

wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 04:15 pm BST

PDB ID : 8B1G

Title : DtpB-Nb132-AW

Authors: Killer, M.; Finocchio, G.; Lei, J.; Jungnickel, K.; Kotov, V.; Steinke, J.; Bar-

tels, K.; Strauss, J.; Dupeux, F.; Humm, A.S.; Cornaciu, I.; Marquez, J.;

Pardon, E.; Steyeart, J.; Loew, C.

Deposited on : 2022-09-09

Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.34

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

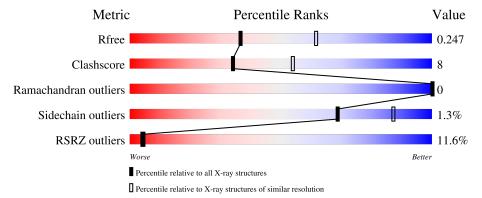
Validation Pipeline (wwPDB-VP) : 2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 2.50 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 $(\# \mathrm{Entries})$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries}, ext{ resolution range}(\mathring{A})) \end{aligned}$		
R_{free}	130704	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	5231 (2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

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	489	76%	16% 8%					
2	В	127	9% 77%	23%					
3	С	2	50%	50%					

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
11	HEX	A	814	-	-	-	X
11	HEX	A	815	-	-	-	X
7	1PE	A	804	-	-	-	X
7	1PE	A	811	-	-	-	X
8	D12	A	809	-	-	-	X



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 4786 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 Dipeptide and tripeptide permease B.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	451	Total 3480	C 2349	N 531	O 573	S 27	4	0	0

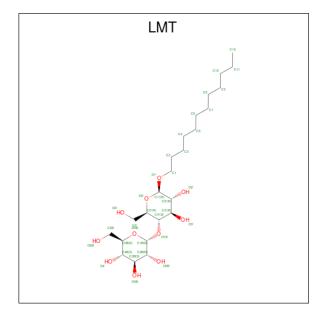
• Molecule 2 is a protein called Nanobody 132.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	127	Total 976	C 613	N 178	O 181	S 4	5	1	0

• Molecule 3 is a protein called ALA-TRP.

Mol	Chain	Residues	A	tom	ıs		ZeroOcc	AltConf	Trace
3	С	2	Total 20	C 14	N 3	O 3	0	0	0

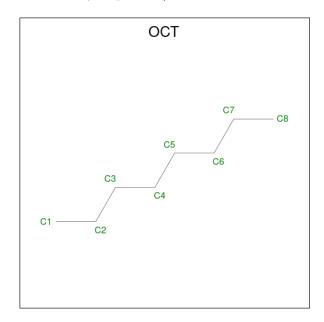
• Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).





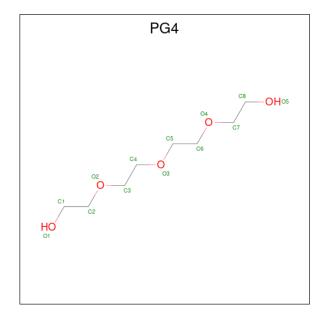
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total 35	C 24	O 11	0	0

• Molecule 5 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Aton	ıs	ZeroOcc	AltConf
5	A	1	Total 8	C 8	0	0

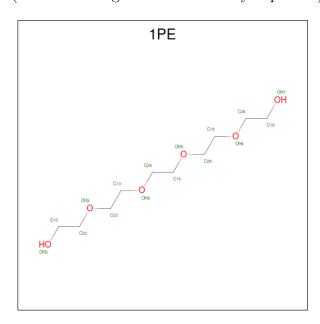
 \bullet Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5)$ (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0

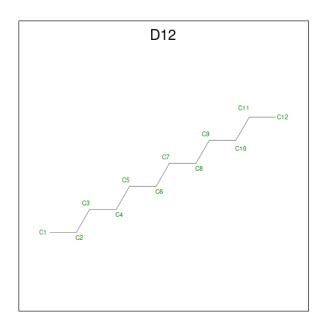
• Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0
7	A	1	Total C O 16 10 6	0	0

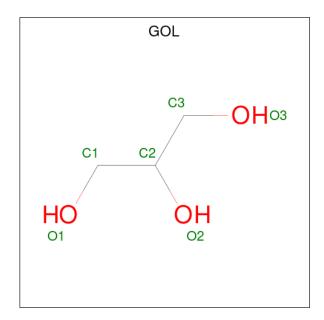
• Molecule 8 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 12 12	0	0

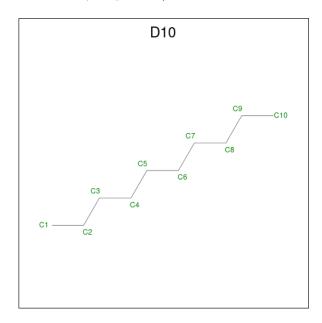
• Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

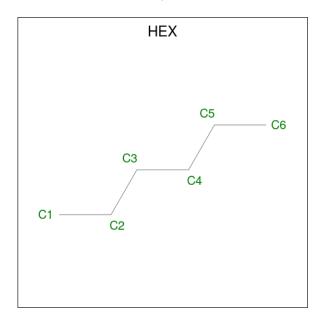


• Molecule 10 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 10 10	0	0

• Molecule 11 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C 6 6	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C 6 6	0	0

• Molecule 12 is water.

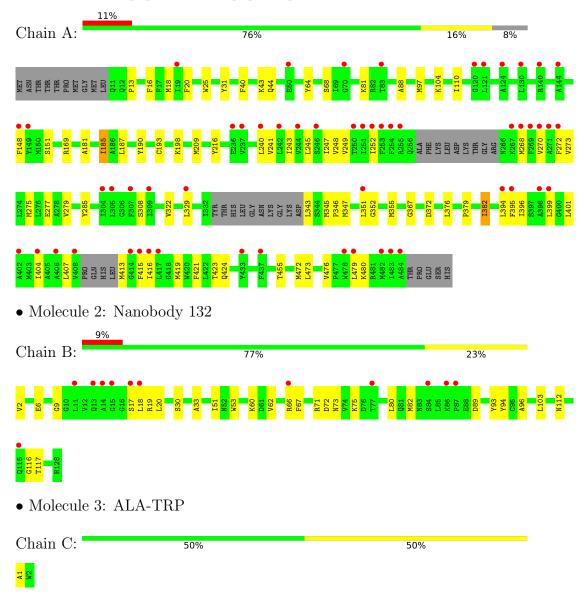
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	64	Total O 64 64	0	0
12	В	59	Total O 59 59	0	0
12	С	1	Total O 1 1	0	0



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: Dipeptide and tripeptide permease B





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	54.61Å 126.41Å 168.04Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.97 - 2.50	Depositor
resolution (A)	69.97 - 2.50	EDS
% Data completeness	99.1 (69.97-2.50)	Depositor
(in resolution range)	91.0 (69.97-2.50)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
P.P.	0.225 , 0.249	Depositor
R, R_{free}	0.225 , 0.247	DCC
R_{free} test set	2017 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29, 69.2	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4786	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 1PE, D10, GOL, LMT, OCT, D12, PG4, HEX

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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.53	0/3572	0.74	5/4859 (0.1%)
2	В	0.54	0/1004	0.74	0/1361
3	С	0.66	0/21	0.70	0/27
All	All	0.53	0/4597	0.74	5/6247 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	240	LEU	CB-CG-CD2	-9.03	95.64	111.00
1	A	407	LEU	CA-CB-CG	7.26	132.00	115.30
1	A	401	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	268	MET	CG-SD-CE	5.47	108.96	100.20
1	A	382	ILE	CG1-CB-CG2	-5.05	100.29	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	A	3480	0	3605	59	0
2	В	976	0	939	19	0
3	С	20	0	17	2	0

Continued on next page...



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	45	3	0
5	A	8	0	18	0	0
6	A	65	0	90	1	0
7	A	32	0	44	2	0
8	A	12	0	26	0	0
9	A	12	0	16	0	0
10	A	10	0	22	2	0
11	A	12	0	28	1	0
12	A	64	0	0	0	0
12	В	59	0	0	1	0
12	С	1	0	0	0	0
All	All	4786	0	4850	80	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 8.

The worst 5 of 80 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:346:PRO:HG3	1:A:479:LEU:HD22	1.52	0.89
1:A:25:TRP:CE2	1:A:185:ILE:HD11	2.20	0.77
1:A:64:TYR:CE2	1:A:424:GLN:HB2	2.26	0.70
2:B:19:ARG:NH1	12:B:201:HOH:O	2.18	0.69
2:B:60:LYS:HD3	2:B:62:VAL:HG22	1.74	0.68

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		
1	A	443/489 (91%)	436 (98%)	7 (2%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$_{ m ntiles}$
2	В	126/127 (99%)	122 (97%)	4 (3%)	0	100	100
All	All	569/616 (92%)	558 (98%)	11 (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	Perce	ntiles
1	A	368/401 (92%)	364 (99%)	4 (1%)	73	89
2	В	102/101 (101%)	100 (98%)	2 (2%)	55	79
3	С	1/1 (100%)	1 (100%)	0	100	100
All	All	471/503 (94%)	465 (99%)	6 (1%)	69	87

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	MET
2	В	30	SER
2	В	53	TRP
1	A	209	MET
1	A	185	ILE

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

Mol	Chain	Res	Type	
1	A	389	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)

15 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).

N / - 1	Т	Clasica	Das	T : 1-	Во	ond leng	ths	В	ond ang	gles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OCT	A	802	-	7,7,7	0.39	0	6,6,6	0.67	0
9	GOL	A	810	-	5,5,5	1.07	0	5,5,5	0.86	0
10	D10	A	812	-	9,9,9	0.39	0	8,8,8	0.98	1 (12%)
11	HEX	A	815	-	5,5,5	0.40	0	4,4,4	0.45	0
6	PG4	A	807	-	12,12,12	0.28	0	11,11,11	0.44	0
7	1PE	A	804	-	15,15,15	0.22	0	14,14,14	0.27	0
6	PG4	A	803	-	12,12,12	0.18	0	11,11,11	0.60	0
6	PG4	A	808	-	12,12,12	0.27	0	11,11,11	0.50	0
7	1PE	A	811	-	15,15,15	0.14	0	14,14,14	0.22	0
11	HEX	A	814	-	5,5,5	0.37	0	4,4,4	0.65	0
6	PG4	A	805	-	12,12,12	0.17	0	11,11,11	0.65	0
9	GOL	A	813	-	5,5,5	1.26	0	5,5,5	0.84	0
6	PG4	A	806	-	12,12,12	0.29	0	11,11,11	0.48	0
4	LMT	A	801	-	36,36,36	1.18	3 (8%)	47,47,47	1.63	10 (21%)
8	D12	A	809	-	11,11,11	0.47	0	10,10,10	0.66	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
5	OCT	A	802	-	-	2/5/5/5	-
9	GOL	A	810	-	-	2/4/4/4	-
10	D10	A	812	-	-	1/7/7/7	-
11	HEX	A	815	-	ı	0/3/3/3	-
6	PG4	A	807	_	-	5/10/10/10	-
7	1PE	A	804	-	-	7/13/13/13	-
6	PG4	A	803	-	-	4/10/10/10	-
6	PG4	A	808	-	-	4/10/10/10	-
7	1PE	A	811	-	-	6/13/13/13	-
11	HEX	A	814	-	-	0/3/3/3	
6	PG4	A	805	-	-	4/10/10/10	-
9	GOL	A	813	-	-	0/4/4/4	-
6	PG4	A	806	-	-	6/10/10/10	-
4	LMT	A	801	-	-	14/21/61/61	0/2/2/2
8	D12	A	809	-	-	3/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	A	801	LMT	O2B-C2B	-3.53	1.34	1.43
4	A	801	LMT	O3B-C3B	-2.32	1.37	1.43
4	A	801	LMT	O2'-C2'	-2.00	1.38	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
4	A	801	LMT	O5B-C5B-C4B	4.06	117.06	109.69
4	A	801	LMT	C1B-O1B-C4'	4.04	127.97	117.96
4	A	801	LMT	C1'-O5'-C5'	-3.15	107.50	113.69
4	A	801	LMT	O1B-C4'-C3'	2.82	114.79	107.28
4	A	801	LMT	O1'-C1'-C2'	2.48	112.17	108.30

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C2'-C1'-O1'-C1
4	A	801	LMT	O5'-C1'-O1'-C1
4	A	801	LMT	O5'-C5'-C6'-O6'
6	A	803	PG4	O3-C5-C6-O4

Continued on next page...



Continued from previous page...

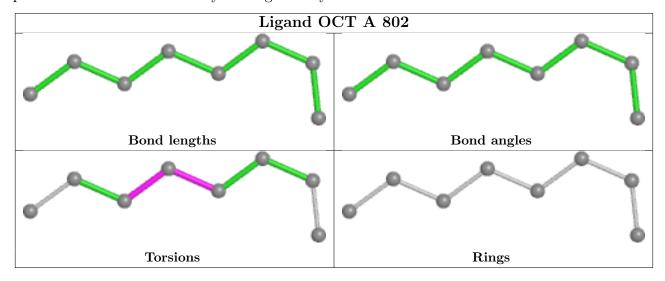
Mol	Chain	Res	Type	Atoms
6	A	806	PG4	O2-C3-C4-O3

There are no ring outliers.

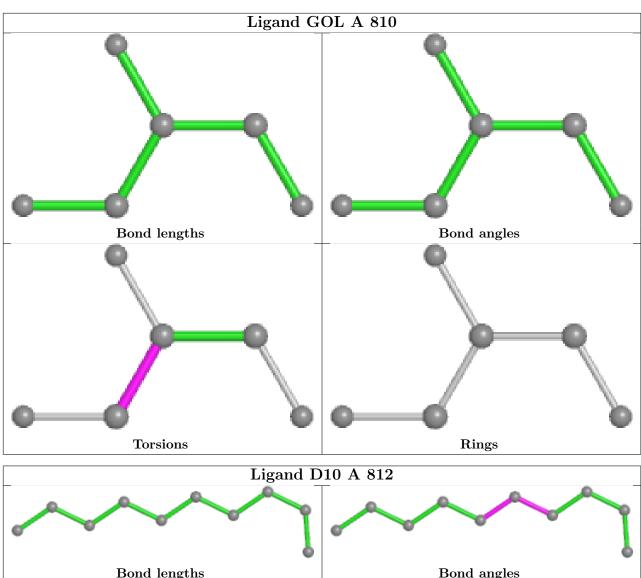
5 monomers are involved in 8 short contacts:

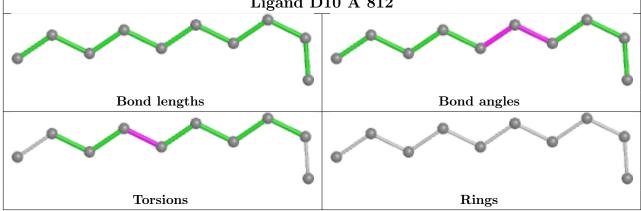
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	812	D10	2	0
6	A	807	PG4	1	0
7	A	811	1PE	2	0
11	A	814	HEX	1	0
4	A	801	LMT	3	0

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.

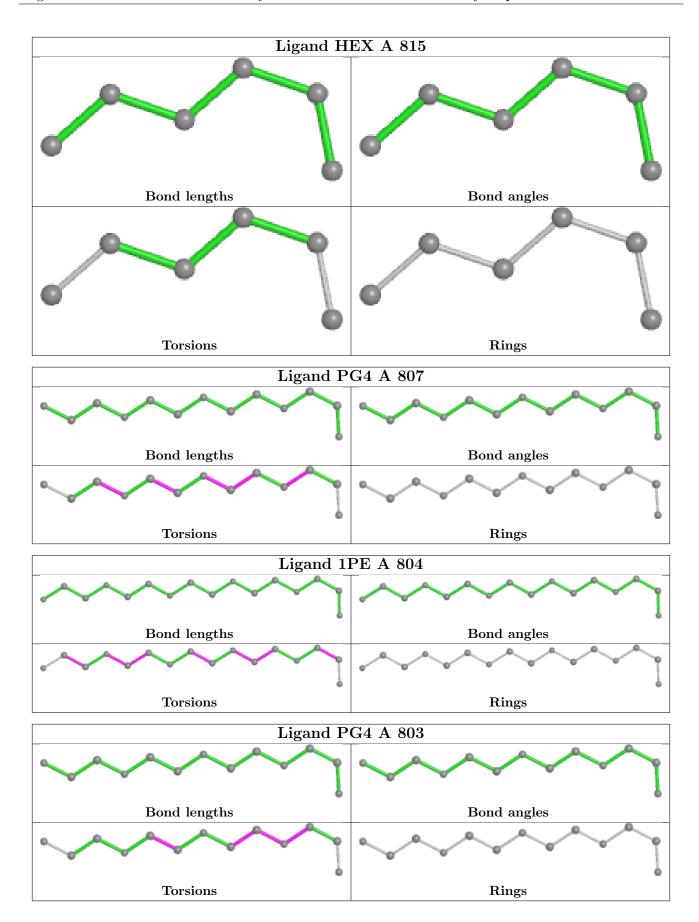




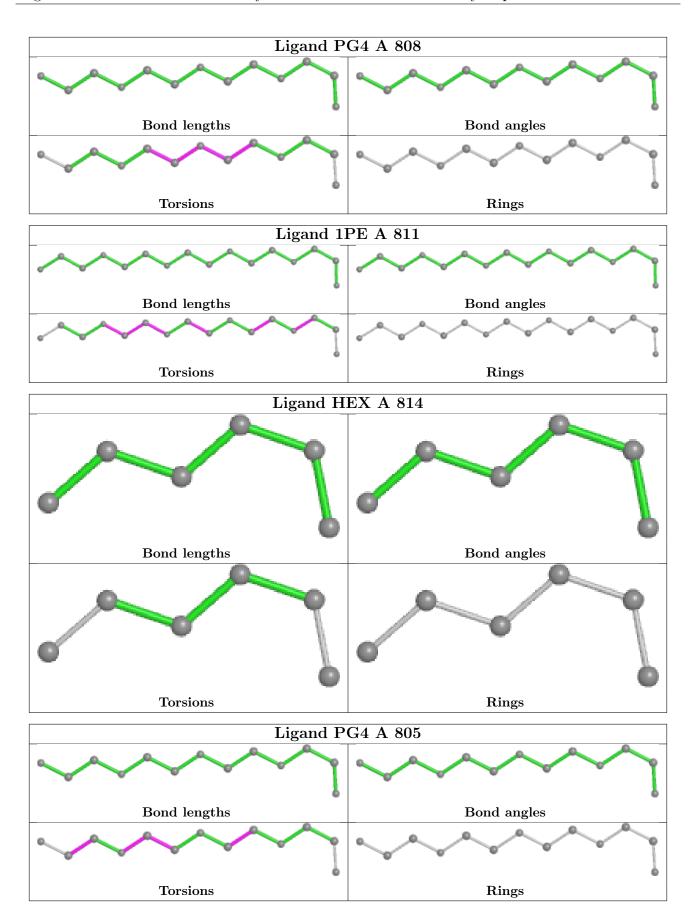




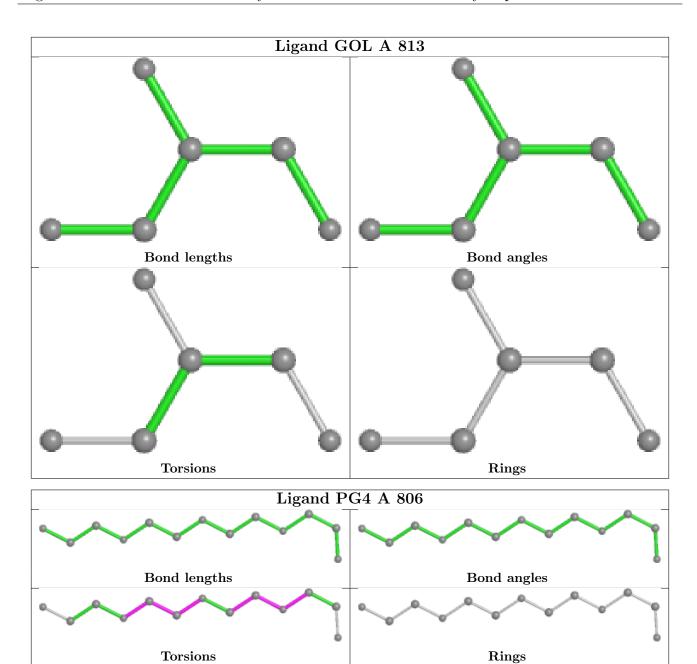




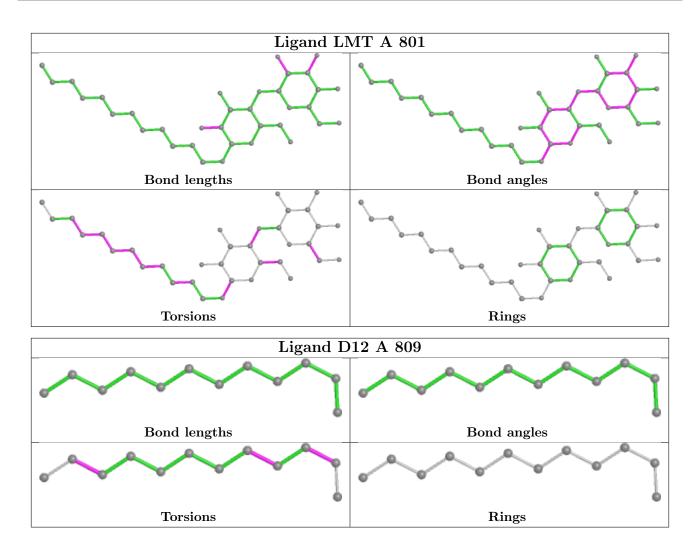












5.7 Other polymers (i)

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, 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	451/489 (92%)	0.82	55 (12%) 4 3	52, 70, 131, 160	1 (0%)
2	В	127/127 (100%)	0.44	12 (9%) 8 8	53, 66, 101, 110	1 (0%)
3	С	2/2 (100%)	0.76	0 100 100	67, 67, 67, 80	0
All	All	580/618 (93%)	0.74	67 (11%) 4 4	52, 69, 124, 160	2 (0%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	ALA	9.0
1	A	399	LEU	7.8
1	A	240	LEU	7.2
1	A	253	PHE	7.1
1	A	144	ALA	6.9

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 monosaccharides in this entry.

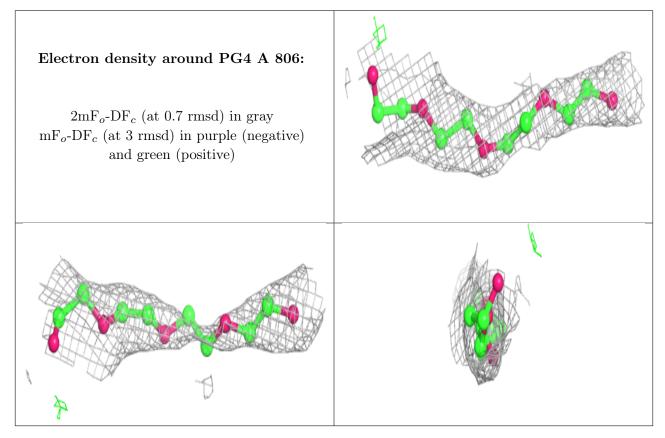
6.4 Ligands (i)

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	$\operatorname{B-factors}({\rm \AA}^2)$	Q<0.9
6	PG4	A	806	13/13	0.26	0.35	89,98,108,110	0
8	D12	A	809	12/12	0.36	1.14	86,90,95,98	0
10	D10	A	812	10/10	0.47	0.37	74,81,93,101	0
9	GOL	A	810	6/6	0.48	0.39	111,116,120,121	0
6	PG4	A	805	13/13	0.51	0.26	79,93,104,109	0
7	1PE	A	811	16/16	0.54	0.50	93,96,101,109	0
6	PG4	A	807	13/13	0.62	0.40	83,91,99,102	0
9	GOL	A	813	6/6	0.62	0.20	87,93,94,102	0
6	PG4	A	808	13/13	0.62	0.23	75,85,101,104	0
11	HEX	A	815	6/6	0.68	0.50	72,77,86,87	0
11	HEX	A	814	6/6	0.73	0.48	82,85,89,89	0
7	1PE	A	804	16/16	0.73	0.60	70,85,109,111	0
5	OCT	A	802	8/8	0.78	0.25	73,76,82,85	0
6	PG4	A	803	13/13	0.84	0.18	71,80,101,103	0
4	LMT	A	801	35/35	0.85	0.35	67,87,110,112	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.





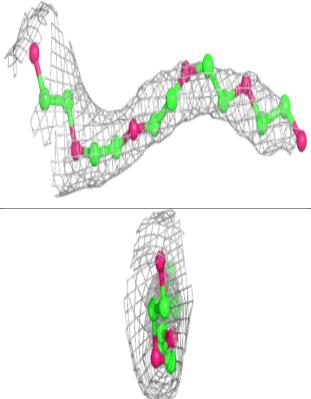


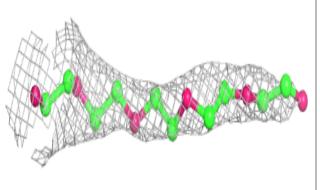
Electron density around GOL A 810: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



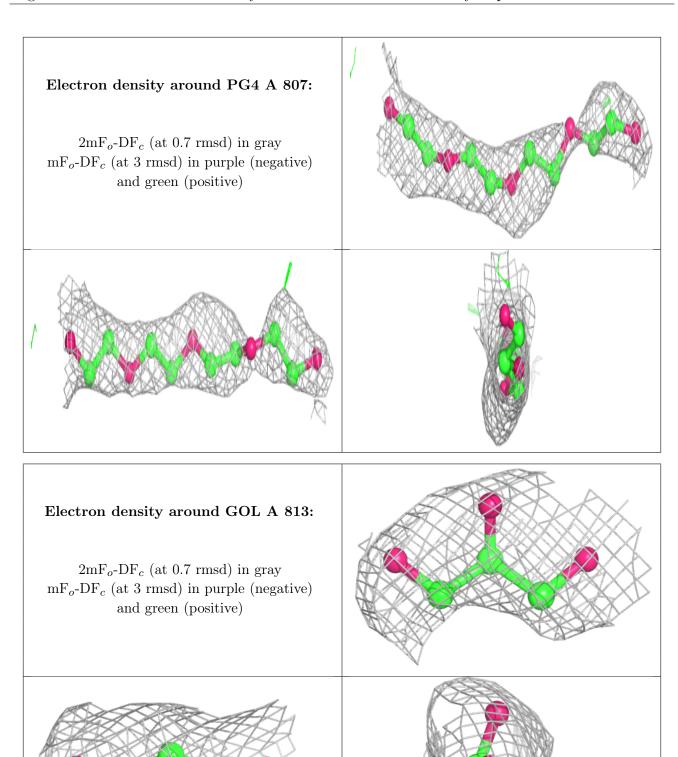
Electron density around 1PE A 811: $2mF_o$ -DF_c (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative)

and green (positive)





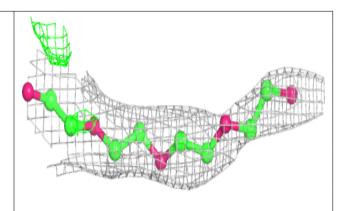


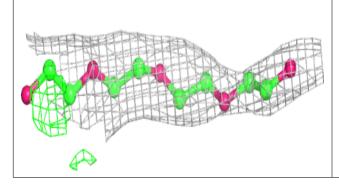


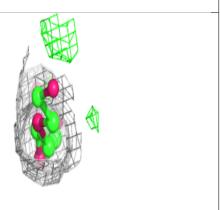


Electron density around PG4 A 808:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

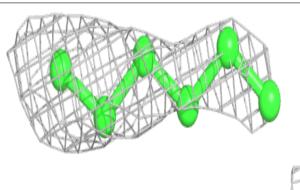


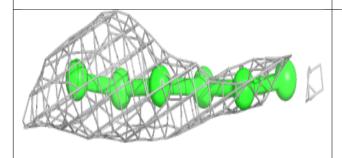


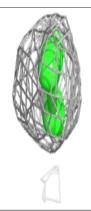


Electron density around HEX A 815:

 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

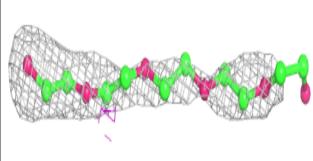


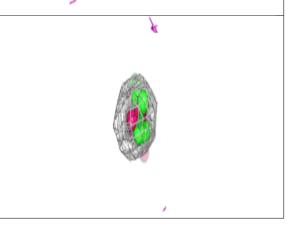






Electron density around HEX A 814: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around 1PE A 804: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)

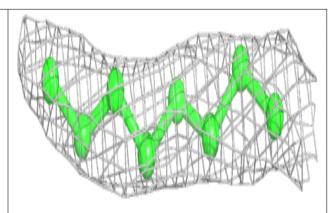


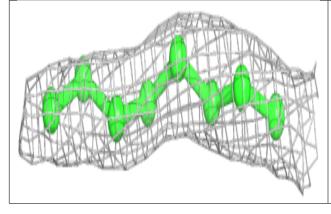


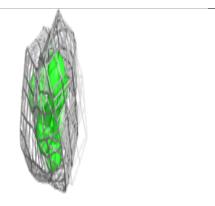


Electron density around OCT A 802:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

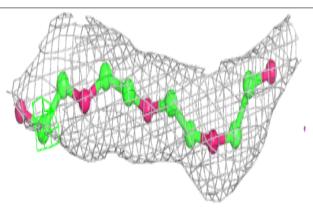


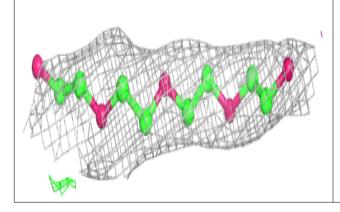


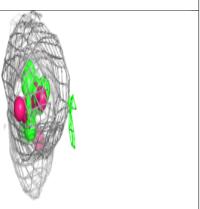


Electron density around PG4 A 803:

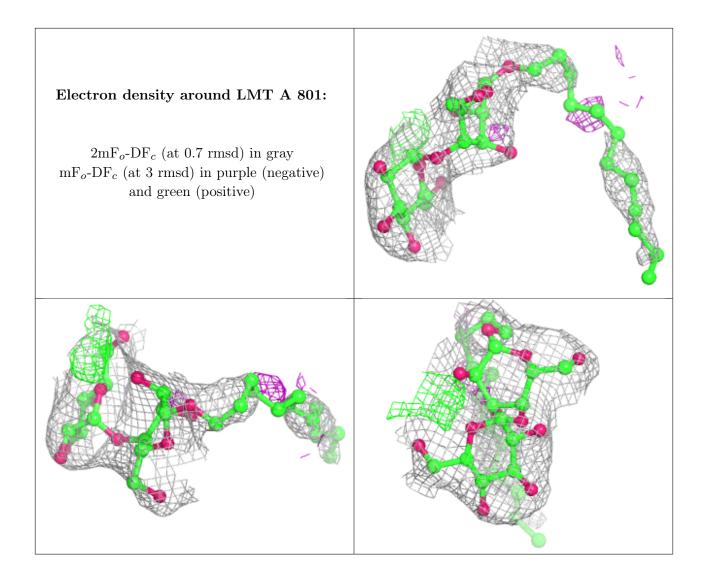
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

