Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:17 am BST

PDB ID	:	5JEI
Title	:	Crystal structure of the GluA2 LBD in complex with FW
Authors	:	Eibl, C.; Salazar, H.; Chebli, M.; Plested, A.J.R.
Deposited on	:	2016-04-18
Resolution	:	1.23 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:

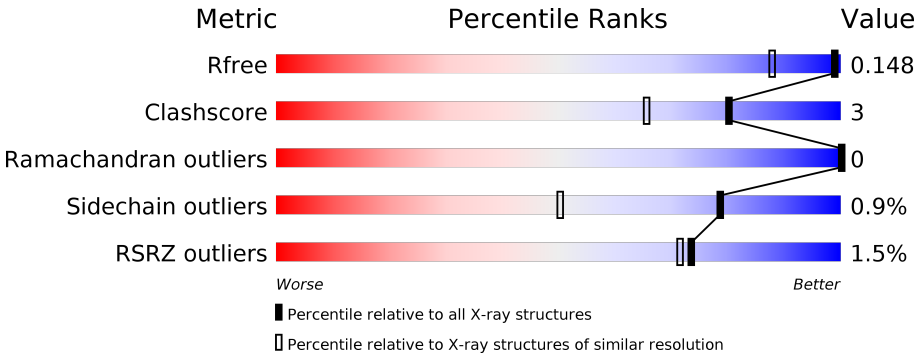
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.23 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	1232 (1.24-1.20)
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)
RSRZ outliers	127900	1209 (1.24-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	264	2% 96%

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	PO4	A	303	-	X	-	-
9	EDO	A	312	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4797 atoms, of which 2229 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.

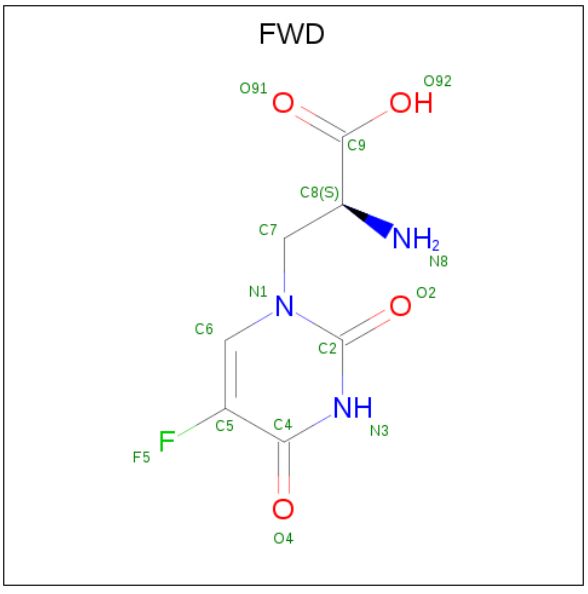
- Molecule 1 is a protein called Glutamate receptor 2,Glutamate receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	264	4174	1317	2099	348	395	15	0	5	0

There are 5 discrepancies between the modelled and reference sequences:

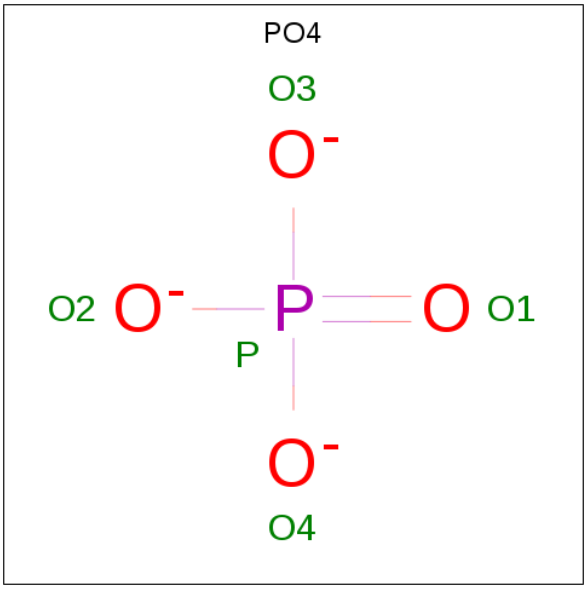
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P19491
A	2	ALA	-	expression tag	UNP P19491
A	118	GLY	-	linker	UNP P19491
A	119	THR	-	linker	UNP P19491
A	154	CYS	VAL	conflict	UNP P19491

- Molecule 2 is 2-AMINO-3-(5-FLUORO-2,4-DIOXO-3,4-DIHYDRO-2H-PYRIMIDIN-1-YL) -PROPIONIC ACID (three-letter code: FWD) (formula: $C_7H_8FN_3O_4$).



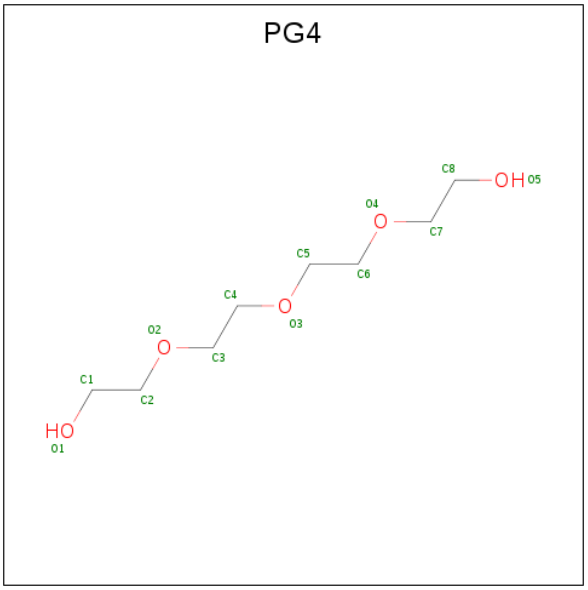
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			22	7	1	7	3	4		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



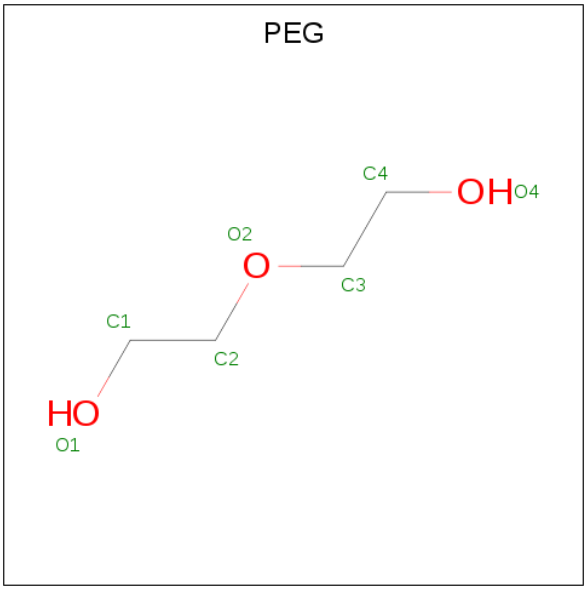
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

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



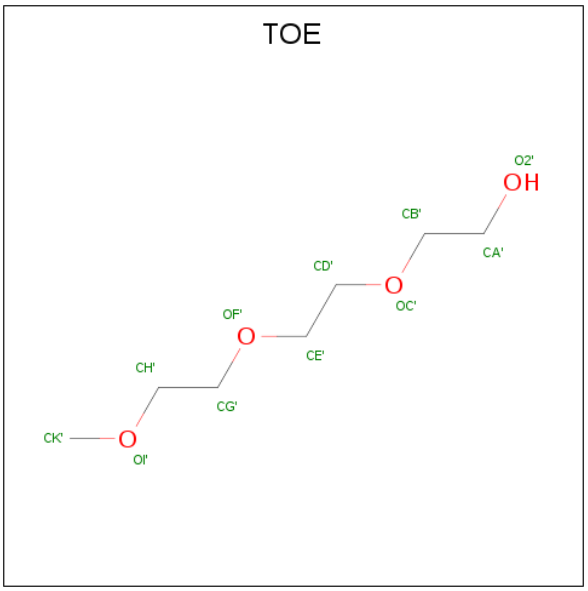
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			29	8	16	5		
4	A	1	Total	C	H	O	0	0
			15	4	8	3		

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



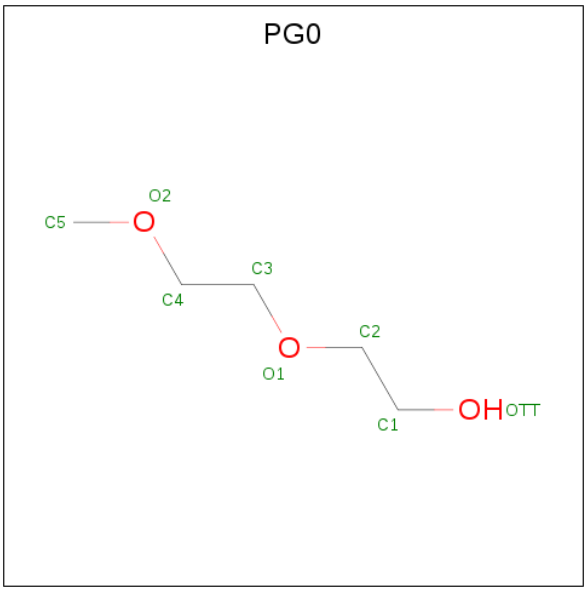
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			15	4	8	3		
5	A	1	Total	C	H	O	0	0
			16	4	9	3		
5	A	1	Total	C	H	O	0	0
			16	4	9	3		

- Molecule 6 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: $C_7H_{16}O_4$).



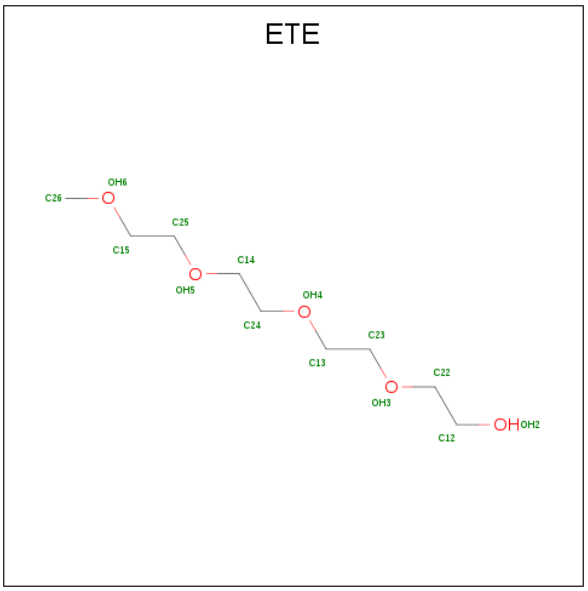
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	27	7	16	4	0	0

- Molecule 7 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



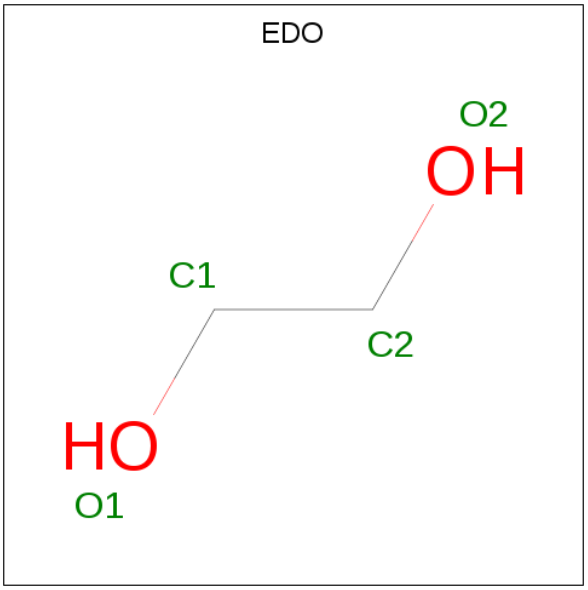
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	20	5	12	3	0	0

- Molecule 8 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: $C_9H_{20}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			34	9	20	5		
8	A	1	Total	C	H	O	0	0
			33	9	19	5		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 11 is water.

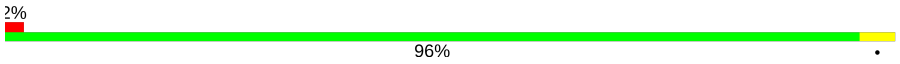
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	375	Total O 375 375	0	0

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: Glutamate receptor 2,Glutamate receptor 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.47Å 44.42Å 47.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.37 – 1.23 47.28 – 1.23	Depositor EDS
% Data completeness (in resolution range)	96.7 (32.37-1.23) 96.7 (47.28-1.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.23Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.121 , 0.147 0.122 , 0.148	Depositor DCC
R_{free} test set	3792 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	9.9	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 50.4	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	0.98	EDS
Total number of atoms	4797	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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: FWD, NA, PO4, EDO, PG4, PG0, ETE, PEG, TOE

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	0.59	0/2127	0.66	0/2857

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	2075	2099	2088	9	0
2	A	15	7	7	0	0
3	A	10	0	0	0	0
4	A	20	24	27	1	0
5	A	21	26	30	1	0
6	A	11	16	16	1	0
7	A	8	12	12	0	0
8	A	28	39	40	0	0
9	A	4	6	6	4	0
10	A	1	0	0	0	0
11	A	375	0	0	6	3
All	All	2568	2229	2226	12	3

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 3.

All (12) 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:243[A]:GLU:HG3	11:A:586:HOH:O	2.05	0.56
5:A:313:PEG:H32	11:A:456:HOH:O	2.08	0.54
1:A:81:GLY:HA2	11:A:441:HOH:O	2.08	0.53
1:A:52:LYS:NZ	11:A:403:HOH:O	2.41	0.53
1:A:14:SER:H	9:A:312:EDO:H11	1.75	0.52
1:A:100:ILE:O	1:A:226:LYS:NZ	2.36	0.49
6:A:306:TOE:H13	11:A:431:HOH:O	2.15	0.46
1:A:14:SER:H	9:A:312:EDO:C1	2.30	0.45
1:A:97:GLU:O	1:A:226:LYS:NZ	2.46	0.44
1:A:14:SER:HB2	9:A:312:EDO:H11	2.00	0.43
9:A:312:EDO:C1	11:A:466:HOH:O	2.68	0.41
1:A:144:LYS:HE2	4:A:307:PG4:H71	2.03	0.40

All (3) 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)
11:A:679:HOH:O	11:A:679:HOH:O[2_785]	2.00	0.20
11:A:649:HOH:O	11:A:649:HOH:O[2_775]	2.06	0.14
11:A:482:HOH:O	11:A:505:HOH:O[1_554]	2.13	0.07

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	267/264 (101%)	266 (100%)	1 (0%)	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	224/219 (102%)	221 (99%)	3 (1%)	69 34

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LEU
1	A	116[A]	LYS
1	A	116[B]	LYS

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\#\|Z\| > 2$
7	PG0	A	308	-	7,7,7	0.58	0	6,6,6	0.35	0
5	PEG	A	305	-	6,6,6	0.48	0	5,5,5	0.95	0
8	ETE	A	310	-	13,13,13	0.56	0	12,12,12	0.58	0
6	TOE	A	306	-	10,10,10	0.77	0	9,9,9	0.39	0
5	PEG	A	311	-	6,6,6	0.49	0	5,5,5	0.48	0
8	ETE	A	309	-	13,13,13	0.90	0	12,12,12	1.12	2 (16%)
2	FWD	A	301	-	9,15,15	0.76	0	7,21,21	3.94	2 (28%)
4	PG4	A	304	-	12,12,12	0.77	0	11,11,11	0.49	0
3	PO4	A	303	-	4,4,4	0.75	0	6,6,6	2.13	4 (66%)
9	EDO	A	312	-	3,3,3	0.74	0	2,2,2	0.64	0
5	PEG	A	313	-	6,6,6	0.49	0	5,5,5	0.82	0
4	PG4	A	307	-	6,6,12	0.56	0	5,5,11	0.50	0
3	PO4	A	302	-	4,4,4	0.61	0	6,6,6	0.97	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	PEG	A	305	-	-	1/4/4/4	-
8	ETE	A	310	-	-	0/11/11/11	-
6	TOE	A	306	-	-	6/8/8/8	-
5	PEG	A	311	-	-	3/4/4/4	-
8	ETE	A	309	-	-	3/11/11/11	-
2	FWD	A	301	-	-	0/4/8/8	0/1/1/1
4	PG4	A	304	-	-	0/10/10/10	-
5	PEG	A	313	-	-	2/4/4/4	-
9	EDO	A	312	-	-	0/1/1/1	-
4	PG4	A	307	-	-	3/4/4/10	-
7	PG0	A	308	-	-	0/5/5/5	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	FWD	C4-N3-C2	9.16	122.88	115.14
2	A	301	FWD	C5-C4-N3	-4.56	117.57	122.39
3	A	303	PO4	O4-P-O1	-2.72	100.95	110.89
8	A	309	ETE	C24-OH4-C13	2.47	123.99	113.29
3	A	303	PO4	O3-P-O2	2.40	115.69	107.97
3	A	303	PO4	O4-P-O3	2.33	115.45	107.97
8	A	309	ETE	OH5-C14-C24	2.08	119.75	110.39
3	A	303	PO4	O3-P-O1	-2.03	103.45	110.89

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	309	ETE	OH5-C14-C24-OH4
4	A	307	PG4	O3-C5-C6-O4
6	A	306	TOE	O2'-CA'-CB'-OC'
4	A	307	PG4	O4-C7-C8-O5
5	A	311	PEG	C1-C2-O2-C3
5	A	311	PEG	C4-C3-O2-C2
8	A	309	ETE	C14-C24-OH4-C13
5	A	313	PEG	C1-C2-O2-C3
5	A	305	PEG	C4-C3-O2-C2
4	A	307	PG4	C8-C7-O4-C6
6	A	306	TOE	CE'-CD'-OC'-CB'
6	A	306	TOE	OF'-CG'-CH'-OI'
5	A	311	PEG	O2-C3-C4-O4
5	A	313	PEG	O1-C1-C2-O2
6	A	306	TOE	CG'-CH'-OI'-CK'
6	A	306	TOE	CA'-CB'-OC'-CD'
6	A	306	TOE	OC'-CD'-CE'-OF'
8	A	309	ETE	OH6-C15-C25-OH5

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	306	TOE	1	0
9	A	312	EDO	4	0
5	A	313	PEG	1	0
4	A	307	PG4	1	0

5.7 Other polymers

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

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	264/264 (100%)	-0.62	4 (1%)	73	71	6, 10, 22, 42	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	ALA	5.1
1	A	67	ASP	3.4
1	A	264	GLY	2.9
1	A	68	THR	2.5

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	PO4	A	303	5/5	0.65	0.22	17,26,29,31	0
5	PEG	A	313	7/7	0.73	0.27	22,27,29,31	0
4	PG4	A	304	13/13	0.82	0.20	23,30,37,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	A	311	7/7	0.85	0.16	31,38,43,43	0
9	EDO	A	312	4/4	0.85	0.26	24,29,31,36	0
6	TOE	A	306	11/11	0.88	0.10	19,29,37,40	0
4	PG4	A	307	7/13	0.88	0.12	38,43,51,51	0
5	PEG	A	305	7/7	0.89	0.15	19,32,38,38	0
8	ETE	A	309	14/14	0.93	0.11	18,25,44,44	0
7	PG0	A	308	8/8	0.96	0.12	13,19,30,30	0
8	ETE	A	310	14/14	0.97	0.07	14,19,32,32	0
10	NA	A	314	1/1	0.98	0.10	39,39,39,39	0
2	FWD	A	301	15/15	0.99	0.05	5,6,8,8	0
3	PO4	A	302	5/5	1.00	0.05	8,9,12,14	0

6.5 Other polymers (i)

There are no such residues in this entry.