Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2023 – 01:20 AM EDT

PDB ID	:	3HHL
Title	:	Crystal structure of methylated RPA0582 protein
Authors	:	Sledz, P.; Niedzialkowska, E.; Chruszcz, M.; Porebski, P.; Yim, V.; Kudritska, M.; Zimmerman, M.D.; Evdokimova, E.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Minor, W.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-05-15
Resolution	:	2.65 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

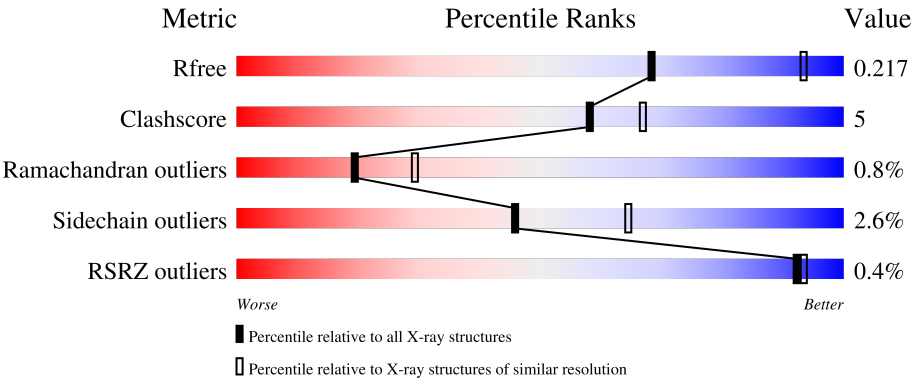
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	143	85% 8% · 6%
2	B	143	78% 17% 6%
3	C	143	83% 10% · 6%
4	D	143	80% 13% · 6%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 4944 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 RPA0582.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	135	1098	696	203	195	4	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q6NC90
A	61	SER	PHE	SEE REMARK 999	UNP Q6NC90

- Molecule 2 is a protein called RPA0582.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	135	1103	698	208	194	3	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q6NC90
B	61	SER	PHE	SEE REMARK 999	UNP Q6NC90

- Molecule 3 is a protein called RPA0582.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
3	C	135	1119	710	210	195	4	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q6NC90
C	61	SER	PHE	SEE REMARK 999	UNP Q6NC90

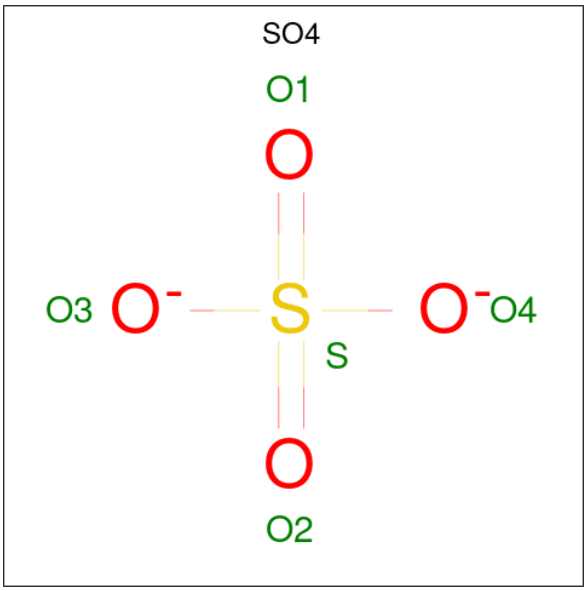
- Molecule 4 is a protein called RPA0582.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	135	Total	C	N	O	Se	0	3	0
			1103	697	205	198	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP Q6NC90
D	61	SER	PHE	SEE REMARK 999	UNP Q6NC90

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- 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		

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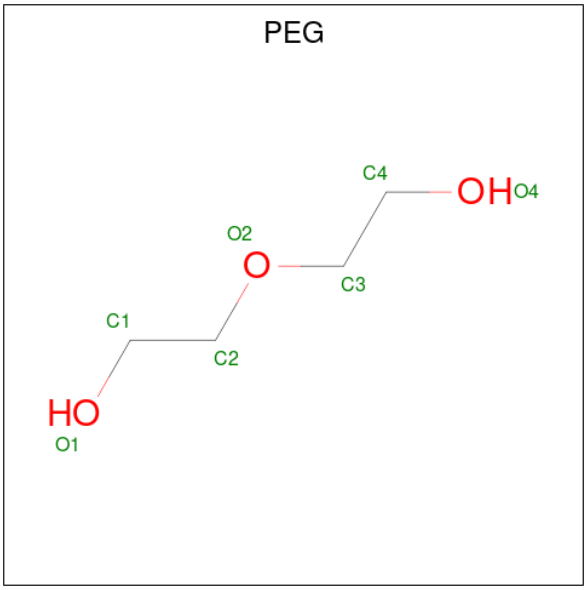
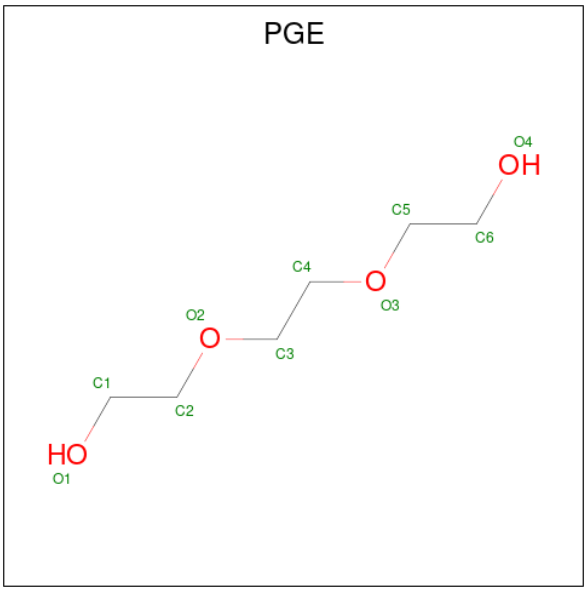
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



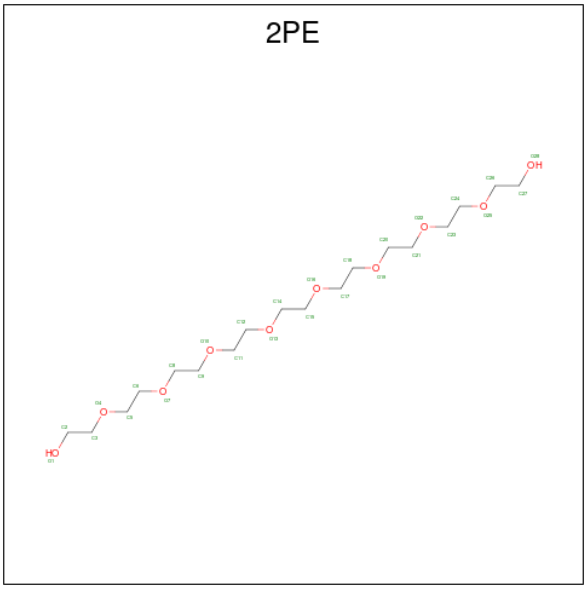
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			10	6	4		
8	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			28	18	10		

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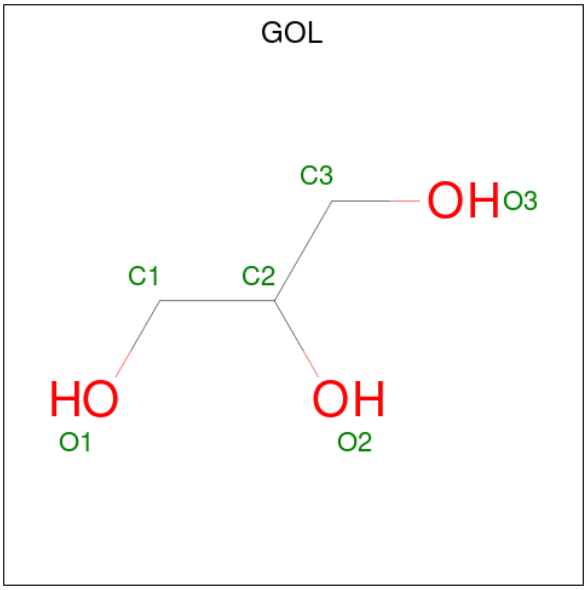
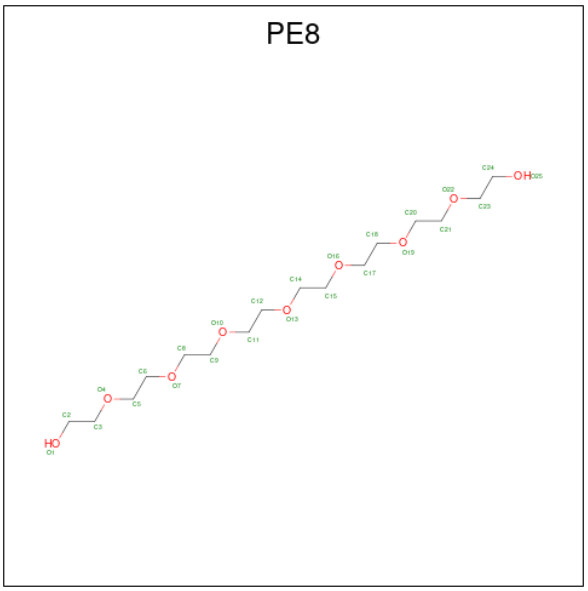
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 28 18 10	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



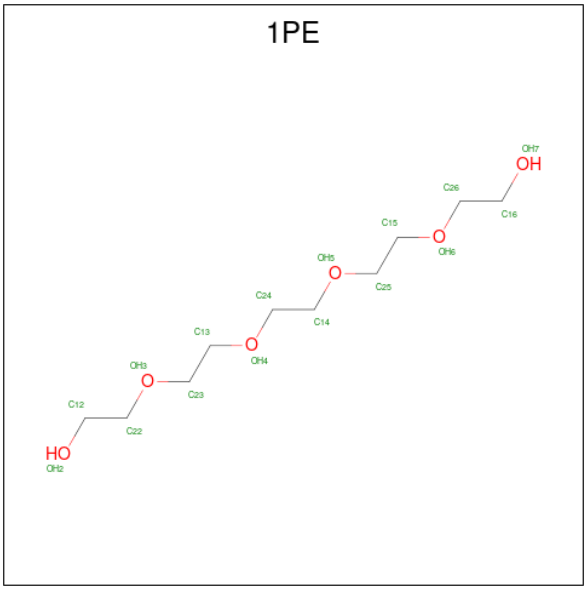
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0
10	C	1	Total C O 6 3 3	0	0
10	D	1	Total C O 6 3 3	0	0

- Molecule 11 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



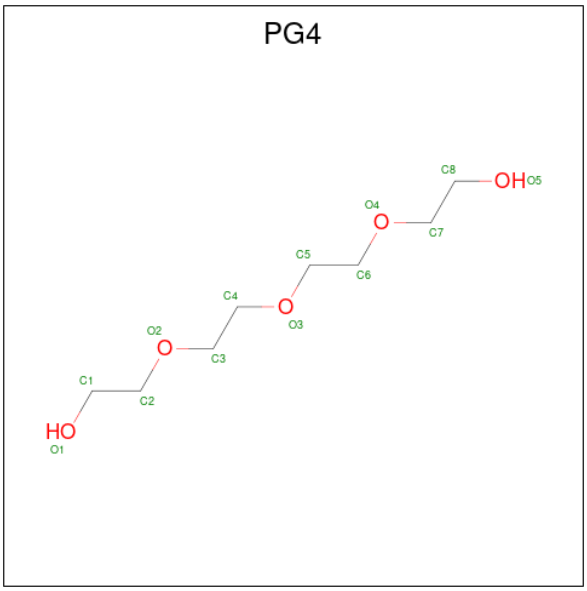
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C O 25 16 9	0	0
11	C	1	Total C O 25 16 9	0	0

- Molecule 12 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 16 10 6	0	0

- Molecule 13 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 14 is water.

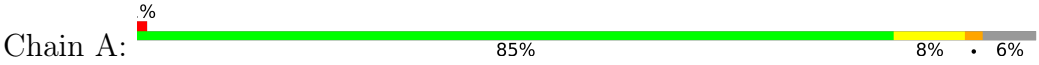
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	57	Total O 57 57	0	0
14	B	66	Total O 66 66	0	0
14	C	70	Total O 70 70	0	0
14	D	58	Total O 58 58	0	0

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: RPA0582

Chain A:

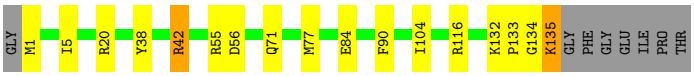


- Molecule 2: RPA0582

Chain B:

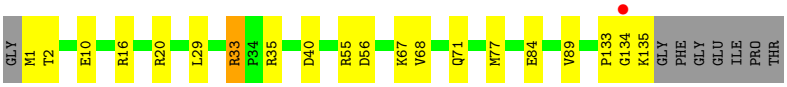
- Molecule 3: RPA0582

Chain C:



- Molecule 4: RPA0582

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	193.01Å 193.01Å 117.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.17 – 2.65 32.17 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.17-2.65) 99.2 (32.17-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.178 , 0.206 0.190 , 0.217	Depositor DCC
R_{free} test set	2400 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 24.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.015 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.012 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.014 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.470 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.477 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.470 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.016 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4944	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: 1PE, CL, SO4, PEG, GOL, PG4, MLY, MLZ, PE8, PGE, 2PE

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	0.82	0/1090	0.78	0/1471
2	B	0.83	1/1112 (0.1%)	0.77	0/1500
3	C	0.78	0/1109	0.79	0/1494
4	D	0.84	2/1105 (0.2%)	0.82	1/1494 (0.1%)
All	All	0.82	3/4416 (0.1%)	0.79	1/5959 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	10	GLU	CG-CD	6.83	1.62	1.51
4	D	10[A]	GLU	CG-CD	5.35	1.59	1.51
4	D	10[B]	GLU	CG-CD	5.35	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	33	ARG	NE-CZ-NH1	5.64	123.12	120.30

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	1098	0	1076	9	0
2	B	1103	0	1089	20	0
3	C	1119	0	1111	9	0
4	D	1103	0	1071	11	0
5	A	10	0	0	0	0
5	C	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
6	C	1	0	0	1	0
6	D	1	0	0	0	0
7	A	14	0	20	0	0
7	B	21	0	30	0	0
7	C	7	0	10	0	0
7	D	7	0	10	0	0
8	A	10	0	14	0	0
8	B	10	0	14	0	0
8	C	10	0	14	0	0
9	A	28	0	38	1	0
9	D	28	0	38	1	0
10	A	6	0	8	0	0
10	B	6	0	8	0	0
10	C	6	0	8	0	0
10	D	6	0	8	0	0
11	B	25	0	34	2	0
11	C	25	0	34	1	0
12	B	16	0	22	0	0
13	C	13	0	18	0	0
13	D	13	0	18	0	0
14	A	57	0	0	1	0
14	B	66	0	0	0	0
14	C	70	0	0	1	0
14	D	58	0	0	1	0
All	All	4944	0	4693	45	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 5.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16[B]:ARG:HG2	2:B:16[B]:ARG:HH11	1.09	1.15
4:D:16[B]:ARG:HH11	4:D:16[B]:ARG:HG2	1.20	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16[B]:ARG:HG2	2:B:16[B]:ARG:NH1	1.90	0.85
4:D:16[B]:ARG:HG2	4:D:16[B]:ARG:NH1	1.95	0.76
2:B:16[B]:ARG:HH11	2:B:16[B]:ARG:CG	1.95	0.75
2:B:1:MSE:O	2:B:2:THR:HG22	1.89	0.73
1:A:44:THR:HG22	1:A:48:GLU:OE1	1.92	0.69
2:B:100:PHE:CE2	2:B:104:ILE:HD12	2.32	0.65
1:A:77:MSE:HE3	1:A:84:GLU:HB3	1.80	0.64
4:D:33:ARG:HG3	4:D:35:ARG:O	1.98	0.63
2:B:1:MSE:O	2:B:2:THR:CG2	2.47	0.62
2:B:68:VAL:HG23	11:B:148:PE8:H231	1.82	0.60
6:C:144:CL:CL	11:C:148:PE8:H172	2.40	0.59
4:D:55[A]:ARG:NH1	4:D:56:ASP:OD1	2.37	0.58
4:D:77:MSE:HE3	4:D:84:GLU:HB3	1.85	0.58
2:B:132:LYS:O	2:B:134:GLY:N	2.35	0.57
3:C:77:MSE:HE3	3:C:84:GLU:HB3	1.85	0.57
3:C:5:ILE:O	3:C:116:ARG:NH2	2.37	0.56
2:B:131:LEU:HD12	3:C:71:GLN:HG2	1.91	0.53
4:D:68:VAL:HG23	9:D:146:2PE:H262	1.91	0.50
2:B:77:MSE:HE3	2:B:84:GLU:HB3	1.94	0.50
2:B:135:MLY:HH11	3:C:90:PHE:CD1	2.46	0.50
3:C:1:MSE:N	14:C:233:HOH:O	2.46	0.49
3:C:55[A]:ARG:NH1	3:C:56:ASP:OD1	2.46	0.47
1:A:68:VAL:HG23	9:A:148:2PE:H261	1.96	0.47
2:B:16[B]:ARG:NH1	2:B:16[B]:ARG:CG	2.64	0.47
2:B:135:MLY:HH12	2:B:135:MLY:HD2	1.60	0.47
1:A:132:LYS:O	1:A:134:GLY:N	2.43	0.46
1:A:2:THR:HG22	14:A:238:HOH:O	2.14	0.46
4:D:134:GLY:O	4:D:135:MLY:C	2.65	0.45
1:A:2:THR:HG23	1:A:2:THR:O	2.17	0.45
2:B:5:ILE:O	2:B:116:ARG:NH2	2.50	0.45
2:B:90:PHE:CD1	3:C:135:MLY:HH11	2.52	0.45
3:C:132:LYS:O	3:C:134:GLY:N	2.43	0.44
6:B:143:CL:CL	11:B:148:PE8:H171	2.54	0.44
2:B:40:ASP:O	2:B:40:ASP:CG	2.57	0.43
2:B:135:MLY:HB2	2:B:135:MLY:HE3	1.57	0.43
3:C:38:TYR:CD1	3:C:42:ARG:HD2	2.54	0.43
1:A:133:PRO:HB3	4:D:68:VAL:HG12	2.00	0.42
4:D:29:LEU:HD23	4:D:89:VAL:HG13	2.01	0.42
2:B:100:PHE:CE2	2:B:104:ILE:CD1	3.02	0.42
1:A:135:MLY:HD2	4:D:71:GLN:HE22	1.86	0.41
1:A:14:GLN:NE2	2:B:63:ARG:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:MSE:N	14:D:189:HOH:O	2.54	0.41
2:B:35:ARG:HD2	2:B:43:GLU:OE2	2.20	0.41

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	133/143 (93%)	129 (97%)	3 (2%)	1 (1%)	19	29
2	B	135/143 (94%)	131 (97%)	3 (2%)	1 (1%)	22	33
3	C	135/143 (94%)	130 (96%)	4 (3%)	1 (1%)	22	33
4	D	135/143 (94%)	130 (96%)	4 (3%)	1 (1%)	22	33
All	All	538/572 (94%)	520 (97%)	14 (3%)	4 (1%)	19	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	PRO
3	C	133	PRO
4	D	133	PRO
1	A	133	PRO

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	107/108 (99%)	104 (97%)	3 (3%)	43	61
2	B	109/109 (100%)	107 (98%)	2 (2%)	59	75
3	C	109/107 (102%)	106 (97%)	3 (3%)	43	61
4	D	108/109 (99%)	105 (97%)	3 (3%)	43	61
All	All	433/433 (100%)	422 (98%)	11 (2%)	46	66

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

Mol	Chain	Res	Type
1	A	20	ARG
1	A	42	ARG
1	A	44	THR
2	B	20	ARG
2	B	44	THR
3	C	20	ARG
3	C	42	ARG
3	C	104	ILE
4	D	2	THR
4	D	20	ARG
4	D	40	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
4	D	4	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

11 non-standard protein/DNA/RNA residues 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MLZ	C	114	3	8,9,10	0.97	0	4,9,11	0.61	0
3	MLY	C	67	3	9,10,11	0.65	0	6,11,13	0.40	0
1	MLY	A	135	1	9,10,11	1.18	1 (11%)	6,11,13	0.35	0
4	MLY	D	67	4	9,10,11	0.67	0	6,11,13	1.04	1 (16%)
2	MLY	B	135	2	9,10,11	0.52	0	6,11,13	0.44	0
4	MLY	D	135	4	9,10,11	0.89	0	6,11,13	0.40	0
3	MLY	C	135	3	9,10,11	1.10	1 (11%)	6,11,13	0.72	0
1	MLZ	A	129	1	8,9,10	1.68	2 (25%)	4,9,11	1.18	0
1	MLY	A	67	1	9,10,11	0.61	0	6,11,13	0.49	0
3	MLZ	C	129	3	8,9,10	1.06	0	4,9,11	0.61	0
2	MLZ	B	67	2	8,9,10	1.38	1 (12%)	4,9,11	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
3	MLZ	C	114	3	-	0/7/8/10	-
3	MLY	C	67	3	-	2/8/9/11	-
1	MLY	A	135	1	-	1/8/9/11	-
4	MLY	D	67	4	-	2/8/9/11	-
2	MLY	B	135	2	-	4/8/9/11	-
4	MLY	D	135	4	-	2/8/9/11	-
3	MLY	C	135	3	-	4/8/9/11	-
1	MLZ	A	129	1	-	3/7/8/10	-
1	MLY	A	67	1	-	3/8/9/11	-
3	MLZ	C	129	3	-	2/7/8/10	-
2	MLZ	B	67	2	-	1/7/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	67	MLZ	CB-CA	-2.82	1.49	1.53
1	A	129	MLZ	CD-CE	-2.77	1.40	1.51
1	A	129	MLZ	CB-CA	-2.71	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	MLY	CB-CA	2.62	1.57	1.53
3	C	135	MLY	CB-CA	2.49	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	67	MLY	CD-CE-NZ	2.34	120.12	113.79

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	135	MLY	O-C-CA-CB
3	C	135	MLY	C-CA-CB-CG
4	D	67	MLY	O-C-CA-CB
2	B	135	MLY	CE-CD-CG-CB
3	C	129	MLZ	CG-CD-CE-NZ
1	A	129	MLZ	CG-CD-CE-NZ
3	C	135	MLY	CD-CE-NZ-CH2
1	A	67	MLY	CG-CD-CE-NZ
1	A	129	MLZ	CD-CE-NZ-CM
3	C	135	MLY	CD-CE-NZ-CH1
1	A	135	MLY	CG-CD-CE-NZ
4	D	135	MLY	CA-CB-CG-CD
3	C	67	MLY	CG-CD-CE-NZ
2	B	135	MLY	CD-CE-NZ-CH1
4	D	135	MLY	CE-CD-CG-CB
2	B	135	MLY	CG-CD-CE-NZ
3	C	67	MLY	CE-CD-CG-CB
1	A	67	MLY	CE-CD-CG-CB
3	C	135	MLY	CG-CD-CE-NZ
2	B	67	MLZ	CD-CE-NZ-CM
3	C	129	MLZ	CE-CD-CG-CB
4	D	67	MLY	CG-CD-CE-NZ
1	A	67	MLY	CA-CB-CG-CD
1	A	129	MLZ	CE-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	135	MLY	1	0
2	B	135	MLY	3	0
4	D	135	MLY	1	0
3	C	135	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
13	PG4	C	145	-	12,12,12	0.59	0	11,11,11	0.34	0
9	2PE	D	146	-	27,27,27	0.61	0	26,26,26	0.43	0
9	2PE	A	148	-	27,27,27	0.65	0	26,26,26	0.48	0
11	PE8	B	148	-	24,24,24	0.70	0	23,23,23	0.54	0
7	PEG	A	146	-	6,6,6	0.46	0	5,5,5	0.23	0
5	SO4	A	143	-	4,4,4	0.35	0	6,6,6	0.34	0
8	PGE	A	147	-	9,9,9	0.66	0	8,8,8	0.42	0
7	PEG	B	145	-	6,6,6	0.47	0	5,5,5	0.41	0
10	GOL	D	147	-	5,5,5	0.27	0	5,5,5	0.31	0
8	PGE	C	147	-	9,9,9	0.61	0	8,8,8	0.52	0
13	PG4	D	144	-	12,12,12	0.70	0	11,11,11	0.55	0
10	GOL	A	150	-	5,5,5	0.33	0	5,5,5	0.15	0
11	PE8	C	148	-	24,24,24	0.75	0	23,23,23	0.72	1 (4%)
5	SO4	A	144	-	4,4,4	0.14	0	6,6,6	0.13	0
7	PEG	A	149	-	6,6,6	0.40	0	5,5,5	0.40	0
7	PEG	D	145	-	6,6,6	0.50	0	5,5,5	0.23	0
10	GOL	C	149	-	5,5,5	0.31	0	5,5,5	0.36	0
7	PEG	C	146	-	6,6,6	0.49	0	5,5,5	0.19	0
5	SO4	C	143	-	4,4,4	0.20	0	6,6,6	0.23	0
10	GOL	B	149	-	5,5,5	0.50	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PEG	B	146	-	6,6,6	0.40	0	5,5,5	0.45	0
7	PEG	B	144	-	6,6,6	0.54	0	5,5,5	0.23	0
8	PGE	B	147	-	9,9,9	0.59	0	8,8,8	0.67	0
12	1PE	B	150	-	15,15,15	0.60	0	14,14,14	0.39	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
13	PG4	C	145	-	-	2/10/10/10	-
9	2PE	D	146	-	-	13/25/25/25	-
9	2PE	A	148	-	-	13/25/25/25	-
11	PE8	B	148	-	-	12/22/22/22	-
7	PEG	A	146	-	-	3/4/4/4	-
8	PGE	A	147	-	-	3/7/7/7	-
7	PEG	B	145	-	-	3/4/4/4	-
10	GOL	D	147	-	-	0/4/4/4	-
8	PGE	C	147	-	-	1/7/7/7	-
13	PG4	D	144	-	-	6/10/10/10	-
10	GOL	A	150	-	-	4/4/4/4	-
11	PE8	C	148	-	-	13/22/22/22	-
7	PEG	A	149	-	-	3/4/4/4	-
7	PEG	D	145	-	-	2/4/4/4	-
10	GOL	C	149	-	-	0/4/4/4	-
7	PEG	C	146	-	-	2/4/4/4	-
10	GOL	B	149	-	-	4/4/4/4	-
7	PEG	B	146	-	-	2/4/4/4	-
7	PEG	B	144	-	-	2/4/4/4	-
8	PGE	B	147	-	-	4/7/7/7	-
12	1PE	B	150	-	-	8/13/13/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	148	PE8	O19-C18-C17	2.18	120.21	110.39

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	150	GOL	C1-C2-C3-O3
10	B	149	GOL	C1-C2-C3-O3
9	D	146	2PE	O25-C26-C27-O28
9	D	146	2PE	O19-C20-C21-O22
11	B	148	PE8	O4-C5-C6-O7
11	C	148	PE8	O7-C8-C9-O10
9	A	148	2PE	O13-C14-C15-O16
12	B	150	1PE	OH6-C15-C25-OH5
8	A	147	PGE	O3-C5-C6-O4
9	A	148	2PE	O19-C20-C21-O22
9	A	148	2PE	O7-C8-C9-O10
8	A	147	PGE	O2-C3-C4-O3
9	D	146	2PE	O7-C8-C9-O10
7	D	145	PEG	O1-C1-C2-O2
7	D	145	PEG	O2-C3-C4-O4
8	B	147	PGE	O3-C5-C6-O4
11	C	148	PE8	O22-C23-C24-O25
9	D	146	2PE	O13-C14-C15-O16
9	A	148	2PE	O22-C23-C24-O25
7	A	146	PEG	O1-C1-C2-O2
7	A	149	PEG	O1-C1-C2-O2
7	B	144	PEG	O2-C3-C4-O4
11	B	148	PE8	O1-C2-C3-O4
11	B	148	PE8	O22-C23-C24-O25
12	B	150	1PE	OH2-C12-C22-OH3
11	C	148	PE8	O4-C5-C6-O7
11	B	148	PE8	O16-C17-C18-O19
13	D	144	PG4	O2-C3-C4-O3
7	B	145	PEG	O2-C3-C4-O4
13	D	144	PG4	O1-C1-C2-O2
11	B	148	PE8	O13-C14-C15-O16
10	A	150	GOL	O2-C2-C3-O3
10	B	149	GOL	O2-C2-C3-O3
9	A	148	2PE	O10-C11-C12-O13
8	B	147	PGE	O1-C1-C2-O2
12	B	150	1PE	OH4-C13-C23-OH3
8	B	147	PGE	O2-C3-C4-O3
7	A	146	PEG	O2-C3-C4-O4
7	B	144	PEG	O1-C1-C2-O2
7	B	146	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
7	C	146	PEG	O2-C3-C4-O4
11	C	148	PE8	O1-C2-C3-O4
13	C	145	PG4	O1-C1-C2-O2
13	D	144	PG4	O3-C5-C6-O4
10	B	149	GOL	O1-C1-C2-O2
9	A	148	2PE	O4-C5-C6-O7
9	D	146	2PE	O4-C5-C6-O7
8	C	147	PGE	C6-C5-O3-C4
12	B	150	1PE	OH7-C16-C26-OH6
9	D	146	2PE	C21-C20-O19-C18
9	A	148	2PE	C27-C26-O25-C24
11	B	148	PE8	C20-C21-O22-C23
13	D	144	PG4	C3-C4-O3-C5
9	D	146	2PE	C18-C17-O16-C15
11	C	148	PE8	C20-C21-O22-C23
11	C	148	PE8	C24-C23-O22-C21
9	A	148	2PE	C18-C17-O16-C15
11	C	148	PE8	C18-C17-O16-C15
9	A	148	2PE	C21-C20-O19-C18
12	B	150	1PE	C14-C24-OH4-C13
7	B	146	PEG	C4-C3-O2-C2
9	D	146	2PE	C14-C15-O16-C17
8	B	147	PGE	C4-C3-O2-C2
9	A	148	2PE	C14-C15-O16-C17
13	D	144	PG4	C5-C6-O4-C7
7	A	149	PEG	C4-C3-O2-C2
7	B	145	PEG	C1-C2-O2-C3
9	D	146	2PE	C6-C5-O4-C3
10	A	150	GOL	O1-C1-C2-O2
9	A	148	2PE	C24-C23-O22-C21
10	A	150	GOL	O1-C1-C2-C3
13	D	144	PG4	C4-C3-O2-C2
7	A	146	PEG	C1-C2-O2-C3
11	C	148	PE8	C11-C12-O13-C14
11	B	148	PE8	C17-C18-O19-C20
11	C	148	PE8	O16-C17-C18-O19
7	A	149	PEG	O2-C3-C4-O4
12	B	150	1PE	OH5-C14-C24-OH4
9	A	148	2PE	O1-C2-C3-O4
9	D	146	2PE	C2-C3-O4-C5
11	C	148	PE8	C9-C8-O7-C6
11	B	148	PE8	C9-C8-O7-C6

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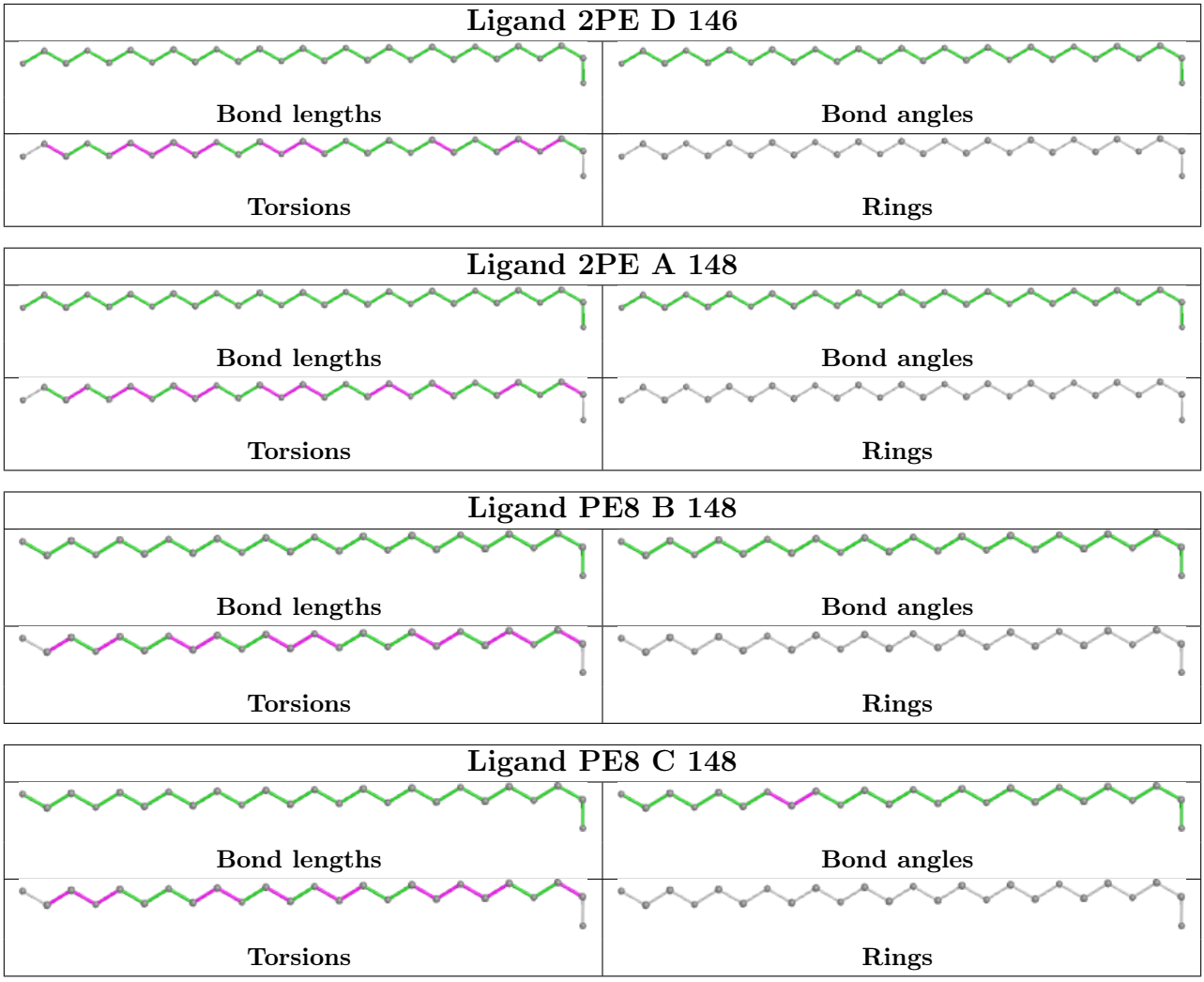
Mol	Chain	Res	Type	Atoms
11	B	148	PE8	C11-C12-O13-C14
11	B	148	PE8	O7-C8-C9-O10
11	B	148	PE8	C6-C5-O4-C3
9	A	148	2PE	C12-C11-O10-C9
11	C	148	PE8	C5-C6-O7-C8
11	C	148	PE8	O13-C14-C15-O16
9	D	146	2PE	C24-C23-O22-C21
7	C	146	PEG	O1-C1-C2-O2
7	B	145	PEG	C4-C3-O2-C2
9	D	146	2PE	O22-C23-C24-O25
10	B	149	GOL	O1-C1-C2-C3
8	A	147	PGE	C3-C4-O3-C5
11	C	148	PE8	O10-C11-C12-O13
12	B	150	1PE	C25-C15-OH6-C26
11	B	148	PE8	C15-C14-O13-C12
12	B	150	1PE	C24-C14-OH5-C25
9	D	146	2PE	C20-C21-O22-C23
13	C	145	PG4	C1-C2-O2-C3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	146	2PE	1	0
9	A	148	2PE	1	0
11	B	148	PE8	2	0
11	C	148	PE8	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

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	128/143 (89%)	-0.09	1 (0%) 86 85	26, 37, 55, 79	0
2	B	129/143 (90%)	-0.14	0 100 100	26, 37, 55, 79	0
3	C	127/143 (88%)	-0.10	0 100 100	25, 37, 53, 77	0
4	D	129/143 (90%)	-0.10	1 (0%) 86 85	26, 37, 55, 79	0
All	All	513/572 (89%)	-0.11	2 (0%) 92 93	25, 37, 55, 79	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	GLY	5.1
4	D	134	GLY	2.3

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

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
4	MLY	D	135	11/12	0.65	0.25	72,79,82,82	0
3	MLY	C	135	11/12	0.69	0.28	73,77,79,79	0
1	MLY	A	135	11/12	0.71	0.31	74,80,82,82	0
2	MLY	B	135	11/12	0.71	0.22	74,78,81,81	0
1	MLY	A	67	11/12	0.96	0.22	37,38,69,69	0
3	MLY	C	67	11/12	0.97	0.18	36,38,62,64	0
3	MLZ	C	114	10/11	0.98	0.21	35,37,47,50	0
3	MLZ	C	129	10/11	0.98	0.20	33,34,59,61	0
1	MLZ	A	129	10/11	0.98	0.16	33,34,62,62	0
4	MLY	D	67	11/12	0.98	0.24	38,39,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLZ	B	67	10/11	0.98	0.22	38,38,60,60	0

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
7	PEG	A	149	7/7	0.65	0.24	105,107,108,109	0
9	2PE	A	148	28/28	0.78	0.27	102,107,116,116	0
8	PGE	C	147	10/10	0.79	0.18	88,89,92,92	0
7	PEG	B	144	7/7	0.79	0.23	127,128,129,130	0
13	PG4	D	144	13/13	0.79	0.27	110,113,116,116	0
8	PGE	B	147	10/10	0.80	0.16	89,96,100,100	0
11	PE8	B	148	25/25	0.81	0.22	93,100,107,108	0
7	PEG	D	145	7/7	0.81	0.22	110,111,111,112	0
9	2PE	D	146	28/28	0.82	0.24	99,105,116,117	0
13	PG4	C	145	13/13	0.84	0.27	110,114,118,118	0
11	PE8	C	148	25/25	0.84	0.23	97,104,111,112	0
12	1PE	B	150	16/16	0.85	0.22	108,111,116,116	0
8	PGE	A	147	10/10	0.87	0.14	84,85,87,88	0
10	GOL	D	147	6/6	0.89	0.15	82,86,87,88	0
10	GOL	C	149	6/6	0.89	0.20	77,78,79,79	0
10	GOL	B	149	6/6	0.90	0.17	73,76,80,82	0
10	GOL	A	150	6/6	0.91	0.22	77,79,80,80	0
7	PEG	C	146	7/7	0.92	0.19	76,77,79,80	0
7	PEG	A	146	7/7	0.92	0.19	77,78,81,82	0
5	SO4	A	144	5/5	0.93	0.27	125,125,125,126	0
7	PEG	B	145	7/7	0.93	0.15	76,76,78,78	0
7	PEG	B	146	7/7	0.94	0.15	80,81,84,85	0
6	CL	B	143	1/1	0.98	0.11	54,54,54,54	0
6	CL	C	144	1/1	0.98	0.07	55,55,55,55	0
6	CL	D	143	1/1	0.98	0.08	54,54,54,54	0
5	SO4	A	143	5/5	0.99	0.14	55,57,57,58	0
5	SO4	C	143	5/5	0.99	0.15	51,52,53,53	5

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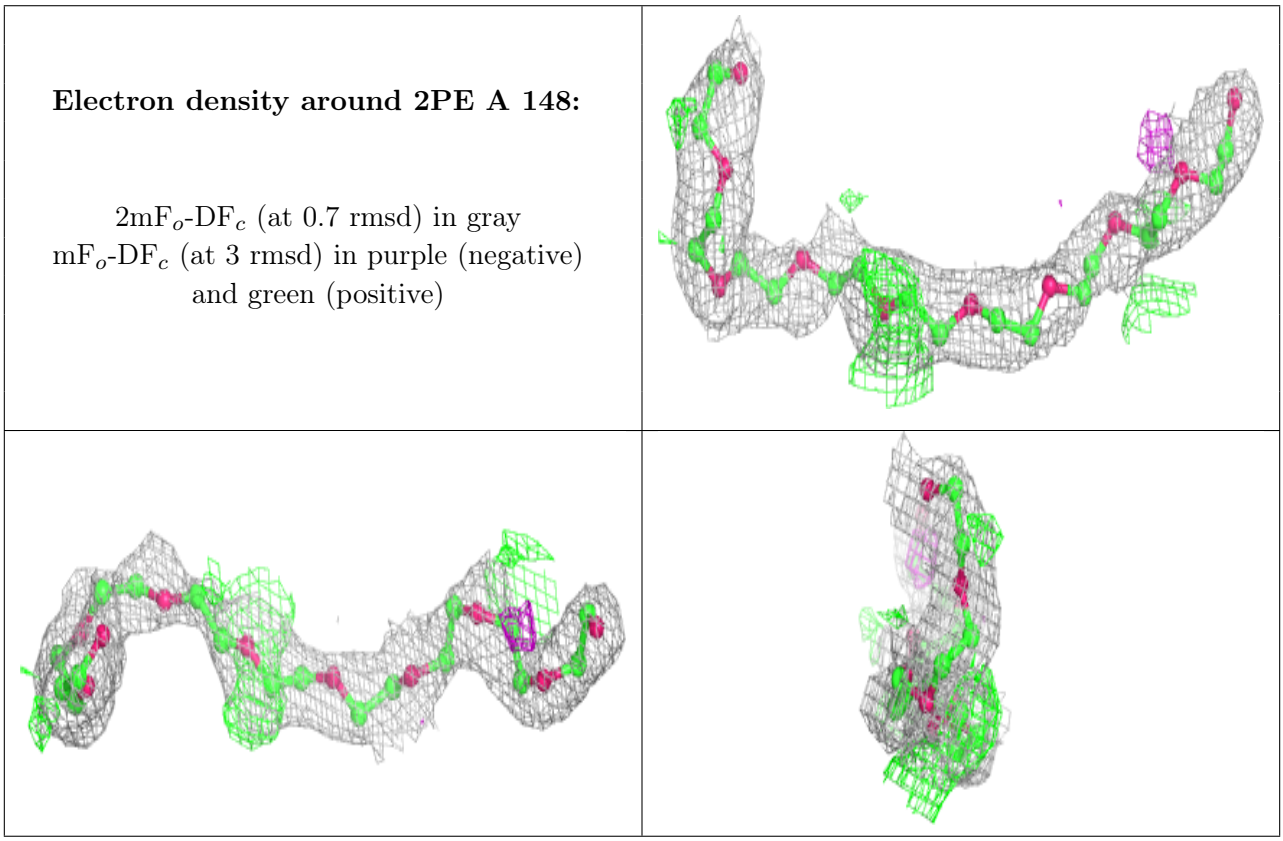
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	A	145	1/1	0.99	0.12	54,54,54,54	0

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.

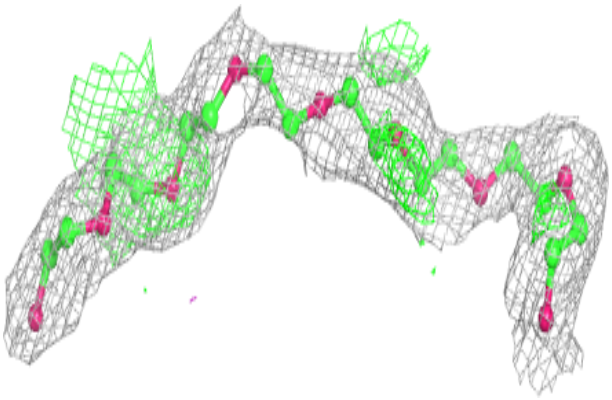
Electron density around 2PE A 148:

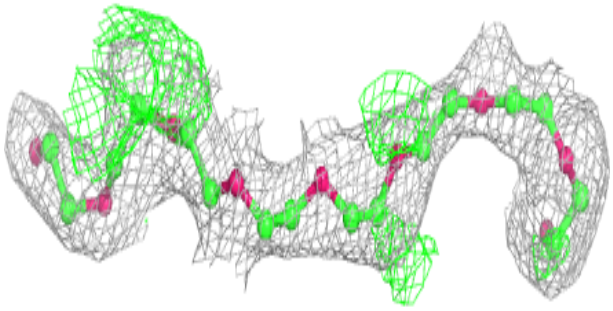
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

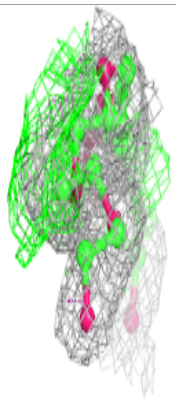


Electron density around PE8 B 148:

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

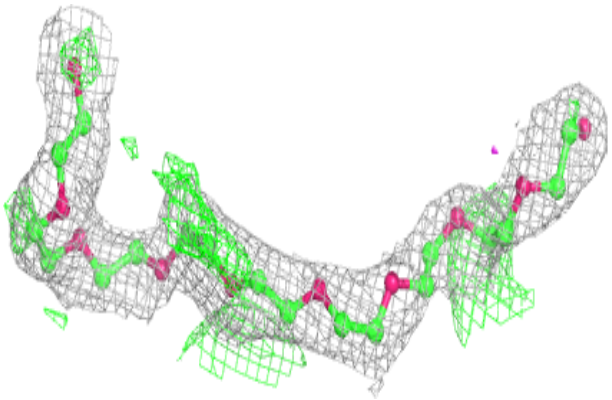


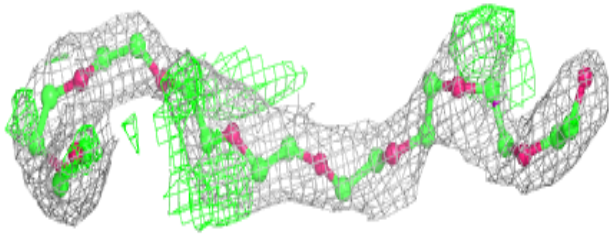


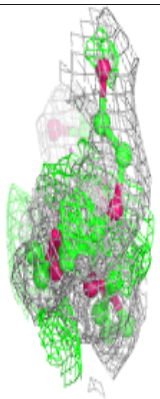


Electron density around 2PE D 146:

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

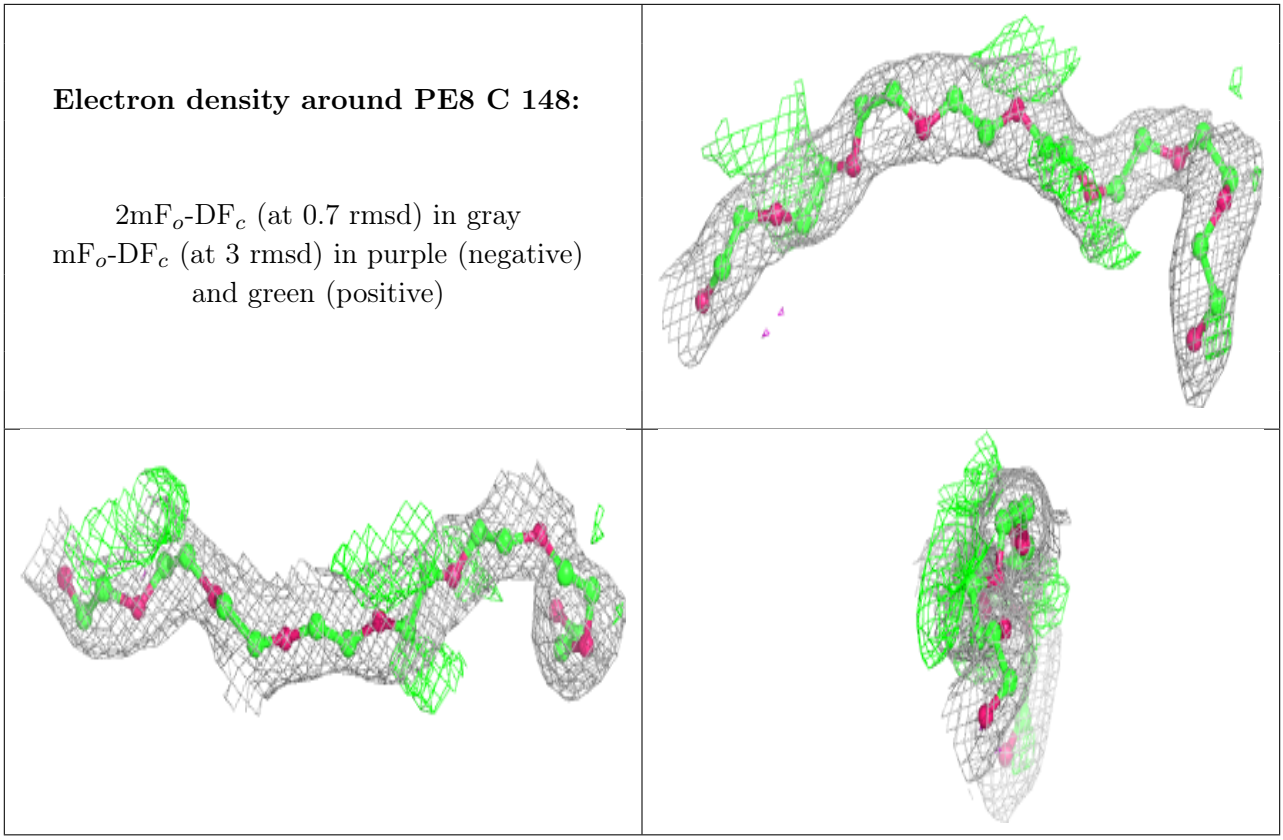






Electron density around PE8 C 148:

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



6.5 Other polymers (i)

There are no such residues in this entry.