LEU:HD11	2.00	0.43
1:B:352:MET:HE1	4:B:1007:EDO:C1	2.48	0.43
1:D:174:VAL:HG12	8:D:1012:PEG:H41	1.99	0.43
1:A:323:THR:HB	1:A:395:ILE:HG23	2.01	0.43
1:D:155:ALA:HB2	5:D:1014:DTT:H2	2.00	0.42
1:B:323:THR:HB	1:B:395:ILE:HG23	2.01	0.42
1:B:182:GLU:O	1:B:297:VAL:HG21	2.21	0.41
1:B:105[B]:HIS:HE1	1:B:107:PHE:HB2	1.85	0.41
1:B:184:VAL:HG22	1:B:297:VAL:HG13	2.03	0.41
1:C:323:THR:HB	1:C:395:ILE:HG23	2.02	0.41
1:B:262:LYS:HG3	4:B:1005:EDO:H21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:SER:O	1:C:258:GLN:NE2[4_479]	2.11	0.09

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	329/364 (90%)	324 (98%)	5 (2%)	0	100	100
1	B	324/364 (89%)	320 (99%)	4 (1%)	0	100	100
1	C	321/364 (88%)	316 (98%)	5 (2%)	0	100	100
1	D	323/364 (89%)	319 (99%)	4 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1297/1456 (89%)	1279 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	302/331 (91%)	295 (98%)	7 (2%)	50	59
1	B	298/331 (90%)	290 (97%)	8 (3%)	44	54
1	C	295/331 (89%)	286 (97%)	9 (3%)	40	49
1	D	297/331 (90%)	294 (99%)	3 (1%)	76	84
All	All	1192/1324 (90%)	1165 (98%)	27 (2%)	50	59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	PHE
1	A	84	VAL
1	A	116	ARG
1	A	178	THR
1	A	298	LEU
1	A	338	GLU
1	A	404	GLU
1	B	89	GLU
1	B	108	ARG
1	B	128	GLU
1	B	133	LYS
1	B	239	LYS
1	B	298	LEU
1	B	348	ARG
1	B	367	LYS
1	C	89	GLU
1	C	133	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	LEU
1	C	254	LYS
1	C	258	GLN
1	C	259	SER
1	C	298	LEU
1	C	330	ARG
1	C	338	GLU
1	D	133	LYS
1	D	178	THR
1	D	298	LEU

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

Mol	Chain	Res	Type
1	B	231	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 8 are monoatomic - leaving 39 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
4	EDO	D	1007	-	3,3,3	0.36	0	2,2,2	0.71	0
6	6M5	C	1008	-	48,48,48	0.41	0	55,65,65	1.02	4 (7%)
4	EDO	D	1010	-	3,3,3	0.43	0	2,2,2	0.95	0
4	EDO	D	1011	-	3,3,3	0.79	0	2,2,2	0.52	0
8	PEG	D	1012	-	6,6,6	0.83	0	5,5,5	0.90	0
4	EDO	B	1005	-	3,3,3	0.69	0	2,2,2	0.33	0
7	EPE	B	1010	-	15,15,15	1.92	1 (6%)	18,20,20	1.54	4 (22%)
4	EDO	C	1006	-	3,3,3	0.70	0	2,2,2	0.65	0
4	EDO	B	1007	-	3,3,3	0.70	0	2,2,2	0.55	0
4	EDO	C	1004	-	3,3,3	0.39	0	2,2,2	0.60	0
4	EDO	B	1006	-	3,3,3	0.57	0	2,2,2	0.17	0
4	EDO	C	1005	-	3,3,3	0.67	0	2,2,2	0.28	0
4	EDO	B	1009	-	3,3,3	0.17	0	2,2,2	1.09	0
4	EDO	A	1007	-	3,3,3	0.59	0	2,2,2	0.50	0
6	6M5	D	1015	-	48,48,48	0.39	0	55,65,65	1.10	4 (7%)
4	EDO	D	1003	-	3,3,3	0.84	0	2,2,2	0.56	0
4	EDO	D	1008	-	3,3,3	0.52	0	2,2,2	0.35	0
5	DTT	D	1014	-	7,7,7	1.54	1 (14%)	4,8,8	3.51	1 (25%)
4	EDO	A	1005	-	3,3,3	0.26	0	2,2,2	0.70	0
4	EDO	B	1004	-	3,3,3	0.50	0	2,2,2	0.56	0
4	EDO	D	1004	-	3,3,3	0.49	0	2,2,2	0.89	0
4	EDO	D	1009	-	3,3,3	0.21	0	2,2,2	0.87	0
4	EDO	A	1003	-	3,3,3	0.49	0	2,2,2	1.13	0
7	EPE	C	1007	-	15,15,15	1.85	1 (6%)	18,20,20	1.63	2 (11%)
4	EDO	C	1003	-	3,3,3	0.27	0	2,2,2	1.32	0
4	EDO	D	1006	-	3,3,3	0.30	0	2,2,2	0.81	0
5	DTT	A	1013	-	7,7,7	1.59	2 (28%)	4,8,8	3.47	4 (100%)
4	EDO	A	1009	-	3,3,3	0.84	0	2,2,2	0.22	0
4	EDO	A	1004	-	3,3,3	0.64	0	2,2,2	0.87	0
6	6M5	B	1011	-	48,48,48	0.41	0	55,65,65	1.21	4 (7%)
4	EDO	D	1005	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	A	1012	-	3,3,3	0.59	0	2,2,2	0.42	0
4	EDO	A	1008	-	3,3,3	0.72	0	2,2,2	0.14	0
8	PEG	D	1013	-	6,6,6	1.09	0	5,5,5	1.47	1 (20%)
6	6M5	A	1011	-	48,48,48	0.61	0	55,65,65	1.20	4 (7%)
4	EDO	B	1008	-	3,3,3	0.50	0	2,2,2	0.27	0
4	EDO	A	1006	-	3,3,3	0.42	0	2,2,2	0.22	0
5	DTT	A	1010	-	7,7,7	0.62	0	4,8,8	2.69	3 (75%)
4	EDO	B	1003	-	3,3,3	0.52	0	2,2,2	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	1007	-	-	1/1/1/1	-
6	6M5	C	1008	-	-	3/21/59/59	0/6/6/6
4	EDO	D	1010	-	-	1/1/1/1	-
4	EDO	D	1011	-	-	1/1/1/1	-
8	PEG	D	1012	-	-	3/4/4/4	-
4	EDO	B	1005	-	-	1/1/1/1	-
7	EPE	B	1010	-	-	2/9/19/19	0/1/1/1
4	EDO	C	1006	-	-	0/1/1/1	-
4	EDO	B	1007	-	-	1/1/1/1	-
4	EDO	C	1004	-	-	1/1/1/1	-
4	EDO	B	1006	-	-	1/1/1/1	-
4	EDO	C	1005	-	-	1/1/1/1	-
4	EDO	B	1009	-	-	1/1/1/1	-
4	EDO	A	1007	-	-	1/1/1/1	-
6	6M5	D	1015	-	-	3/21/59/59	0/6/6/6
4	EDO	D	1003	-	-	0/1/1/1	-
4	EDO	D	1008	-	-	1/1/1/1	-
5	DTT	D	1014	-	-	8/8/8/8	-
4	EDO	A	1005	-	-	1/1/1/1	-
4	EDO	B	1004	-	-	1/1/1/1	-
4	EDO	D	1004	-	-	0/1/1/1	-
4	EDO	D	1009	-	-	1/1/1/1	-
4	EDO	A	1003	-	-	0/1/1/1	-
7	EPE	C	1007	-	-	1/9/19/19	0/1/1/1
4	EDO	C	1003	-	-	0/1/1/1	-
4	EDO	D	1006	-	-	1/1/1/1	-
5	DTT	A	1013	-	-	3/8/8/8	-
4	EDO	A	1009	-	-	1/1/1/1	-
4	EDO	A	1004	-	-	1/1/1/1	-
6	6M5	B	1011	-	-	3/21/59/59	0/6/6/6
4	EDO	D	1005	-	-	0/1/1/1	-
4	EDO	A	1012	-	-	0/1/1/1	-
4	EDO	A	1008	-	-	1/1/1/1	-
8	PEG	D	1013	-	-	0/4/4/4	-
6	6M5	A	1011	-	-	7/21/59/59	0/6/6/6
4	EDO	B	1008	-	-	0/1/1/1	-
4	EDO	A	1006	-	-	1/1/1/1	-
5	DTT	A	1010	-	-	5/8/8/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1003	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1010	EPE	C10-S	-6.96	1.67	1.77
7	C	1007	EPE	C10-S	-6.22	1.68	1.77
5	D	1014	DTT	C3-C2	3.01	1.60	1.52
5	A	1013	DTT	C3-C2	2.57	1.59	1.52
5	A	1013	DTT	C4-C3	2.08	1.57	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1014	DTT	O3-C3-C2	6.89	123.87	109.72
6	A	1011	6M5	C13-N-N1	4.55	108.92	104.87
6	B	1011	6M5	C13-N-N1	4.40	108.79	104.87
6	B	1011	6M5	N-N1-N2	-4.37	106.68	109.53
5	A	1013	DTT	O3-C3-C2	4.20	118.36	109.72
6	A	1011	6M5	N-N1-N2	-4.14	106.83	109.53
6	D	1015	6M5	C13-N-N1	4.05	108.47	104.87
7	C	1007	EPE	O3S-S-C10	4.02	112.26	105.77
5	A	1010	DTT	C2-C1-S1	3.99	126.09	114.47
7	C	1007	EPE	O1S-S-C10	3.93	111.65	106.92
6	D	1015	6M5	N-N1-N2	-3.89	106.99	109.53
5	A	1013	DTT	C3-C4-S4	3.65	125.09	114.47
5	A	1013	DTT	O2-C2-C3	3.60	117.12	109.72
6	C	1008	6M5	C13-N-N1	3.58	108.05	104.87
6	A	1011	6M5	N-C13-N3	-3.47	107.52	111.39
6	C	1008	6M5	N-N1-N2	-3.30	107.38	109.53
6	B	1011	6M5	N-C13-N3	-3.08	107.95	111.39
8	D	1013	PEG	O2-C2-C1	3.01	123.28	110.07
7	B	1010	EPE	C6-N1-C2	2.94	115.44	108.83
7	B	1010	EPE	O2S-S-O1S	-2.80	104.27	113.95
6	D	1015	6M5	N-C13-N3	-2.77	108.29	111.39
5	A	1010	DTT	O3-C3-C2	2.73	115.34	109.72
6	C	1008	6M5	N-C13-N3	-2.71	108.36	111.39
6	B	1011	6M5	C16-C15-C18	2.50	123.71	120.75
6	C	1008	6M5	C16-C15-C18	2.47	123.68	120.75
7	B	1010	EPE	O3S-S-C10	2.30	109.49	105.77
6	D	1015	6M5	C32-C31-C30	2.22	115.33	111.73
5	A	1010	DTT	C3-C4-S4	-2.20	108.06	114.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1011	6M5	C18-N4-N5	-2.18	116.69	118.97
7	B	1010	EPE	C6-C5-N4	-2.08	106.38	110.64
5	A	1013	DTT	C2-C1-S1	2.07	120.49	114.47

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1014	DTT	S1-C1-C2-O2
5	D	1014	DTT	S1-C1-C2-C3
5	D	1014	DTT	C2-C3-C4-S4
4	D	1009	EDO	O1-C1-C2-O2
5	A	1013	DTT	O3-C3-C4-S4
5	A	1010	DTT	S1-C1-C2-O2
5	A	1010	DTT	C2-C3-C4-S4
5	A	1010	DTT	O3-C3-C4-S4
4	D	1010	EDO	O1-C1-C2-O2
7	B	1010	EPE	N4-C7-C8-O8
7	C	1007	EPE	N4-C7-C8-O8
8	D	1012	PEG	C4-C3-O2-C2
6	A	1011	6M5	C1-C2-O1-C3
4	D	1007	EDO	O1-C1-C2-O2
4	B	1005	EDO	O1-C1-C2-O2
4	A	1007	EDO	O1-C1-C2-O2
4	D	1008	EDO	O1-C1-C2-O2
4	D	1006	EDO	O1-C1-C2-O2
4	A	1004	EDO	O1-C1-C2-O2
4	A	1008	EDO	O1-C1-C2-O2
6	A	1011	6M5	C4-C5-C6-O2
8	D	1012	PEG	O1-C1-C2-O2
6	B	1011	6M5	C4-C3-O1-C2
6	B	1011	6M5	C1-C2-O1-C3
6	D	1015	6M5	C4-C3-O1-C2
6	C	1008	6M5	C1-C2-O1-C3
8	D	1012	PEG	O2-C3-C4-O4
4	B	1007	EDO	O1-C1-C2-O2
6	A	1011	6M5	O1-C3-C4-C5
6	C	1008	6M5	C4-C3-O1-C2
6	D	1015	6M5	C1-C2-O1-C3
6	A	1011	6M5	C14-C2-O1-C3
4	D	1011	EDO	O1-C1-C2-O2
4	B	1006	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1005	EDO	O1-C1-C2-O2
4	A	1009	EDO	O1-C1-C2-O2
6	A	1011	6M5	C4-C3-O1-C2
5	D	1014	DTT	C1-C2-C3-C4
5	A	1010	DTT	C1-C2-C3-C4
4	C	1004	EDO	O1-C1-C2-O2
6	C	1008	6M5	C14-C2-O1-C3
5	D	1014	DTT	O3-C3-C4-S4
5	A	1013	DTT	S1-C1-C2-O2
6	B	1011	6M5	C14-C2-O1-C3
6	D	1015	6M5	C14-C2-O1-C3
4	B	1009	EDO	O1-C1-C2-O2
5	D	1014	DTT	C1-C2-C3-O3
5	D	1014	DTT	O2-C2-C3-C4
5	A	1013	DTT	C2-C3-C4-S4
4	A	1005	EDO	O1-C1-C2-O2
4	B	1004	EDO	O1-C1-C2-O2
4	B	1003	EDO	O1-C1-C2-O2
7	B	1010	EPE	C8-C7-N4-C3
5	D	1014	DTT	O2-C2-C3-O3
4	A	1006	EDO	O1-C1-C2-O2
5	A	1010	DTT	O2-C2-C3-O3
6	A	1011	6M5	C8-C7-O2-C6
6	A	1011	6M5	C12-C7-O2-C6

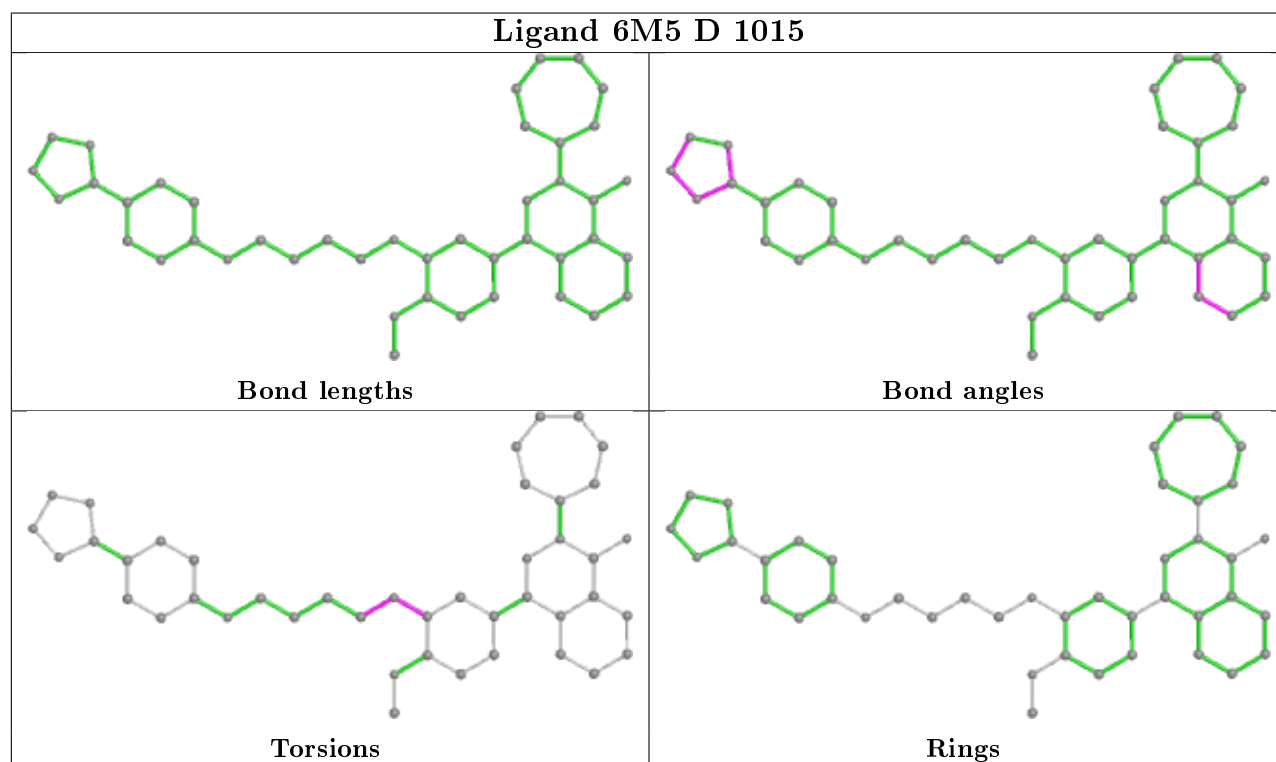
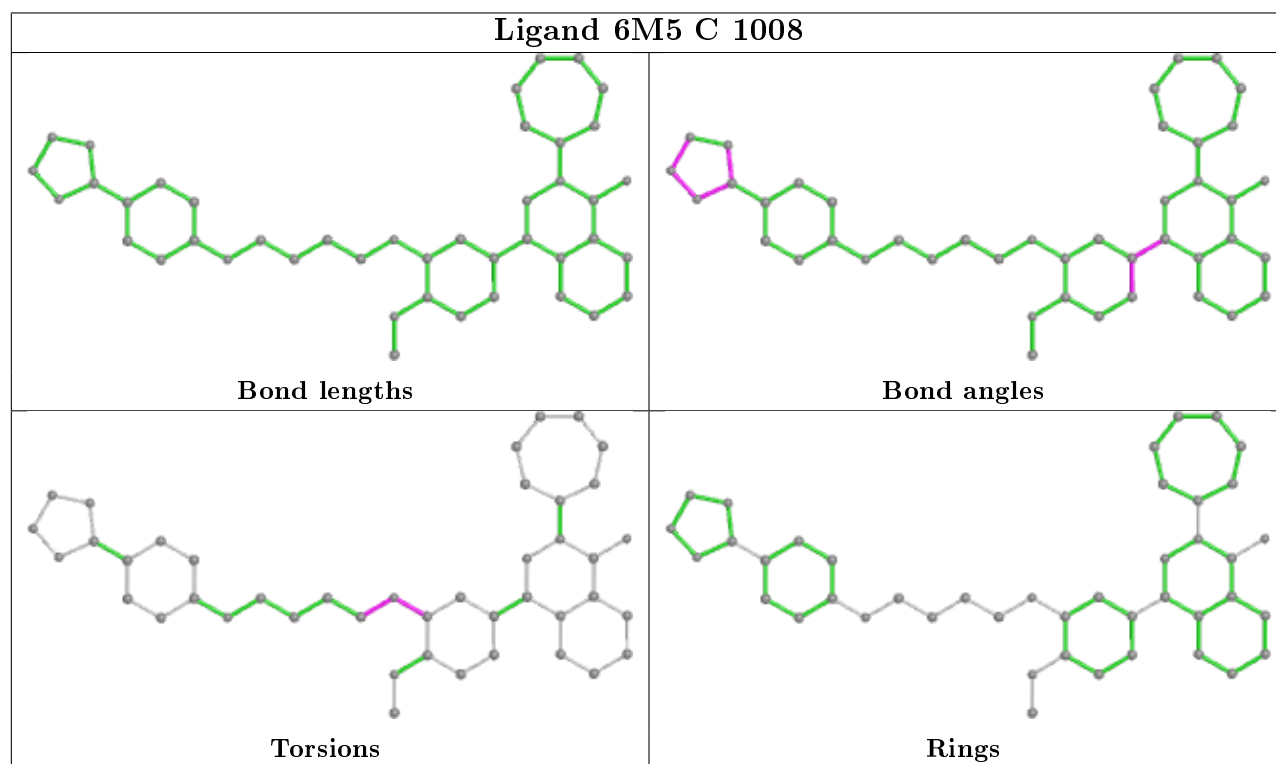
There are no ring outliers.

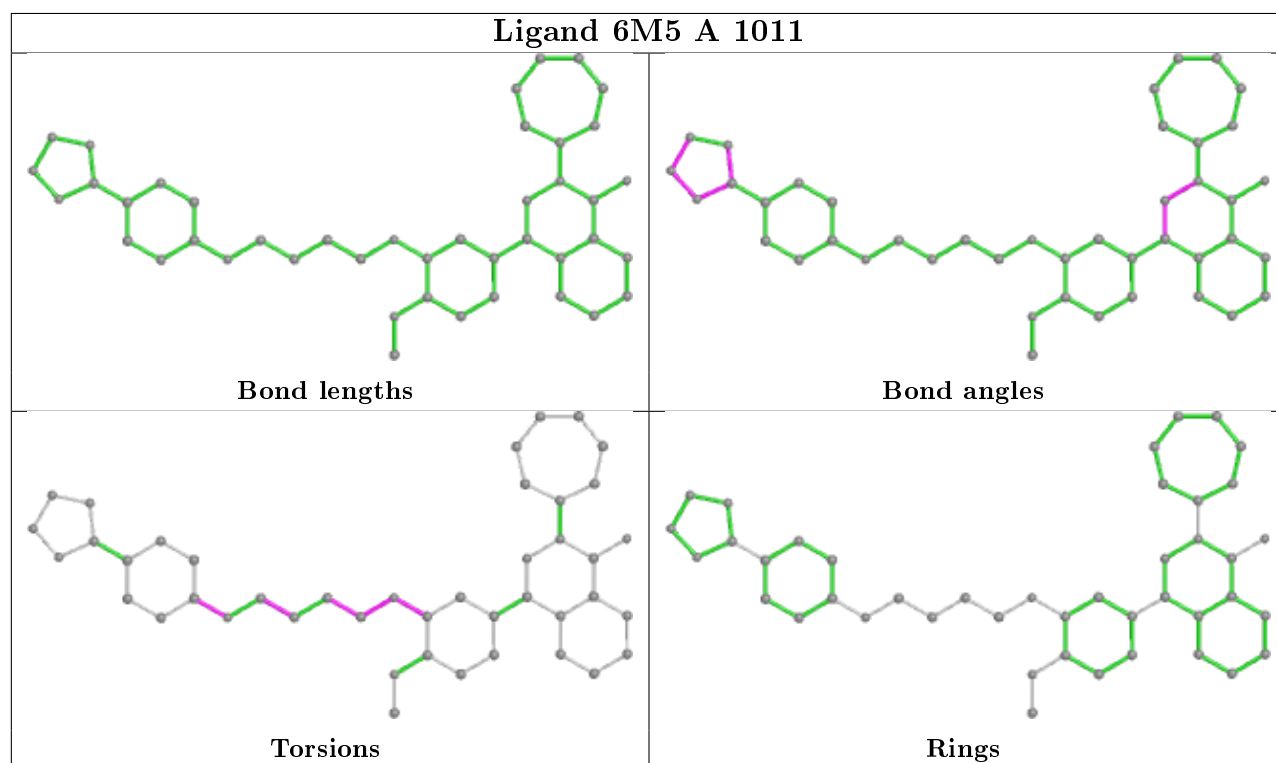
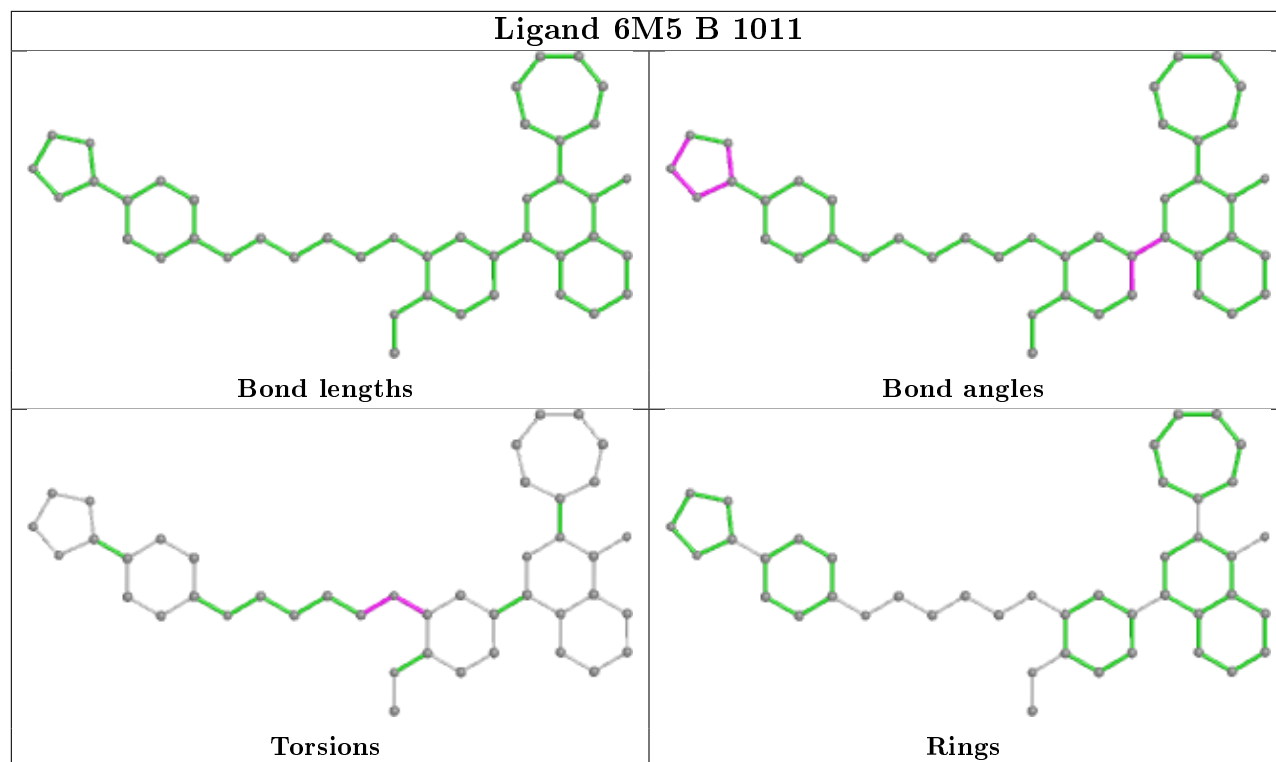
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1012	PEG	1	0
4	B	1005	EDO	1	0
4	B	1007	EDO	2	0
5	D	1014	DTT	2	0
5	A	1013	DTT	4	0
5	A	1010	DTT	1	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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/364 (90%)	-0.16	3 (0%) 84 85	24, 40, 79, 110	0
1	B	324/364 (89%)	-0.19	1 (0%) 94 94	25, 47, 73, 113	0
1	C	323/364 (88%)	-0.17	1 (0%) 94 94	25, 45, 80, 110	0
1	D	324/364 (89%)	-0.25	1 (0%) 94 94	20, 33, 64, 90	0
All	All	1301/1456 (89%)	-0.19	6 (0%) 91 91	20, 41, 75, 113	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	SER	4.3
1	D	362	ASN	3.6
1	B	90	ASP	3.1
1	A	353	GLU	3.0
1	C	297	VAL	2.8
1	A	362	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

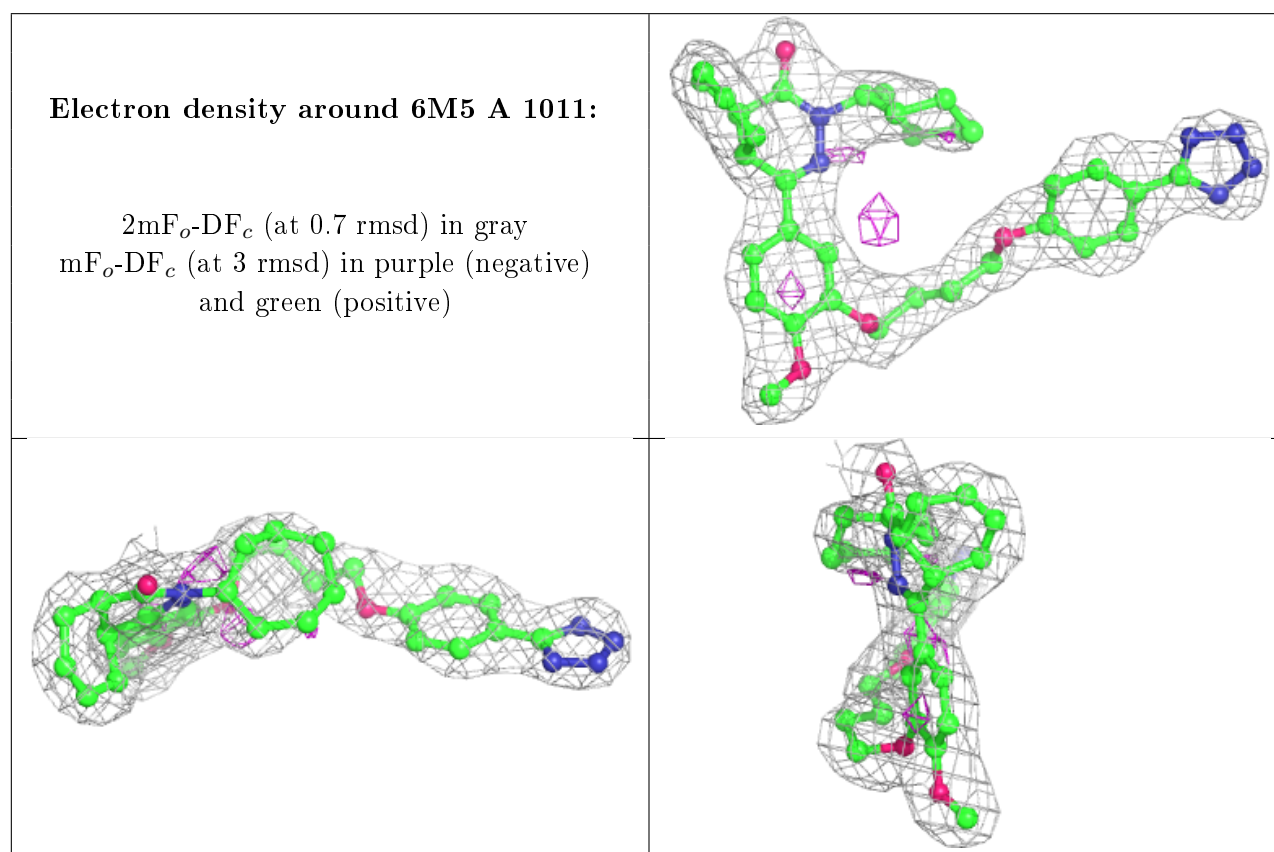
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DTT	A	1010	8/8	0.65	0.27	78,94,101,109	0
4	EDO	A	1012	4/4	0.78	0.18	58,60,64,66	0
4	EDO	D	1003	4/4	0.79	0.19	57,59,65,65	0
4	EDO	A	1009	4/4	0.80	0.14	54,65,72,74	0
4	EDO	B	1007	4/4	0.81	0.34	52,60,61,68	0
4	EDO	A	1008	4/4	0.83	0.11	64,70,72,73	0
8	PEG	D	1013	7/7	0.84	0.19	43,46,55,57	0
4	EDO	B	1006	4/4	0.84	0.19	62,73,74,81	0
5	DTT	A	1013	8/8	0.85	0.21	62,76,78,97	0
5	DTT	D	1014	8/8	0.86	0.24	67,84,96,113	0
4	EDO	C	1005	4/4	0.87	0.15	60,63,64,69	0
4	EDO	D	1007	4/4	0.87	0.22	72,75,77,89	0
4	EDO	D	1011	4/4	0.87	0.18	45,47,57,59	0
4	EDO	B	1005	4/4	0.88	0.21	58,67,67,69	0
7	EPE	B	1010	15/15	0.88	0.21	67,96,104,106	0
4	EDO	D	1006	4/4	0.89	0.19	64,65,67,71	0
4	EDO	D	1004	4/4	0.89	0.16	53,58,59,65	0
4	EDO	C	1004	4/4	0.90	0.16	59,59,63,73	0
4	EDO	B	1008	4/4	0.90	0.23	49,50,60,64	0
4	EDO	D	1008	4/4	0.90	0.20	47,53,54,66	0
4	EDO	A	1004	4/4	0.92	0.21	54,55,57,60	0
4	EDO	D	1009	4/4	0.92	0.19	52,53,61,66	0
4	EDO	C	1003	4/4	0.92	0.20	58,59,65,70	0
4	EDO	B	1003	4/4	0.92	0.15	50,50,50,55	0
4	EDO	A	1003	4/4	0.93	0.17	54,55,57,64	0
4	EDO	B	1004	4/4	0.93	0.28	55,61,64,70	0
6	6M5	A	1011	43/43	0.93	0.19	40,47,68,74	0
6	6M5	C	1008	43/43	0.93	0.15	37,49,65,70	0
4	EDO	D	1010	4/4	0.93	0.21	63,73,74,74	0
8	PEG	D	1012	7/7	0.93	0.19	42,43,53,55	0
4	EDO	A	1007	4/4	0.94	0.18	58,62,63,74	0
4	EDO	A	1006	4/4	0.95	0.17	45,46,47,51	0
6	6M5	D	1015	43/43	0.95	0.11	34,40,64,75	0
4	EDO	B	1009	4/4	0.95	0.20	49,51,53,58	0
4	EDO	D	1005	4/4	0.96	0.13	44,49,49,57	0
4	EDO	C	1006	4/4	0.96	0.14	61,63,69,70	0
6	6M5	B	1011	43/43	0.96	0.14	35,40,59,66	0
7	EPE	C	1007	15/15	0.97	0.13	48,63,75,76	0
4	EDO	A	1005	4/4	0.97	0.16	40,53,54,55	0
3	MG	D	1002	1/1	0.99	0.12	20,20,20,20	0
3	MG	B	1002	1/1	0.99	0.14	24,24,24,24	0

Continued on next page...

Continued from previous page...

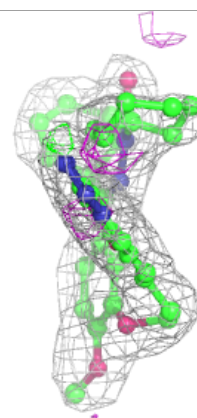
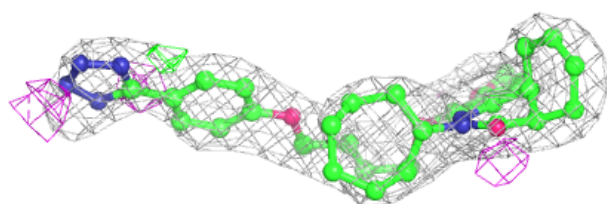
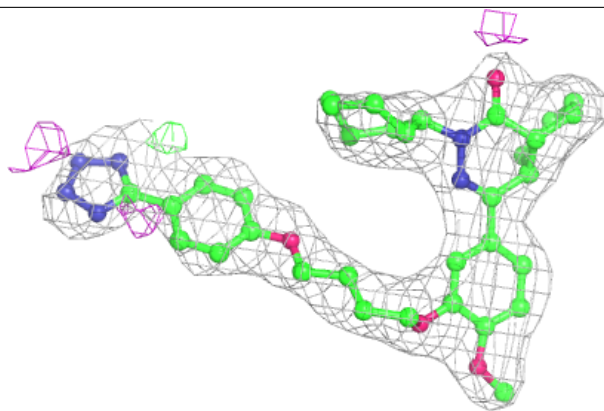
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	C	1002	1/1	0.99	0.12	22,22,22,22	0
2	ZN	A	1001	1/1	0.99	0.13	35,35,35,35	0
2	ZN	B	1001	1/1	0.99	0.12	39,39,39,39	0
3	MG	A	1002	1/1	0.99	0.12	23,23,23,23	0
2	ZN	D	1001	1/1	1.00	0.13	32,32,32,32	0
2	ZN	C	1001	1/1	1.00	0.12	38,38,38,38	0

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.

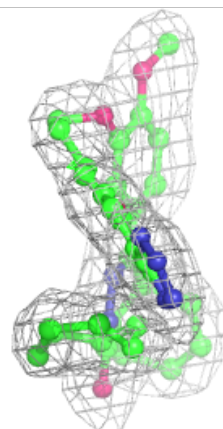
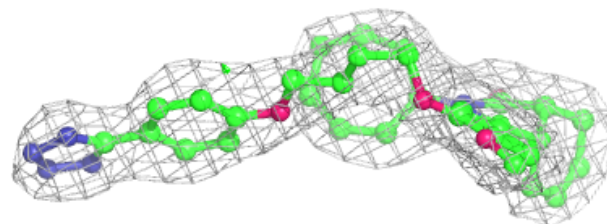
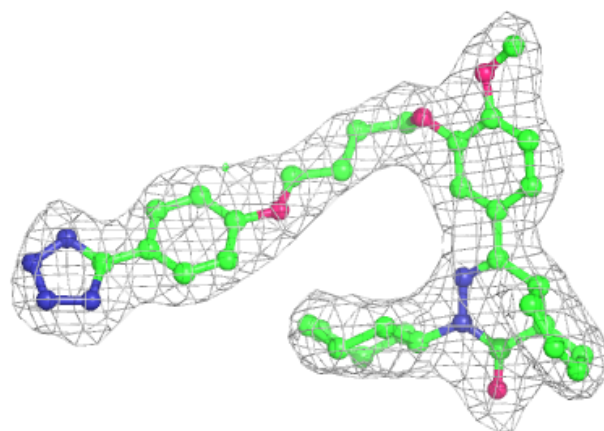


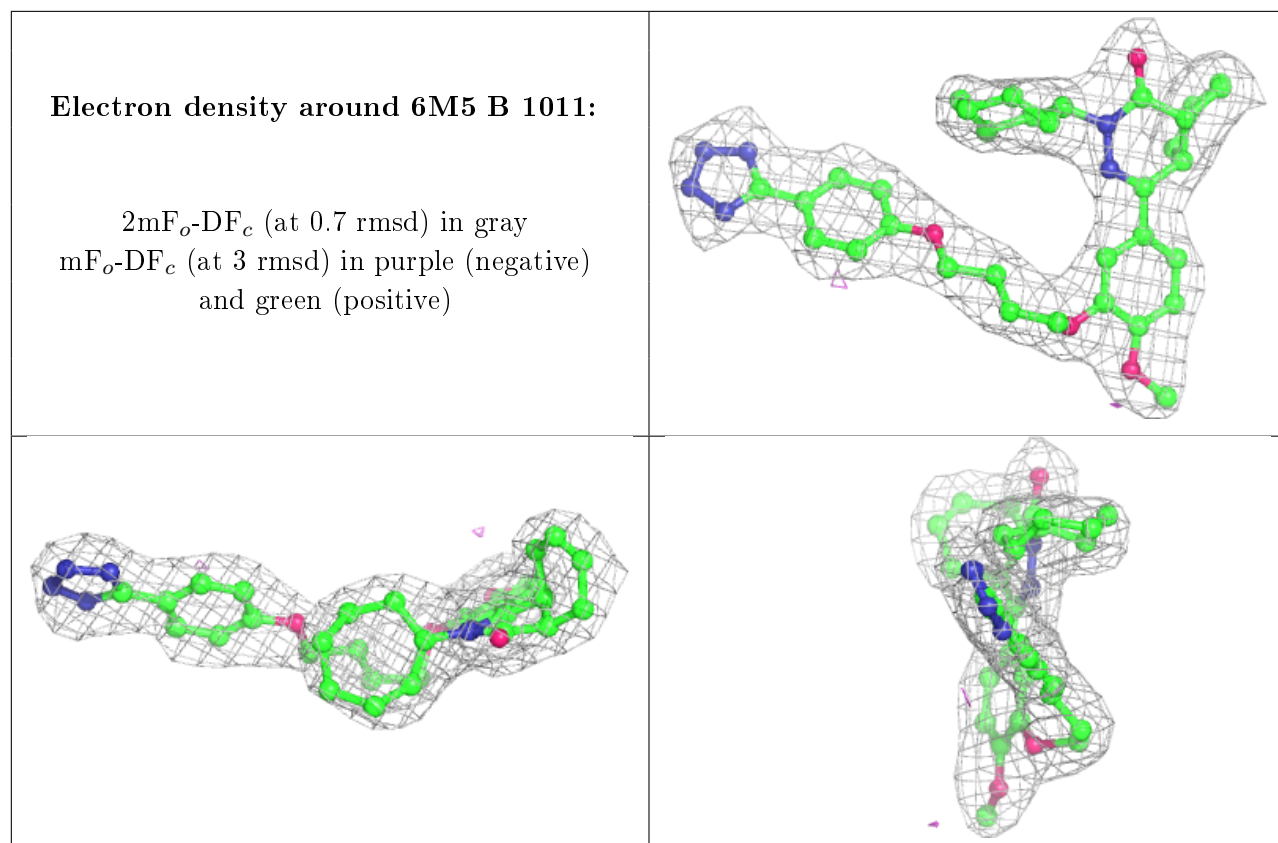
Electron density around 6M5 C 1008:

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

**Electron density around 6M5 D 1015:**

$2mF_o-DF_c$ (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.