



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:17 PM BST

PDB ID : 5W4D
Title : C. japonica N-domain, Selenomethionine mutant
Authors : Aoki, S.T.; Bingman, C.A.; Kimble, J.
Deposited on : 2017-06-10
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	:	2.13.1
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)	:	2.13.1

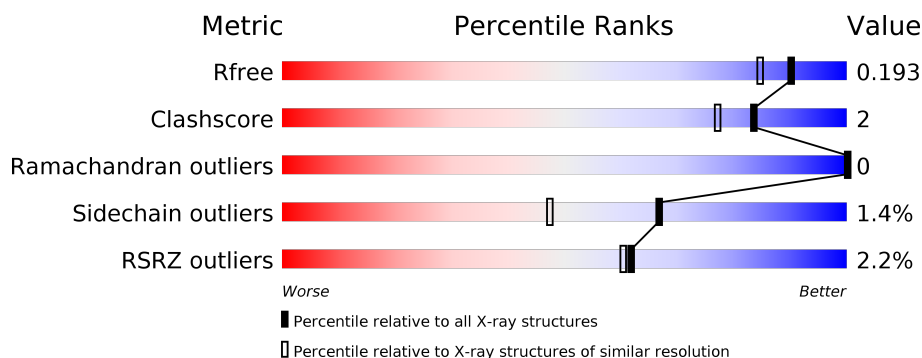
1 Overall quality at a glance

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 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	216	<div> <div></div> <div>94%</div> <div></div> </div>
1	B	216	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
1	C	216	<div> <div>2%</div> <div>89%</div> <div>7%</div> </div>
1	D	216	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14603 atoms, of which 7025 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 P-granule scaffold protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	211	Total	C	H	N	O	S	Se	0	4	0
			3381	1072	1696	274	333	1	5			
1	B	215	Total	C	H	N	O	S	Se	0	7	0
			3487	1102	1753	284	342	1	5			
1	C	208	Total	C	H	N	O	S	Se	0	4	0
			3343	1059	1678	271	329	1	5			
1	D	212	Total	C	H	N	O	S	Se	0	2	0
			3375	1070	1691	276	332	1	5			

There are 8 discrepancies between the modelled and reference sequences:

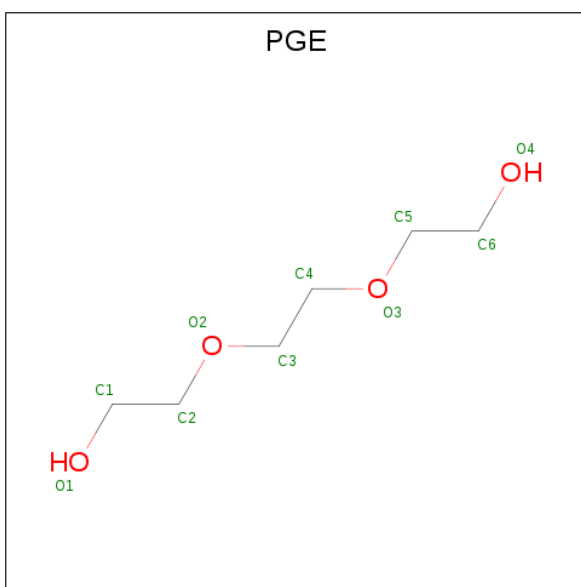
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MSE	ILE	engineered mutation	UNP H2W791
A	212	MSE	ILE	engineered mutation	UNP H2W791
B	63	MSE	ILE	engineered mutation	UNP H2W791
B	212	MSE	ILE	engineered mutation	UNP H2W791
C	63	MSE	ILE	engineered mutation	UNP H2W791
C	212	MSE	ILE	engineered mutation	UNP H2W791
D	63	MSE	ILE	engineered mutation	UNP H2W791
D	212	MSE	ILE	engineered mutation	UNP H2W791

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



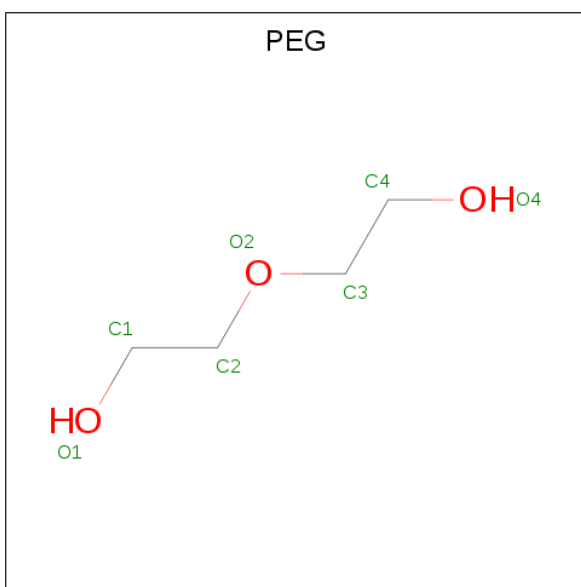
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



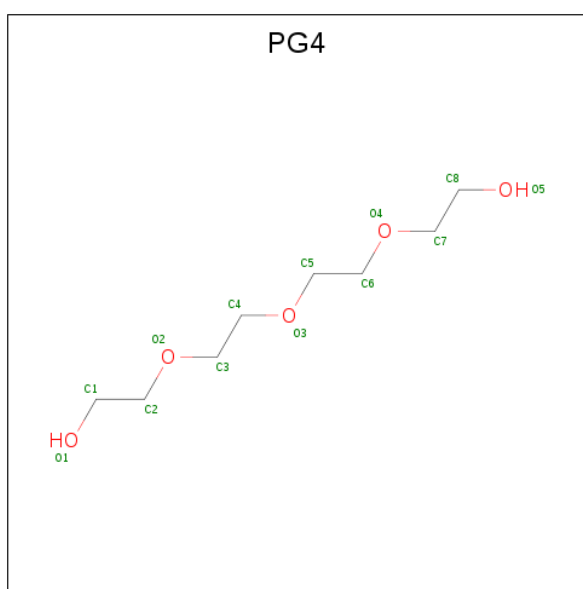
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

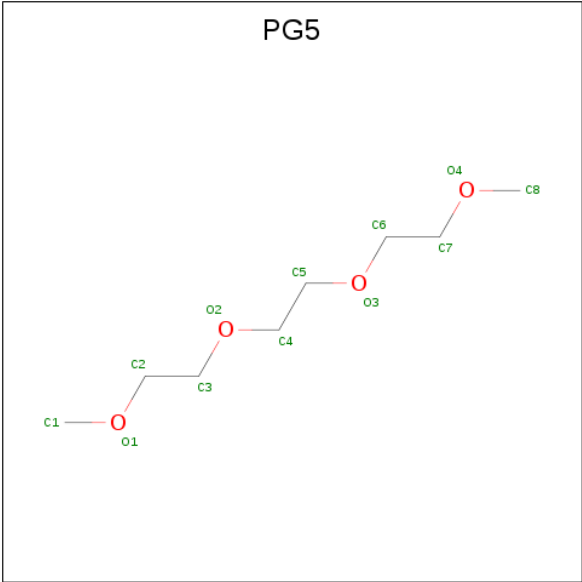
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	N	0	0
			10	3	5	2		
7	B	1	Total	C	H	N	0	0
			10	3	5	2		
7	B	1	Total	C	H	N	0	0
			10	3	5	2		
7	C	1	Total	C	H	N	0	0
			10	3	5	2		
7	D	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 8 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (three-letter code: PG5) (formula: C₈H₁₈O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	H	O	0	0
			30	8	18	4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	186	Total	O	0	0
			186	186		
9	B	158	Total	O	0	0
			158	158		
9	C	166	Total	O	0	0
			166	166		
9	D	147	Total	O	0	0
			147	147		

- Molecule 1: P-granule scaffold protein



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- | Year | Number of Publications |
|------|------------------------|
| 2011 | 1 |
| 2012 | 0 |
| 2013 | 1 |
| 2014 | 0 |
| 2015 | 1 |
| 2016 | 0 |
| 2017 | 1 |
| 2018 | 0 |
| 2019 | 1 |
| 2020 | 0 |

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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.30Å 94.80Å 72.50Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	48.47 – 1.60 48.47 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.47-1.60) 91.3 (48.47-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.157 , 0.190 0.161 , 0.193	Depositor DCC
R_{free} test set	1424 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14603	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9752e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PGE, IMD, CL, EDO, PG4, PG5, 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	0.54	0/1717	0.70	3/2308 (0.1%)
1	B	0.48	0/1775	0.61	1/2386 (0.0%)
1	C	0.50	0/1696	0.66	1/2279 (0.0%)
1	D	0.46	0/1710	0.61	1/2299 (0.0%)
All	All	0.50	0/6898	0.65	6/9272 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	B	79	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	43	PHE	CB-CG-CD1	5.38	124.57	120.80
1	C	128	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	194	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	128	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1685	1696	1698	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1734	1753	1759	14	0
1	C	1665	1678	1680	8	1
1	D	1684	1691	1693	4	0
2	A	8	12	12	0	0
2	B	4	6	6	0	0
2	C	8	12	12	0	0
2	D	4	6	6	0	0
3	A	10	14	14	0	0
3	B	10	14	14	0	0
3	D	10	14	14	0	0
4	A	14	20	20	0	0
4	B	7	10	10	0	0
4	C	14	20	20	0	0
5	A	13	18	18	1	0
5	B	13	18	18	2	0
6	A	1	0	0	1	0
7	B	15	15	15	3	0
7	C	5	5	5	1	0
7	D	5	5	5	2	0
8	C	12	18	18	1	0
9	A	186	0	0	1	0
9	B	158	0	0	11	0
9	C	166	0	0	4	0
9	D	147	0	0	2	0
All	All	7578	7025	7037	34	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 (34) 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)
7:D:302:IMD:N1	9:D:401:HOH:O	1.99	0.85
1:B:10:GLU:OE2	9:B:401:HOH:O	2.00	0.80
5:A:305:PG4:O4	9:A:401:HOH:O	2.04	0.75
1:B:58:ASP:OD2	9:B:402:HOH:O	2.05	0.75
7:B:303:IMD:H4	9:B:465:HOH:O	1.91	0.70
1:B:107:ASP:OD1	7:B:303:IMD:H2	1.91	0.69
1:C:7:GLU:OE1	9:C:401:HOH:O	2.14	0.66
7:C:303:IMD:H2	9:C:506:HOH:O	1.98	0.63
1:B:117:ASP:OD2	1:B:121:LYS:NZ	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASP:OD1	1:C:214:ASN:ND2	2.36	0.58
1:B:126:MSE:SE	9:B:547:HOH:O	2.74	0.54
1:B:126:MSE:HB2	9:B:547:HOH:O	2.12	0.50
1:B:64:LEU:HD22	9:B:445:HOH:O	2.11	0.49
1:A:98:ASP:OD1	1:A:101:ARG:NH1	2.47	0.47
1:C:36:ASP:OD2	1:C:39:LYS:HD3	2.15	0.47
1:B:185:ASP:OD2	7:B:304:IMD:H2	2.15	0.47
1:C:34:VAL:CG2	1:C:211:ILE:HD11	2.45	0.47
1:A:124:ASN:ND2	6:A:306:CL:CL	2.78	0.46
1:D:4:ASN:OD1	7:D:302:IMD:H4	2.16	0.46
1:B:131[B]:LYS:NZ	9:B:416:HOH:O	2.46	0.45
1:B:110:ILE:HG23	9:B:452:HOH:O	2.17	0.45
1:D:93:LYS:NZ	9:D:403:HOH:O	2.29	0.45
1:B:131[B]:LYS:NZ	9:B:411:HOH:O	2.41	0.45
1:B:28:ASN:HB3	5:B:301:PG4:H72	1.99	0.44
1:B:156:LYS:NZ	9:B:409:HOH:O	2.38	0.44
1:D:198:LEU:HD13	1:D:213:ARG:HG3	2.00	0.44
1:A:131:LYS:NZ	1:C:162:GLU:OE2	2.50	0.44
1:C:1:MSE:O	1:C:72:GLY:HA3	2.18	0.43
1:C:200:ARG:NH1	9:C:406:HOH:O	2.45	0.43
8:C:306:PG5:H62	9:C:402:HOH:O	2.17	0.43
5:B:301:PG4:H52	9:B:403:HOH:O	2.19	0.42
1:D:173:TYR:CE2	1:D:212:MSE:HE3	2.55	0.42
1:B:12:LEU:HG	1:B:204:THR:HB	2.03	0.41
1:C:117:ASP:O	1:C:121:LYS:HG2	2.22	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:A:39:LYS:HZ1	1:C:98:ASP:OD2[1_554]	1.58	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	213/216 (99%)	211 (99%)	2 (1%)	0	100	100
1	B	220/216 (102%)	217 (99%)	3 (1%)	0	100	100
1	C	208/216 (96%)	204 (98%)	4 (2%)	0	100	100
1	D	212/216 (98%)	210 (99%)	2 (1%)	0	100	100
All	All	853/864 (99%)	842 (99%)	11 (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	187/183 (102%)	185 (99%)	2 (1%)	73	57
1	B	194/183 (106%)	191 (98%)	3 (2%)	65	44
1	C	186/183 (102%)	183 (98%)	3 (2%)	62	41
1	D	186/183 (102%)	183 (98%)	3 (2%)	62	41
All	All	753/732 (103%)	742 (98%)	11 (2%)	67	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	151	GLU
1	B	115	ASP
1	B	116	GLU
1	B	214	ASN
1	C	39	LYS
1	C	152[A]	GLU
1	C	152[B]	GLU
1	D	7	GLU
1	D	42	SER

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Mol	Chain	Res	Type
1	D	67	SER

Some 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 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	$\# Z > 2$
5	PG4	B	301	-	12,12,12	0.50	0	11,11,11	0.50	0
4	PEG	A	307	-	6,6,6	0.47	0	5,5,5	0.45	0
3	PGE	B	306	-	9,9,9	0.37	0	8,8,8	0.37	0
3	PGE	A	303	-	9,9,9	0.31	0	8,8,8	0.30	0
3	PGE	D	303	-	9,9,9	0.28	0	8,8,8	0.50	0
4	PEG	C	305	-	6,6,6	0.47	0	5,5,5	0.32	0
2	EDO	C	301	-	3,3,3	0.60	0	2,2,2	0.03	0
7	IMD	D	302	-	3,5,5	0.24	0	4,5,5	1.07	0
8	PG5	C	306	-	11,11,11	0.53	0	10,10,10	0.66	0
2	EDO	D	301	-	3,3,3	0.48	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	B	307	-	6,6,6	0.45	0	5,5,5	0.30	0
7	IMD	C	303	-	3,5,5	0.39	0	4,5,5	0.91	0
4	PEG	A	304	-	6,6,6	0.48	0	5,5,5	0.45	0
2	EDO	B	302	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	C	302	-	3,3,3	0.49	0	2,2,2	0.27	0
2	EDO	A	301	-	3,3,3	0.41	0	2,2,2	0.32	0
5	PG4	A	305	-	12,12,12	0.55	0	11,11,11	0.46	0
7	IMD	B	303	-	3,5,5	0.48	0	4,5,5	0.50	0
4	PEG	C	304	-	6,6,6	0.52	0	5,5,5	0.34	0
2	EDO	A	302	-	3,3,3	0.46	0	2,2,2	0.24	0
7	IMD	B	304	-	3,5,5	0.41	0	4,5,5	0.60	0
7	IMD	B	305	-	3,5,5	0.44	0	4,5,5	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	B	301	-	-	7/10/10/10	-
4	PEG	A	307	-	-	4/4/4/4	-
3	PGE	B	306	-	-	3/7/7/7	-
3	PGE	A	303	-	-	2/7/7/7	-
3	PGE	D	303	-	-	5/7/7/7	-
4	PEG	C	305	-	-	2/4/4/4	-
2	EDO	C	301	-	-	0/1/1/1	-
7	IMD	D	302	-	-	-	0/1/1/1
8	PG5	C	306	-	-	5/9/9/9	-
2	EDO	D	301	-	-	1/1/1/1	-
4	PEG	B	307	-	-	1/4/4/4	-
7	IMD	C	303	-	-	-	0/1/1/1
4	PEG	A	304	-	-	2/4/4/4	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	C	302	-	-	0/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
5	PG4	A	305	-	-	2/10/10/10	-
7	IMD	B	303	-	-	-	0/1/1/1
4	PEG	C	304	-	-	2/4/4/4	-
2	EDO	A	302	-	-	0/1/1/1	-
7	IMD	B	304	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IMD	B	305	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	PEG	C1-C2-O2-C3
5	B	301	PG4	O2-C3-C4-O3
8	C	306	PG5	O2-C4-C5-O3
3	B	306	PGE	O1-C1-C2-O2
3	A	303	PGE	O1-C1-C2-O2
4	C	304	PEG	O1-C1-C2-O2
5	B	301	PG4	O1-C1-C2-O2
2	D	301	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
8	C	306	PG5	O1-C2-C3-O2
4	A	307	PEG	O2-C3-C4-O4
3	D	303	PGE	O1-C1-C2-O2
5	A	305	PG4	O3-C5-C6-O4
3	D	303	PGE	C6-C5-O3-C4
8	C	306	PG5	C2-C3-O2-C4
4	A	307	PEG	C4-C3-O2-C2
4	B	307	PEG	O2-C3-C4-O4
3	B	306	PGE	C4-C3-O2-C2
5	B	301	PG4	C4-C3-O2-C2
8	C	306	PG5	C6-C7-O4-C8
8	C	306	PG5	O3-C6-C7-O4
4	C	305	PEG	C1-C2-O2-C3
5	A	305	PG4	O1-C1-C2-O2
3	B	306	PGE	O2-C3-C4-O3
5	B	301	PG4	C3-C4-O3-C5
4	A	307	PEG	C1-C2-O2-C3
4	A	307	PEG	O1-C1-C2-O2
4	C	304	PEG	C1-C2-O2-C3
3	D	303	PGE	C1-C2-O2-C3
5	B	301	PG4	C6-C5-O3-C4
5	B	301	PG4	C1-C2-O2-C3
5	B	301	PG4	C5-C6-O4-C7
3	A	303	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	D	303	PGE	O3-C5-C6-O4
4	A	304	PEG	O1-C1-C2-O2
4	C	305	PEG	O1-C1-C2-O2
3	D	303	PGE	O2-C3-C4-O3

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	PG4	2	0
7	D	302	IMD	2	0
8	C	306	PG5	1	0
7	C	303	IMD	1	0
5	A	305	PG4	1	0
7	B	303	IMD	2	0
7	B	304	IMD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	207/216 (95%)	-0.25	1 (0%) 91 90	14, 22, 48, 73	0
1	B	210/216 (97%)	-0.12	7 (3%) 46 43	16, 27, 55, 93	0
1	C	203/216 (93%)	-0.22	4 (1%) 65 64	16, 25, 49, 79	0
1	D	208/216 (96%)	-0.10	6 (2%) 51 49	17, 28, 61, 78	0
All	All	828/864 (95%)	-0.17	18 (2%) 62 60	14, 25, 54, 93	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ASP	4.9
1	D	53	LYS	4.4
1	C	215	GLY	3.5
1	B	214	ASN	3.3
1	B	111	LEU	3.3
1	D	38	ASN	3.2
1	B	116	GLU	3.1
1	B	151	GLU	2.7
1	C	117	ASP	2.7
1	D	4	ASN	2.6
1	C	4	ASN	2.5
1	D	39	LYS	2.5
1	B	115	ASP	2.4
1	B	114	GLY	2.3
1	B	86	PRO	2.2
1	A	214	ASN	2.2
1	D	151	GLU	2.0
1	D	211	ILE	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(\AA^2)	Q<0.9
3	PGE	B	306	10/10	0.56	0.17	57,74,85,90	0
2	EDO	C	301	4/4	0.56	0.15	51,65,70,78	0
4	PEG	C	304	7/7	0.59	0.21	40,54,64,75	0
2	EDO	D	301	4/4	0.74	0.13	41,51,63,67	0
4	PEG	C	305	7/7	0.74	0.14	58,70,74,78	0
8	PG5	C	306	12/12	0.75	0.15	43,60,67,81	0
5	PG4	B	301	13/13	0.76	0.15	46,57,73,74	0
4	PEG	A	307	7/7	0.76	0.12	54,65,75,83	0
7	IMD	B	304	5/5	0.78	0.24	67,74,84,89	0
3	PGE	A	303	10/10	0.79	0.12	56,68,77,78	0
4	PEG	A	304	7/7	0.79	0.12	48,58,74,85	0
4	PEG	B	307	7/7	0.82	0.13	33,50,62,62	0
7	IMD	D	302	5/5	0.83	0.16	21,38,52,55	10
2	EDO	A	302	4/4	0.83	0.10	40,58,70,74	0
2	EDO	C	302	4/4	0.83	0.13	44,60,72,77	0
2	EDO	B	302	4/4	0.85	0.11	52,63,72,83	0
3	PGE	D	303	10/10	0.86	0.11	47,63,71,80	0
5	PG4	A	305	13/13	0.89	0.12	32,47,65,78	0
7	IMD	B	305	5/5	0.89	0.26	51,56,66,67	10
7	IMD	C	303	5/5	0.92	0.12	24,36,44,45	0
2	EDO	A	301	4/4	0.94	0.10	40,48,55,66	0
7	IMD	B	303	5/5	0.96	0.08	19,28,34,35	0
6	CL	A	306	1/1	1.00	0.04	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.