wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2026 – 02:21 am BST

PDB ID	:	2YNM / pdb_00002ynm
Title	:	Structure of the ADPxAlF3-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 wwPDB X-ray Structure Validation Summary 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:

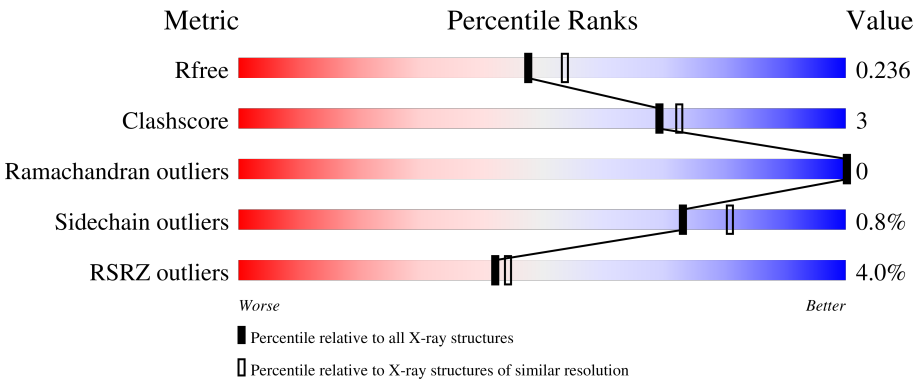
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.10 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 <=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	80% 9% 11%
1	B	301	2% 81% 7% 11%
2	C	426	3% 90% 8% •
3	D	530	7% 83% 9% 8%

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 (i)

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
			Total	C	N	O	S			
1	A	267	2056	1304	347	393	12	0	0	0
1	B	268	2069	1311	349	397	12	0	1	0

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
			Total	C	N	O	S			
2	C	417	3238	2061	564	599	14	0	0	0

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

Continued on next page...

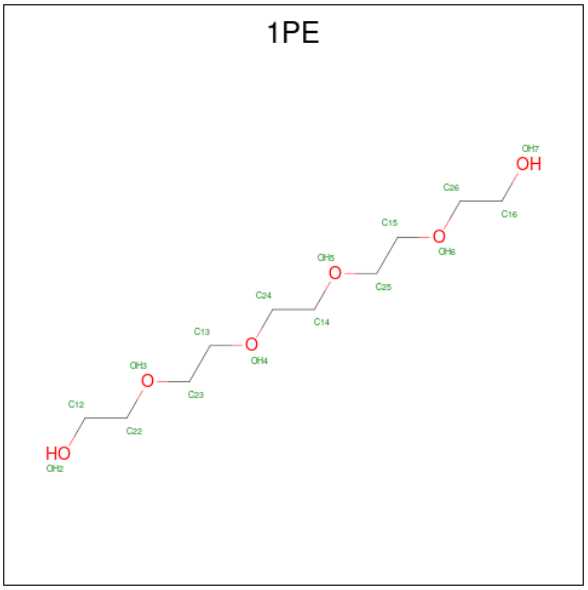
Continued from previous page...

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.

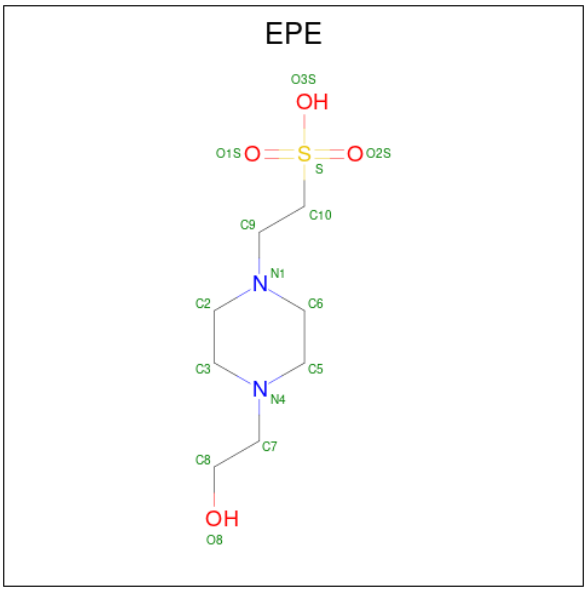
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	488	3854	2449	661	723	21	0	2	0

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



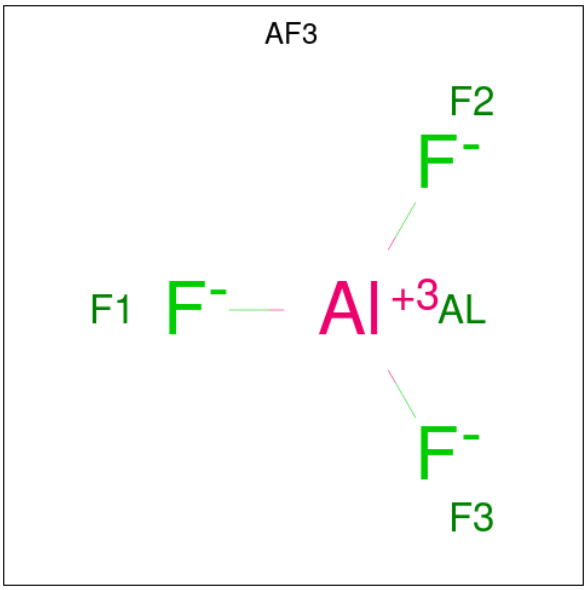
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	16	10	6	0	0

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



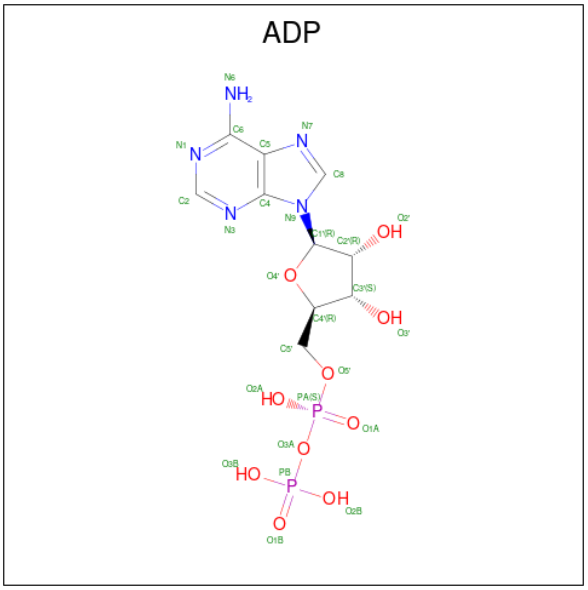
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	B	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	D	1	15	8	2	4	1	0	0

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



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

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

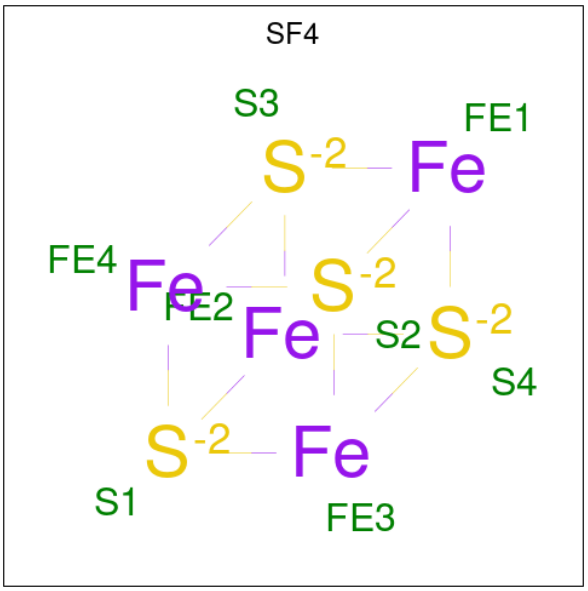


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	27	10	5	10	2	0	0
7	B	1	27	10	5	10	2	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

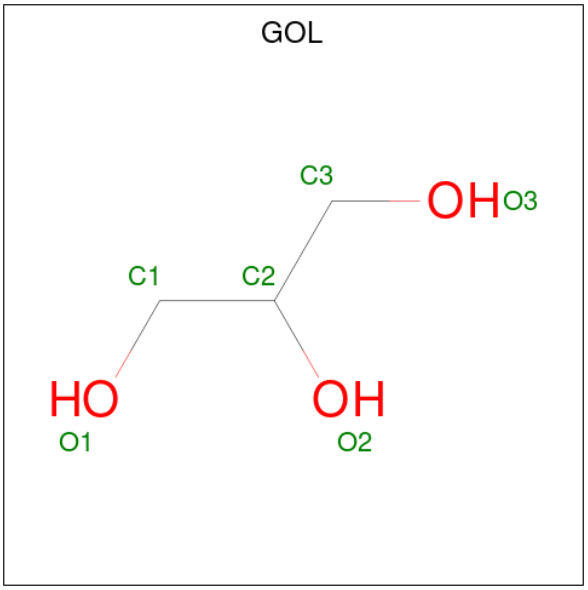
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	A	1	1	1	0	0
8	B	1	1	1	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



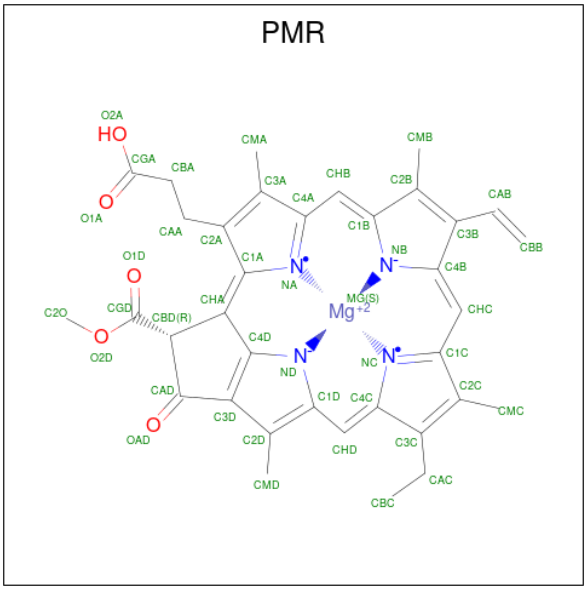
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0

Continued on next page...

Continued from previous page...

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

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



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

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

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

- Molecule 13 is water.

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

Continued on next page...

Continued from previous page...

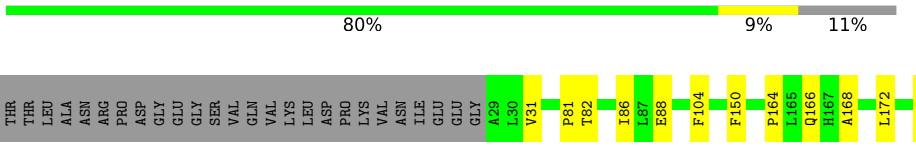
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	D	127	127	127	0	0

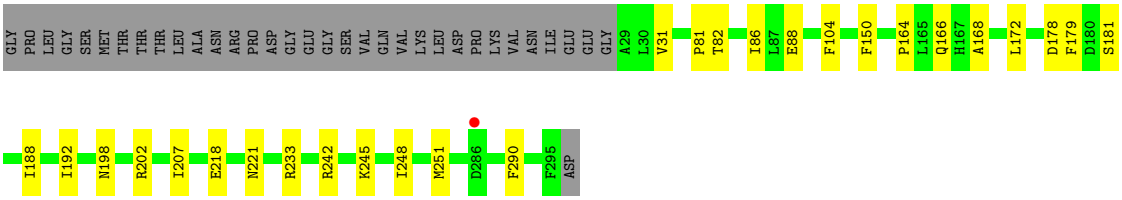
3 Residue-property plots (i)

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: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE IRON-SULFUR ATP-BINDING PROTEIN

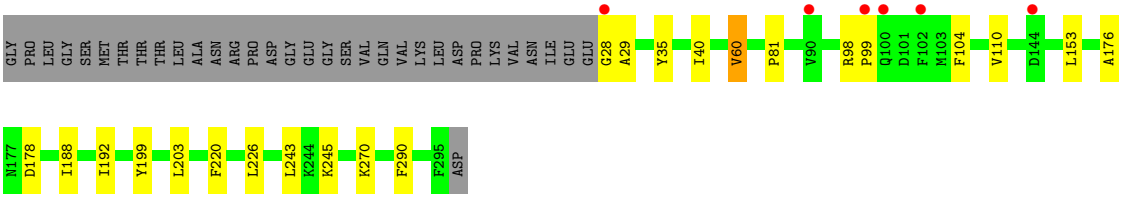
Chain A:





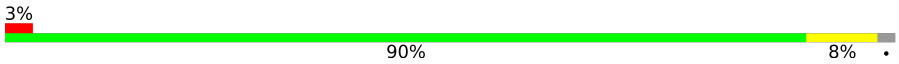
• Molecule 1: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE IRON-SULFUR ATP-BINDING PROTEIN

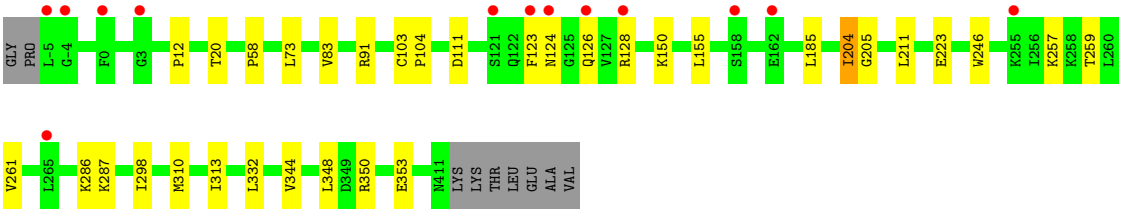
Chain B:



• Molecule 2: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT N

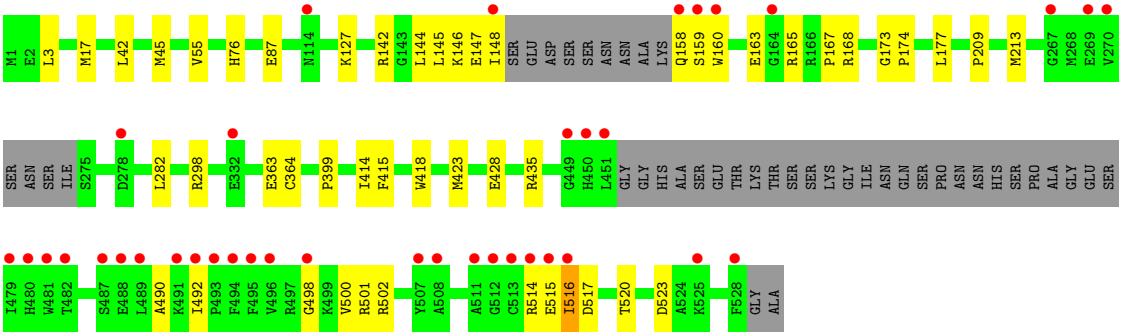
Chain C:





• Molecule 3: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B

Chain D:


M1 E2 L3 M17 L42 M45 V55 H76 E87 N114 K127 R142 G143 L144 L145 K146 E147 I148 SER GLU ASP SER SER ASN ASN ALA LYS Q158 S159 W160 E163 G164 R165 R166 P167 R168 G173 P174 L177 P209 M213 G267 M268 E269 V270
SER ASN SER ILE S275 D278 L282 R298 E332 E363 C364 P399 I414 F415 W418 M423 E428 R435 G449 H450 L451 GLY GLY HIS ALA SER GLU THR LYS THR SER SER LYS GLY ILE ASN GLN SER PRO ASN ASN HIS SER PRO ALA GLY GLU SER
I479 H480 W481 T482 S487 E488 L489 A490 R491 I492 P493 F494 F495 V496 R497 G498 K499 V500 R501 R502 Y507 A508 A511 G512 C513 R514 E515 I516 D517 T520 D523 A524 K525 F528 GLY ALA

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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 (i)

5.1 Standard geometry (i)

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

Continued on next page...

Continued from previous page...

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.

The worst 5 of 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

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
All	All	1429/1558 (92%)	1387 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	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

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	144	LEU
3	D	158	GLN
3	D	516	ILE
1	B	270	LYS
2	C	124	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	407	GLN
2	C	411	ASN
3	D	480	HIS
3	D	158	GLN
2	C	343	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	$\#\|Z\| > 2$
6	AF3	B	1298	7,13	0,3,3	-	-	-		
5	EPE	D	1529	-	15,15,15	0.73	1 (6%)	18,20,20	1.80	4 (22%)
7	ADP	A	1300	8,6	27,29,29	1.38	4 (14%)	42,45,45	1.92	11 (26%)
10	GOL	D	1532	-	5,5,5	0.24	0	5,5,5	0.25	0
7	ADP	B	1299	8,6	27,29,29	1.36	4 (14%)	42,45,45	1.92	11 (26%)
10	GOL	C	1412	-	5,5,5	0.21	0	5,5,5	0.37	0
10	GOL	A	1303	-	5,5,5	0.26	0	5,5,5	0.39	0
10	GOL	D	1530	-	5,5,5	0.25	0	5,5,5	0.34	0
6	AF3	A	1299	7,13	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	PMR	C	1414	13	49,53,53	2.37	17 (34%)	62,89,89	3.37	29 (46%)
4	1PE	A	1296	-	15,15,15	0.44	0	14,14,14	0.44	0
9	SF4	A	1302	1	0,12,12	-	-	-		
5	EPE	A	1297	-	15,15,15	0.84	1 (6%)	18,20,20	1.79	5 (27%)
5	EPE	A	1298	-	15,15,15	0.86	1 (6%)	18,20,20	1.75	5 (27%)
5	EPE	B	1296	-	15,15,15	0.80	1 (6%)	18,20,20	1.67	5 (27%)
9	SF4	C	1413	2,3	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	D	1529	-	-	4/9/19/19	0/1/1/1
7	ADP	A	1300	8,6	-	2/16/32/32	0/3/3/3
10	GOL	D	1532	-	-	3/4/4/4	-
7	ADP	B	1299	8,6	-	0/16/32/32	0/3/3/3
10	GOL	C	1412	-	-	0/4/4/4	-
11	PMR	C	1414	13	3/3/6/10	8/15/71/71	-
10	GOL	A	1303	-	-	3/4/4/4	-
10	GOL	D	1530	-	-	0/4/4/4	-
4	1PE	A	1296	-	-	3/13/13/13	-
9	SF4	A	1302	1	-	-	0/6/5/5
5	EPE	A	1297	-	-	4/9/19/19	0/1/1/1
5	EPE	A	1298	-	-	2/9/19/19	0/1/1/1
5	EPE	B	1296	-	-	4/9/19/19	0/1/1/1
9	SF4	C	1413	2,3	-	-	0/6/5/5

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1414	PMR	C3C-C2C	5.45	1.48	1.36
11	C	1414	PMR	O2D-CGD	5.15	1.45	1.33
11	C	1414	PMR	C3B-C2B	4.75	1.46	1.37
11	C	1414	PMR	C2A-C3A	4.69	1.46	1.36
7	A	1300	ADP	C5-C4	4.68	1.47	1.39

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	1414	PMR	C1A-NA-C4A	-9.28	102.54	106.71
11	C	1414	PMR	C2B-C1B-NB	9.09	116.80	110.10
11	C	1414	PMR	CMD-C2D-C1D	8.95	139.00	125.37
11	C	1414	PMR	C3C-C4C-NC	7.12	116.58	109.88
11	C	1414	PMR	C3B-C2B-C1B	-6.62	100.75	107.08

All (3) chirality outliers are listed below:

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

5 of 33 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

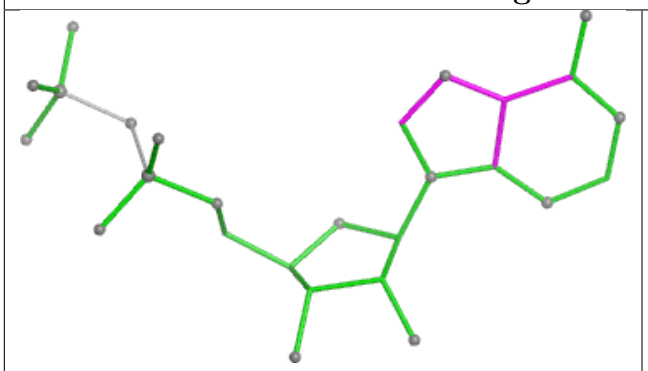
There are no ring outliers.

4 monomers are involved in 10 short contacts:

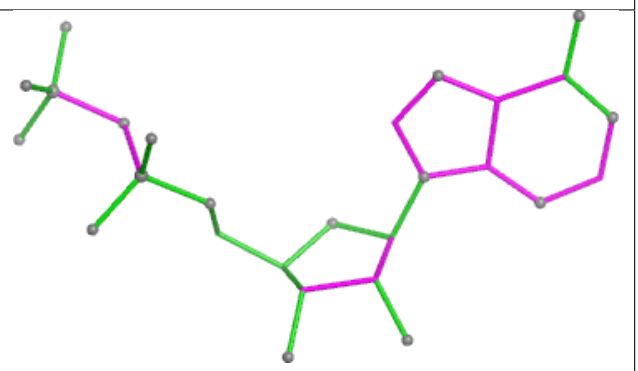
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1529	EPE	2	0
10	A	1303	GOL	2	0
11	C	1414	PMR	3	0
4	A	1296	1PE	3	0

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.

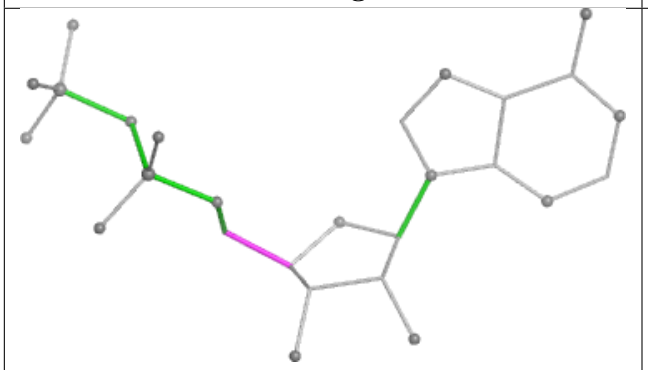
Ligand ADP A 1300



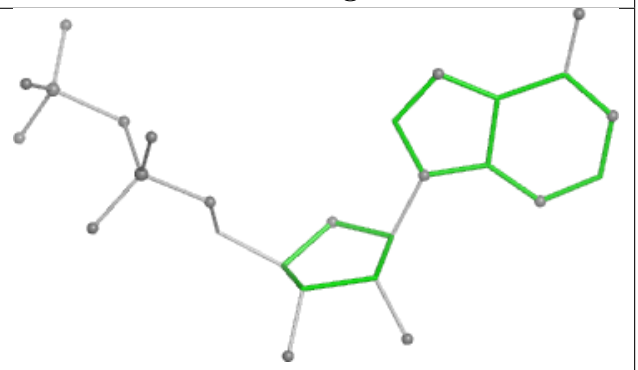
Bond lengths



Bond angles

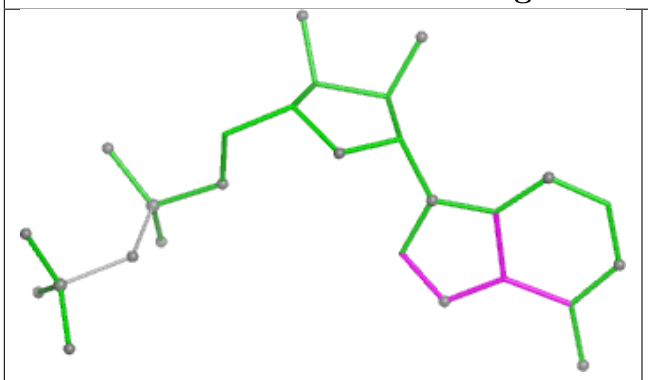


Torsions

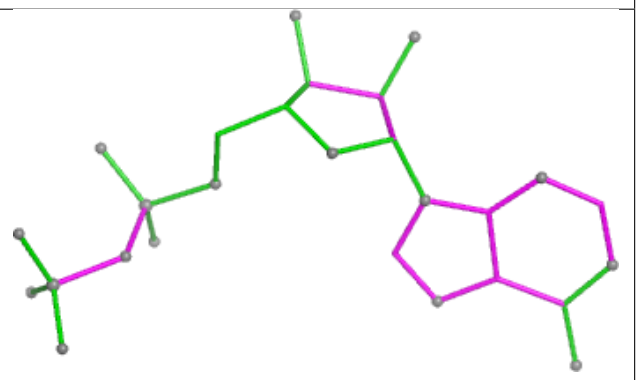


Rings

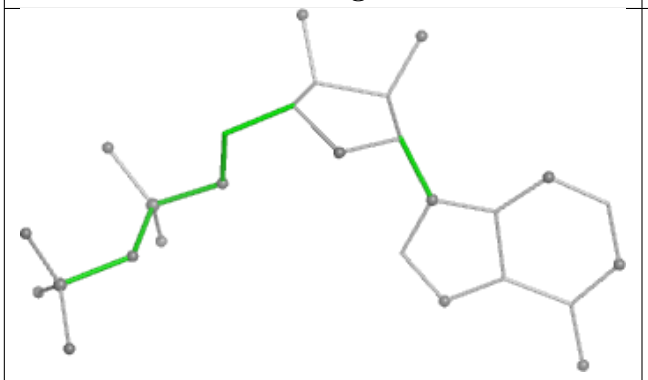
Ligand ADP B 1299



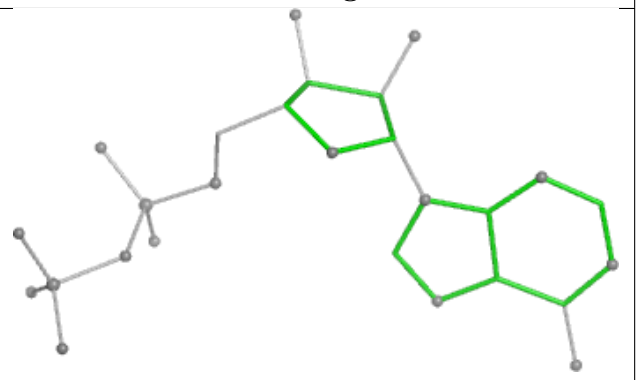
Bond lengths



Bond angles

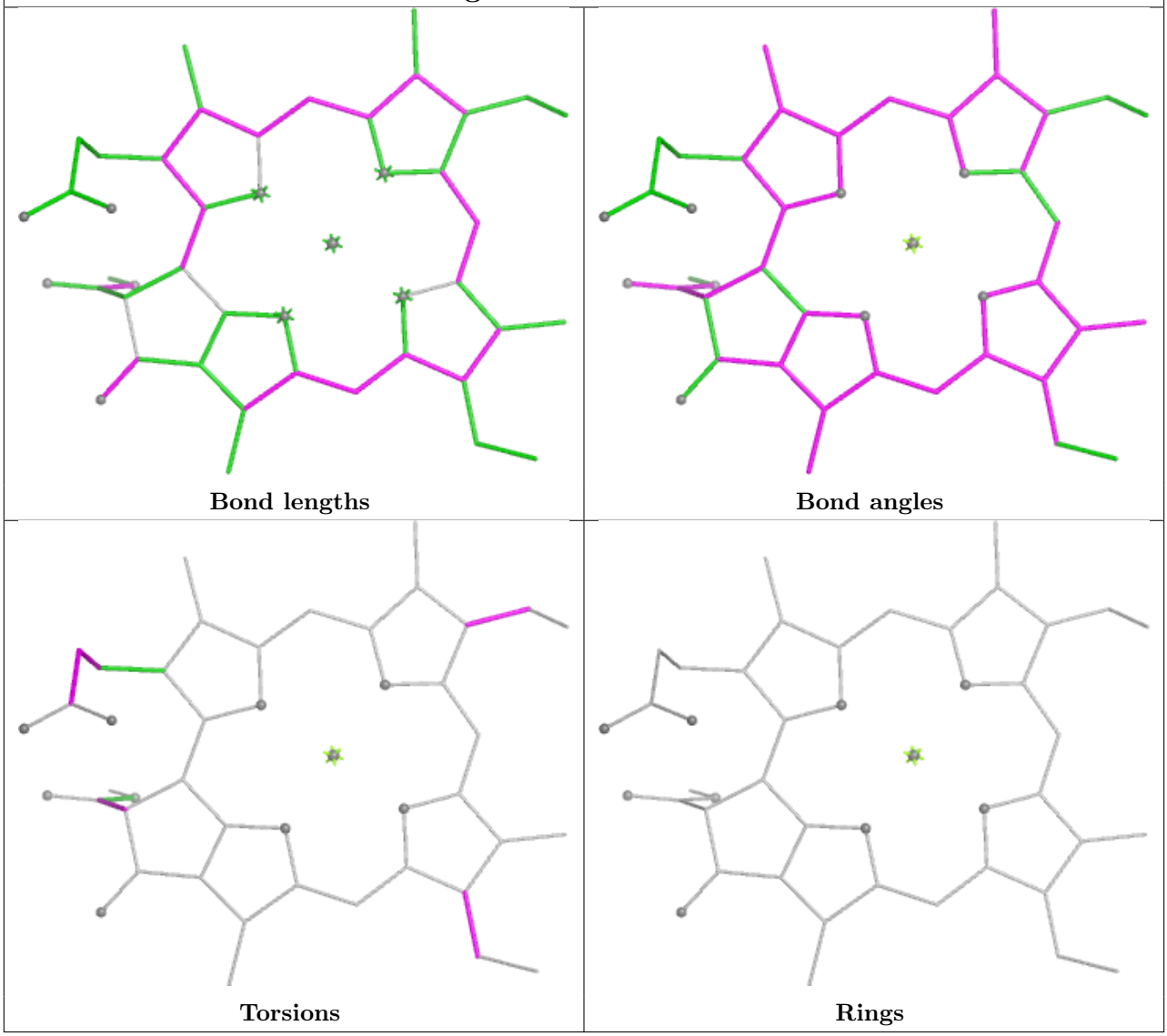


Torsions



Rings

Ligand PMR C 1414



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)

The worst 5 of 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

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

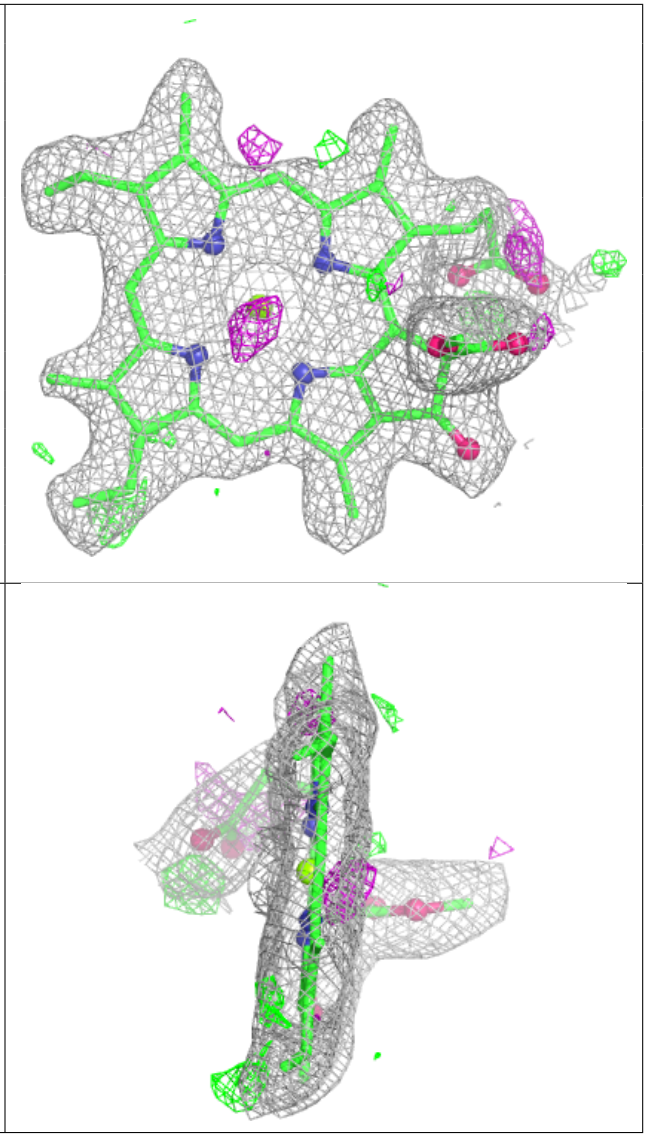
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.

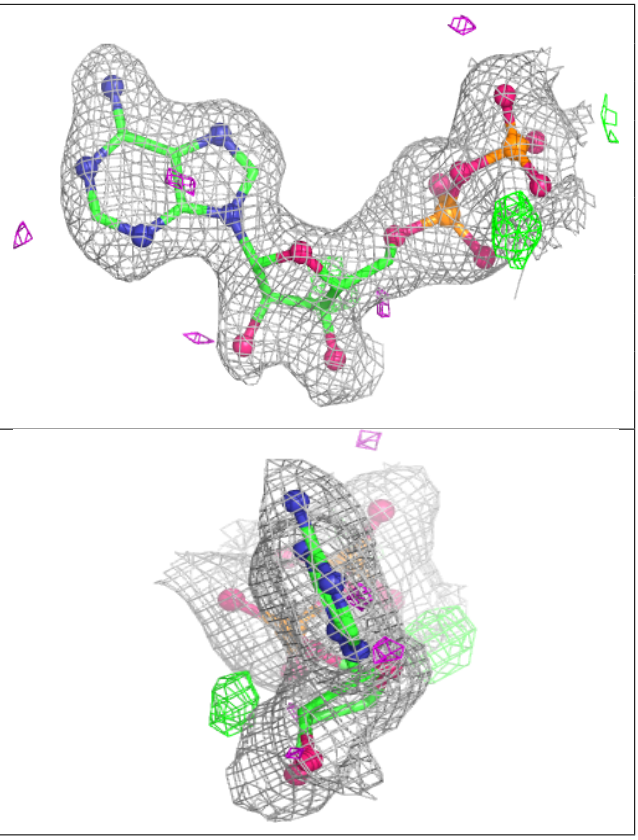
Electron density around PMR C 1414:

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



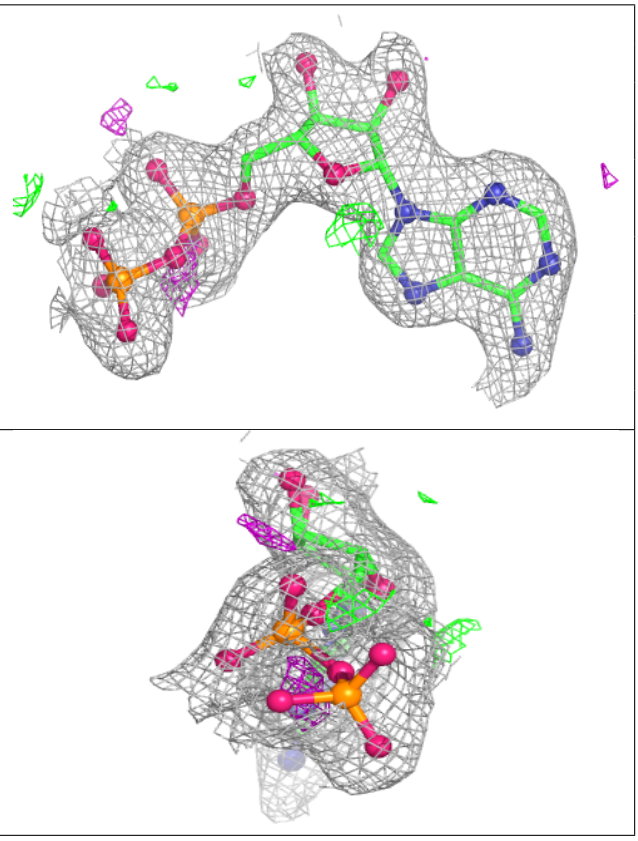
Electron density around ADP A 1300:

$2mF_o$-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.