Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2024 – 11:56 pm GMT

PDB ID	:	6H30
Title	:	The crystal structure of SBD1-SBD2 tandem of GlnPQ transporter
Authors	:	Schuurman-Wolters, G.K.; Guskov, A.; Poolman, B.
Deposited on	:	2018-07-17
Resolution	:	2.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

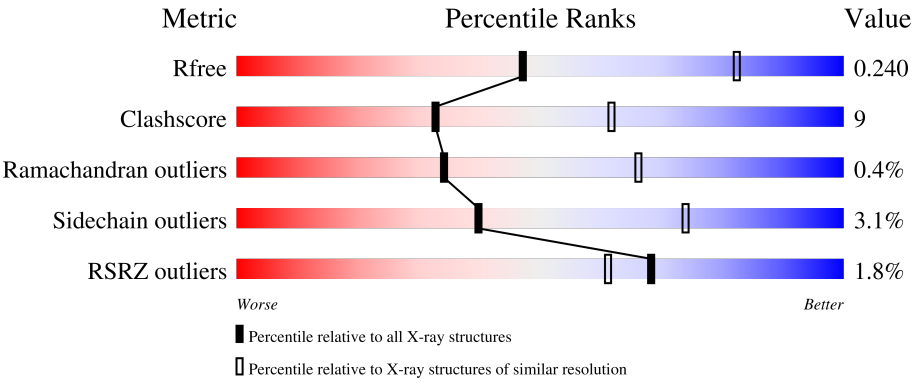
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

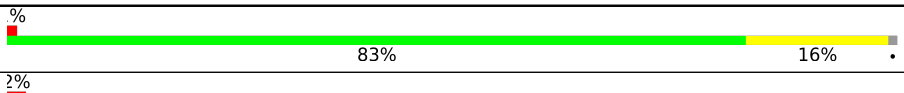
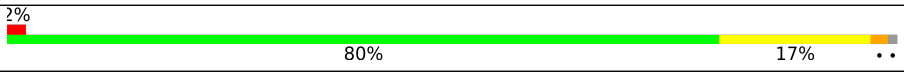
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	460	
1	B	460	

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
2	PEG	A	513	-	-	X	-
4	PG4	A	531	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7710 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.

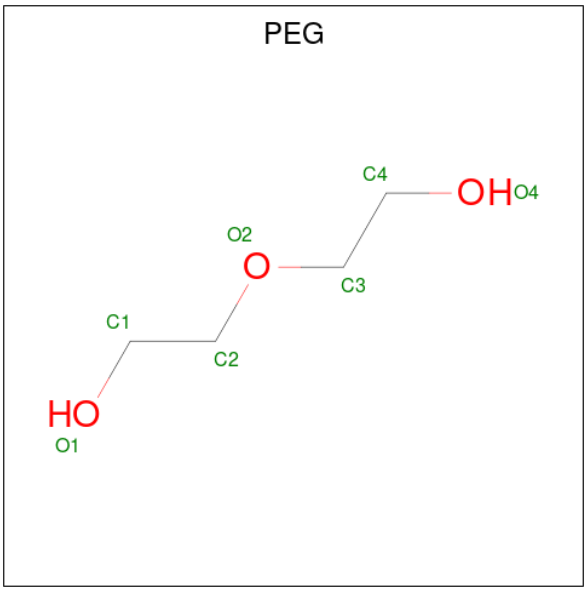
- Molecule 1 is a protein called Glutamine ABC transporter permease and substrate binding protein protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	3	0
			3533	2244	572	702	15			
1	B	454	Total	C	N	O	S	0	0	0
			3498	2222	567	694	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP Q9CES5
A	26	MET	-	expression tag	UNP Q9CES5
B	25	GLY	-	expression tag	UNP Q9CES5
B	26	MET	-	expression tag	UNP Q9CES5

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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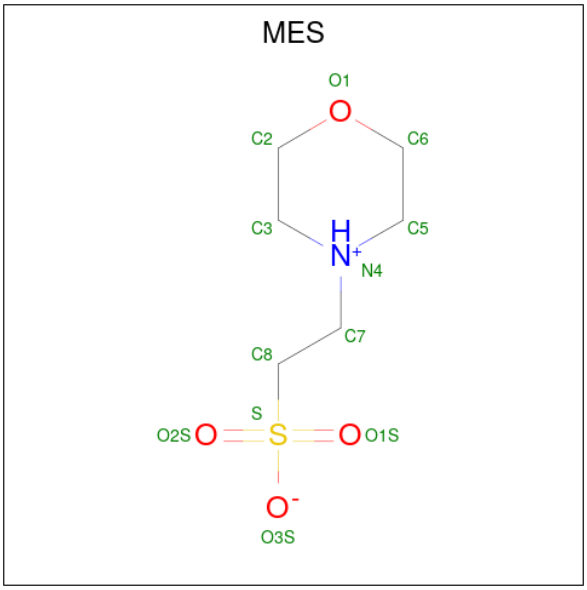
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 12 6 1 4 1	0	0
3	A	1	Total C N O S 12 6 1 4 1	0	0
3	B	1	Total C N O S 12 6 1 4 1	0	0

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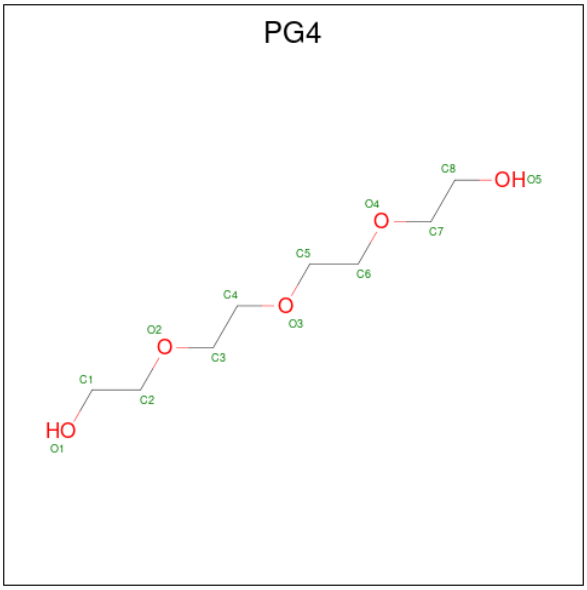
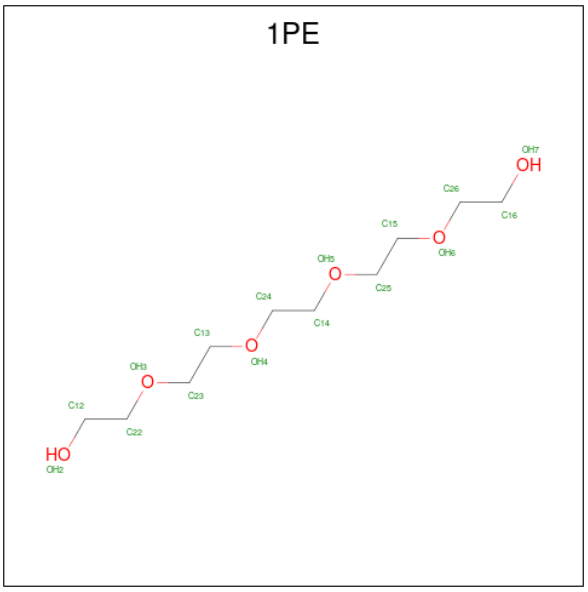
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O S 12 6 1 4 1	0	0
3	B	1	Total C N O S 12 6 1 4 1	0	0

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



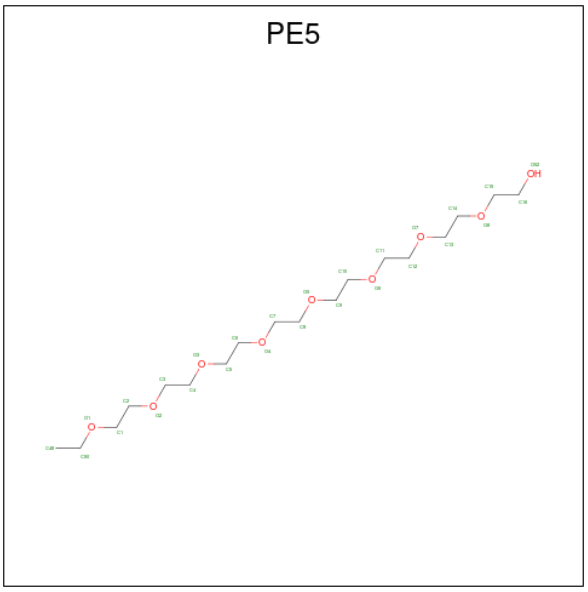
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



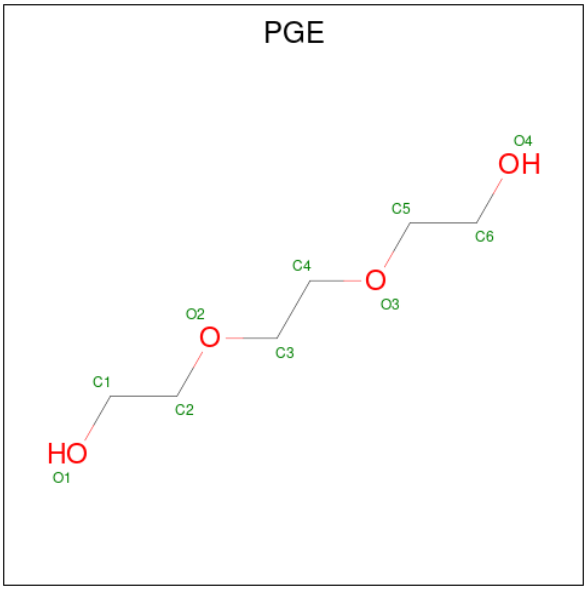
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 16 10 6	0	0

- Molecule 6 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: $C_{18}H_{38}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 27 18 9	0	0
6	A	1	Total C O 27 18 9	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

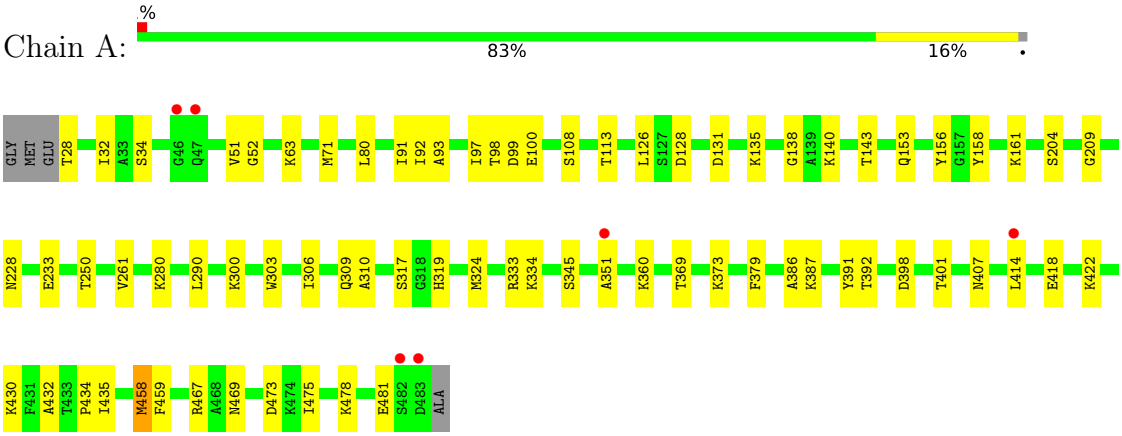
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	151	Total O 151 151	0	0
8	B	83	Total O 83 83	0	0

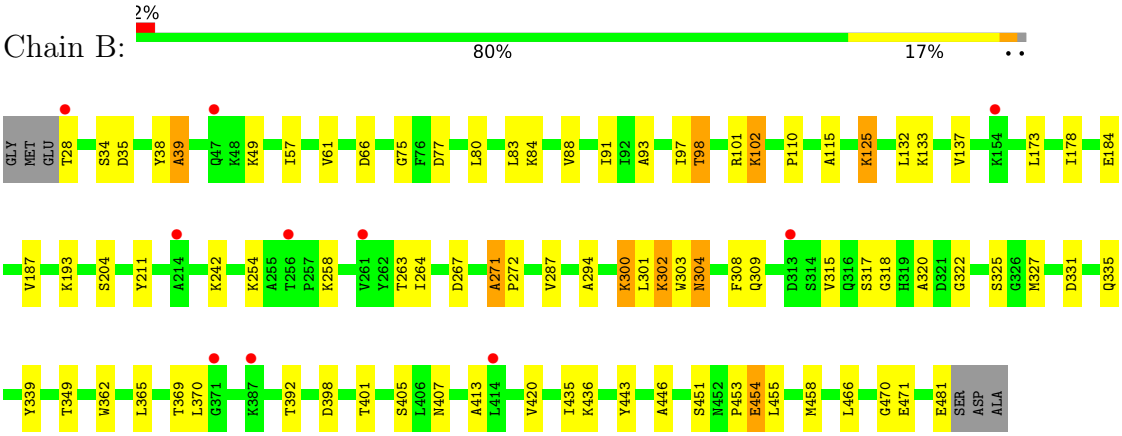
3 Residue-property plots (i)

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: Glutamine ABC transporter permease and substrate binding protein protein



• Molecule 1: Glutamine ABC transporter permease and substrate binding protein protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	93.56Å 187.03Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.80 19.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.80) 100.0 (19.97-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.79Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.164 , 0.240 0.164 , 0.240	Depositor DCC
R_{free} test set	1490 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.8	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	0.95	EDS
Total number of atoms	7710	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: PE5, PEG, 1PE, PG4, MES, PGE

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	0.45	0/3612	0.60	0/4875
1	B	0.41	0/3570	0.60	1/4818 (0.0%)
All	All	0.43	0/7182	0.60	1/9693 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	451	SER	C-N-CA	-6.65	105.07	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	38	TYR	Peptide

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	3533	0	3456	62	0
1	B	3498	0	3424	59	0
2	A	154	0	220	16	0
2	B	56	0	80	3	0
3	A	24	0	26	1	0
3	B	36	0	39	1	0
4	A	52	0	72	7	0
4	B	13	0	18	0	0
5	A	16	0	22	3	0
6	A	54	0	76	19	0
7	A	10	0	14	5	0
7	B	30	0	42	1	0
8	A	151	0	0	8	0
8	B	83	0	0	4	0
All	All	7710	0	7489	130	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 9.

All (130) 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:B:98:THR:HG22	1:B:101:ARG:H	1.33	0.92
6:A:530:PE5:H101	1:B:242:LYS:HZ2	1.36	0.88
1:A:126:LEU:HD22	1:A:131:ASP:HB3	1.59	0.83
1:B:88:VAL:O	8:B:601:HOH:O	2.00	0.78
1:A:333:ARG:HH21	7:A:532:PGE:H52	1.51	0.74
1:B:300:LYS:HD3	1:B:301:LEU:H	1.55	0.72
1:B:258:LYS:HE3	1:B:454:GLU:HG2	1.74	0.70
1:A:153:GLN:NE2	1:A:158:TYR:O	2.23	0.69
1:A:309:GLN:H	2:A:513:PEG:H32	1.58	0.69
1:A:209:GLY:HA2	6:A:529:PE5:H111	1.74	0.68
1:A:333:ARG:HG2	7:A:532:PGE:H3	1.75	0.66
1:A:317:SER:HG	1:A:319[B]:HIS:HD1	1.41	0.66
1:B:83:LEU:HD22	1:B:91:ILE:HG13	1.79	0.65
1:A:63:LYS:O	1:B:436:LYS:HB2	1.98	0.64
6:A:530:PE5:H152	1:B:242:LYS:HZ3	1.61	0.64
1:B:300:LYS:HA	1:B:300:LYS:HE2	1.81	0.63
1:A:99:ASP:HB2	6:A:529:PE5:H162	1.81	0.62
1:B:97:ILE:HG21	2:B:502:PEG:H12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PHE:CZ	3:B:510:MES:H81	2.35	0.61
1:B:254:LYS:NZ	8:B:605:HOH:O	2.35	0.60
1:B:369:THR:HG22	1:B:392:THR:HB	1.85	0.59
1:A:99:ASP:H	6:A:529:PE5:H142	1.67	0.59
1:A:309:GLN:HB3	2:A:513:PEG:H11	1.85	0.58
1:A:434:PRO:HG2	1:A:435:ILE:HD12	1.85	0.58
1:A:334:LYS:HZ1	4:A:526:PG4:H52	1.69	0.58
6:A:530:PE5:H102	8:A:605:HOH:O	2.04	0.58
1:A:128:ASP:OD1	8:A:601:HOH:O	2.18	0.56
1:A:333:ARG:HE	7:A:532:PGE:H42	1.69	0.56
1:A:309:GLN:HB2	2:A:513:PEG:H32	1.86	0.56
1:B:264:ILE:HA	1:B:322:GLY:O	2.06	0.55
1:B:300:LYS:HD3	1:B:301:LEU:N	2.19	0.55
1:A:97:ILE:HG21	6:A:529:PE5:H502	1.87	0.55
1:B:317:SER:OG	1:B:318:GLY:N	2.38	0.55
1:A:398:ASP:OD2	1:A:401:THR:HG23	2.06	0.55
1:A:280:LYS:HD2	2:A:516:PEG:H21	1.89	0.55
1:B:303:TRP:O	1:B:304:ASN:HB2	2.06	0.55
1:A:469:ASN:O	1:B:193:LYS:NZ	2.40	0.54
1:B:35:ASP:HA	1:B:75:GLY:HA2	1.88	0.54
1:B:132:LEU:HD13	1:B:137:VAL:HG21	1.89	0.54
1:B:315:VAL:HA	1:B:320:ALA:HB3	1.90	0.53
1:A:306:ILE:HD12	1:A:310:ALA:HB1	1.90	0.53
1:A:369:THR:HG22	1:A:392:THR:HB	1.90	0.53
1:B:102:LYS:HE3	2:B:502:PEG:H31	1.91	0.53
1:B:125:LYS:H	1:B:125:LYS:HE2	1.74	0.53
1:A:300:LYS:HD3	2:A:517:PEG:H21	1.91	0.53
1:A:303:TRP:CD1	2:A:515:PEG:H12	2.45	0.52
1:B:339:TYR:CE1	1:B:446:ALA:HB2	2.45	0.51
1:A:261:VAL:HG23	1:A:300:LYS:HG2	1.93	0.51
1:B:466:LEU:HD22	1:B:471:GLU:HB2	1.93	0.51
6:A:530:PE5:H101	1:B:242:LYS:NZ	2.18	0.50
1:A:309:GLN:H	2:A:513:PEG:H22	1.76	0.50
1:B:80:LEU:HD23	1:B:91:ILE:HD12	1.94	0.50
1:A:310:ALA:H	2:A:513:PEG:H11	1.76	0.50
1:A:32:ILE:HG21	1:A:92:ILE:HG22	1.94	0.50
1:B:271:ALA:HB1	1:B:272:PRO:HD3	1.94	0.50
1:B:365:LEU:HD22	1:B:370:LEU:HD21	1.94	0.49
1:A:98:THR:HA	6:A:529:PE5:H142	1.95	0.49
1:A:345:SER:HB2	6:A:530:PE5:H41	1.95	0.49
1:B:184:GLU:HB2	1:B:187:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ARG:NH1	8:A:609:HOH:O	2.45	0.48
5:A:528:1PE:H221	5:A:528:1PE:H251	1.96	0.48
1:A:334:LYS:NZ	4:A:526:PG4:H72	2.30	0.47
1:A:473:ASP:HB3	1:B:242:LYS:HE3	1.96	0.47
1:A:113:THR:H	2:A:519:PEG:H22	1.79	0.47
1:A:98:THR:HB	6:A:529:PE5:H151	1.97	0.47
1:B:173:LEU:HA	1:B:178:ILE:HG13	1.96	0.47
1:B:370:LEU:HG	1:B:413:ALA:HB3	1.97	0.46
1:B:263:THR:HA	1:B:302:LYS:HG3	1.98	0.46
1:A:373:LYS:O	1:A:379:PHE:HB2	2.16	0.46
4:A:525:PG4:H82	4:A:525:PG4:H41	1.97	0.46
6:A:529:PE5:H21	6:A:529:PE5:H41	1.50	0.46
1:B:401:THR:O	1:B:405:SER:OG	2.21	0.46
6:A:530:PE5:H131	1:B:242:LYS:HD3	1.99	0.45
1:A:156:TYR:OH	5:A:528:1PE:H222	2.16	0.45
8:A:603:HOH:O	1:B:49:LYS:NZ	2.49	0.45
1:A:481[B]:GLU:HG2	6:A:530:PE5:H162	1.97	0.45
1:B:264:ILE:HD11	1:B:301:LEU:HD22	1.98	0.45
1:A:261:VAL:HG11	2:A:517:PEG:H32	1.97	0.45
4:A:525:PG4:H52	8:A:652:HOH:O	2.17	0.45
3:A:523:MES:H72	8:A:627:HOH:O	2.16	0.44
4:A:525:PG4:H32	8:A:652:HOH:O	2.17	0.44
1:A:80:LEU:HD23	1:A:91[B]:ILE:CD1	2.48	0.44
1:B:39:ALA:HB1	1:B:187:VAL:HG22	1.99	0.44
1:B:287:VAL:HA	1:B:303:TRP:CZ2	2.52	0.44
1:B:398:ASP:OD2	1:B:401:THR:HG23	2.18	0.44
1:A:71:MET:HB2	2:A:501:PEG:H31	1.99	0.44
1:A:467:ARG:HH22	6:A:530:PE5:H501	1.82	0.43
1:B:331:ASP:O	1:B:335:GLN:HG2	2.18	0.43
1:B:327:MET:O	1:B:443:TYR:HA	2.18	0.43
1:B:362:TRP:CD1	1:B:435:ILE:HD12	2.53	0.43
1:A:34:SER:HA	1:A:93:ALA:HB2	2.00	0.43
1:B:455:LEU:HD12	1:B:455:LEU:HA	1.92	0.43
1:A:138:GLY:HA2	1:A:161:LYS:O	2.19	0.43
1:A:432:ALA:HB1	8:A:706:HOH:O	2.18	0.43
1:A:351:ALA:HB3	1:A:414:LEU:HG	2.00	0.43
2:A:509:PEG:H21	1:B:470:GLY:HA3	1.99	0.43
1:B:98:THR:HG21	8:B:664:HOH:O	2.19	0.43
1:B:264:ILE:O	1:B:303:TRP:O	2.36	0.42
1:A:309:GLN:CB	2:A:513:PEG:H32	2.48	0.42
5:A:528:1PE:H251	5:A:528:1PE:H231	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ARG:NH2	6:A:530:PE5:H501	2.33	0.42
1:A:51:VAL:HG22	1:A:52:GLY:H	1.84	0.42
1:B:84:LYS:NZ	7:B:512:PGE:O3	2.52	0.42
1:B:57:ILE:O	1:B:61:VAL:HG23	2.20	0.42
1:B:110:PRO:HA	1:B:211:TYR:O	2.19	0.42
1:A:99:ASP:OD1	6:A:529:PE5:H72	2.18	0.42
1:A:386:ALA:HA	1:A:391:TYR:CZ	2.54	0.42
1:B:133:LYS:HE2	8:B:679:HOH:O	2.19	0.41
2:A:511:PEG:H32	2:A:511:PEG:H11	1.67	0.41
1:B:294:ALA:HB2	1:B:301:LEU:HD11	2.01	0.41
1:A:140:LYS:HB2	1:A:143:THR:HG21	2.02	0.41
1:A:475:ILE:O	1:A:478:LYS:HB3	2.21	0.41
1:B:34:SER:HA	1:B:93:ALA:HB2	2.01	0.41
2:B:505:PEG:H11	2:B:505:PEG:H31	1.90	0.41
1:A:290:LEU:HD22	1:A:324:MET:HB2	2.03	0.41
1:A:333:ARG:NE	7:A:532:PGE:H42	2.33	0.41
4:A:526:PG4:H52	4:A:526:PG4:H72	1.57	0.41
6:A:530:PE5:H131	1:B:242:LYS:NZ	2.36	0.41
1:A:418:GLU:HG2	1:A:422:LYS:HD2	2.02	0.41
1:B:267:ASP:H	1:B:325:SER:HB2	1.87	0.40
1:A:108:SER:HB2	1:A:228:ASN:OD1	2.21	0.40
1:A:360:LYS:HE2	1:B:66:ASP:OD2	2.21	0.40
1:A:458:MET:HG3	1:A:459:PHE:N	2.35	0.40
4:A:527:PG4:H41	4:A:527:PG4:H61	1.60	0.40
1:A:333:ARG:NH2	7:A:532:PGE:H52	2.27	0.40
6:A:529:PE5:H141	6:A:529:PE5:H122	1.63	0.40
1:B:115:ALA:O	1:B:184:GLU:HA	2.20	0.40
1:B:271:ALA:HB1	1:B:420:VAL:HG22	2.03	0.40
1:A:113:THR:N	2:A:519:PEG:H22	2.37	0.40
1:A:135:LYS:HD3	2:A:522:PEG:H42	2.03	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	457/460 (99%)	443 (97%)	14 (3%)	0	100 100
1	B	452/460 (98%)	429 (95%)	19 (4%)	4 (1%)	17 46
All	All	909/920 (99%)	872 (96%)	33 (4%)	4 (0%)	34 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ALA
1	B	271	ALA
1	B	453	PRO
1	B	304	ASN

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	376/375 (100%)	367 (98%)	9 (2%)	49 81
1	B	371/375 (99%)	357 (96%)	14 (4%)	33 67
All	All	747/750 (100%)	724 (97%)	23 (3%)	40 74

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	100	GLU
1	A	204	SER
1	A	233	GLU
1	A	250	THR
1	A	387	LYS
1	A	407	ASN
1	A	430	LYS
1	A	458	MET

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Mol	Chain	Res	Type
1	B	28	THR
1	B	77	ASP
1	B	98	THR
1	B	102	LYS
1	B	125	LYS
1	B	204	SER
1	B	300	LYS
1	B	302	LYS
1	B	309	GLN
1	B	349	THR
1	B	407	ASN
1	B	454	GLU
1	B	458	MET
1	B	481	GLU

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)

47 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PEG	A	503	-	6,6,6	0.50	0	5,5,5	0.22	0
2	PEG	A	509	-	6,6,6	0.49	0	5,5,5	0.32	0
2	PEG	A	514	-	6,6,6	0.49	0	5,5,5	0.23	0
2	PEG	B	501	-	6,6,6	0.49	0	5,5,5	0.28	0
2	PEG	B	503	-	6,6,6	0.51	0	5,5,5	0.27	0
2	PEG	A	518	-	6,6,6	0.50	0	5,5,5	0.36	0
2	PEG	A	505	-	6,6,6	0.49	0	5,5,5	0.34	0
2	PEG	A	515	-	6,6,6	0.47	0	5,5,5	0.41	0
2	PEG	A	517	-	6,6,6	0.54	0	5,5,5	0.62	0
2	PEG	A	507	-	6,6,6	0.52	0	5,5,5	0.20	0
7	PGE	B	512	-	9,9,9	0.57	0	8,8,8	0.45	0
2	PEG	B	505	-	6,6,6	0.49	0	5,5,5	0.27	0
7	PGE	A	532	-	9,9,9	0.42	0	8,8,8	0.34	0
4	PG4	A	527	-	12,12,12	0.57	0	11,11,11	0.39	0
7	PGE	B	514	-	9,9,9	0.55	0	8,8,8	0.67	0
2	PEG	B	507	-	6,6,6	0.51	0	5,5,5	0.22	0
3	MES	B	511	-	12,12,12	2.27	1 (8%)	14,16,16	1.22	3 (21%)
2	PEG	A	521	-	6,6,6	0.52	0	5,5,5	0.40	0
2	PEG	A	506	-	6,6,6	0.48	0	5,5,5	0.25	0
6	PE5	A	530	-	26,26,26	0.57	0	25,25,25	0.39	0
2	PEG	B	502	-	6,6,6	0.49	0	5,5,5	0.26	0
2	PEG	B	506	-	6,6,6	0.52	0	5,5,5	0.28	0
2	PEG	A	513	-	6,6,6	0.56	0	5,5,5	0.32	0
2	PEG	B	508	-	6,6,6	0.47	0	5,5,5	0.33	0
6	PE5	A	529	-	26,26,26	0.58	0	25,25,25	0.35	0
2	PEG	A	501	-	6,6,6	0.52	0	5,5,5	0.51	0
2	PEG	A	522	-	6,6,6	0.53	0	5,5,5	0.30	0
3	MES	A	523	-	12,12,12	2.28	1 (8%)	14,16,16	1.24	3 (21%)
3	MES	B	509	-	12,12,12	2.25	1 (8%)	14,16,16	1.22	3 (21%)
4	PG4	A	525	-	12,12,12	0.54	0	11,11,11	0.42	0
2	PEG	A	502	-	6,6,6	0.52	0	5,5,5	0.41	0
4	PG4	A	531	-	12,12,12	0.54	0	11,11,11	0.24	0
3	MES	A	524	-	12,12,12	2.28	1 (8%)	14,16,16	1.23	3 (21%)
2	PEG	A	516	-	6,6,6	0.49	0	5,5,5	0.34	0
2	PEG	A	520	-	6,6,6	0.50	0	5,5,5	0.53	0
4	PG4	B	513	-	12,12,12	0.54	0	11,11,11	0.37	0
5	1PE	A	528	-	15,15,15	0.63	0	14,14,14	0.84	0
2	PEG	A	511	-	6,6,6	0.49	0	5,5,5	0.36	0
3	MES	B	510	-	12,12,12	2.28	1 (8%)	14,16,16	1.22	3 (21%)
2	PEG	A	508	-	6,6,6	0.48	0	5,5,5	0.29	0
7	PGE	B	515	-	9,9,9	0.37	0	8,8,8	0.35	0
2	PEG	A	504	-	6,6,6	0.52	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PEG	A	510	-	6,6,6	0.49	0	5,5,5	0.36	0
4	PG4	A	526	-	12,12,12	0.54	0	11,11,11	0.52	0
2	PEG	A	519	-	6,6,6	0.53	0	5,5,5	0.35	0
2	PEG	B	504	-	6,6,6	0.46	0	5,5,5	0.33	0
2	PEG	A	512	-	6,6,6	0.53	0	5,5,5	0.22	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
2	PEG	A	503	-	-	3/4/4/4	-
2	PEG	A	509	-	-	2/4/4/4	-
2	PEG	A	514	-	-	3/4/4/4	-
2	PEG	B	501	-	-	4/4/4/4	-
2	PEG	B	503	-	-	1/4/4/4	-
2	PEG	A	518	-	-	3/4/4/4	-
2	PEG	A	505	-	-	2/4/4/4	-
2	PEG	A	515	-	-	3/4/4/4	-
2	PEG	A	517	-	-	3/4/4/4	-
2	PEG	A	507	-	-	4/4/4/4	-
7	PGE	B	512	-	-	2/7/7/7	-
2	PEG	B	505	-	-	2/4/4/4	-
7	PGE	A	532	-	-	3/7/7/7	-
4	PG4	A	527	-	-	5/10/10/10	-
7	PGE	B	514	-	-	3/7/7/7	-
2	PEG	B	507	-	-	3/4/4/4	-
3	MES	B	511	-	-	5/6/14/14	0/1/1/1
2	PEG	A	521	-	-	3/4/4/4	-
2	PEG	A	506	-	-	2/4/4/4	-
6	PE5	A	530	-	-	17/24/24/24	-
2	PEG	B	502	-	-	3/4/4/4	-
2	PEG	B	506	-	-	2/4/4/4	-
2	PEG	A	513	-	-	2/4/4/4	-
2	PEG	B	508	-	-	2/4/4/4	-
6	PE5	A	529	-	-	15/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	501	-	-	1/4/4/4	-
2	PEG	A	522	-	-	3/4/4/4	-
3	MES	A	523	-	-	3/6/14/14	0/1/1/1
3	MES	B	509	-	-	2/6/14/14	0/1/1/1
4	PG4	A	525	-	-	9/10/10/10	-
2	PEG	A	502	-	-	2/4/4/4	-
4	PG4	A	531	-	-	7/10/10/10	-
3	MES	A	524	-	-	2/6/14/14	0/1/1/1
2	PEG	A	516	-	-	3/4/4/4	-
2	PEG	A	520	-	-	2/4/4/4	-
4	PG4	B	513	-	-	5/10/10/10	-
5	1PE	A	528	-	-	10/13/13/13	-
2	PEG	A	511	-	-	3/4/4/4	-
3	MES	B	510	-	-	3/6/14/14	0/1/1/1
2	PEG	A	508	-	-	3/4/4/4	-
7	PGE	B	515	-	-	2/7/7/7	-
2	PEG	A	504	-	-	3/4/4/4	-
2	PEG	A	510	-	-	2/4/4/4	-
4	PG4	A	526	-	-	5/10/10/10	-
2	PEG	A	519	-	-	2/4/4/4	-
2	PEG	B	504	-	-	2/4/4/4	-
2	PEG	A	512	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	523	MES	C8-S	-7.67	1.66	1.77
3	A	524	MES	C8-S	-7.66	1.66	1.77
3	B	510	MES	C8-S	-7.65	1.66	1.77
3	B	511	MES	C8-S	-7.62	1.66	1.77
3	B	509	MES	C8-S	-7.57	1.66	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	523	MES	O3S-S-C8	2.31	109.50	105.77
3	B	509	MES	O3S-S-C8	2.30	109.49	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	510	MES	O3S-S-C8	2.30	109.48	105.77
3	B	511	MES	O3S-S-C8	2.29	109.47	105.77
3	A	524	MES	O3S-S-C8	2.27	109.43	105.77
3	A	523	MES	O1S-S-C8	2.17	109.53	106.92
3	A	524	MES	O1S-S-C8	2.17	109.53	106.92
3	B	510	MES	O2S-S-C8	2.16	109.51	106.92
3	A	523	MES	O2S-S-C8	2.15	109.51	106.92
3	A	524	MES	O2S-S-C8	2.15	109.51	106.92
3	B	511	MES	O2S-S-C8	2.14	109.49	106.92
3	B	511	MES	O1S-S-C8	2.11	109.46	106.92
3	B	509	MES	O2S-S-C8	2.11	109.45	106.92
3	B	509	MES	O1S-S-C8	2.10	109.45	106.92
3	B	510	MES	O1S-S-C8	2.10	109.44	106.92

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	523	MES	C7-C8-S-O2S
3	A	523	MES	C7-C8-S-O3S
3	A	524	MES	C7-C8-S-O1S
3	B	509	MES	C8-C7-N4-C3
3	B	510	MES	N4-C7-C8-S
3	B	511	MES	C7-C8-S-O1S
3	B	511	MES	C7-C8-S-O3S
7	A	532	PGE	C1-C2-O2-C3
4	A	526	PG4	C5-C6-O4-C7
5	A	528	1PE	C14-C24-OH4-C13
5	A	528	1PE	C24-C14-OH5-C25
6	A	529	PE5	C4-C3-O2-C2
2	A	507	PEG	O2-C3-C4-O4
2	A	517	PEG	O2-C3-C4-O4
4	B	513	PG4	O1-C1-C2-O2
4	B	513	PG4	O2-C3-C4-O3
6	A	530	PE5	O3-C5-C6-O4
4	A	527	PG4	O2-C3-C4-O3
6	A	530	PE5	O7-C13-C14-O8
6	A	530	PE5	O2-C3-C4-O3
5	A	528	1PE	OH4-C13-C23-OH3
2	A	516	PEG	O2-C3-C4-O4
7	B	515	PGE	O1-C1-C2-O2
4	A	525	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	A	527	PG4	C6-C5-O3-C4
7	A	532	PGE	O2-C3-C4-O3
4	A	526	PG4	O3-C5-C6-O4
4	A	531	PG4	O3-C5-C6-O4
6	A	530	PE5	O4-C7-C8-O5
6	A	529	PE5	O4-C7-C8-O5
4	A	526	PG4	O2-C3-C4-O3
2	A	503	PEG	O1-C1-C2-O2
2	A	507	PEG	O1-C1-C2-O2
2	A	512	PEG	O2-C3-C4-O4
2	A	514	PEG	O2-C3-C4-O4
2	A	516	PEG	O1-C1-C2-O2
2	A	520	PEG	O2-C3-C4-O4
2	B	501	PEG	O1-C1-C2-O2
4	A	531	PG4	O4-C7-C8-O5
6	A	530	PE5	C7-C8-O5-C9
2	A	502	PEG	O2-C3-C4-O4
2	A	503	PEG	O2-C3-C4-O4
2	A	506	PEG	O2-C3-C4-O4
2	B	502	PEG	O1-C1-C2-O2
2	B	507	PEG	O2-C3-C4-O4
4	A	527	PG4	O1-C1-C2-O2
4	B	513	PG4	O4-C7-C8-O5
7	B	512	PGE	O1-C1-C2-O2
2	B	505	PEG	C1-C2-O2-C3
2	A	510	PEG	O1-C1-C2-O2
4	A	531	PG4	C6-C5-O3-C4
6	A	529	PE5	C14-C13-O7-C12
2	A	504	PEG	O1-C1-C2-O2
2	A	505	PEG	O1-C1-C2-O2
2	A	513	PEG	O1-C1-C2-O2
2	A	521	PEG	O1-C1-C2-O2
7	B	514	PGE	O1-C1-C2-O2
2	A	506	PEG	O1-C1-C2-O2
2	A	509	PEG	O1-C1-C2-O2
2	A	518	PEG	O2-C3-C4-O4
7	B	514	PGE	O2-C3-C4-O3
6	A	530	PE5	O1-C1-C2-O2
6	A	530	PE5	C6-C5-O3-C4
2	A	511	PEG	O1-C1-C2-O2
2	A	515	PEG	O2-C3-C4-O4
4	A	525	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
6	A	530	PE5	C48-C50-O1-C1
4	A	527	PG4	O3-C5-C6-O4
6	A	529	PE5	C8-C7-O4-C6
6	A	529	PE5	O1-C1-C2-O2
2	A	501	PEG	O1-C1-C2-O2
6	A	530	PE5	O6-C10-C9-O5
6	A	529	PE5	C48-C50-O1-C1
7	B	514	PGE	O3-C5-C6-O4
2	A	511	PEG	C1-C2-O2-C3
2	A	514	PEG	C4-C3-O2-C2
2	B	501	PEG	O2-C3-C4-O4
2	B	508	PEG	O2-C3-C4-O4
5	A	528	1PE	OH6-C15-C25-OH5
4	A	525	PG4	C3-C4-O3-C5
2	A	507	PEG	C4-C3-O2-C2
2	B	504	PEG	O1-C1-C2-O2
2	B	506	PEG	O1-C1-C2-O2
4	B	513	PG4	C5-C6-O4-C7
2	A	521	PEG	C1-C2-O2-C3
4	A	525	PG4	C5-C6-O4-C7
6	A	530	PE5	C9-C10-O6-C11
2	A	508	PEG	C4-C3-O2-C2
4	A	525	PG4	C1-C2-O2-C3
4	B	513	PG4	C1-C2-O2-C3
2	A	517	PEG	C1-C2-O2-C3
2	A	522	PEG	C4-C3-O2-C2
6	A	529	PE5	C6-C5-O3-C4
6	A	530	PE5	C10-C9-O5-C8
7	B	515	PGE	C1-C2-O2-C3
2	A	522	PEG	C1-C2-O2-C3
6	A	530	PE5	C3-C4-O3-C5
2	A	502	PEG	C4-C3-O2-C2
2	B	503	PEG	C4-C3-O2-C2
2	A	509	PEG	C1-C2-O2-C3
2	A	512	PEG	C1-C2-O2-C3
2	A	519	PEG	C4-C3-O2-C2
2	B	507	PEG	C1-C2-O2-C3
2	A	514	PEG	O1-C1-C2-O2
2	B	505	PEG	O1-C1-C2-O2
2	A	508	PEG	C1-C2-O2-C3
7	B	512	PGE	C1-C2-O2-C3
2	B	507	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
2	A	521	PEG	C4-C3-O2-C2
4	A	525	PG4	C6-C5-O3-C4
4	A	531	PG4	C5-C6-O4-C7
2	B	508	PEG	C4-C3-O2-C2
6	A	530	PE5	C8-C7-O4-C6
2	A	515	PEG	O1-C1-C2-O2
2	A	519	PEG	O2-C3-C4-O4
4	A	525	PG4	O2-C3-C4-O3
2	B	502	PEG	C1-C2-O2-C3
3	A	523	MES	C7-C8-S-O1S
3	A	524	MES	C7-C8-S-O2S
3	B	511	MES	C7-C8-S-O2S
6	A	530	PE5	C14-C13-O7-C12
2	B	501	PEG	C1-C2-O2-C3
5	A	528	1PE	C13-C23-OH3-C22
2	A	520	PEG	C1-C2-O2-C3
2	A	507	PEG	C1-C2-O2-C3
4	A	526	PG4	C8-C7-O4-C6
5	A	528	1PE	C25-C15-OH6-C26
2	A	511	PEG	O2-C3-C4-O4
2	B	506	PEG	O2-C3-C4-O4
5	A	528	1PE	C12-C22-OH3-C23
6	A	529	PE5	O6-C11-C12-O7
2	A	516	PEG	C1-C2-O2-C3
2	A	517	PEG	C4-C3-O2-C2
6	A	529	PE5	C3-C4-O3-C5
6	A	529	PE5	O7-C13-C14-O8
2	A	505	PEG	C1-C2-O2-C3
4	A	525	PG4	C4-C3-O2-C2
4	A	531	PG4	C4-C3-O2-C2
6	A	529	PE5	C10-C9-O5-C8
2	A	522	PEG	O1-C1-C2-O2
2	A	510	PEG	C1-C2-O2-C3
2	A	513	PEG	C1-C2-O2-C3
2	A	504	PEG	O2-C3-C4-O4
6	A	529	PE5	C1-C2-O2-C3
2	A	504	PEG	C4-C3-O2-C2
3	B	510	MES	C8-C7-N4-C5
3	B	511	MES	C8-C7-N4-C3
3	B	511	MES	C8-C7-N4-C5
5	A	528	1PE	OH5-C14-C24-OH4
6	A	529	PE5	C11-C12-O7-C13

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Mol	Chain	Res	Type	Atoms
6	A	530	PE5	C11-C12-O7-C13
4	A	527	PG4	C4-C3-O2-C2
4	A	531	PG4	C3-C4-O3-C5
5	A	528	1PE	C16-C26-OH6-C15
2	A	503	PEG	C1-C2-O2-C3
2	B	504	PEG	C4-C3-O2-C2
5	A	528	1PE	C23-C13-OH4-C24
7	A	532	PGE	O3-C5-C6-O4
2	A	515	PEG	C4-C3-O2-C2
2	A	518	PEG	C1-C2-O2-C3
6	A	529	PE5	C9-C10-O6-C11
3	B	509	MES	C7-C8-S-O3S
6	A	529	PE5	C16-C15-O8-C14
4	A	531	PG4	C1-C2-O2-C3
2	A	518	PEG	C4-C3-O2-C2
2	B	501	PEG	C4-C3-O2-C2
4	A	526	PG4	C4-C3-O2-C2
2	A	508	PEG	O1-C1-C2-O2
2	B	502	PEG	O2-C3-C4-O4
4	A	525	PG4	C8-C7-O4-C6
6	A	530	PE5	C12-C11-O6-C10
6	A	530	PE5	O6-C11-C12-O7
3	B	510	MES	C8-C7-N4-C3

There are no ring outliers.

21 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	509	PEG	1	0
2	A	515	PEG	1	0
2	A	517	PEG	2	0
7	B	512	PGE	1	0
2	B	505	PEG	1	0
7	A	532	PGE	5	0
4	A	527	PG4	1	0
6	A	530	PE5	10	0
2	B	502	PEG	2	0
2	A	513	PEG	6	0
6	A	529	PE5	9	0
2	A	501	PEG	1	0
2	A	522	PEG	1	0
3	A	523	MES	1	0

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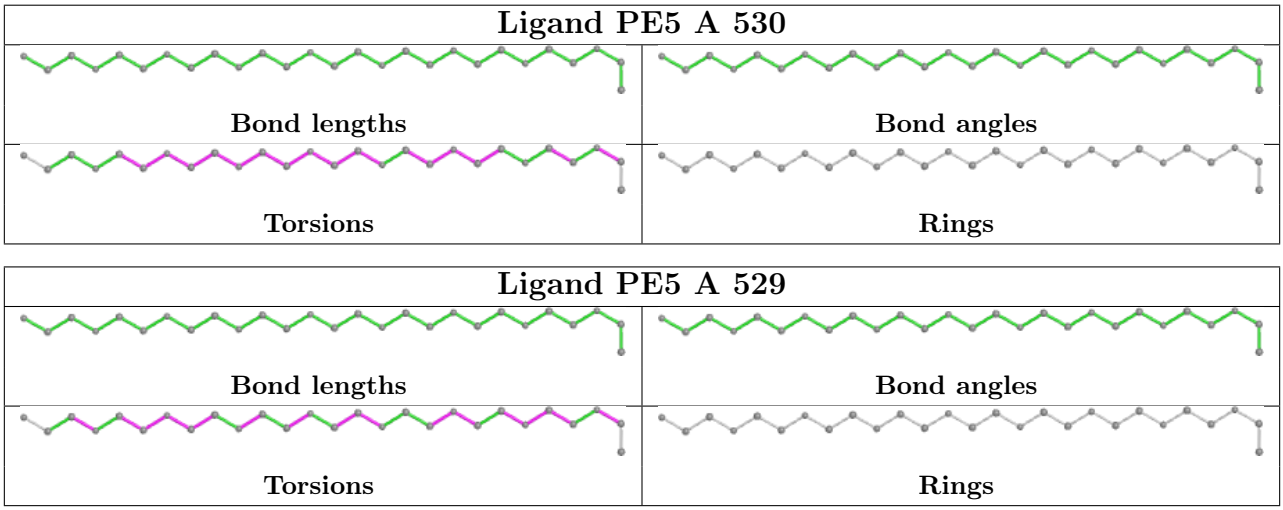
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	525	PG4	3	0
2	A	516	PEG	1	0
5	A	528	1PE	3	0
2	A	511	PEG	1	0
3	B	510	MES	1	0
4	A	526	PG4	3	0
2	A	519	PEG	2	0

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	456/460 (99%)	-0.60	6 (1%)	77	72	26, 41, 69, 102	0
1	B	454/460 (98%)	-0.23	10 (2%)	62	52	31, 62, 111, 140	0
All	All	910/920 (98%)	-0.42	16 (1%)	68	61	26, 49, 102, 140	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	GLY	3.5
1	A	47	GLN	3.0
1	B	261	VAL	2.6
1	B	387	LYS	2.5
1	A	482	SER	2.4
1	B	47	GLN	2.3
1	B	154	LYS	2.3
1	B	256	THR	2.2
1	B	214	ALA	2.1
1	B	28	THR	2.0
1	A	414	LEU	2.0
1	B	313	ASP	2.0
1	B	371	GLY	2.0
1	B	414	LEU	2.0
1	A	483	ASP	2.0
1	A	351	ALA	2.0

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG4	A	531	13/13	0.76	0.41	98,108,111,111	0
2	PEG	B	508	7/7	0.80	0.34	84,92,96,96	0
2	PEG	A	514	7/7	0.80	0.21	88,97,101,105	0
2	PEG	A	518	7/7	0.81	0.29	84,88,98,99	0
2	PEG	A	509	7/7	0.83	0.31	77,78,84,84	0
2	PEG	A	506	7/7	0.84	0.33	77,78,83,84	0
2	PEG	B	506	7/7	0.84	0.34	70,75,79,81	0
2	PEG	B	507	7/7	0.85	0.25	85,95,102,104	0
2	PEG	A	513	7/7	0.85	0.34	59,66,81,85	0
2	PEG	A	515	7/7	0.85	0.24	58,61,76,80	0
7	PGE	A	532	10/10	0.85	0.40	61,66,75,76	0
2	PEG	A	522	7/7	0.86	0.30	66,82,91,91	0
2	PEG	A	510	7/7	0.86	0.29	108,109,110,110	7
2	PEG	B	501	7/7	0.87	0.20	82,84,91,91	0
3	MES	B	511	12/12	0.87	0.23	118,123,125,126	0
4	PG4	A	525	13/13	0.87	0.32	65,77,87,88	0
2	PEG	A	519	7/7	0.87	0.25	79,86,90,91	0
2	PEG	A	501	7/7	0.87	0.32	54,69,79,81	0
2	PEG	B	502	7/7	0.88	0.25	70,85,90,91	0
2	PEG	A	521	7/7	0.88	0.15	52,63,71,72	0
2	PEG	A	511	7/7	0.88	0.29	75,86,98,100	0
6	PE5	A	529	27/27	0.88	0.30	58,77,96,99	0
2	PEG	A	503	7/7	0.88	0.20	66,67,79,81	0
5	1PE	A	528	16/16	0.89	0.23	52,74,83,84	0
2	PEG	A	508	7/7	0.89	0.26	85,86,98,98	0
6	PE5	A	530	27/27	0.89	0.24	50,71,95,101	0
2	PEG	A	520	7/7	0.89	0.22	43,61,72,74	0
2	PEG	B	503	7/7	0.90	0.19	78,82,91,91	0
2	PEG	B	505	7/7	0.90	0.25	76,78,87,88	0
2	PEG	A	504	7/7	0.91	0.20	55,65,75,77	0
4	PG4	B	513	13/13	0.91	0.20	37,66,82,82	0
2	PEG	A	517	7/7	0.91	0.18	30,41,54,55	0

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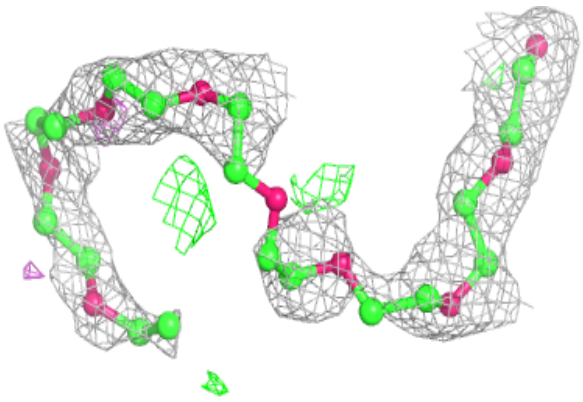
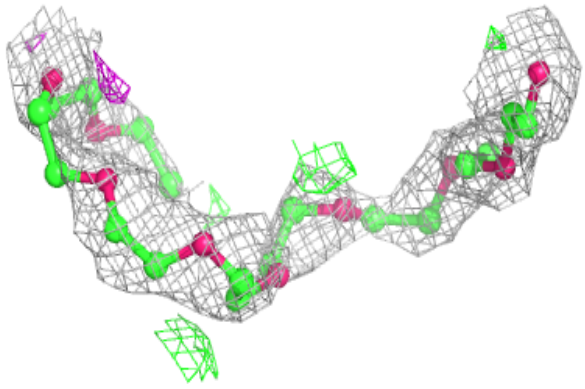
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	A	512	7/7	0.92	0.20	67,73,86,88	0
2	PEG	B	504	7/7	0.92	0.24	59,65,85,86	0
2	PEG	A	507	7/7	0.92	0.37	60,67,73,74	0
3	MES	B	510	12/12	0.92	0.20	96,106,111,113	0
7	PGE	B	514	10/10	0.92	0.13	31,46,52,53	0
4	PG4	A	526	13/13	0.93	0.20	49,67,72,76	0
7	PGE	B	512	10/10	0.93	0.18	46,54,60,62	0
3	MES	A	524	12/12	0.93	0.17	71,80,90,91	0
2	PEG	A	505	7/7	0.94	0.14	54,57,70,75	0
4	PG4	A	527	13/13	0.94	0.15	41,49,73,77	0
2	PEG	A	502	7/7	0.95	0.17	33,51,65,67	0
2	PEG	A	516	7/7	0.95	0.15	48,57,66,66	0
7	PGE	B	515	10/10	0.95	0.16	64,70,75,75	0
3	MES	A	523	12/12	0.98	0.11	27,45,52,53	0
3	MES	B	509	12/12	0.98	0.09	32,43,51,56	0

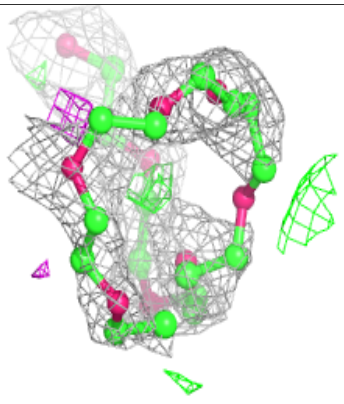
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PE5 A 529:

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

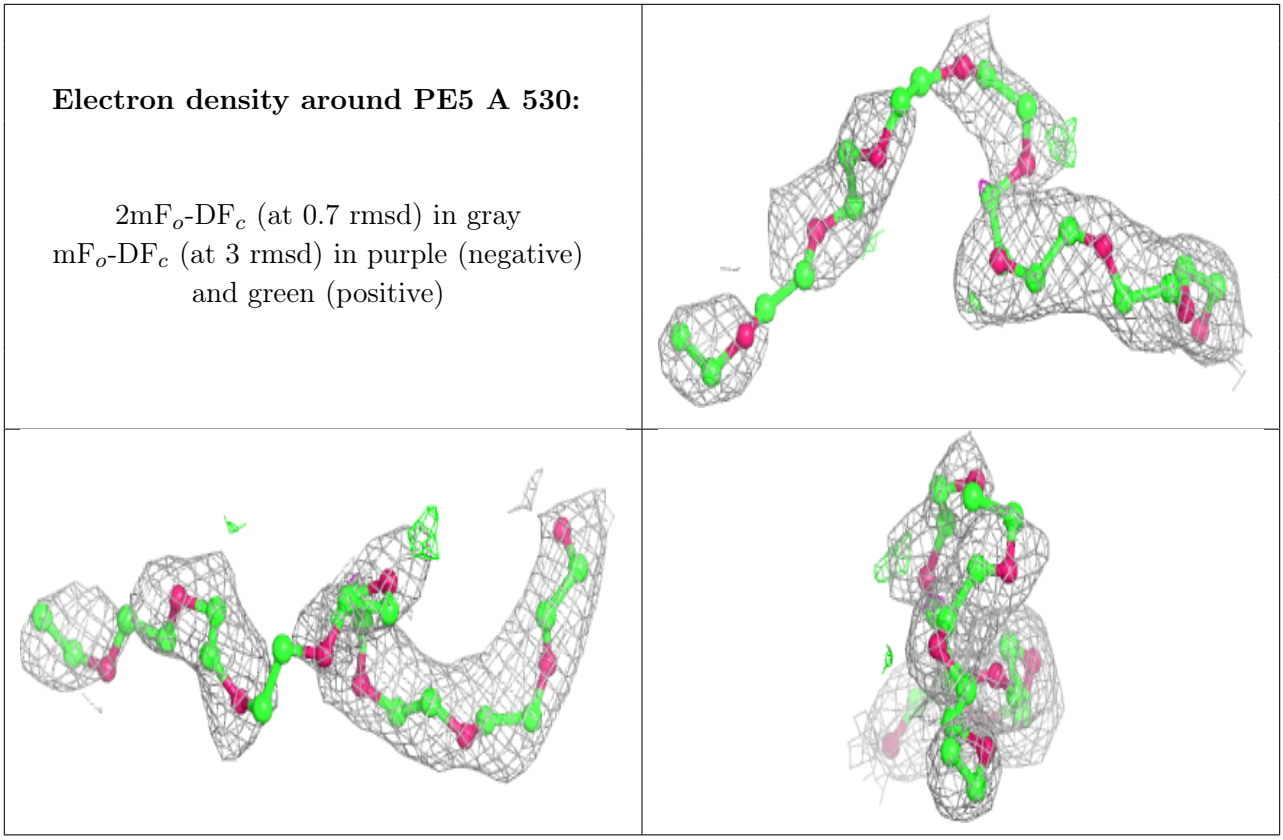






Electron density around PE5 A 530:

$2mF_o$-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.