



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:26 PM UTC

PDB ID : 2YNM / pdb_00002ynm
Title : Structure of the ADP $\times$ AlF₃-Stabilized Transition State of the Nitrogenase-like Dark-Operative Protochlorophyllide Oxidoreductase Complex from *Prochlorococcus marinus* with Its Substrate Protochlorophyllide a
Authors : Krausze, J.; Lange, C.; Heinz, D.W.; Moser, J.
Deposited on : 2012-10-16
Resolution : 2.10 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

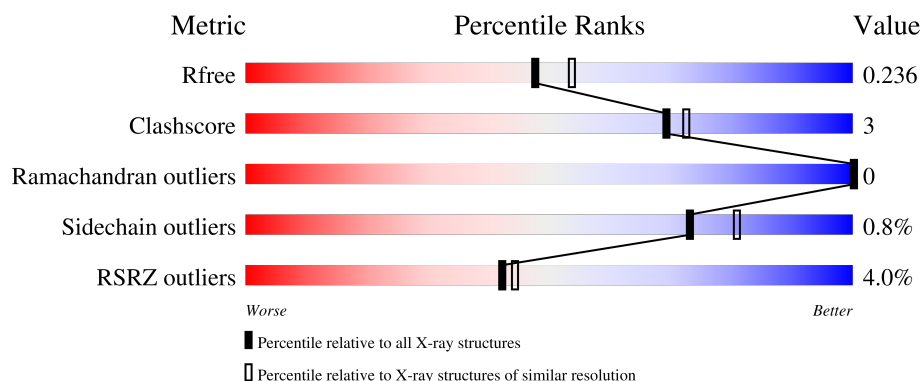
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
2	C	426	
3	D	530	

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
11	PMR	C	1414	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 11825 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 LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE IRON-SULFUR ATP-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2056	1304	347	393	12			
1	B	268	Total	C	N	O	S	0	1	0
			2069	1311	349	397	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q7VD39
A	-3	PRO	-	expression tag	UNP Q7VD39
A	-2	LEU	-	expression tag	UNP Q7VD39
A	-1	GLY	-	expression tag	UNP Q7VD39
A	0	SER	-	expression tag	UNP Q7VD39
B	-4	GLY	-	expression tag	UNP Q7VD39
B	-3	PRO	-	expression tag	UNP Q7VD39
B	-2	LEU	-	expression tag	UNP Q7VD39
B	-1	GLY	-	expression tag	UNP Q7VD39
B	0	SER	-	expression tag	UNP Q7VD39

- Molecule 2 is a protein called LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	417	Total	C	N	O	S	0	0	0
			3238	2061	564	599	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP Q7VD37
C	-6	PRO	-	expression tag	UNP Q7VD37

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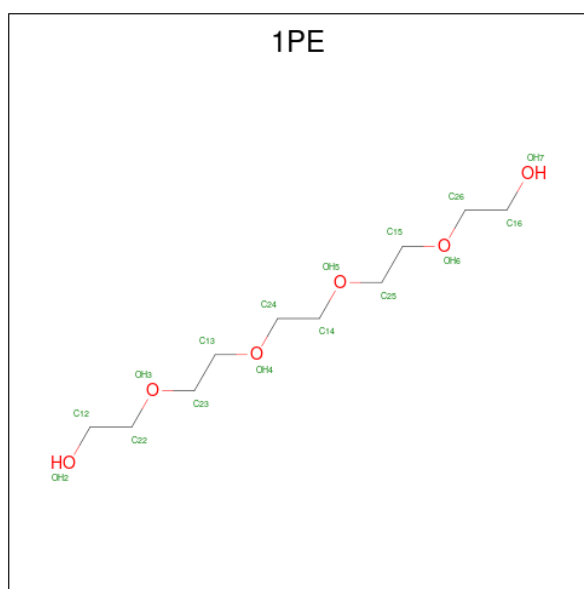
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	expression tag	UNP Q7VD37
C	-4	GLY	-	expression tag	UNP Q7VD37
C	-3	SER	-	expression tag	UNP Q7VD37
C	-2	PRO	-	expression tag	UNP Q7VD37
C	-1	GLU	-	expression tag	UNP Q7VD37
C	0	PHE	-	expression tag	UNP Q7VD37

- Molecule 3 is a protein called LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	488	Total	C	N	O	S	0	2	0
			3854	2449	661	723	21			

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



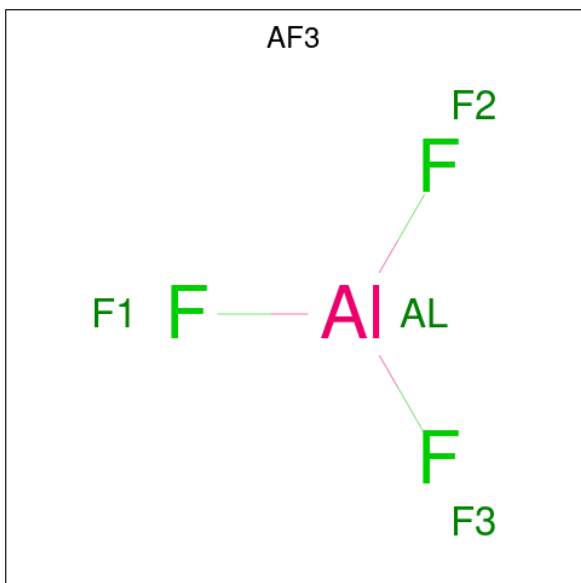
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



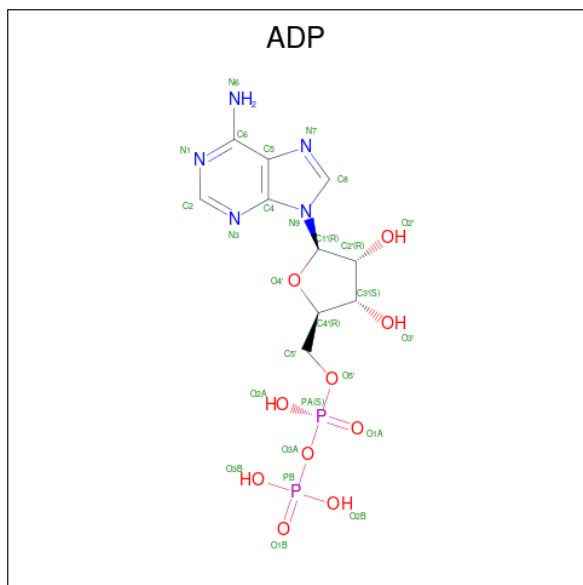
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

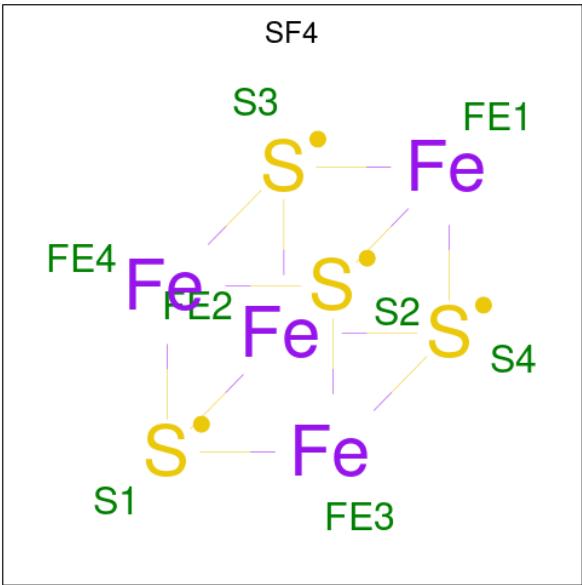
- Molecule 6 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	B	1	Total	Al	F	0	0
			4	1	3		

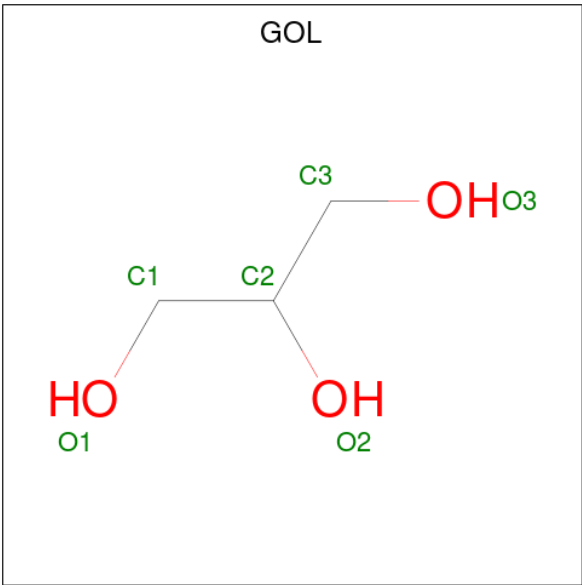
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



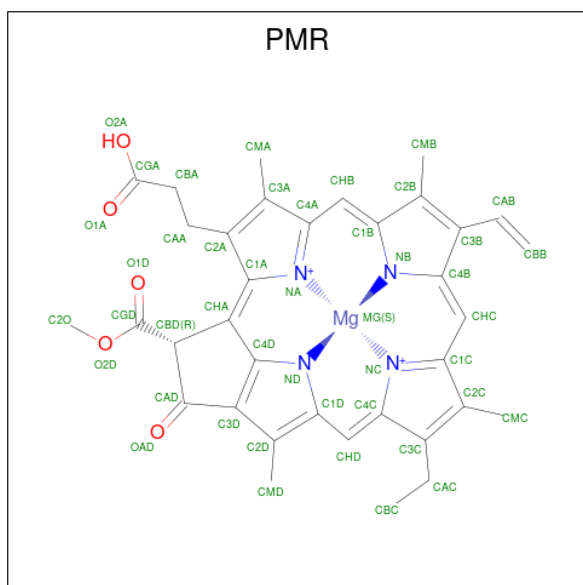
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 11 is Protochlorophyllide (CCD ID: PMR) (formula: $C_{35}H_{32}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 12 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	1	Total	K	0	0
			1	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	89	Total	O	0	0
			89	89		
13	B	63	Total	O	0	0
			63	63		
13	C	103	Total	O	0	0
			103	103		

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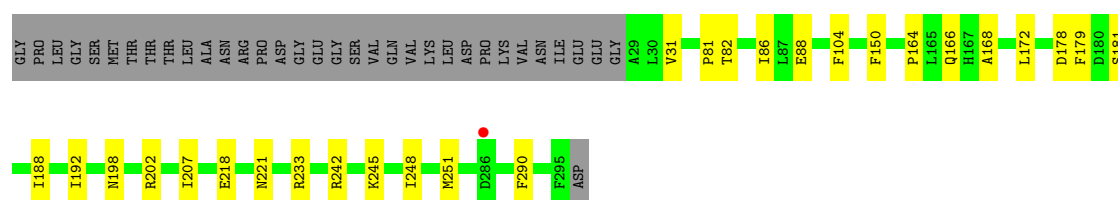
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	127	Total 127	O 127	0	0

3 Residue-property plots

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.

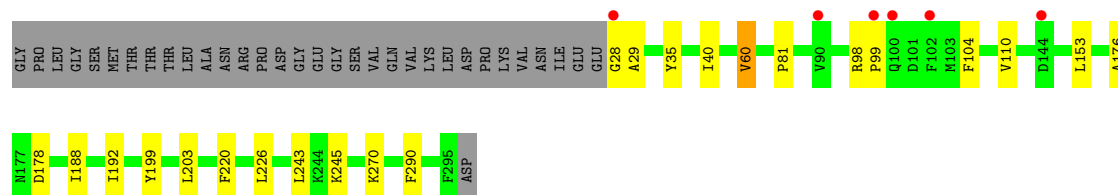
• Molecule 1: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE IRON-SULFUR ATP-BINDING PROTEIN

Chain A: 

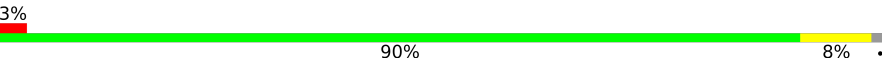


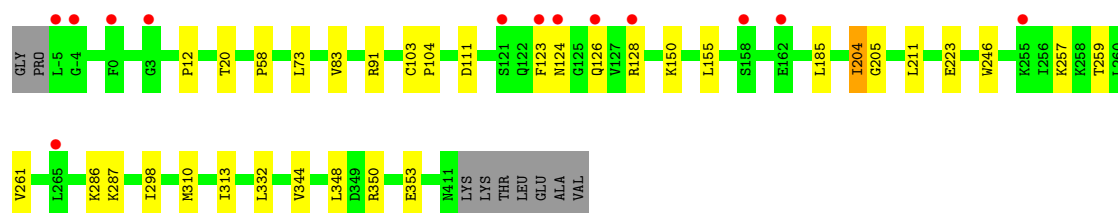
• Molecule 1: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE IRON-SULFUR ATP-BINDING PROTEIN

Chain B: 



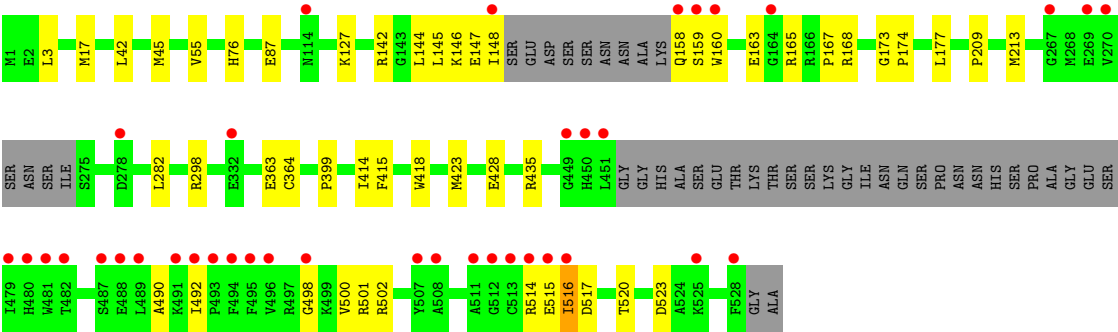
• Molecule 2: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT N

Chain C: 



• Molecule 3: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	308.40Å 74.11Å 74.23Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	34.51 – 2.10 34.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (34.51-2.10) 83.1 (34.51-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.199 , 0.233 0.201 , 0.236	Depositor DCC
R_{free} test set	4030 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11825	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 1PE, PMR, GOL, MG, SF4, K, ADP, AF3

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	0.28	0/2091	0.70	0/2821
1	B	0.29	0/2104	0.70	0/2838
2	C	0.31	0/3300	0.73	0/4469
3	D	0.30	0/3942	0.72	0/5335
All	All	0.30	0/11437	0.71	0/15463

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2056	0	2056	19	0
1	B	2069	0	2064	15	0
2	C	3238	0	3321	20	0
3	D	3854	0	3808	30	0
4	A	16	0	22	3	0
5	A	30	0	34	0	0
5	B	15	0	17	0	0
5	D	15	0	17	2	0
6	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	0	0	0
7	A	27	0	12	0	0
7	B	27	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	8	0	0	0	0
9	C	8	0	0	0	0
10	A	6	0	8	2	0
10	C	6	0	8	0	0
10	D	12	0	16	0	0
11	C	45	0	31	3	0
12	D	1	0	0	0	0
13	A	89	0	0	3	0
13	B	63	0	0	0	0
13	C	103	0	0	1	0
13	D	127	0	0	1	0
All	All	11825	0	11426	79	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 3.

All (79) 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)
3:D:399:PRO:HG3	5:D:1529:EPE:H82	1.71	0.71
1:A:202:ARG:HH22	4:A:1296:1PE:H121	1.56	0.69
3:D:147:GLU:HG3	3:D:148:ILE:HG13	1.79	0.65
3:D:514:ARG:O	3:D:515:GLU:HG2	1.99	0.62
1:B:199:TYR:OH	2:C:111:ASP:OD2	2.17	0.61
2:C:150:LYS:HG3	2:C:223:GLU:HG3	1.82	0.61
2:C:287:LYS:NZ	13:C:2069:HOH:O	2.37	0.57
1:A:290:PHE:CZ	1:B:245:LYS:HG2	2.40	0.56
3:D:501:ARG:HH22	3:D:502:ARG:HH21	1.53	0.56
1:A:172:LEU:HD13	1:A:207:ILE:HD11	1.88	0.56
1:A:88:GLU:HG3	2:C:73:LEU:HD13	1.88	0.54
2:C:58:PRO:O	2:C:91:ARG:NH1	2.39	0.54
3:D:363:GLU:HA	3:D:502:ARG:HH12	1.72	0.54
3:D:42:LEU:HB3	3:D:177:LEU:HD11	1.90	0.54
2:C:287:LYS:HB3	2:C:313:ILE:HD11	1.89	0.53
1:A:81:PRO:HG2	1:A:104:PHE:CZ	2.43	0.53
13:A:2077:HOH:O	1:B:178:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:TYR:HB3	1:B:188:ILE:HD13	1.92	0.50
1:B:203:LEU:HD13	1:B:226:LEU:HD21	1.94	0.50
11:C:1414:PMR:HMA	3:D:45:MET:HB3	1.94	0.50
2:C:185:LEU:HD22	2:C:261:VAL:HG12	1.93	0.50
3:D:517:ASP:H	3:D:520:THR:HG22	1.78	0.48
3:D:282:LEU:HD12	3:D:415:PHE:HB2	1.95	0.48
2:C:12:PRO:HB2	2:C:344:VAL:HG12	1.95	0.48
2:C:211:LEU:HB3	2:C:246:TRP:CZ2	2.49	0.48
3:D:498:GLY:O	3:D:502:ARG:HG2	2.13	0.48
2:C:123:PHE:HB3	2:C:126:GLN:HG3	1.97	0.47
2:C:12:PRO:HG3	3:D:76:HIS:NE2	2.29	0.47
3:D:515:GLU:O	3:D:516:ILE:HG13	2.15	0.47
1:A:31:VAL:HB	1:A:168:ALA:HA	1.97	0.47
3:D:159:SER:OG	3:D:163:GLU:OE2	2.27	0.47
3:D:423:MET:HE3	3:D:428:GLU:HG3	1.96	0.47
1:A:181:SER:HB3	10:A:1303:GOL:H11	1.97	0.47
1:A:233:ARG:NH1	13:A:2075:HOH:O	2.48	0.47
3:D:87:GLU:HB2	3:D:209:PRO:HG2	1.96	0.47
1:B:60:VAL:HG13	1:B:110:VAL:HG22	1.98	0.46
3:D:145:LEU:HD21	3:D:213:MET:HA	1.97	0.46
1:B:40:ILE:HD11	1:B:176:ALA:HB2	1.97	0.46
1:B:192:ILE:HG21	1:B:203:LEU:HG	1.97	0.46
2:C:103:CYS:HB2	2:C:104:PRO:HD3	1.97	0.46
2:C:204:ILE:HG12	2:C:205:GLY:H	1.81	0.46
1:A:150:PHE:CG	1:A:164:PRO:HB3	2.51	0.46
2:C:257:LYS:HE3	2:C:259:THR:HG23	1.97	0.46
3:D:492:ILE:HG13	3:D:500:VAL:HG11	1.99	0.45
2:C:83:VAL:HG13	3:D:3:LEU:HB2	1.98	0.45
3:D:17:MET:HG3	3:D:55:VAL:HG21	1.97	0.45
11:C:1414:PMR:CGD	11:C:1414:PMR:HAA	2.47	0.45
2:C:298:ILE:HG23	2:C:332:LEU:HD11	1.98	0.45
3:D:142:ARG:O	3:D:146:LYS:HB2	2.17	0.44
3:D:502:ARG:NH1	13:D:2127:HOH:O	2.50	0.44
2:C:350:ARG:HA	2:C:353:GLU:HG2	1.98	0.44
3:D:160:TRP:CE2	3:D:167:PRO:HG3	2.53	0.44
2:C:286:LYS:HB2	2:C:310:MET:HE3	1.99	0.44
3:D:435:ARG:NH1	3:D:490:ALA:O	2.43	0.43
1:A:179:PHE:HB2	1:B:243:LEU:HD23	2.00	0.43
1:B:188:ILE:O	1:B:192:ILE:HG12	2.19	0.43
1:A:245:LYS:HG2	1:B:290:PHE:CE2	2.53	0.43
3:D:173:GLY:N	3:D:174:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:414:ILE:HG23	3:D:418:TRP:CD2	2.55	0.42
5:D:1529:EPE:H101	5:D:1529:EPE:H61	1.66	0.42
1:A:198:ASN:HD21	4:A:1296:1PE:H162	1.84	0.42
2:C:20:THR:HB	11:C:1414:PMR:HBCB	2.02	0.42
3:D:298:ARG:NH2	3:D:364:CYS:O	2.42	0.42
1:A:178:ASP:OD2	10:A:1303:GOL:H12	2.20	0.42
1:A:218:GLU:HA	1:A:221:ASN:HB2	2.01	0.42
1:A:188:ILE:O	1:A:192:ILE:HG12	2.20	0.42
1:B:98:ARG:HG3	1:B:99:PRO:HD2	2.02	0.42
1:A:248:ILE:HD12	1:A:251:MET:HG3	2.01	0.41
2:C:128:ARG:HD3	2:C:155:LEU:HD23	2.00	0.41
1:B:81:PRO:HG2	1:B:104:PHE:CZ	2.55	0.41
1:A:242:ARG:HB2	13:A:2077:HOH:O	2.20	0.41
1:B:28:GLY:HA2	1:B:29:ALA:HA	1.83	0.41
3:D:520:THR:HA	3:D:523:ASP:HB2	2.02	0.41
3:D:165:ARG:NH1	3:D:168:ARG:HG2	2.36	0.41
1:A:202:ARG:HH12	4:A:1296:1PE:H122	1.86	0.40
3:D:127:LYS:HA	3:D:127:LYS:HD3	1.86	0.40
1:B:220:PHE:HE2	1:B:226:LEU:HD12	1.86	0.40
3:D:17:MET:HE3	3:D:17:MET:HB2	1.87	0.40
1:A:82:THR:O	1:A:86:ILE:HG12	2.22	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	265/301 (88%)	258 (97%)	7 (3%)	0	100	100
1	B	267/301 (89%)	259 (97%)	8 (3%)	0	100	100
2	C	415/426 (97%)	402 (97%)	13 (3%)	0	100	100
3	D	482/530 (91%)	468 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1429/1558 (92%)	1387 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/252 (89%)	223 (100%)	1 (0%)	84	89
1	B	225/252 (89%)	222 (99%)	3 (1%)	61	69
2	C	354/361 (98%)	351 (99%)	3 (1%)	73	81
3	D	412/443 (93%)	409 (99%)	3 (1%)	76	83
All	All	1215/1308 (93%)	1205 (99%)	10 (1%)	73	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	B	60	VAL
1	B	153	LEU
1	B	270	LYS
2	C	124	ASN
2	C	204	ILE
2	C	348	LEU
3	D	144	LEU
3	D	158	GLN
3	D	516	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	B	275	ASN

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Mol	Chain	Res	Type
2	C	343	HIS
2	C	407	GLN
2	C	411	ASN
3	D	158	GLN
3	D	480	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\# Z > 2$
10	GOL	A	1303	-	5,5,5	0.26	0	5,5,5	0.42	0
10	GOL	D	1530	-	5,5,5	0.25	0	5,5,5	0.38	0
6	AF3	A	1299	13,7	0,3,3	-	-	-	-	-
10	GOL	C	1412	-	5,5,5	0.21	0	5,5,5	0.41	0
11	PMR	C	1414	13	37,53,53	3.84	16 (43%)	36,89,89	2.60	15 (41%)
9	SF4	A	1302	1	0,12,12	-	-	-	-	-
4	1PE	A	1296	-	15,15,15	0.44	0	14,14,14	0.43	0
7	ADP	A	1300	6,8	28,29,29	1.47	5 (17%)	43,45,45	1.81	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EPE	A	1298	-	15,15,15	0.85	1 (6%)	19,20,20	1.65	5 (26%)
9	SF4	C	1413	2,3	0,12,12	-	-	-		
10	GOL	D	1532	-	5,5,5	0.25	0	5,5,5	0.29	0
5	EPE	A	1297	-	15,15,15	0.83	1 (6%)	19,20,20	1.68	4 (21%)
5	EPE	D	1529	-	15,15,15	0.73	1 (6%)	19,20,20	1.70	4 (21%)
7	ADP	B	1299	6,8	28,29,29	1.41	4 (14%)	43,45,45	1.80	9 (20%)
5	EPE	B	1296	-	15,15,15	0.79	1 (6%)	19,20,20	1.57	5 (26%)
6	AF3	B	1298	13,7,8	0,3,3	-	-	-		

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
10	GOL	A	1303	-	-	2/4/4/4	-
10	GOL	D	1530	-	-	0/4/4/4	-
10	GOL	C	1412	-	-	0/4/4/4	-
11	PMR	C	1414	13	3/3/16/20	6/13/111/111	-
9	SF4	A	1302	1	-	-	0/6/5/5
4	1PE	A	1296	-	-	4/13/13/13	-
7	ADP	A	1300	6,8	-	2/16/32/32	0/3/3/3
5	EPE	A	1298	-	-	2/9/19/19	0/1/1/1
10	GOL	D	1532	-	-	3/4/4/4	-
9	SF4	C	1413	2,3	-	-	0/6/5/5
5	EPE	A	1297	-	-	4/9/19/19	0/1/1/1
5	EPE	D	1529	-	-	4/9/19/19	0/1/1/1
7	ADP	B	1299	6,8	-	0/16/32/32	0/3/3/3
5	EPE	B	1296	-	-	4/9/19/19	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1414	PMR	C1D-C2D	9.45	1.50	1.39
11	C	1414	PMR	C1A-CHA	8.92	1.49	1.39
11	C	1414	PMR	C1B-C2B	8.70	1.49	1.39
11	C	1414	PMR	C3B-C4B	7.27	1.48	1.41
11	C	1414	PMR	O2D-CGD	5.10	1.45	1.33
11	C	1414	PMR	OAD-CAD	5.08	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1300	ADP	C5-C4	4.86	1.47	1.39
11	C	1414	PMR	C3B-C2B	4.81	1.46	1.40
7	B	1299	ADP	C5-C4	4.73	1.47	1.39
11	C	1414	PMR	CHB-C1B	4.60	1.47	1.39
11	C	1414	PMR	CHC-C4B	4.51	1.46	1.39
11	C	1414	PMR	CHD-C1D	4.47	1.46	1.39
11	C	1414	PMR	C3D-C4D	-4.28	1.35	1.41
11	C	1414	PMR	C3D-C2D	4.22	1.46	1.39
11	C	1414	PMR	CHD-C4C	4.19	1.47	1.39
11	C	1414	PMR	CHB-C4A	4.09	1.47	1.39
11	C	1414	PMR	CHC-C1C	3.91	1.46	1.39
11	C	1414	PMR	C1A-C2A	3.90	1.49	1.45
5	A	1298	EPE	C10-S	2.96	1.81	1.77
5	A	1297	EPE	C10-S	2.84	1.81	1.77
7	A	1300	ADP	C5-C6	2.78	1.48	1.41
7	B	1299	ADP	C5-C6	2.77	1.48	1.41
5	B	1296	EPE	C10-S	2.60	1.81	1.77
7	A	1300	ADP	PA-O3A	2.47	1.62	1.59
5	D	1529	EPE	C10-S	2.43	1.81	1.77
7	A	1300	ADP	C8-N7	2.38	1.36	1.31
7	B	1299	ADP	C5-N7	-2.26	1.35	1.39
7	B	1299	ADP	C8-N7	2.21	1.35	1.31
7	A	1300	ADP	C5-N7	-2.19	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1414	PMR	O2D-CGD-CBD	8.41	120.19	110.95
11	C	1414	PMR	CHA-C1A-C2A	-7.09	119.86	132.84
7	B	1299	ADP	C5-C4-N3	-5.64	118.95	126.72
7	A	1300	ADP	C5-C4-N3	-5.59	119.02	126.72
5	D	1529	EPE	C5-N4-C3	4.55	118.64	108.84
7	B	1299	ADP	N3-C4-N9	4.54	134.90	127.17
5	A	1298	EPE	C5-N4-C3	4.49	118.51	108.84
5	A	1297	EPE	C5-N4-C3	4.48	118.50	108.84
7	A	1300	ADP	N3-C4-N9	4.45	134.74	127.17
5	B	1296	EPE	C5-N4-C3	3.74	116.90	108.84
7	A	1300	ADP	C2-N3-C4	3.65	120.74	111.83
7	B	1299	ADP	C2-N3-C4	3.58	120.57	111.83
7	A	1300	ADP	C4-C5-N7	-3.49	106.59	110.58
7	B	1299	ADP	C4-C5-N7	-3.43	106.66	110.58
7	A	1300	ADP	N3-C2-N1	-3.33	123.55	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1529	EPE	C7-N4-C5	3.21	119.80	111.24
7	B	1299	ADP	N3-C2-N1	-3.14	123.83	128.58
11	C	1414	PMR	C4A-CHB-C1B	3.08	127.07	116.07
11	C	1414	PMR	C1C-CHC-C4B	3.04	126.94	116.07
11	C	1414	PMR	CAC-C3C-C2C	3.00	133.06	127.56
11	C	1414	PMR	C4C-C3C-C2C	-2.98	101.60	113.37
11	C	1414	PMR	C1A-CHA-C4D	-2.96	116.49	119.15
5	D	1529	EPE	C7-N4-C3	2.91	119.00	111.24
11	C	1414	PMR	C4D-CHA-CBD	-2.85	106.10	108.97
11	C	1414	PMR	O2D-CGD-O1D	-2.83	118.34	123.85
7	B	1299	ADP	C4-N9-C8	2.77	108.65	105.74
7	A	1300	ADP	C4-N9-C8	2.75	108.62	105.74
5	A	1297	EPE	C7-N4-C3	2.73	118.53	111.24
5	A	1297	EPE	C7-N4-C5	2.69	118.40	111.24
5	B	1296	EPE	C7-N4-C3	2.60	118.17	111.24
5	B	1296	EPE	C7-N4-C5	2.59	118.13	111.24
7	A	1300	ADP	C5-N7-C8	2.58	107.51	103.45
7	B	1299	ADP	C5-N7-C8	2.52	107.41	103.45
11	C	1414	PMR	CMB-C2B-C3B	2.43	129.55	124.68
11	C	1414	PMR	CMA-C3A-C4A	2.42	129.09	124.73
5	A	1298	EPE	C7-N4-C5	2.30	117.37	111.24
5	B	1296	EPE	O2S-S-C10	2.29	110.19	106.73
5	A	1297	EPE	O3S-S-C10	2.29	110.48	106.00
11	C	1414	PMR	C4C-CHD-C1D	2.29	124.25	116.07
7	A	1300	ADP	C6-C5-N7	2.26	136.45	132.09
7	A	1300	ADP	C3'-C2'-C1'	2.24	105.71	101.46
5	A	1298	EPE	O1S-S-C10	2.17	110.00	106.73
11	C	1414	PMR	O1D-CGD-CBD	-2.14	121.47	124.72
11	C	1414	PMR	C3A-C4A-NA	2.14	116.51	110.46
5	D	1529	EPE	O3S-S-C10	2.13	110.18	106.00
11	C	1414	PMR	C2C-C1C-NC	2.12	116.46	110.46
5	B	1296	EPE	O1S-S-C10	2.10	109.91	106.73
7	B	1299	ADP	C3'-C2'-C1'	2.08	105.40	101.46
7	B	1299	ADP	C6-C5-N7	2.08	136.10	132.09
7	A	1300	ADP	N9-C8-N7	-2.05	111.03	113.94
5	A	1298	EPE	C3-C2-N1	-2.02	106.57	110.65
5	A	1298	EPE	C7-N4-C3	2.02	116.63	111.24
7	A	1300	ADP	C2-N1-C6	2.02	122.04	118.73

All (3) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
11	C	1414	PMR	NC
11	C	1414	PMR	NB
11	C	1414	PMR	NA

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1297	EPE	C8-C7-N4-C3
5	A	1297	EPE	C9-C10-S-O1S
5	A	1298	EPE	C10-C9-N1-C6
5	D	1529	EPE	C10-C9-N1-C6
5	D	1529	EPE	S-C10-C9-N1
10	A	1303	GOL	O1-C1-C2-C3
11	C	1414	PMR	C4C-C3C-CAC-CBC
11	C	1414	PMR	C2C-C3C-CAC-CBC
4	A	1296	1PE	OH5-C14-C24-OH4
10	D	1532	GOL	C1-C2-C3-O3
10	A	1303	GOL	O1-C1-C2-O2
5	A	1297	EPE	C9-C10-S-O3S
10	D	1532	GOL	O2-C2-C3-O3
5	B	1296	EPE	C8-C7-N4-C5
5	D	1529	EPE	N4-C7-C8-O8
5	B	1296	EPE	C9-C10-S-O3S
5	A	1297	EPE	C9-C10-S-O2S
5	B	1296	EPE	C9-C10-S-O2S
4	A	1296	1PE	C13-C23-OH3-C22
7	A	1300	ADP	O4'-C4'-C5'-O5'
7	A	1300	ADP	C3'-C4'-C5'-O5'
5	A	1298	EPE	C10-C9-N1-C2
10	D	1532	GOL	O1-C1-C2-O2
4	A	1296	1PE	C23-C13-OH4-C24
11	C	1414	PMR	CAA-CBA-CGA-O2A
11	C	1414	PMR	CAA-CBA-CGA-O1A
11	C	1414	PMR	C2A-CAA-CBA-CGA
5	B	1296	EPE	C8-C7-N4-C3
5	D	1529	EPE	C8-C7-N4-C3
4	A	1296	1PE	C15-C25-OH5-C14
11	C	1414	PMR	CAD-CBD-CGD-O2D

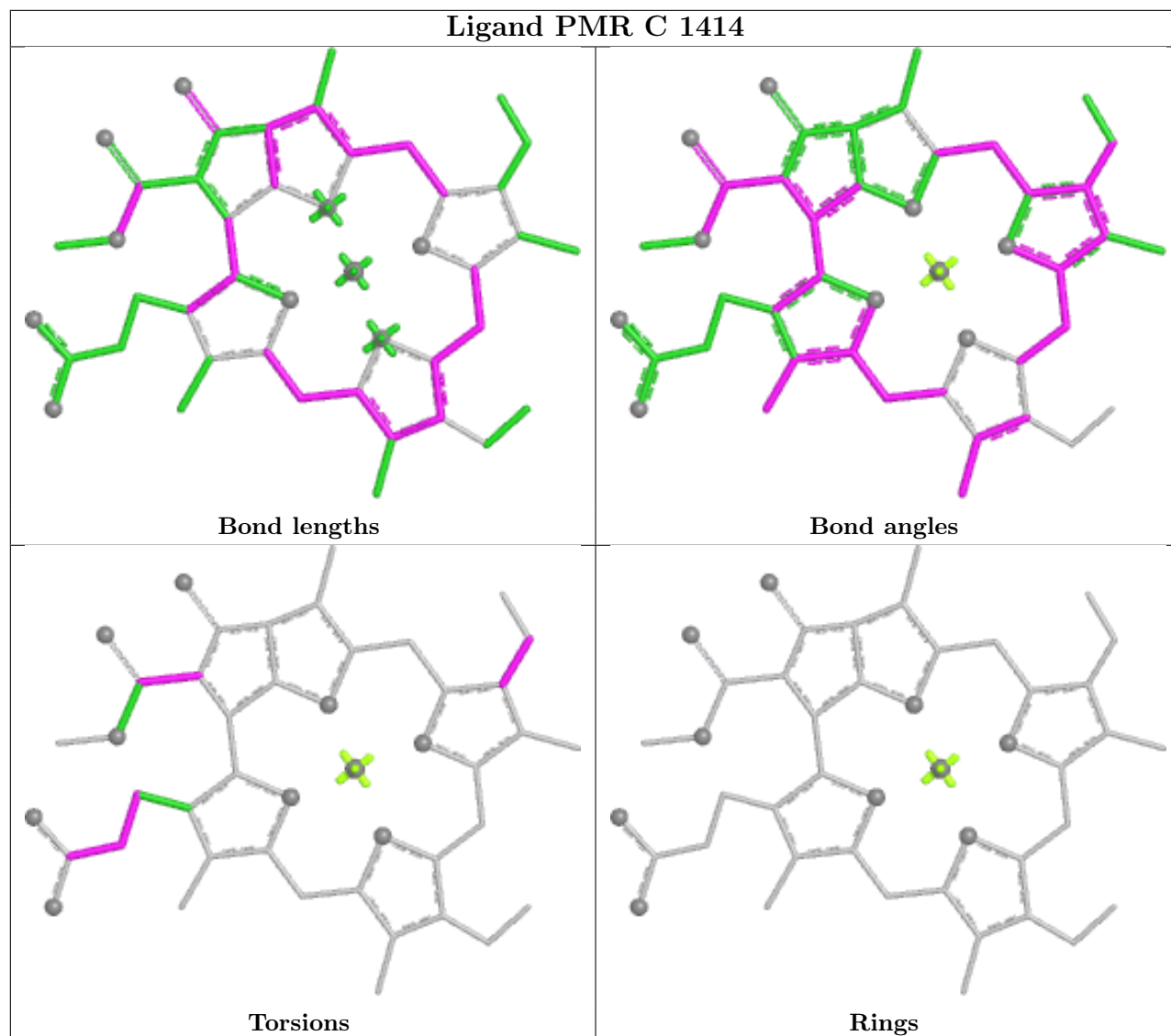
There are no ring outliers.

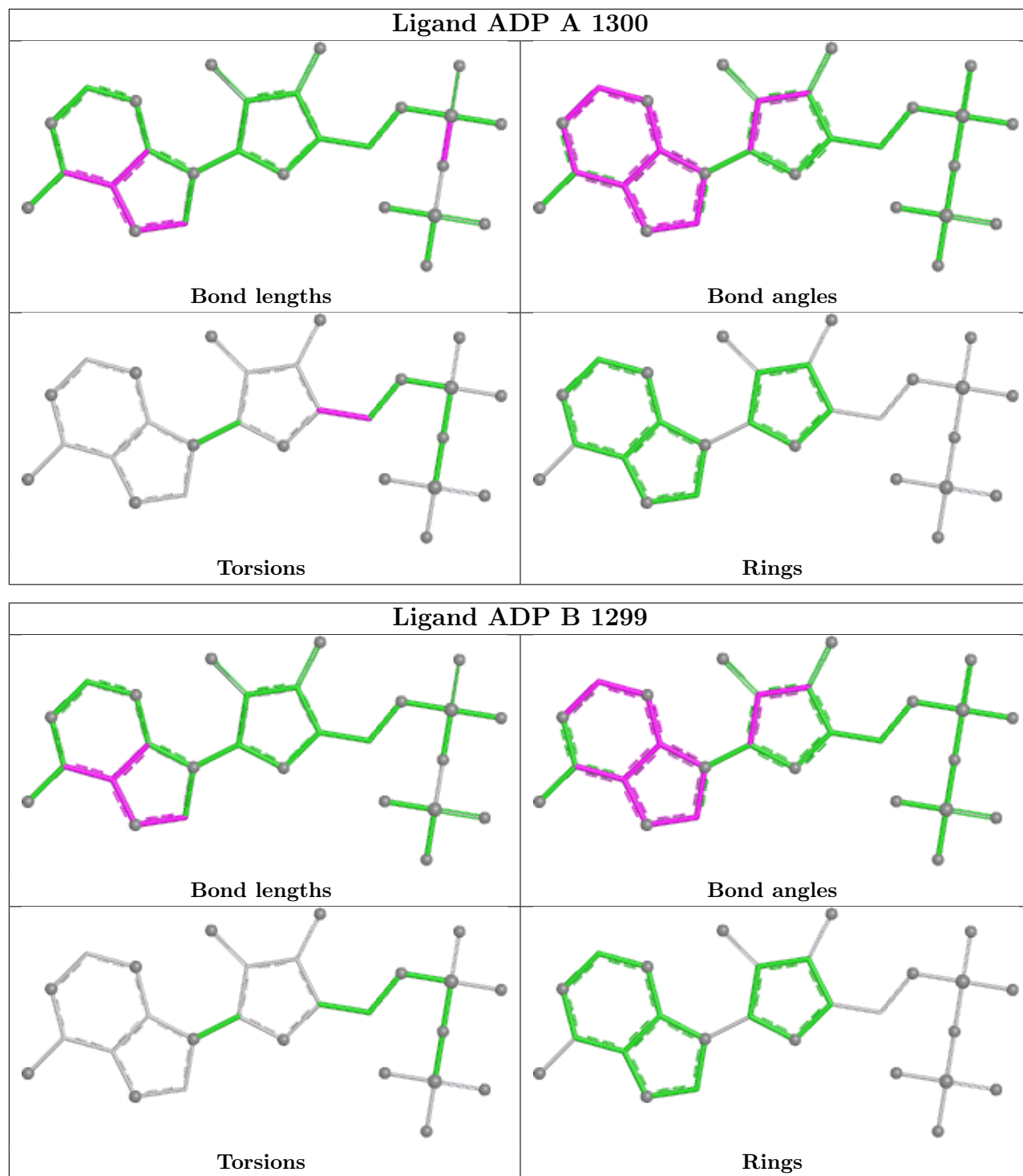
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1303	GOL	2	0
11	C	1414	PMR	3	0
4	A	1296	1PE	3	0
5	D	1529	EPE	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PMR C 1414





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	267/301 (88%)	0.22	1 (0%) 88 90	19, 35, 63, 78	0
1	B	268/301 (89%)	0.31	6 (2%) 62 65	18, 37, 64, 83	1 (0%)
2	C	417/426 (97%)	0.38	13 (3%) 51 54	19, 42, 71, 96	0
3	D	488/530 (92%)	0.43	38 (7%) 19 20	16, 35, 83, 133	2 (0%)
All	All	1440/1558 (92%)	0.36	58 (4%) 42 44	16, 38, 72, 133	3 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	479	ILE	6.9
3	D	493	PRO	5.3
1	B	99	PRO	5.1
3	D	494	PHE	4.8
3	D	451	LEU	4.7
3	D	270	VAL	4.6
3	D	516	ILE	4.3
3	D	495	PHE	4.1
3	D	528	PHE	3.9
3	D	449	GLY	3.8
3	D	480	HIS	3.7
3	D	514	ARG	3.7
3	D	148	ILE	3.6
3	D	492	ILE	3.6
3	D	487	SER	3.3
3	D	450	HIS	3.3
3	D	158	GLN	3.2
1	B	28	GLY	3.1
3	D	512	GLY	3.0
3	D	278[A]	ASP	3.0
3	D	511	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	162	GLU	2.9
3	D	496	VAL	2.9
3	D	481	TRP	2.9
3	D	489	LEU	2.7
2	C	3	GLY	2.7
2	C	123	PHE	2.7
2	C	265	LEU	2.7
3	D	513	CYS	2.7
2	C	124	ASN	2.6
1	A	286	ASP	2.6
1	B	90	VAL	2.6
3	D	267	GLY	2.5
3	D	332	GLU	2.4
3	D	114	ASN	2.4
3	D	488	GLU	2.4
1	B	144	ASP	2.4
3	D	482	THR	2.4
3	D	515	GLU	2.3
3	D	508	ALA	2.3
2	C	-5	LEU	2.3
3	D	269	GLU	2.2
3	D	164	GLY	2.2
3	D	498	GLY	2.2
3	D	159	SER	2.2
2	C	158	SER	2.2
2	C	126	GLN	2.1
2	C	-4	GLY	2.1
3	D	525	LYS	2.1
1	B	102	PHE	2.1
3	D	160	TRP	2.1
3	D	491	LYS	2.1
2	C	0	PHE	2.1
1	B	100	GLN	2.0
2	C	255	LYS	2.0
3	D	507	TYR	2.0
2	C	121	SER	2.0
2	C	128	ARG	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

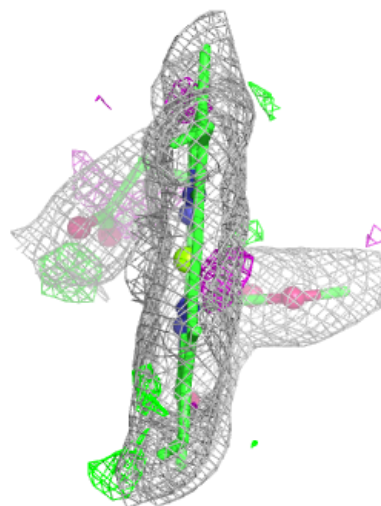
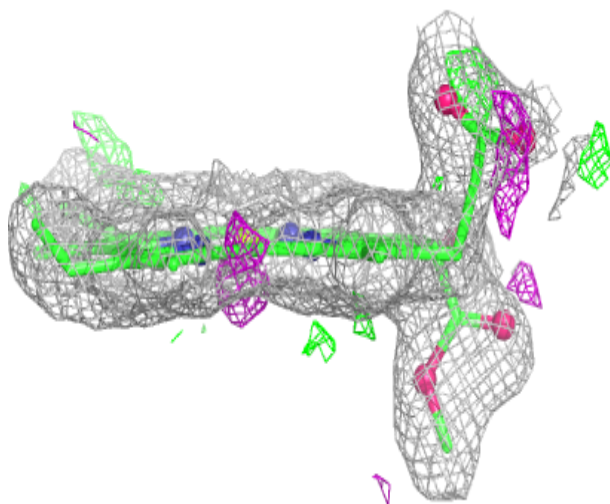
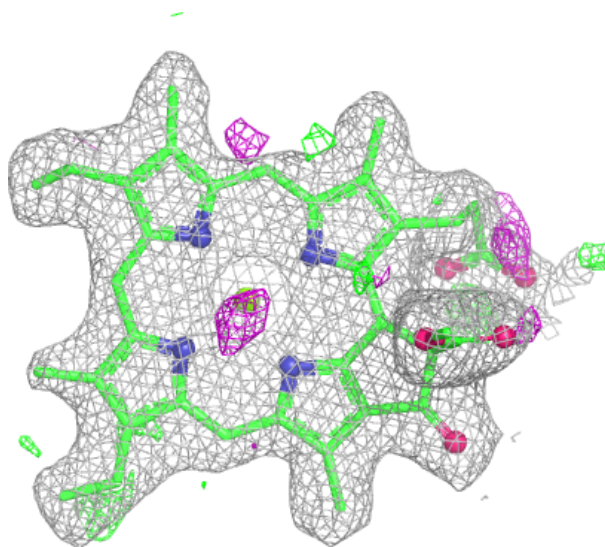
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	1PE	A	1296	16/16	0.76	0.20	49,64,71,72	0
10	GOL	A	1303	6/6	0.76	0.29	63,69,71,71	0
5	EPE	D	1529	15/15	0.78	0.27	60,66,74,75	0
12	K	D	1531	1/1	0.83	0.19	66,66,66,66	0
5	EPE	A	1298	15/15	0.85	0.14	39,41,51,52	0
10	GOL	D	1532	6/6	0.87	0.15	38,42,45,46	0
11	PMR	C	1414	45/45	0.91	0.09	14,23,28,39	0
5	EPE	B	1296	15/15	0.93	0.14	35,58,60,60	0
6	AF3	B	1298	4/4	0.94	0.06	25,27,29,44	0
5	EPE	A	1297	15/15	0.94	0.12	32,46,53,54	0
10	GOL	C	1412	6/6	0.94	0.08	25,33,36,38	0
10	GOL	D	1530	6/6	0.95	0.07	20,30,33,35	0
6	AF3	A	1299	4/4	0.96	0.06	17,27,32,39	0
7	ADP	A	1300	27/27	0.96	0.07	20,31,34,38	0
8	MG	B	1297	1/1	0.96	0.07	34,34,34,34	0
7	ADP	B	1299	27/27	0.97	0.07	20,29,38,39	0
8	MG	A	1301	1/1	0.98	0.04	26,26,26,26	0
9	SF4	A	1302	8/8	0.99	0.03	17,19,21,22	0
9	SF4	C	1413	8/8	0.99	0.03	19,22,25,26	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.

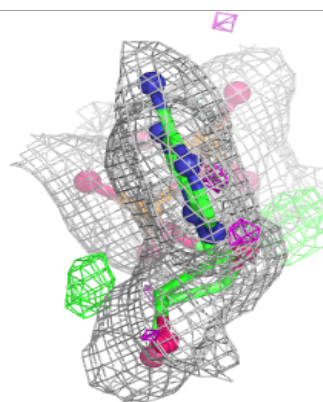
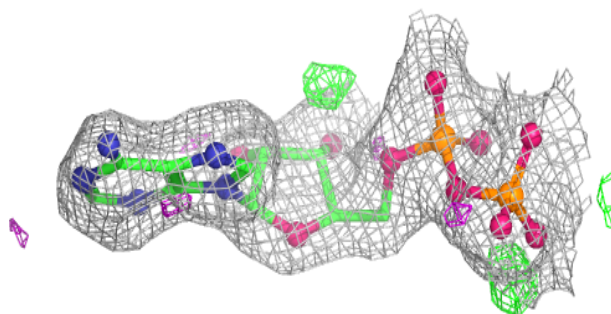
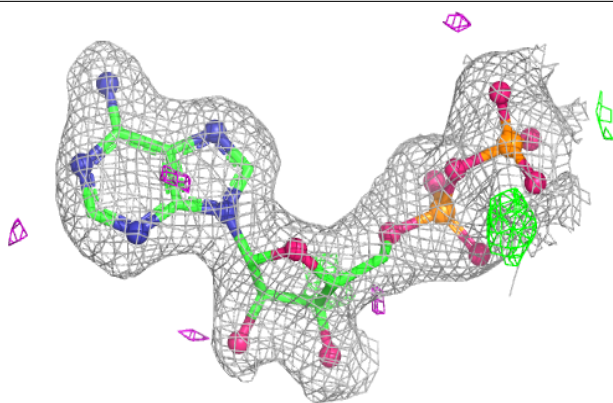
Electron density around PMR C 1414:

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

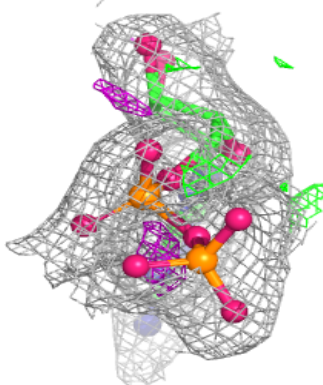
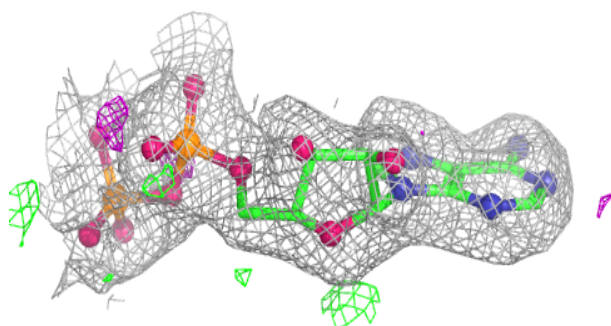
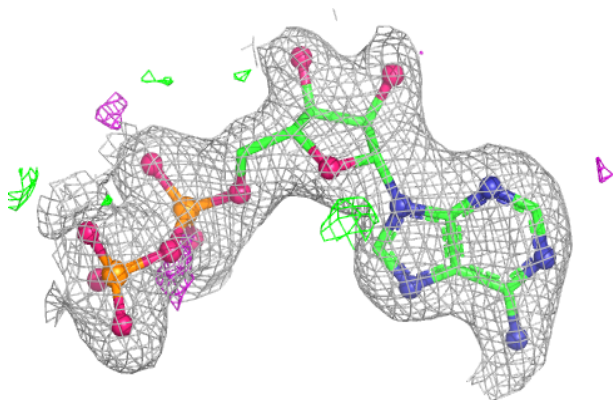


Electron density around ADP A 1300:

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

**Electron density around ADP B 1299:**

$2mF_o-DF_c$ (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.