Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:52 AM GMT

PDB ID	:	2YNM
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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

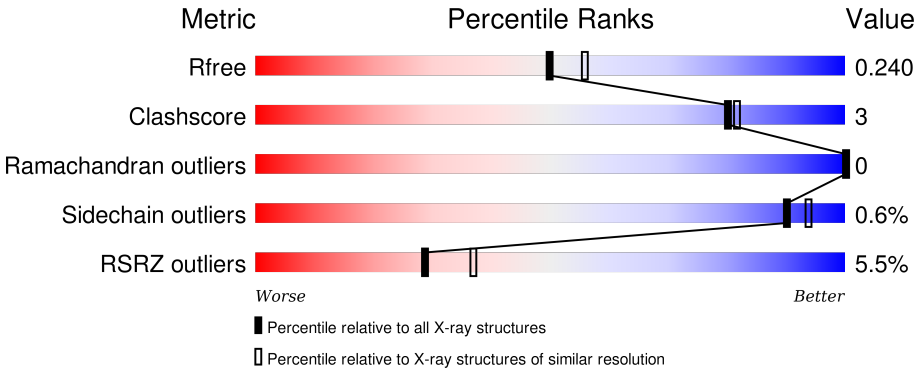
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 79% 10% 11%
1	B	301	3% 81% 8% 11%
2	C	426	6% 90% 7%
3	D	530	7% 84% 8% 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
10	GOL	A	1303	-	-	-	X
4	1PE	A	1296	-	-	-	X
5	EPE	D	1529	-	-	-	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
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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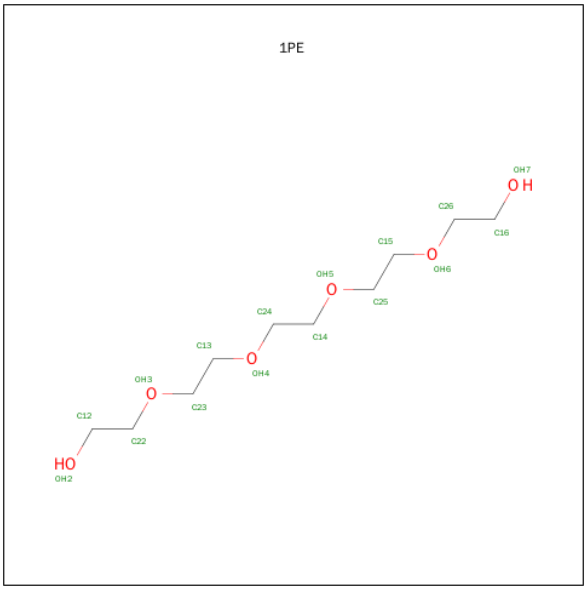
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	EXPRESSION TAG	UNP Q7VD37
C	-4	GLY	-	EXPRESSION TAG	UNP Q7VD37
C	-3	SER	-	EXPRESSION TAG	UNP Q7VD37
C	-2	PRO	-	EXPRESSION TAG	UNP Q7VD37
C	-1	GLU	-	EXPRESSION TAG	UNP Q7VD37
C	0	PHE	-	EXPRESSION TAG	UNP Q7VD37

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

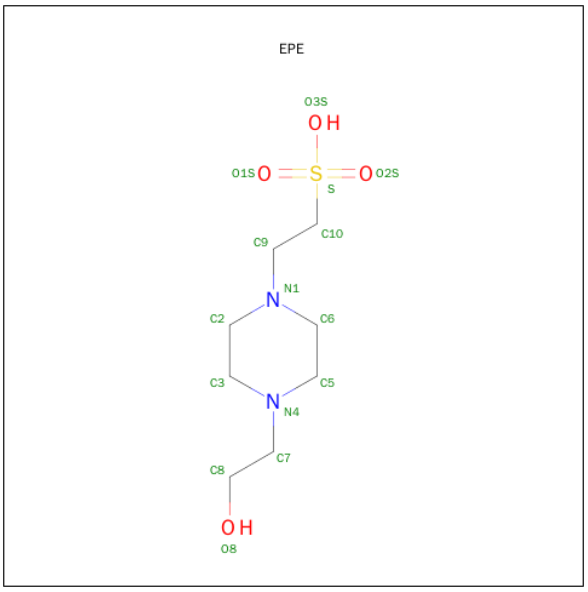
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	488	Total	C	N	O	S	0	2	0
			3854	2449	661	723	21			

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



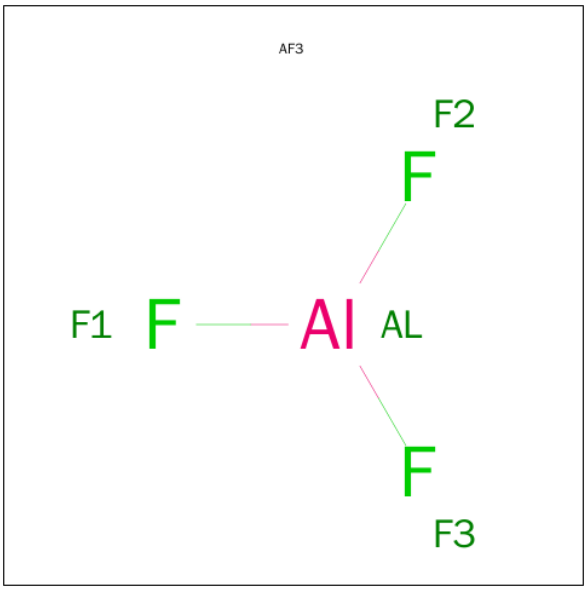
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			16	10	6			

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



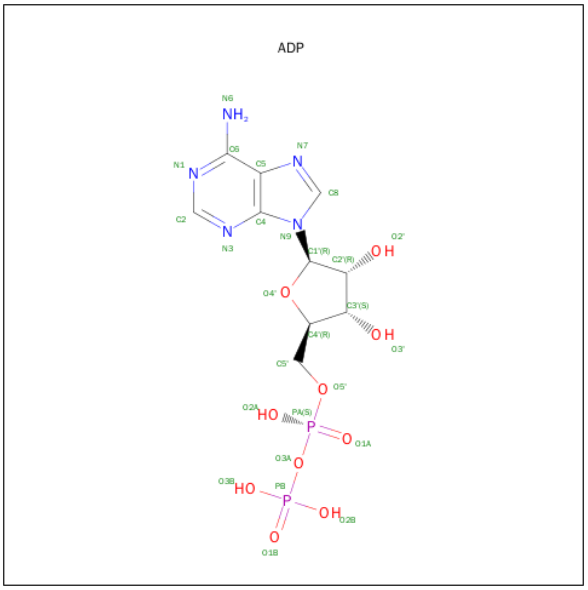
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



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

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

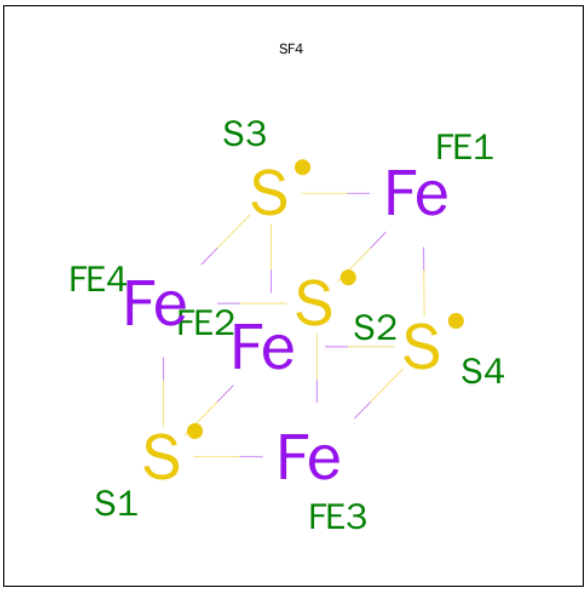


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 27 10 5 10 2	0	0
7	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

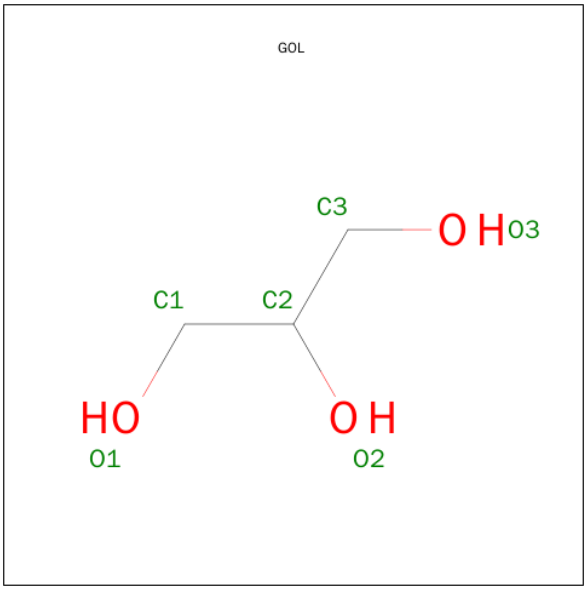
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	A	1	Total Mg 1 1	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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



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

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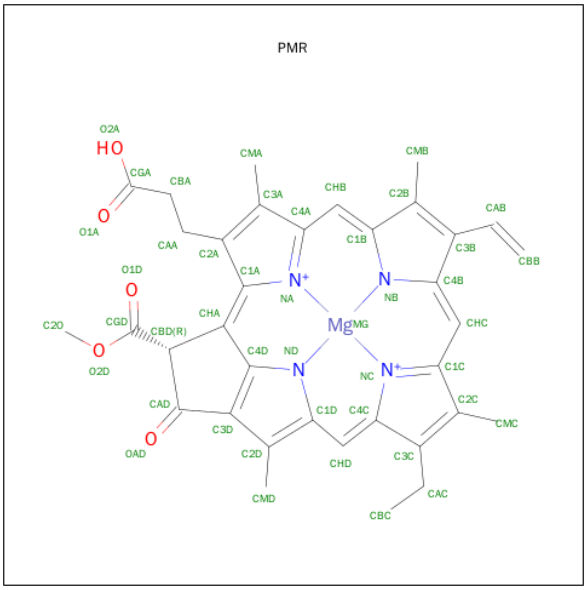
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total C O 6 3 3	0	0
10	D	1	Total C O 6 3 3	0	0

- Molecule 11 is PROTOCHLOROPHYLLIDE (three-letter code: PMR) (formula: $C_{35}H_{32}MgN_4O_5$).



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

- Molecule 12 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 13 is water.

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

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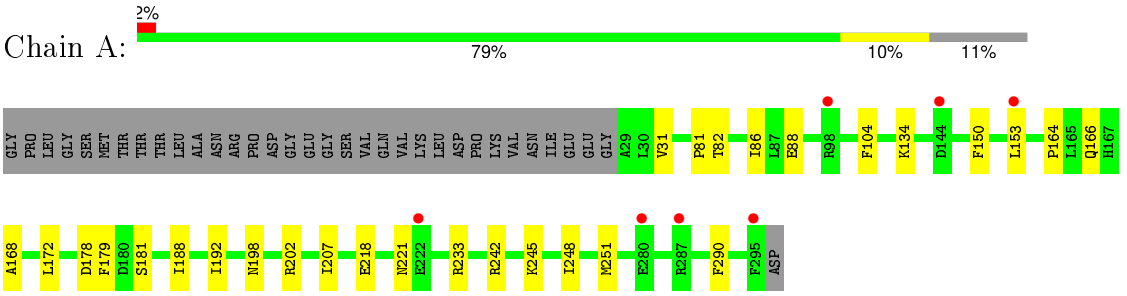
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	127	Total	O	0	0
			127	127		

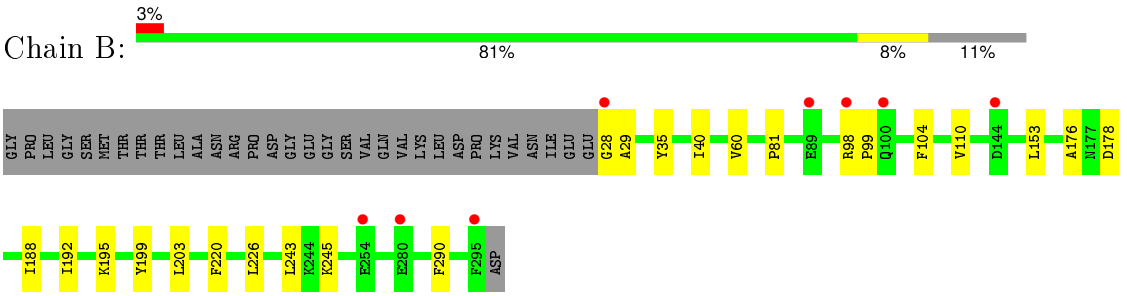
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

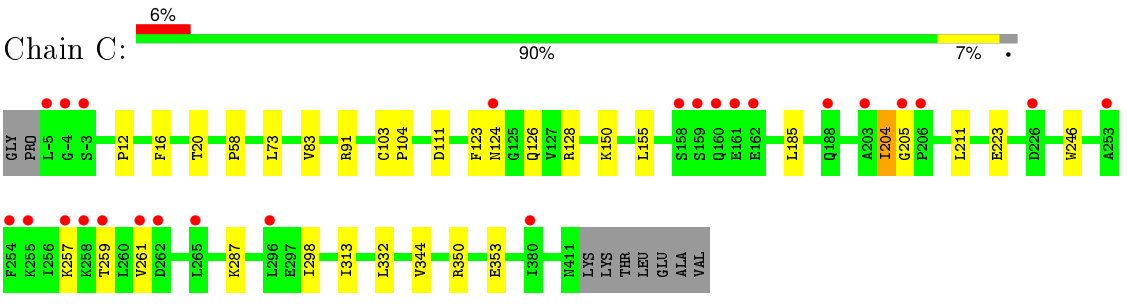
• Molecule 1: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE IRON-SULFUR ATP-BINDING PROTEIN



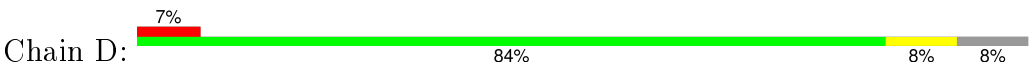
• Molecule 1: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE IRON-SULFUR ATP-BINDING PROTEIN

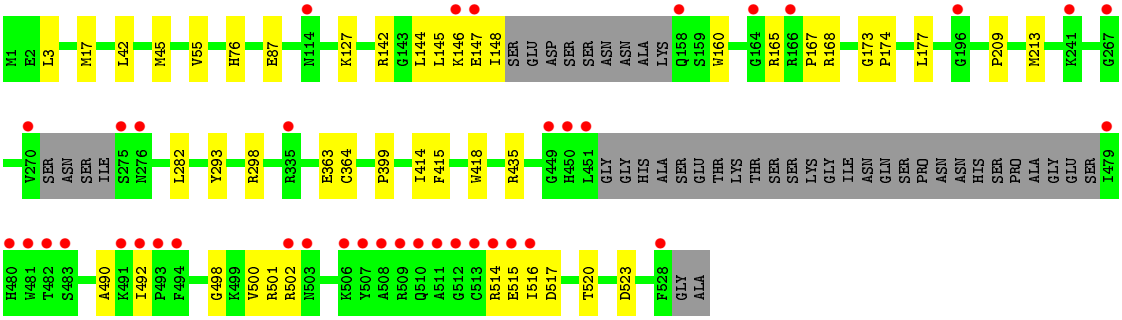


• Molecule 2: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT N



• Molecule 3: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B




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 G164 R165 R166 P167 R168 G173 P174 L177 G196 P209 M213 K241 G267
V270 SER ASN SER ILE S275 N276 L282 Y293 R298 R335 E363 C364 P399 I414 F415 W418 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 S483 A490 K491 I492 P493 F494 G498 K499 V500 R501 R502 N503 K506 Y507 A508 R509 Q510 A511 G512 C513 R514 E515 I516 D517 T520 D523 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 0.208 , 0.240	Depositor DCC
R_{free} test set	4030 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.7	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 81370 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, ADP, PMR, SF4, 1PE, EPE, K, 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	0.22	0/2091	0.40	0/2821
1	B	0.23	0/2104	0.40	0/2838
2	C	0.22	0/3300	0.42	0/4469
3	D	0.22	0/3942	0.41	0/5335
All	All	0.22	0/11437	0.41	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

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	20	0
1	B	2069	0	2064	16	0
2	C	3238	0	3321	19	0
3	D	3854	0	3808	27	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	5	0
12	D	1	0	0	0	0
13	A	89	0	0	5	0
13	B	63	0	0	0	0
13	C	103	0	0	0	0
13	D	127	0	0	1	0
All	All	11825	0	11426	78	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 (78) 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
11:C:1414:PMR:HMAA	3:D:45:MET:HB3	1.73	0.70
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
2:C:150:LYS:HG3	2:C:223:GLU:HG3	1.82	0.61
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:B:199:TYR:OH	2:C:111:ASP:OD2	2.17	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
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
3:D:498:GLY:O	3:D:502:ARG:HG2	2.13	0.48
2:C:211:LEU:HB3	2:C:246:TRP:CZ2	2.49	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
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
3:D:145:LEU:HD21	3:D:213:MET:HA	1.97	0.46
1:B:60:VAL:HG13	1:B:110:VAL:HG22	1.98	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
3:D:17:MET:HG3	3:D:55:VAL:HG21	1.97	0.45
2:C:83:VAL:HG13	3:D:3:LEU:HB2	1.98	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
11:C:1414:PMR:HMC	11:C:1414:PMR:HBCB	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
13:A:2040:HOH:O	1:B:195:LYS:NZ	2.38	0.43
5:D:1529:EPE:H101	5:D:1529:EPE:H61	1.66	0.42
3:D:173:GLY:N	3:D:174:PRO:HD2	2.34	0.42
3:D:414:ILE:HG23	3:D:418:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:THR:HB	11:C:1414:PMR:HBCB	2.02	0.42
1:A:198:ASN:HD21	4:A:1296:1PE:H162	1.84	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:B:98:ARG:HG3	1:B:99:PRO:HD2	2.02	0.42
1:A:188:ILE:O	1:A:192:ILE:HG12	2.20	0.42
1:A:134:LYS:NZ	13:A:2044:HOH:O	2.39	0.41
1:A:248:ILE:HD12	1:A:251:MET:HG3	2.01	0.41
2:C:16:PHE:CZ	11:C:1414:PMR:HMCB	2.55	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:HD3	3:D:127:LYS:HA	1.86	0.40
1:B:220:PHE:HE2	1:B:226:LEU:HD12	1.86	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
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%)	222 (99%)	2 (1%)	84 89
1	B	225/252 (89%)	224 (100%)	1 (0%)	93 96
2	C	354/361 (98%)	352 (99%)	2 (1%)	90 94
3	D	412/443 (93%)	410 (100%)	2 (0%)	92 95
All	All	1215/1308 (93%)	1208 (99%)	7 (1%)	90 94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LEU
1	A	166	GLN
1	B	153	LEU
2	C	124	ASN
2	C	204	ILE
3	D	144	LEU
3	D	293	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	343	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
4	1PE	A	1296	-	15,15,15	0.45	0	14,14,14	0.45	0
5	EPE	A	1297	-	14,15,15	0.37	0	18,20,20	1.81	5 (27%)
5	EPE	A	1298	-	14,15,15	0.36	0	18,20,20	1.94	6 (33%)
6	AF3	A	1299	13,7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	A	1300	8,6	22,29,29	1.01	1 (4%)	27,45,45	1.84	5 (18%)
9	SF4	A	1302	1	0,12,12	0.00	-	0,24,24	0.00	-
10	GOL	A	1303	-	5,5,5	0.21	0	5,5,5	0.36	0
5	EPE	B	1296	-	14,15,15	0.41	0	18,20,20	1.87	5 (27%)
6	AF3	B	1298	8,13,7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	B	1299	8,6	22,29,29	0.99	1 (4%)	27,45,45	1.84	4 (14%)
10	GOL	C	1412	-	5,5,5	0.17	0	5,5,5	0.32	0
9	SF4	C	1413	3,2	0,12,12	0.00	-	0,24,24	0.00	-
11	PMR	C	1414	13	36,53,53	2.44	15 (41%)	38,89,89	3.00	21 (55%)
5	EPE	D	1529	-	14,15,15	0.37	0	18,20,20	1.79	5 (27%)
10	GOL	D	1530	-	5,5,5	0.21	0	5,5,5	0.31	0
10	GOL	D	1532	-	5,5,5	0.18	0	5,5,5	0.20	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
4	1PE	A	1296	-	-	0/13/13/13	0/0/0/0
5	EPE	A	1297	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	A	1298	-	-	0/9/19/19	0/1/1/1
6	AF3	A	1299	13,7	-	0/0/0/0	0/0/0/0
7	ADP	A	1300	8,6	-	0/12/32/32	0/3/3/3
9	SF4	A	1302	1	-	0/0/48/48	0/6/5/5
10	GOL	A	1303	-	-	0/4/4/4	0/0/0/0
5	EPE	B	1296	-	-	0/9/19/19	0/1/1/1
6	AF3	B	1298	8,13,7	-	0/0/0/0	0/0/0/0
7	ADP	B	1299	8,6	-	0/12/32/32	0/3/3/3
10	GOL	C	1412	-	-	0/4/4/4	0/0/0/0
9	SF4	C	1413	3,2	-	0/0/48/48	0/6/5/5
11	PMR	C	1414	13	-	0/11/111/111	0/0/9/9
5	EPE	D	1529	-	-	0/9/19/19	0/1/1/1
10	GOL	D	1530	-	-	0/4/4/4	0/0/0/0
10	GOL	D	1532	-	-	0/4/4/4	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1414	PMR	C3D-C4D	-4.23	1.35	1.41
11	C	1414	PMR	C4C-C3C	2.07	1.48	1.45
11	C	1414	PMR	C1A-C2A	2.13	1.49	1.45
11	C	1414	PMR	C4D-CHA	2.19	1.47	1.45
11	C	1414	PMR	CHC-C1C	2.43	1.46	1.41
11	C	1414	PMR	C1D-CHD	2.55	1.46	1.39
11	C	1414	PMR	CHB-C4A	2.58	1.47	1.41
11	C	1414	PMR	C1A-CHA	2.68	1.49	1.40
11	C	1414	PMR	C3D-C2D	2.80	1.46	1.40
7	B	1299	ADP	C5-C4	3.11	1.47	1.40
7	A	1300	ADP	C5-C4	3.22	1.47	1.40
11	C	1414	PMR	CHD-C4C	3.86	1.47	1.35
11	C	1414	PMR	OAD-CAD	4.33	1.29	1.22
11	C	1414	PMR	C2A-C3A	4.63	1.46	1.36
11	C	1414	PMR	O2D-CGD	4.92	1.45	1.33
11	C	1414	PMR	C3B-C2B	4.99	1.46	1.40
11	C	1414	PMR	C3C-C2C	5.36	1.48	1.36

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1300	ADP	N3-C2-N1	-6.98	123.55	128.89
7	B	1299	ADP	N3-C2-N1	-6.61	123.83	128.89
11	C	1414	PMR	C4A-C3A-C2A	-3.50	102.73	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	1414	PMR	C4C-C3C-C2C	-3.29	101.60	106.94
11	C	1414	PMR	C1C-C2C-C3C	-3.29	102.98	106.91
7	B	1299	ADP	PA-O3A-PB	-3.22	121.86	132.67
11	C	1414	PMR	C4C-NC-C1C	-3.21	102.36	106.27
11	C	1414	PMR	CHD-C4C-C3C	-3.18	119.09	125.42
7	A	1300	ADP	C4-C5-N7	-3.14	106.59	109.48
7	B	1299	ADP	C4-C5-N7	-3.07	106.66	109.48
11	C	1414	PMR	CHB-C4A-C3A	-3.02	119.77	124.83
11	C	1414	PMR	C1A-NA-C4A	-3.02	102.54	106.11
7	A	1300	ADP	PA-O3A-PB	-2.95	122.79	132.67
11	C	1414	PMR	CHC-C1C-C2C	-2.75	120.23	124.83
11	C	1414	PMR	O2D-CGD-O1D	-2.64	118.34	123.79
7	B	1299	ADP	C2'-C1'-N9	-2.58	110.35	114.29
11	C	1414	PMR	C3B-CAB-CBB	-2.58	121.04	126.32
11	C	1414	PMR	C1A-C2A-C3A	-2.40	102.73	106.62
11	C	1414	PMR	C1D-CHD-C4C	-2.34	124.25	129.26
5	A	1298	EPE	C3-C2-N1	-2.27	106.57	110.63
11	C	1414	PMR	O1D-CGD-CBD	-2.20	121.47	124.62
7	A	1300	ADP	C2'-C1'-N9	-2.13	111.04	114.29
7	A	1300	ADP	O3B-PB-O2B	2.07	115.28	107.38
5	A	1298	EPE	C7-N4-C3	2.09	116.63	111.27
5	D	1529	EPE	O2S-S-C10	2.18	108.77	106.91
11	C	1414	PMR	CMB-C2B-C3B	2.28	129.55	125.09
5	D	1529	EPE	O1S-S-C10	2.36	108.92	106.91
5	A	1298	EPE	C7-N4-C5	2.38	117.37	111.27
5	A	1297	EPE	O1S-S-C10	2.40	108.96	106.91
11	C	1414	PMR	CMA-C3A-C4A	2.63	129.09	125.02
5	B	1296	EPE	C7-N4-C5	2.68	118.13	111.27
5	B	1296	EPE	C7-N4-C3	2.69	118.17	111.27
5	A	1297	EPE	C7-N4-C5	2.78	118.40	111.27
5	A	1297	EPE	C7-N4-C3	2.83	118.53	111.27
5	A	1297	EPE	O2S-S-C10	2.86	109.34	106.91
11	C	1414	PMR	C4B-CHC-C1C	2.87	126.94	122.60
11	C	1414	PMR	C1B-CHB-C4A	2.95	127.07	122.60
5	D	1529	EPE	C7-N4-C3	3.02	119.00	111.27
11	C	1414	PMR	CAC-C3C-C2C	3.17	133.06	127.51
5	D	1529	EPE	C7-N4-C5	3.33	119.80	111.27
5	A	1298	EPE	O2S-S-C10	3.33	109.75	106.91
5	B	1296	EPE	O1S-S-C10	3.52	109.91	106.91
5	A	1298	EPE	O1S-S-C10	3.63	110.00	106.91
5	B	1296	EPE	C5-N4-C3	3.69	116.90	108.90
5	B	1296	EPE	O2S-S-C10	3.85	110.19	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1297	EPE	C5-N4-C3	4.43	118.50	108.90
5	A	1298	EPE	C5-N4-C3	4.44	118.51	108.90
5	D	1529	EPE	C5-N4-C3	4.50	118.64	108.90
11	C	1414	PMR	CMD-C2D-C1D	6.43	139.00	128.36
11	C	1414	PMR	O2D-CGD-CBD	6.48	120.19	111.30
11	C	1414	PMR	C2A-C1A-NA	9.01	115.48	110.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

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

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, 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	267/301 (88%)	0.05	7 (2%)	59	66	19, 35, 63, 78	0
1	B	268/301 (89%)	0.17	8 (2%)	54	62	18, 37, 64, 83	0
2	C	417/426 (97%)	0.21	25 (5%)	25	33	19, 42, 71, 96	0
3	D	488/530 (92%)	0.29	39 (7%)	15	21	22, 35, 83, 133	0
All	All	1440/1558 (92%)	0.20	79 (5%)	29	37	18, 38, 72, 133	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	512	GLY	6.7
3	D	513	CYS	6.5
3	D	514	ARG	6.1
3	D	515	GLU	5.7
3	D	479	ILE	5.5
3	D	483	SER	5.1
3	D	158	GLN	4.8
3	D	480	HIS	4.7
3	D	450	HIS	4.6
3	D	493	PRO	4.6
1	B	280	GLU	4.2
2	C	-3	SER	4.2
2	C	-4	GLY	4.1
1	B	144	ASP	4.1
3	D	516	ILE	4.1
3	D	528	PHE	4.1
1	B	28	GLY	4.0
3	D	451	LEU	4.0
1	B	98	ARG	3.9
3	D	510	GLN	3.8
3	D	508	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	287	ARG	3.6
2	C	160	GLN	3.5
3	D	114	ASN	3.4
3	D	507	TYR	3.4
2	C	259	THR	3.3
2	C	124	ASN	3.3
2	C	206	PRO	3.3
1	A	295	PHE	3.2
2	C	188	GLN	2.9
3	D	164	GLY	2.9
2	C	258	LYS	2.9
3	D	502	ARG	2.9
2	C	261	VAL	2.8
2	C	203	ALA	2.8
1	A	280	GLU	2.7
1	B	89	GLU	2.7
2	C	158	SER	2.7
2	C	253	ALA	2.7
3	D	449	GLY	2.7
3	D	509	ARG	2.7
3	D	511	ALA	2.7
1	A	144	ASP	2.6
1	B	254	GLU	2.6
3	D	481	TRP	2.6
2	C	162	GLU	2.6
1	B	100	GLN	2.6
2	C	159	SER	2.6
1	A	98	ARG	2.6
2	C	255	LYS	2.5
2	C	-5	LEU	2.5
3	D	270	VAL	2.5
3	D	335	ARG	2.5
1	A	222	GLU	2.3
3	D	494	PHE	2.3
2	C	205	GLY	2.3
3	D	492	ILE	2.3
2	C	226	ASP	2.3
1	A	153	LEU	2.3
2	C	262	ASP	2.3
3	D	147	GLU	2.3
3	D	506	LYS	2.3
3	D	276	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	196	GLY	2.2
2	C	254	PHE	2.2
2	C	265	LEU	2.2
3	D	241	LYS	2.1
3	D	267	GLY	2.1
2	C	380	ILE	2.1
2	C	257	LYS	2.1
3	D	482	THR	2.1
2	C	296	LEU	2.1
1	B	295	PHE	2.1
3	D	146	LYS	2.1
3	D	503	ASN	2.1
3	D	275	SER	2.1
2	C	161	GLU	2.0
3	D	166	ARG	2.0
3	D	491	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	EPE	D	1529	15/15	0.77	0.31	7.93	60,66,74,75	0
10	GOL	A	1303	6/6	0.60	0.44	7.13	63,69,71,71	0
4	1PE	A	1296	16/16	0.74	0.26	3.82	49,64,71,72	0
5	EPE	A	1297	15/15	0.93	0.19	1.51	32,46,53,54	0
5	EPE	A	1298	15/15	0.91	0.15	1.47	39,41,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	GOL	D	1532	6/6	0.88	0.17	1.23	38,42,45,46	0
11	PMR	C	1414	45/45	0.93	0.15	0.88	14,23,28,39	0
5	EPE	B	1296	15/15	0.92	0.17	0.85	35,58,60,60	0
6	AF3	B	1298	4/4	0.96	0.19	0.40	25,27,29,44	0
7	ADP	B	1299	27/27	0.97	0.14	-0.19	20,29,38,39	0
6	AF3	A	1299	4/4	0.97	0.17	-0.23	17,27,32,39	0
10	GOL	C	1412	6/6	0.97	0.12	-0.34	25,33,36,38	0
10	GOL	D	1530	6/6	0.97	0.13	-0.35	20,30,33,35	0
7	ADP	A	1300	27/27	0.96	0.12	-0.43	20,31,34,38	0
9	SF4	A	1302	8/8	0.99	0.11	-1.10	17,19,21,22	0
9	SF4	C	1413	8/8	0.99	0.11	-1.21	19,22,25,26	0
8	MG	A	1301	1/1	0.99	0.11	-1.54	26,26,26,26	0
8	MG	B	1297	1/1	0.92	0.11	-1.85	34,34,34,34	0
12	K	D	1531	1/1	0.73	0.10	-	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.