



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2021 – 12:22 PM GMT

PDB ID : 6YE7
Title : E.coli's Putrescine receptor PotF complexed with Cadaverine
Authors : Shanmugaratnam, S.; Kroeger, P.; Hocker, B.
Deposited on : 2020-03-24
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 ⓘ 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 : 2.16
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) : 2.16

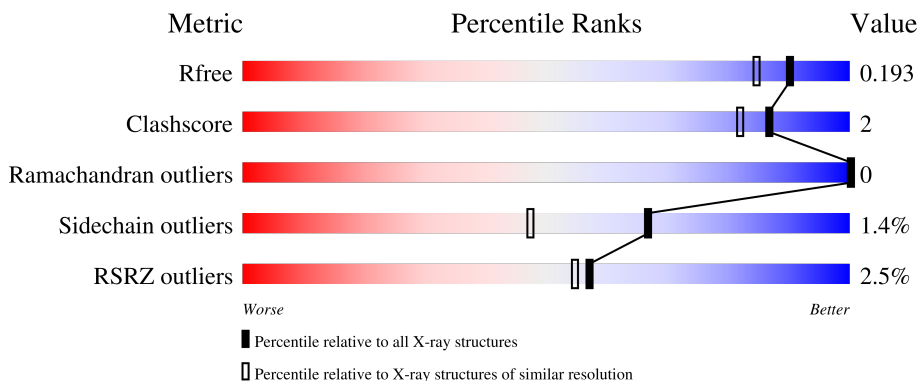
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

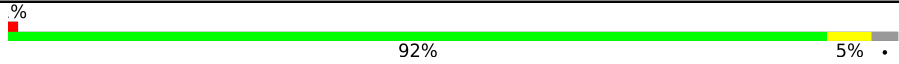
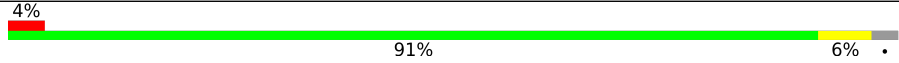
The reported resolution of this entry is 1.60 Å.

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 $\leq 5\%$. 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	352	 92% 5%
1	B	352	 91% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	1112	-	-	-	X
3	EDO	B	1115	-	-	-	X
5	PEG	B	1105	-	-	-	X

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 11830 atoms, of which 5623 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.

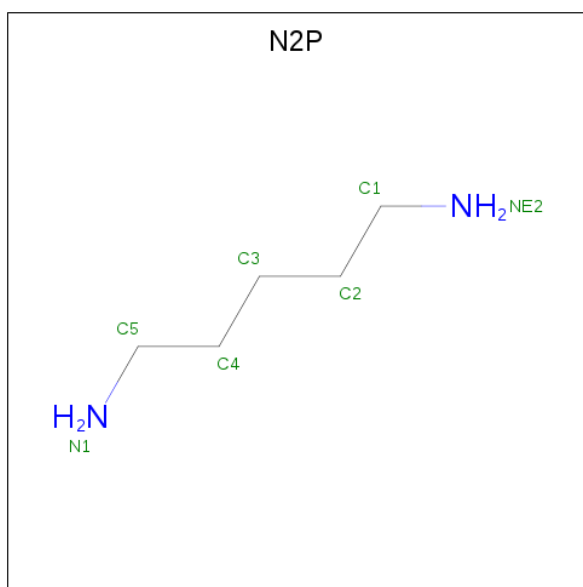
- Molecule 1 is a protein called Putrescine-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	341	Total	C	H	N	O	S	0	2	0
			5352	1730	2661	448	506	7			
1	B	341	Total	C	H	N	O	S	0	1	0
			5337	1727	2651	445	507	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	371	LEU	-	expression tag	UNP P31133
A	372	GLU	-	expression tag	UNP P31133
A	373	HIS	-	expression tag	UNP P31133
A	374	HIS	-	expression tag	UNP P31133
A	375	HIS	-	expression tag	UNP P31133
A	376	HIS	-	expression tag	UNP P31133
A	377	HIS	-	expression tag	UNP P31133
A	378	HIS	-	expression tag	UNP P31133
B	371	LEU	-	expression tag	UNP P31133
B	372	GLU	-	expression tag	UNP P31133
B	373	HIS	-	expression tag	UNP P31133
B	374	HIS	-	expression tag	UNP P31133
B	375	HIS	-	expression tag	UNP P31133
B	376	HIS	-	expression tag	UNP P31133
B	377	HIS	-	expression tag	UNP P31133
B	378	HIS	-	expression tag	UNP P31133

- Molecule 2 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: C₅H₁₄N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	N	0	0
			21	5	14	2		
2	B	1	Total	C	H	N	0	0
			21	5	14	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



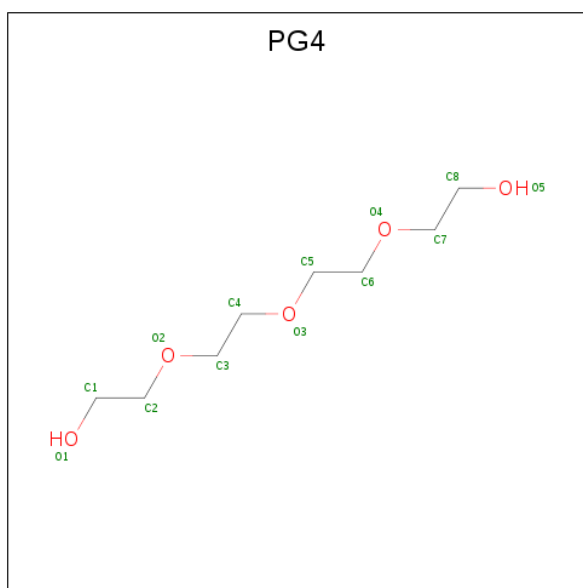
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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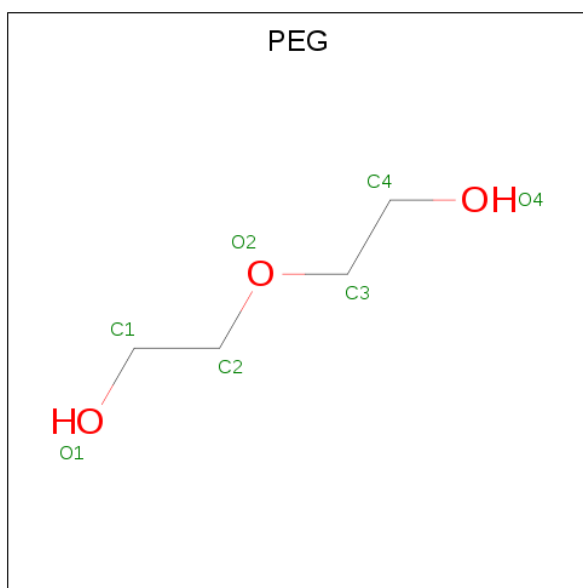
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1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

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



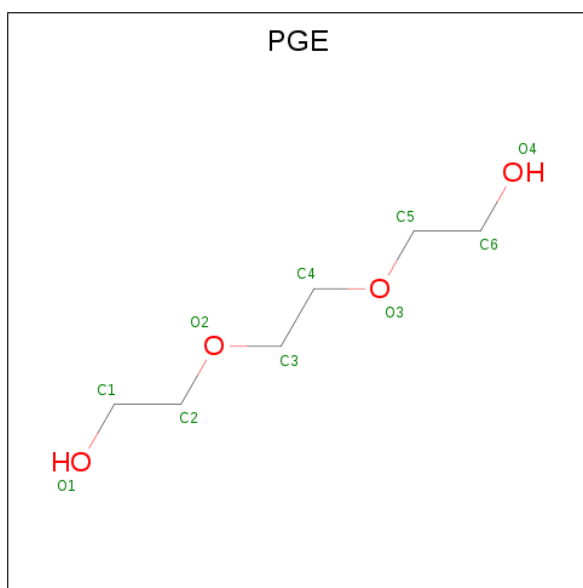
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	31	8	18	5	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



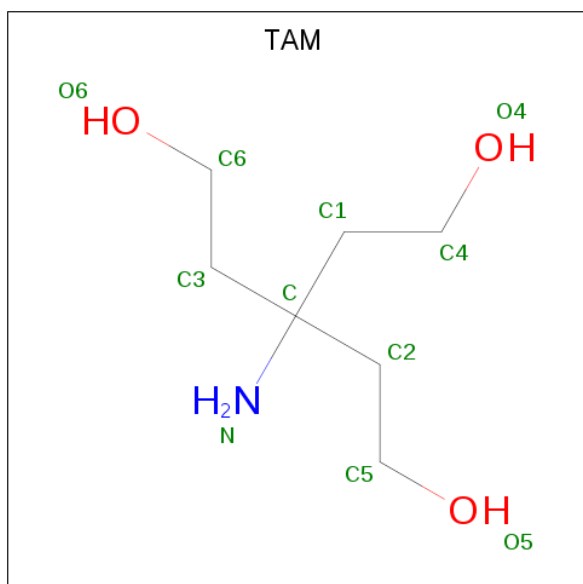
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	17	4	10	3	0	0
5	B	1	17	4	10	3	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 7 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).

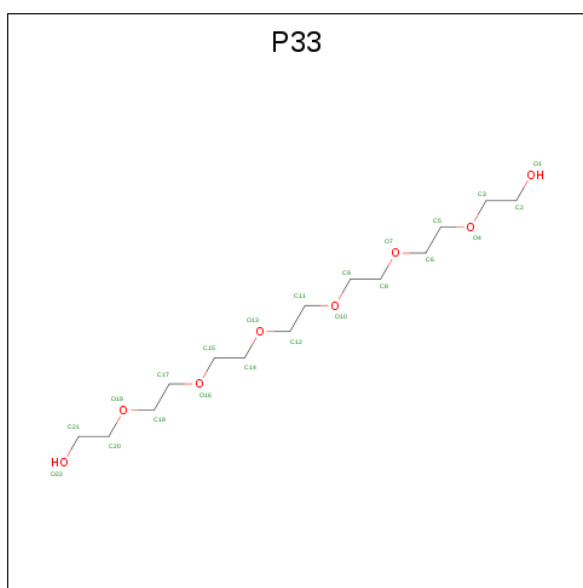


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	A	1	28	7	17	1	3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

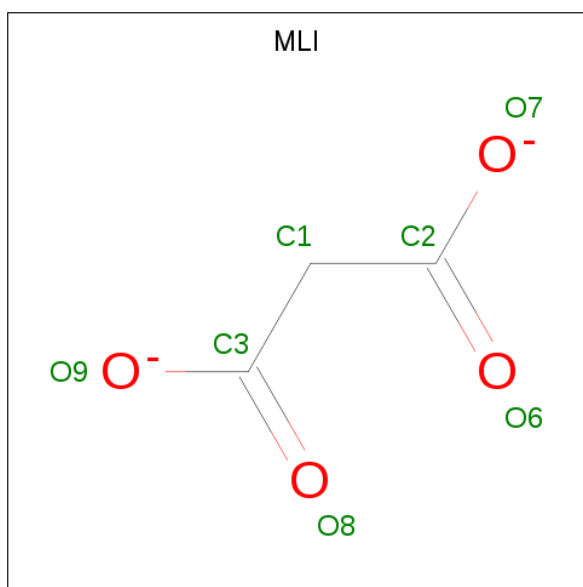
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0
8	A	2	Total Cl 2 2	0	0

- Molecule 9 is 3,6,9,12,15,18-HEXA-OXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: C₁₄H₃₀O₈).



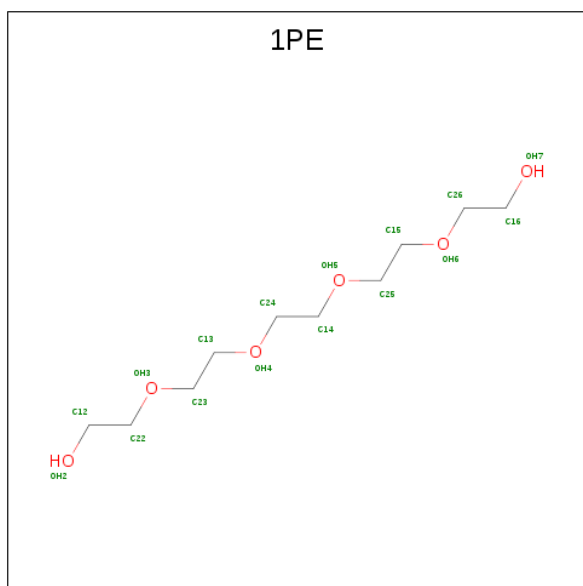
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C H O 52 14 30 8	0	0

- Molecule 10 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
10	B	1	9	3	2	4	0	0

- Molecule 11 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
11	B	1	76	20	44	12	0	1

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	315	Total 323	O 323	0	8
12	B	285	Total 289	O 289	0	4

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.87Å 70.87Å 271.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.50 – 1.60 45.50 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.50-1.60) 99.1 (45.50-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.60Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.168 , 0.194 0.168 , 0.193	Depositor DCC
R_{free} test set	2100 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11830	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, CL, N2P, MLI, EDO, 1PE, PG4, P33, TAM, PEG

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	0.50	0/2765	0.60	0/3763
1	B	0.48	0/2757	0.59	0/3752
All	All	0.49	0/5522	0.59	0/7515

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	2691	2661	2664	11	0
1	B	2686	2651	2652	11	0
2	A	7	14	14	1	0
2	B	7	14	14	1	0
3	A	48	72	72	1	0
3	B	44	66	66	1	0
4	A	13	18	18	0	0
5	A	7	10	10	0	0
5	B	7	10	10	0	0
6	A	10	14	14	0	0
7	A	11	17	17	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	2	0	0	0	0
8	B	1	0	0	0	0
9	B	22	30	30	2	0
10	B	7	2	2	0	0
11	B	32	44	44	0	0
12	A	323	0	0	0	0
12	B	289	0	0	3	0
All	All	6207	5623	5627	23	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 (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:HB3	7:A:516:TAM:H22	1.85	0.58
1:A:105:LYS:HG3	1:A:293:TYR:HB3	1.85	0.57
1:B:169:LEU:HD11	1:B:177:VAL:HG11	1.88	0.56
1:A:169:LEU:HD11	1:A:177:VAL:HG11	1.92	0.52
9:B:1101:P33:H202	12:B:1430:HOH:O	2.09	0.51
1:A:36:ASN:O	1:A:61:VAL:HA	2.11	0.51
1:A:30:LYS:HD2	1:A:291:GLU:OE2	2.12	0.50
1:B:36:ASN:O	1:B:61:VAL:HA	2.12	0.50
1:B:253:ASN:HA	1:B:256:LYS:HE3	1.92	0.50
1:A:368[A]:SER:OG	1:B:58:VAL:HG13	2.11	0.50
1:B:94:THR:HG21	12:B:1452:HOH:O	2.12	0.49
1:A:342:ARG:HB3	7:A:516:TAM:C2	2.42	0.49
1:B:253:ASN:HA	1:B:256:LYS:CE	2.42	0.48
3:A:512:EDO:H12	1:B:71:LYS:HE2	1.97	0.45
1:A:276:PHE:CE1	2:A:501:N2P:H4C2	2.52	0.45
1:A:119:LEU:HD13	7:A:516:TAM:C1	2.49	0.43
1:B:183:PRO:HB3	1:B:363:TRP:CG	2.54	0.43
1:B:276:PHE:CE1	2:B:1108:N2P:H2C1	2.54	0.43
1:B:31:THR:HG22	1:B:32:LEU:N	2.34	0.42
9:B:1101:P33:H112	12:B:1454:HOH:O	2.19	0.42
1:A:324:LEU:HD12	1:A:324:LEU:N	2.35	0.41
1:B:249:TRP:CZ2	1:B:266:PHE:HB3	2.56	0.41
1:A:357:ARG:NH1	3:B:1102:EDO:H21	2.36	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	341/352 (97%)	335 (98%)	6 (2%)	0	100	100
1	B	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
All	All	681/704 (97%)	668 (98%)	13 (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	290/298 (97%)	287 (99%)	3 (1%)	76	61
1	B	289/298 (97%)	284 (98%)	5 (2%)	60	38
All	All	579/596 (97%)	571 (99%)	8 (1%)	67	47

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	TYR
1	A	91	ARG
1	A	118	LYS
1	B	30	LYS
1	B	40	TYR
1	B	153	GLU
1	B	330	ARG
1	B	361	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 37 ligands modelled in this entry, 3 are monoatomic - leaving 34 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

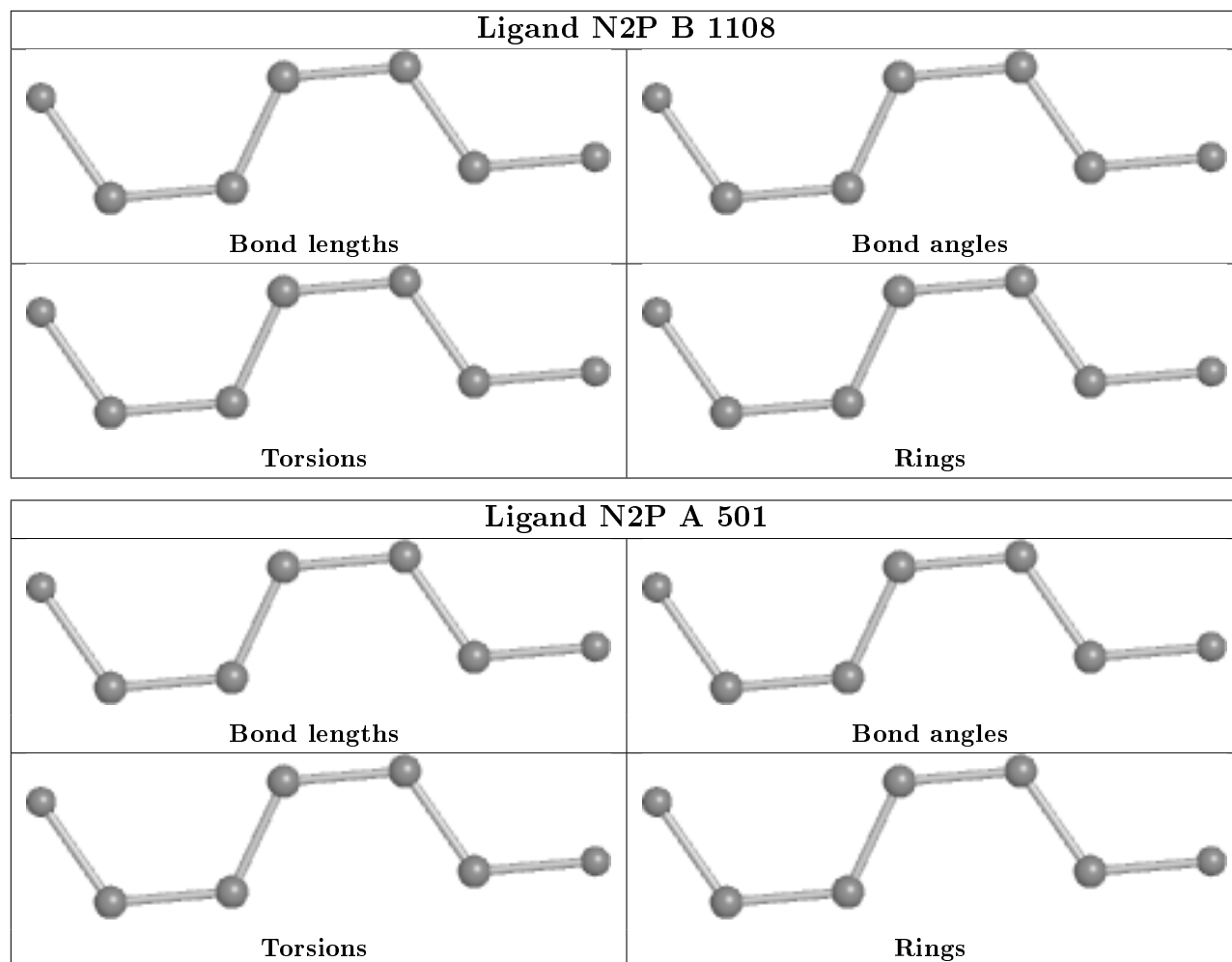
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/352 (96%)	-0.34	4 (1%) 79 78	22, 31, 53, 75	0
1	B	341/352 (96%)	-0.03	13 (3%) 40 37	23, 34, 57, 76	0
All	All	682/704 (96%)	-0.18	17 (2%) 57 55	22, 33, 55, 76	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	LYS	3.9
1	B	29	GLN	3.3
1	B	259	LYS	3.2
1	B	204	ASP	3.2
1	B	257	GLU	2.7
1	B	30	LYS	2.7
1	A	30	LYS	2.6
1	A	369	GLY	2.6
1	B	369	GLY	2.5
1	B	258	ALA	2.4
1	A	31	THR	2.4
1	A	29	GLN	2.3
1	B	256	LYS	2.3
1	B	148	LYS	2.3
1	B	354	LYS	2.2
1	B	98	PHE	2.1
1	B	284	ALA	2.0

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, 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.

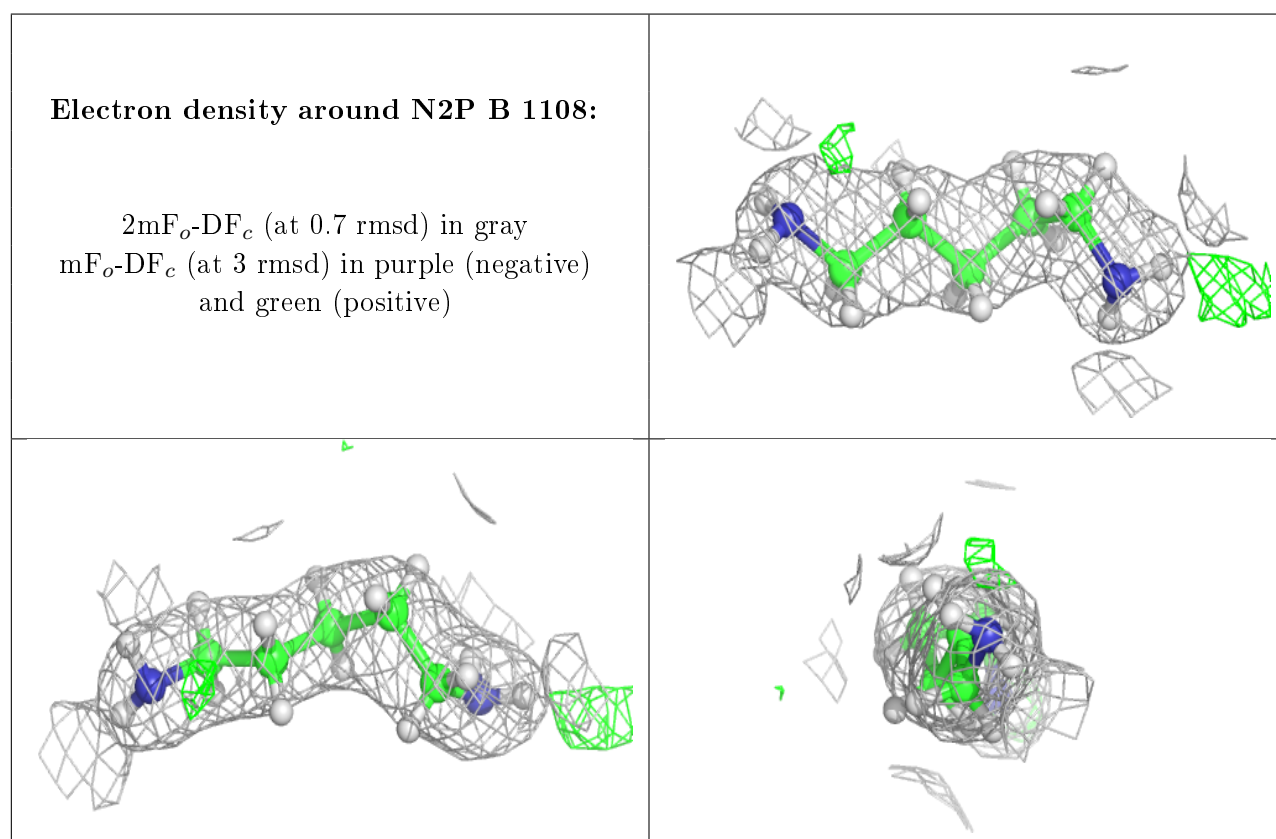
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	510	4/4	0.42	0.25	74,89,92,92	0
3	EDO	B	1112	4/4	0.49	0.84	78,93,100,101	0
3	EDO	B	1117	4/4	0.50	0.22	82,98,103,103	0
3	EDO	B	1115	4/4	0.52	0.48	78,94,99,100	0
11	1PE	B	1111[B]	16/16	0.53	0.27	37,54,66,67	38
11	1PE	B	1111[A]	16/16	0.53	0.27	31,50,67,67	38
4	PG4	A	506	13/13	0.56	0.23	62,78,91,92	0
3	EDO	A	505	4/4	0.62	0.17	50,60,65,65	0
3	EDO	A	512	4/4	0.64	0.29	72,87,89,89	0
3	EDO	B	1104	4/4	0.65	0.13	51,61,66,66	0
3	EDO	B	1107	4/4	0.68	0.28	80,96,98,98	0
3	EDO	A	507	4/4	0.70	0.16	66,79,86,86	0
10	MLI	B	1103	7/7	0.70	0.19	54,58,65,65	0
3	EDO	B	1110	4/4	0.70	0.31	80,96,101,101	0
5	PEG	A	509	7/7	0.71	0.21	66,82,100,100	0
7	TAM	A	516	11/11	0.71	0.22	62,76,85,85	0
8	CL	A	519	1/1	0.71	0.07	72,72,72,72	0
5	PEG	B	1105	7/7	0.73	0.47	67,81,84,85	0
3	EDO	A	508	4/4	0.74	0.11	64,77,85,87	0
3	EDO	B	1114	4/4	0.74	0.21	59,72,85,86	0
6	PGE	A	514	10/10	0.74	0.13	63,78,90,94	0
3	EDO	B	1109	4/4	0.78	0.11	65,78,84,86	0
3	EDO	B	1106	4/4	0.80	0.19	37,47,62,72	0
3	EDO	A	515	4/4	0.81	0.10	69,83,91,94	0
3	EDO	A	503	4/4	0.81	0.08	48,58,65,65	0
3	EDO	A	511	4/4	0.82	0.34	80,96,101,105	0
3	EDO	B	1113	4/4	0.83	0.18	67,80,81,83	0
3	EDO	A	504	4/4	0.86	0.16	45,55,61,66	0
3	EDO	A	513	4/4	0.87	0.12	52,62,70,73	0
9	P33	B	1101	22/22	0.89	0.26	41,52,75,78	0
3	EDO	A	517	4/4	0.90	0.15	53,78,89,94	0
3	EDO	A	502	4/4	0.92	0.16	29,40,57,68	0

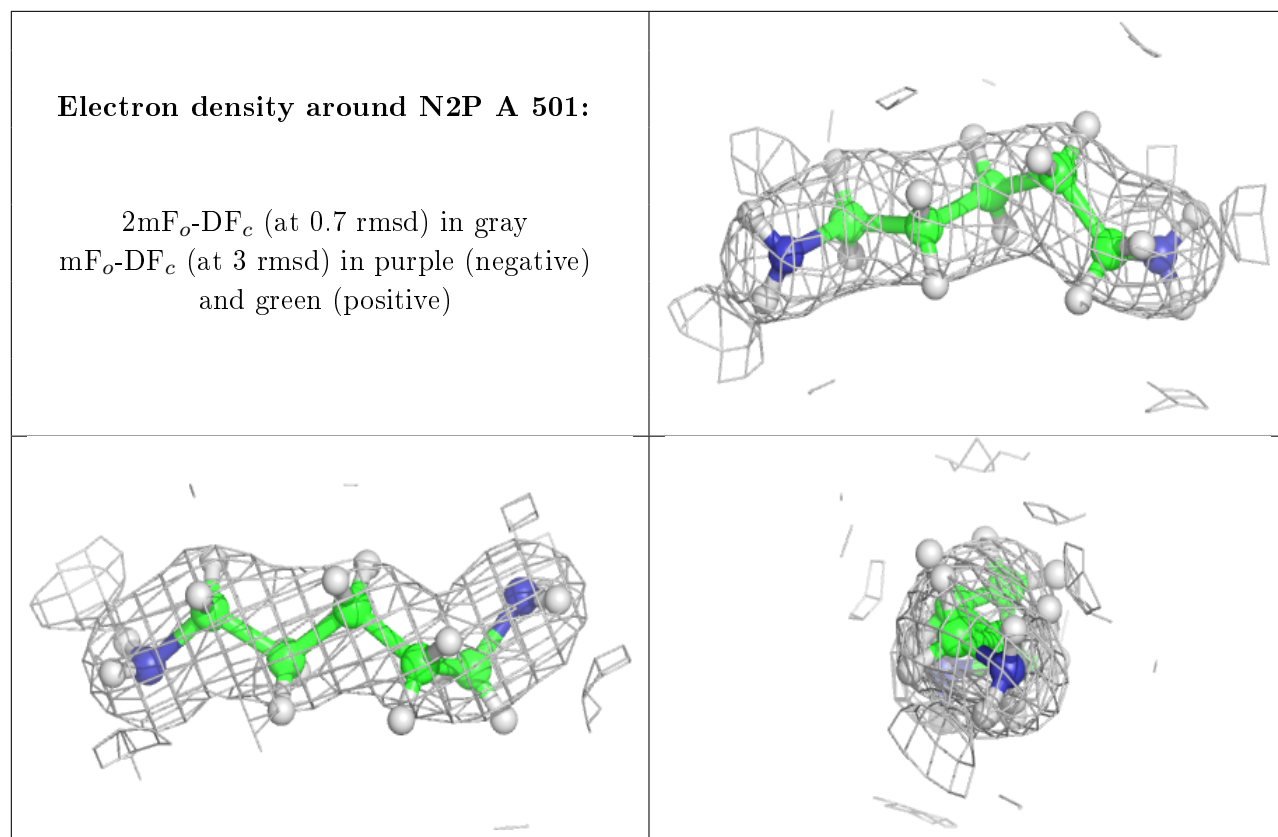
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	N2P	B	1108	7/7	0.97	0.10	26,32,37,37	0
8	CL	B	1116	1/1	0.97	0.21	63,63,63,63	0
8	CL	A	518	1/1	0.97	0.15	63,63,63,63	0
3	EDO	B	1102	4/4	0.97	0.24	33,58,77,89	0
2	N2P	A	501	7/7	0.97	0.08	25,33,34,34	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.