Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 11:03 am BST

PDB ID	:	5AOV
Title	:	Ternary Crystal Structure of Pyrococcus furiosus Glyoxylate Hydroxypyruvate Reductase in presence of glyoxylate
Authors	:	Lassalle, L.; Girard, E.
Deposited on	:	2015-09-12
Resolution	:	1.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

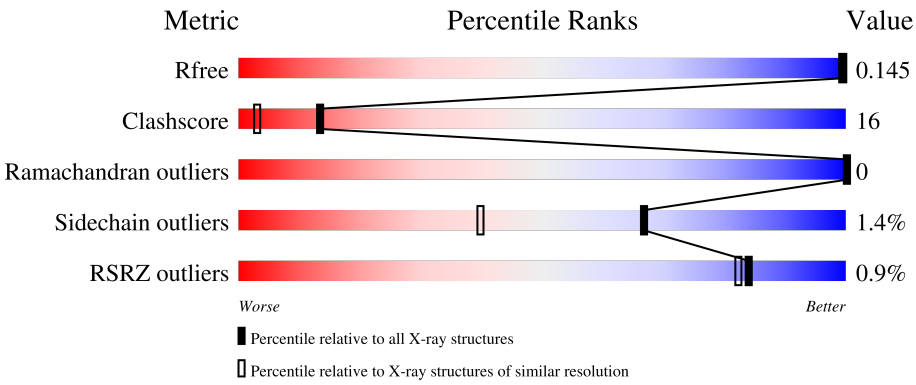
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

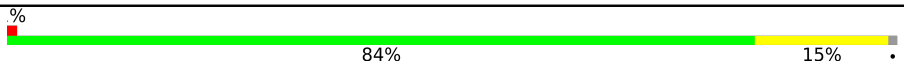
The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	336	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	A	1335[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLV	A	1336	-	X	-	-
3	GLV	A	1356	-	-	X	-
4	1PE	A	1342	-	X	-	-
4	1PE	A	1343	-	-	X	-
4	1PE	A	1345	-	X	-	-
4	1PE	A	1347	-	-	X	-
4	1PE	A	1349	-	-	X	-
4	1PE	A	1359	-	-	X	-

2 Entry composition (i)

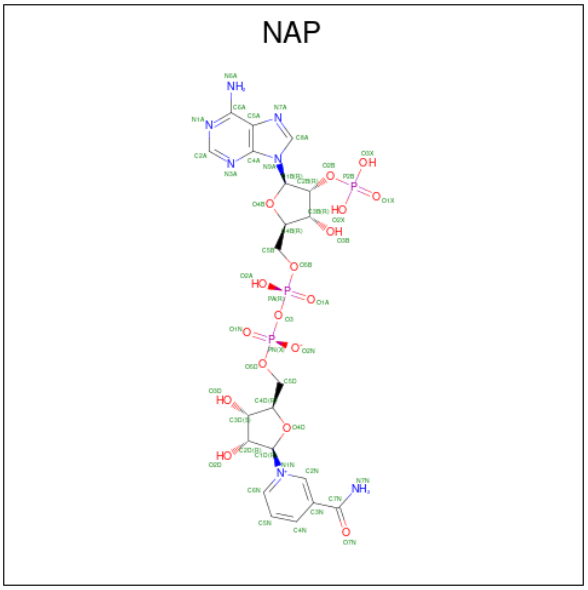
There are 7 unique types of molecules in this entry. The entry contains 6415 atoms, of which 2894 are hydrogens and 0 are deuteriums.

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 GLYOXYLATE REDUCTASE.

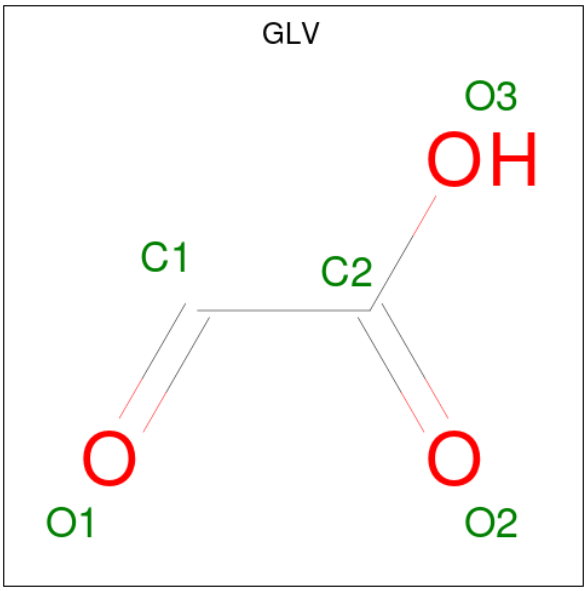
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	334	5676	1810	2858	483	517	8	0	19	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



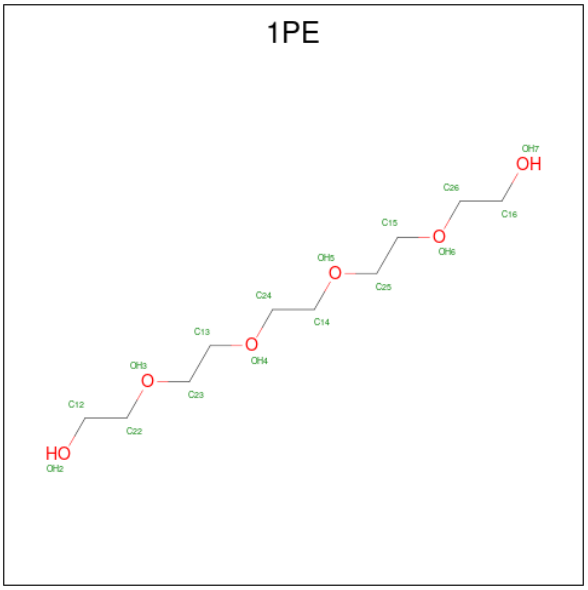
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	96	42	14	34	6	0	1

- Molecule 3 is GLYOXYLIC ACID (three-letter code: GLV) (formula: $C_2H_2O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	5	2	3	0	0
			Total	C	O		
3	A	1	5	2	3	0	0

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



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

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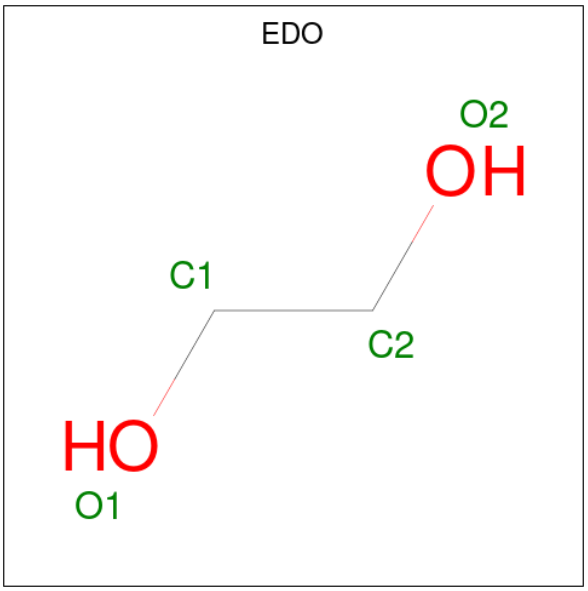
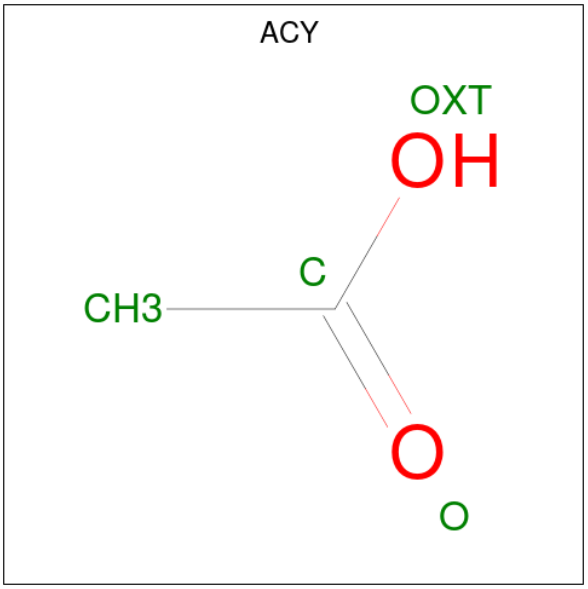
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0
			Total	C	O		
4	A	1	7	4	3	0	0
			Total	C	O		
4	A	1	7	4	3	0	0
			Total	C	O		
4	A	1	7	4	3	0	0
			Total	C	O		
4	A	1	10	6	4	0	0
			Total	C	O		
4	A	1	10	6	4	0	0
			Total	C	O		
4	A	1	10	6	4	0	0
			Total	C	O		
4	A	1	10	6	4	0	0
			Total	C	O		
4	A	1	13	8	5	0	0
			Total	C	O		
4	A	1	16	10	6	0	0
			Total	C	O		
4	A	1	16	10	6	0	0
			Total	C	O		
4	A	1	7	4	3	0	0
			Total	C	O		
4	A	1	13	8	5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	10	2	6	2	0	0
			Total	C	H	O		
5	A	1	10	2	6	2	0	0
			Total	C	H	O		
5	A	1	10	2	6	2	0	0
			Total	C	H	O		
5	A	1	10	2	6	2	0	0
			Total	C	H	O		
5	A	1	10	2	6	2	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 7 is water.

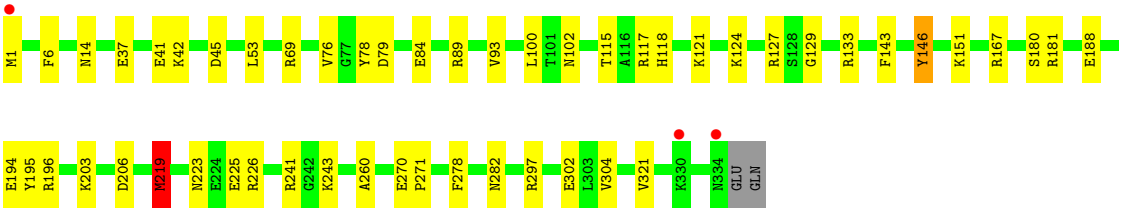
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	422	422	422	0	0

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: GLYOXYLATE REDUCTASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	114.58Å 114.58Å 118.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.51 – 1.40 47.73 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.51-1.40) 99.4 (47.73-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 1.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.131 , 0.143 0.134 , 0.145	Depositor DCC
R_{free} test set	7473 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h 0.023 for -l,-k,-h 0.025 for -h,-l,-k 0.018 for -h,l,k 0.059 for -h,k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: GLV, NAP, EDO, 1PE, ACY

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	1.03	2/2909 (0.1%)	1.13	18/3925 (0.5%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	GLU	CB-CG	5.46	1.62	1.52
1	A	146	TYR	CE1-CZ	-5.05	1.31	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	A	219	MET	CG-SD-CE	-9.50	85.00	100.20
1	A	127	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	A	241[A]	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	241[B]	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	241[A]	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	241[B]	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	226	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	45	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	45	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	206	ASP	CB-CG-OD2	6.92	124.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	304	VAL	CG1-CB-CG2	6.79	121.76	110.90
1	A	127	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	278	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	A	206	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	A	226	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	79	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain

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	2818	2858	2899	71	0
2	A	96	0	49	2	0
3	A	10	0	2	3	0
4	A	147	0	192	76	0
5	A	20	30	30	0	0
6	A	8	6	6	0	0
7	A	422	0	0	25	2
All	All	3521	2894	3178	101	2

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 16.

All (101) 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)
4:A:1359:1PE:H241	7:A:2214:HOH:O	1.34	1.25
1:A:143:PHE:H	4:A:1359:1PE:H132	1.12	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HZ2	4:A:1349:1PE:H132	1.14	1.07
4:A:1359:1PE:H242	7:A:2185:HOH:O	1.58	1.01
1:A:151:LYS:HZ2	4:A:1347:1PE:H132	1.24	1.00
1:A:203:LYS:HZ3	4:A:1348:1PE:H131	1.32	0.91
4:A:1343:1PE:H122	4:A:1343:1PE:H132	1.65	0.77
1:A:243:LYS:NZ	4:A:1349:1PE:H141	2.02	0.74
1:A:102:ASN:HD21	4:A:1346:1PE:H241	1.52	0.74
1:A:14:ASN:ND2	1:A:302[A]:GLU:HG3	2.03	0.73
4:A:1343:1PE:H122	4:A:1343:1PE:C13	2.20	0.72
4:A:1347:1PE:H131	7:A:2285:HOH:O	1.91	0.71
4:A:1343:1PE:C13	4:A:1343:1PE:C12	2.70	0.70
4:A:1343:1PE:C14	4:A:1359:1PE:OH6	2.40	0.70
1:A:118:HIS:HA	4:A:1343:1PE:H221	1.75	0.69
1:A:124[B]:LYS:HG3	7:A:2187:HOH:O	1.92	0.68
1:A:181:ARG:HH21	2:A:1335[A]:NAP:P2B	2.17	0.68
1:A:14:ASN:ND2	1:A:302[A]:GLU:CG	2.57	0.68
1:A:143:PHE:N	4:A:1359:1PE:H132	1.98	0.66
3:A:1336:GLV:H1	7:A:2352:HOH:O	1.96	0.66
4:A:1343:1PE:H222	7:A:2186:HOH:O	1.95	0.66
4:A:1359:1PE:C24	7:A:2185:HOH:O	2.27	0.66
1:A:133:ARG:HH11	4:A:1338:1PE:H131	1.61	0.64
1:A:223:ASN:HD22	4:A:1340:1PE:H121	1.63	0.64
1:A:151:LYS:NZ	4:A:1347:1PE:H141	2.13	0.64
1:A:297[B]:ARG:NH2	7:A:2351:HOH:O	2.32	0.63
4:A:1343:1PE:H141	4:A:1359:1PE:OH6	1.99	0.62
1:A:78:TYR:CZ	1:A:321[A]:VAL:HG11	2.35	0.62
1:A:118:HIS:ND1	4:A:1343:1PE:H122	2.16	0.60
4:A:1359:1PE:H152	7:A:2219:HOH:O	2.01	0.60
1:A:146:TYR:CD1	4:A:1347:1PE:H152	2.36	0.60
1:A:243:LYS:HZ2	4:A:1349:1PE:H141	1.66	0.60
1:A:151:LYS:NZ	4:A:1347:1PE:H221	2.17	0.60
1:A:203:LYS:NZ	4:A:1348:1PE:H131	2.14	0.58
4:A:1343:1PE:H142	4:A:1359:1PE:OH6	2.02	0.58
1:A:118:HIS:CE1	4:A:1343:1PE:H142	2.39	0.58
4:A:1339:1PE:H121	7:A:2401:HOH:O	2.04	0.57
1:A:133:ARG:HG2	4:A:1338:1PE:H121	1.85	0.57
4:A:1349:1PE:H122	7:A:2416:HOH:O	2.04	0.56
1:A:14:ASN:HD21	1:A:302[A]:GLU:HG3	1.70	0.56
1:A:243:LYS:NZ	4:A:1349:1PE:H121	2.21	0.55
1:A:146:TYR:HD1	4:A:1347:1PE:H152	1.71	0.55
1:A:118:HIS:ND1	4:A:1343:1PE:C12	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1349:1PE:H132	4:A:1349:1PE:H121	1.88	0.55
1:A:203:LYS:HZ3	4:A:1348:1PE:H222	1.73	0.54
1:A:243:LYS:HZ3	4:A:1349:1PE:H141	1.70	0.54
1:A:282:ASN:HA	4:A:1343:1PE:H131	1.90	0.54
1:A:93:VAL:O	1:A:321[B]:VAL:HG22	2.07	0.53
4:A:1346:1PE:H231	7:A:2412:HOH:O	2.07	0.53
4:A:1344:1PE:H242	7:A:2194:HOH:O	2.08	0.53
4:A:1349:1PE:H121	4:A:1349:1PE:C13	2.39	0.53
4:A:1345:1PE:H241	7:A:2410:HOH:O	2.08	0.53
1:A:151:LYS:HZ2	4:A:1347:1PE:H141	1.75	0.52
1:A:41[B]:GLU:HG2	7:A:2082:HOH:O	2.09	0.52
1:A:14:ASN:HD22	1:A:302[A]:GLU:CG	2.23	0.51
4:A:1346:1PE:H131	7:A:2413:HOH:O	2.11	0.51
1:A:203:LYS:NZ	4:A:1348:1PE:H222	2.25	0.51
1:A:194:GLU:CD	1:A:196:ARG:HH12	2.15	0.50
1:A:151:LYS:NZ	4:A:1347:1PE:H132	2.10	0.50
4:A:1343:1PE:C12	7:A:2189:HOH:O	2.59	0.50
1:A:6:PHE:CE1	1:A:42:LYS:HD3	2.46	0.49
1:A:194:GLU:HG2	1:A:196:ARG:NH1	2.26	0.49
1:A:37[B]:GLU:O	1:A:41[B]:GLU:HG3	2.14	0.48
1:A:243:LYS:NZ	4:A:1349:1PE:H132	2.03	0.48
1:A:133:ARG:NH1	4:A:1338:1PE:H131	2.27	0.47
3:A:1356:GLV:H1	7:A:2095:HOH:O	2.15	0.47
1:A:121:LYS:CE	4:A:1343:1PE:OH2	2.63	0.47
1:A:219:MET:HE1	4:A:1349:1PE:H241	1.96	0.46
1:A:53:LEU:H	3:A:1356:GLV:C1	2.28	0.46
1:A:118:HIS:ND1	4:A:1343:1PE:H221	2.30	0.46
1:A:118:HIS:CE1	4:A:1359:1PE:H151	2.50	0.46
1:A:84:GLU:OE1	7:A:2149:HOH:O	2.21	0.46
1:A:118:HIS:HE1	4:A:1343:1PE:H142	1.81	0.45
1:A:225:GLU:HG3	7:A:2300:HOH:O	2.15	0.45
1:A:69:ARG:HD3	7:A:2127:HOH:O	2.16	0.45
1:A:282:ASN:HA	4:A:1343:1PE:H232	1.98	0.45
1:A:219:MET:CE	4:A:1349:1PE:H142	2.46	0.45
1:A:118:HIS:CE1	4:A:1343:1PE:H132	2.52	0.44
1:A:129:GLY:HA3	4:A:1338:1PE:H132	1.99	0.44
1:A:203:LYS:HZ3	4:A:1348:1PE:C13	2.16	0.44
4:A:1345:1PE:H121	4:A:1345:1PE:H231	1.79	0.44
1:A:219:MET:HE3	4:A:1349:1PE:H142	1.99	0.44
4:A:1359:1PE:H141	7:A:2185:HOH:O	2.18	0.44
1:A:260:ALA:O	4:A:1343:1PE:H241	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:HA	1:A:271:PRO:C	2.38	0.43
1:A:76:VAL:CG1	2:A:1335[A]:NAP:H6N	2.48	0.43
1:A:118:HIS:ND1	4:A:1343:1PE:C22	2.82	0.43
1:A:195:TYR:CE1	4:A:1341:1PE:H132	2.54	0.43
4:A:1343:1PE:C22	7:A:2186:HOH:O	2.62	0.42
1:A:102:ASN:ND2	4:A:1346:1PE:H241	2.26	0.41
1:A:124[B]:LYS:HE3	7:A:2187:HOH:O	2.20	0.41
1:A:151:LYS:HZ1	4:A:1347:1PE:H141	1.86	0.41
4:A:1349:1PE:H132	4:A:1349:1PE:H141	1.90	0.41
1:A:194:GLU:OE1	1:A:196:ARG:NH2	2.53	0.41
1:A:223:ASN:HB3	4:A:1340:1PE:H121	2.02	0.41
1:A:133:ARG:NH1	4:A:1338:1PE:C13	2.83	0.41
1:A:124[B]:LYS:HE2	7:A:2192:HOH:O	2.21	0.40
4:A:1349:1PE:H122	4:A:1349:1PE:H231	1.88	0.40
1:A:115:THR:O	4:A:1343:1PE:H231	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2059:HOH:O	7:A:2251:HOH:O[3_645]	1.94	0.26
7:A:2220:HOH:O	7:A:2354:HOH:O[6_765]	1.97	0.23

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	351/336 (104%)	342 (97%)	9 (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	301/284 (106%)	297 (99%)	4 (1%)	69 42

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	100	LEU
1	A	180	SER
1	A	219	MET

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

Mol	Chain	Res	Type
1	A	14	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	1PE	A	1346	-	9,9,15	0.62	0	8,8,14	1.91	4 (50%)
5	EDO	A	1354	-	3,3,3	0.61	0	2,2,2	0.12	0
5	EDO	A	1352	-	3,3,3	0.56	0	2,2,2	0.42	0
4	1PE	A	1359	-	12,12,15	0.70	0	11,11,14	2.64	6 (54%)
6	ACY	A	1357	-	3,3,3	1.29	1 (33%)	3,3,3	0.91	0
4	1PE	A	1339	-	6,6,15	0.84	0	5,5,14	1.87	2 (40%)
4	1PE	A	1355	-	6,6,15	0.81	0	5,5,14	1.52	0
3	GLV	A	1356	-	4,4,4	1.74	1 (25%)	3,4,4	0.29	0
5	EDO	A	1350	-	3,3,3	0.53	0	2,2,2	0.19	0
4	1PE	A	1343	-	9,9,15	1.00	0	8,8,14	1.64	2 (25%)
2	NAP	A	1335[A]	-	45,52,52	3.12	11 (24%)	56,80,80	2.21	15 (26%)
4	1PE	A	1344	-	9,9,15	0.51	0	8,8,14	2.34	4 (50%)
4	1PE	A	1337	-	6,6,15	0.43	0	5,5,14	0.82	0
5	EDO	A	1353	-	3,3,3	0.56	0	2,2,2	0.31	0
5	EDO	A	1351	-	3,3,3	0.58	0	2,2,2	0.11	0
3	GLV	A	1336	-	4,4,4	4.46	3 (75%)	3,4,4	4.00	3 (100%)
4	1PE	A	1347	-	12,12,15	0.90	0	11,11,14	1.46	3 (27%)
4	1PE	A	1340	-	6,6,15	0.78	0	5,5,14	1.66	2 (40%)
4	1PE	A	1345	-	9,9,15	0.54	0	8,8,14	2.26	4 (50%)
4	1PE	A	1342	-	6,6,15	0.78	0	5,5,14	1.88	2 (40%)
6	ACY	A	1358	-	3,3,3	0.83	0	3,3,3	0.95	0
4	1PE	A	1348	-	15,15,15	0.82	0	14,14,14	1.74	4 (28%)
2	NAP	A	1335[B]	-	45,52,52	2.84	13 (28%)	56,80,80	2.79	11 (19%)
4	1PE	A	1341	-	6,6,15	0.65	0	5,5,14	1.87	2 (40%)
4	1PE	A	1349	-	15,15,15	0.81	0	14,14,14	1.83	5 (35%)
4	1PE	A	1338	-	6,6,15	0.69	0	5,5,14	1.77	1 (20%)

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	1346	-	-	4/7/7/13	-
5	EDO	A	1354	-	-	0/1/1/1	-
5	EDO	A	1352	-	-	0/1/1/1	-
4	1PE	A	1359	-	-	5/10/10/13	-
4	1PE	A	1339	-	-	0/4/4/13	-
4	1PE	A	1355	-	-	2/4/4/13	-
3	GLV	A	1356	-	-	0/0/2/2	-
5	EDO	A	1350	-	-	0/1/1/1	-
4	1PE	A	1343	-	-	4/7/7/13	-
2	NAP	A	1335[A]	-	-	6/31/67/67	0/5/5/5
4	1PE	A	1344	-	-	4/7/7/13	-
4	1PE	A	1337	-	-	0/4/4/13	-
5	EDO	A	1353	-	-	0/1/1/1	-
5	EDO	A	1351	-	-	0/1/1/1	-
3	GLV	A	1336	-	-	0/0/2/2	-
4	1PE	A	1347	-	-	5/10/10/13	-
4	1PE	A	1340	-	-	2/4/4/13	-
4	1PE	A	1345	-	-	6/7/7/13	-
4	1PE	A	1342	-	-	4/4/4/13	-
4	1PE	A	1348	-	-	5/13/13/13	-
2	NAP	A	1335[B]	-	1/1/12/12	6/31/67/67	0/5/5/5
4	1PE	A	1341	-	-	1/4/4/13	-
4	1PE	A	1349	-	-	6/13/13/13	-
4	1PE	A	1338	-	-	2/4/4/13	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1335[A]	NAP	C2D-C1D	-11.83	1.35	1.53
2	A	1335[A]	NAP	O4D-C1D	11.34	1.56	1.41
2	A	1335[B]	NAP	O4D-C1D	9.44	1.54	1.41
2	A	1335[B]	NAP	C2D-C1D	-9.18	1.39	1.53
3	A	1336	GLV	O3-C2	-7.53	1.10	1.30
2	A	1335[A]	NAP	C3B-C4B	-6.04	1.37	1.53
2	A	1335[B]	NAP	C3B-C4B	-5.34	1.39	1.53
2	A	1335[A]	NAP	O4B-C1B	5.26	1.48	1.41
2	A	1335[B]	NAP	O4B-C1B	5.04	1.48	1.41
2	A	1335[B]	NAP	O4D-C4D	-4.94	1.34	1.45
2	A	1335[B]	NAP	C3B-C2B	4.68	1.63	1.52
2	A	1335[A]	NAP	C3B-C2B	4.66	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1335[B]	NAP	C7N-N7N	4.45	1.41	1.33
2	A	1335[A]	NAP	C7N-N7N	4.39	1.41	1.33
2	A	1335[B]	NAP	C5N-C4N	3.82	1.47	1.38
2	A	1335[B]	NAP	C4N-C3N	3.54	1.45	1.39
3	A	1336	GLV	C1-C2	3.50	1.52	1.44
2	A	1335[A]	NAP	O4D-C4D	-3.42	1.37	1.45
2	A	1335[A]	NAP	O4B-C4B	3.37	1.52	1.45
3	A	1336	GLV	O2-C2	-2.98	1.15	1.23
2	A	1335[B]	NAP	O4B-C4B	2.84	1.51	1.45
3	A	1356	GLV	C1-C2	2.80	1.50	1.44
2	A	1335[A]	NAP	O2D-C2D	2.57	1.49	1.43
2	A	1335[A]	NAP	C4N-C3N	2.41	1.43	1.39
2	A	1335[B]	NAP	P2B-O2X	-2.23	1.46	1.54
2	A	1335[B]	NAP	C6A-N6A	2.21	1.42	1.34
2	A	1335[A]	NAP	C5N-C4N	2.06	1.43	1.38
2	A	1335[B]	NAP	C3N-C7N	2.01	1.53	1.50
6	A	1357	ACY	CH3-C	2.01	1.57	1.49

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1335[B]	NAP	C3D-C2D-C1D	11.58	118.41	100.98
2	A	1335[B]	NAP	O4D-C1D-C2D	-9.84	92.55	106.93
2	A	1335[A]	NAP	C3D-C2D-C1D	9.14	114.74	100.98
2	A	1335[B]	NAP	C2D-C3D-C4D	-8.29	86.54	102.64
3	A	1336	GLV	O3-C2-O2	6.23	135.60	122.67
2	A	1335[B]	NAP	N3A-C2A-N1A	-4.94	120.96	128.68
2	A	1335[A]	NAP	N3A-C2A-N1A	-4.84	121.11	128.68
4	A	1359	1PE	OH4-C24-C14	4.71	131.63	110.39
2	A	1335[A]	NAP	O4D-C1D-C2D	-4.34	100.58	106.93
2	A	1335[B]	NAP	C5N-C4N-C3N	-4.18	115.40	120.34
2	A	1335[A]	NAP	C2D-C3D-C4D	-3.93	95.00	102.64
4	A	1344	1PE	OH3-C22-C12	3.91	127.23	110.07
4	A	1359	1PE	C23-OH3-C22	3.81	129.81	113.29
2	A	1335[A]	NAP	C6N-N1N-C2N	3.67	125.33	121.97
2	A	1335[A]	NAP	O2X-P2B-O1X	-3.64	96.42	110.68
4	A	1359	1PE	OH5-C25-C15	3.53	125.56	110.07
2	A	1335[B]	NAP	O2D-C2D-C1D	3.51	123.82	110.85
2	A	1335[A]	NAP	C1B-N9A-C4A	-3.51	120.48	126.64
4	A	1349	1PE	OH5-C14-C24	3.44	125.92	110.39
2	A	1335[B]	NAP	C4A-C5A-N7A	-3.44	105.82	109.40
2	A	1335[A]	NAP	O3X-P2B-O2X	3.29	120.23	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1335[B]	NAP	C2N-C3N-C4N	3.21	121.90	118.26
2	A	1335[A]	NAP	C3N-C2N-N1N	-3.16	117.34	120.43
4	A	1345	1PE	OH3-C23-C13	3.15	124.60	110.39
4	A	1342	1PE	OH3-C22-C12	3.14	123.87	110.07
4	A	1345	1PE	OH3-C22-C12	3.07	123.57	110.07
4	A	1343	1PE	OH3-C23-C13	3.03	124.06	110.39
4	A	1344	1PE	OH4-C24-C14	3.02	123.36	110.07
4	A	1348	1PE	OH3-C22-C12	2.94	123.00	110.07
4	A	1349	1PE	OH6-C15-C25	2.94	123.64	110.39
2	A	1335[A]	NAP	C3N-C7N-N7N	-2.93	114.23	117.75
4	A	1349	1PE	OH5-C25-C15	2.89	123.43	110.39
4	A	1346	1PE	OH3-C23-C13	2.79	122.98	110.39
4	A	1359	1PE	OH4-C13-C23	2.78	122.95	110.39
4	A	1345	1PE	OH4-C24-C14	2.74	122.10	110.07
4	A	1345	1PE	OH4-C13-C23	2.69	122.53	110.39
4	A	1347	1PE	OH4-C13-C23	2.60	122.09	110.39
4	A	1348	1PE	OH6-C15-C25	2.55	121.90	110.39
4	A	1343	1PE	OH3-C22-C12	2.51	121.08	110.07
4	A	1339	1PE	OH3-C22-C12	2.50	121.07	110.07
4	A	1341	1PE	OH3-C22-C12	2.44	120.80	110.07
2	A	1335[A]	NAP	C2N-C3N-C4N	2.41	121.00	118.26
4	A	1347	1PE	OH3-C22-C12	2.35	120.38	110.07
4	A	1340	1PE	OH3-C23-C13	2.34	120.34	110.07
4	A	1348	1PE	OH6-C26-C16	2.33	120.32	110.07
2	A	1335[B]	NAP	C2A-N1A-C6A	2.32	122.72	118.75
2	A	1335[A]	NAP	C2A-N1A-C6A	2.31	122.70	118.75
4	A	1342	1PE	OH3-C23-C13	2.30	120.16	110.07
4	A	1359	1PE	OH3-C23-C13	2.29	120.72	110.39
2	A	1335[A]	NAP	O3X-P2B-O2B	2.29	116.24	105.99
4	A	1344	1PE	C23-OH3-C22	2.27	123.11	113.29
4	A	1347	1PE	OH3-C23-C13	2.27	120.61	110.39
4	A	1346	1PE	OH4-C13-C23	2.26	120.60	110.39
4	A	1359	1PE	OH6-C15-C25	2.24	124.80	111.81
2	A	1335[B]	NAP	O5B-C5B-C4B	-2.22	101.35	108.99
4	A	1341	1PE	OH3-C23-C13	2.22	119.80	110.07
4	A	1338	1PE	OH3-C23-C13	2.17	119.60	110.07
3	A	1336	GLV	O2-C2-C1	-2.17	116.93	123.83
4	A	1349	1PE	OH6-C26-C16	2.16	119.58	110.07
2	A	1335[A]	NAP	O4B-C4B-C3B	2.16	109.39	105.11
4	A	1339	1PE	OH3-C23-C13	2.15	119.52	110.07
2	A	1335[B]	NAP	C1B-N9A-C4A	-2.15	122.87	126.64
2	A	1335[A]	NAP	N6A-C6A-N1A	2.15	123.03	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1336	GLV	O3-C2-C1	-2.12	107.00	113.52
4	A	1349	1PE	OH3-C23-C13	2.12	119.93	110.39
4	A	1346	1PE	OH5-C14-C24	2.11	124.05	111.81
4	A	1340	1PE	OH3-C22-C12	2.10	119.31	110.07
4	A	1346	1PE	OH3-C22-C12	2.05	119.07	110.07
4	A	1344	1PE	OH3-C23-C13	2.04	119.61	110.39
4	A	1348	1PE	OH5-C25-C15	2.01	119.45	110.39

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1335[B]	NAP	C2D

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1335[A]	NAP	O4D-C1D-N1N-C6N
4	A	1343	1PE	C12-C22-OH3-C23
4	A	1345	1PE	C12-C22-OH3-C23
4	A	1349	1PE	C12-C22-OH3-C23
4	A	1344	1PE	C23-C13-OH4-C24
4	A	1346	1PE	C23-C13-OH4-C24
4	A	1348	1PE	C14-C24-OH4-C13
4	A	1346	1PE	OH5-C14-C24-OH4
4	A	1343	1PE	OH4-C13-C23-OH3
4	A	1349	1PE	OH4-C13-C23-OH3
4	A	1359	1PE	OH4-C13-C23-OH3
4	A	1344	1PE	OH4-C13-C23-OH3
2	A	1335[A]	NAP	C3B-C2B-O2B-P2B
2	A	1335[B]	NAP	C3B-C2B-O2B-P2B
4	A	1342	1PE	OH2-C12-C22-OH3
4	A	1342	1PE	OH4-C13-C23-OH3
4	A	1344	1PE	OH5-C14-C24-OH4
4	A	1345	1PE	OH2-C12-C22-OH3
4	A	1347	1PE	OH6-C15-C25-OH5
4	A	1345	1PE	OH4-C13-C23-OH3
4	A	1348	1PE	C13-C23-OH3-C22
4	A	1343	1PE	C13-C23-OH3-C22
2	A	1335[B]	NAP	C1B-C2B-O2B-P2B
4	A	1340	1PE	OH2-C12-C22-OH3
4	A	1341	1PE	OH2-C12-C22-OH3
4	A	1345	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
2	A	1335[A]	NAP	C1B-C2B-O2B-P2B
4	A	1359	1PE	OH5-C14-C24-OH4
4	A	1346	1PE	OH2-C12-C22-OH3
4	A	1343	1PE	OH5-C14-C24-OH4
4	A	1344	1PE	OH2-C12-C22-OH3
4	A	1359	1PE	OH6-C15-C25-OH5
4	A	1349	1PE	OH6-C15-C25-OH5
4	A	1355	1PE	OH2-C12-C22-OH3
4	A	1359	1PE	C23-C13-OH4-C24
4	A	1342	1PE	C12-C22-OH3-C23
4	A	1348	1PE	OH7-C16-C26-OH6
4	A	1347	1PE	OH4-C13-C23-OH3
4	A	1338	1PE	C13-C23-OH3-C22
4	A	1338	1PE	C12-C22-OH3-C23
4	A	1345	1PE	C13-C23-OH3-C22
4	A	1347	1PE	C13-C23-OH3-C22
4	A	1342	1PE	C13-C23-OH3-C22
4	A	1349	1PE	C15-C25-OH5-C14
4	A	1348	1PE	OH5-C14-C24-OH4
4	A	1340	1PE	OH4-C13-C23-OH3
4	A	1349	1PE	C14-C24-OH4-C13
4	A	1347	1PE	C24-C14-OH5-C25
4	A	1349	1PE	OH5-C14-C24-OH4
4	A	1346	1PE	OH4-C13-C23-OH3
4	A	1359	1PE	OH2-C12-C22-OH3
4	A	1345	1PE	OH5-C14-C24-OH4
4	A	1347	1PE	OH5-C14-C24-OH4
2	A	1335[A]	NAP	C2B-O2B-P2B-O2X
2	A	1335[A]	NAP	C2B-O2B-P2B-O3X
2	A	1335[A]	NAP	O4B-C4B-C5B-O5B
2	A	1335[B]	NAP	O4B-C4B-C5B-O5B
2	A	1335[B]	NAP	PA-O3-PN-O1N
2	A	1335[B]	NAP	PA-O3-PN-O2N
4	A	1355	1PE	OH4-C13-C23-OH3
2	A	1335[B]	NAP	C5B-O5B-PA-O1A
4	A	1348	1PE	OH4-C13-C23-OH3

There are no ring outliers.

15 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1346	1PE	4	0

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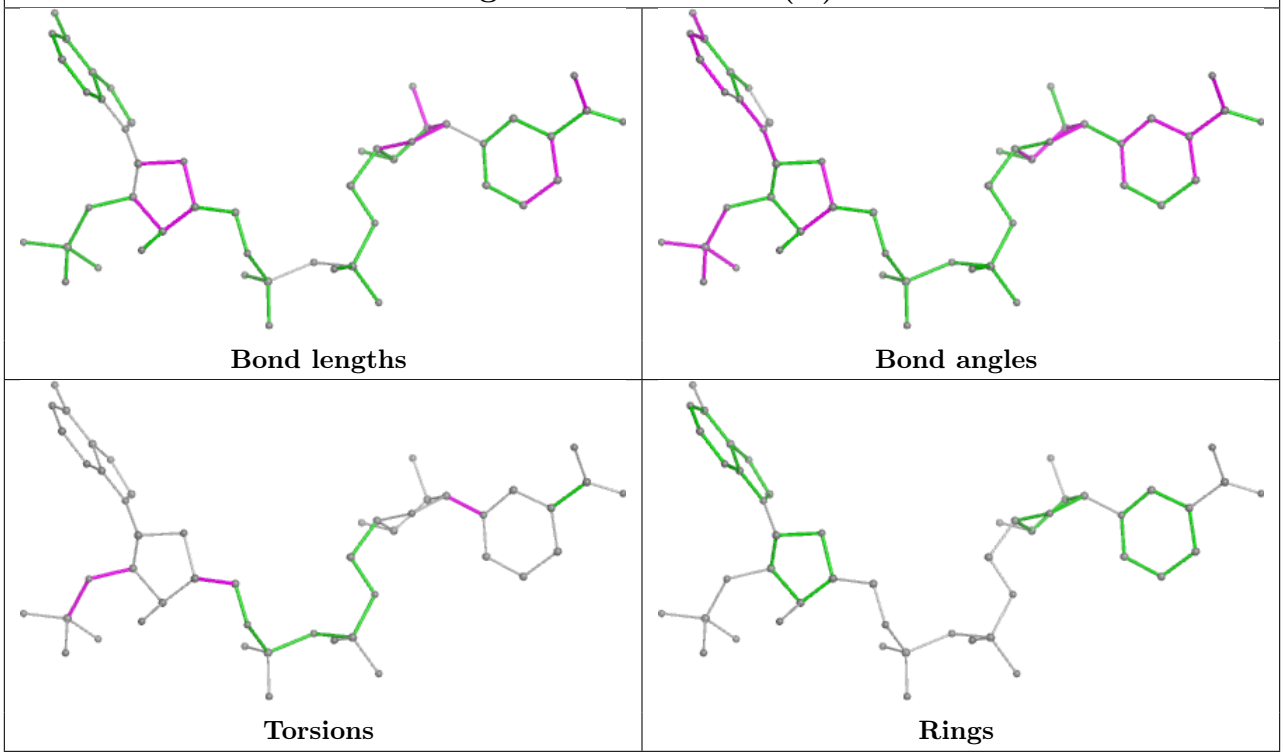
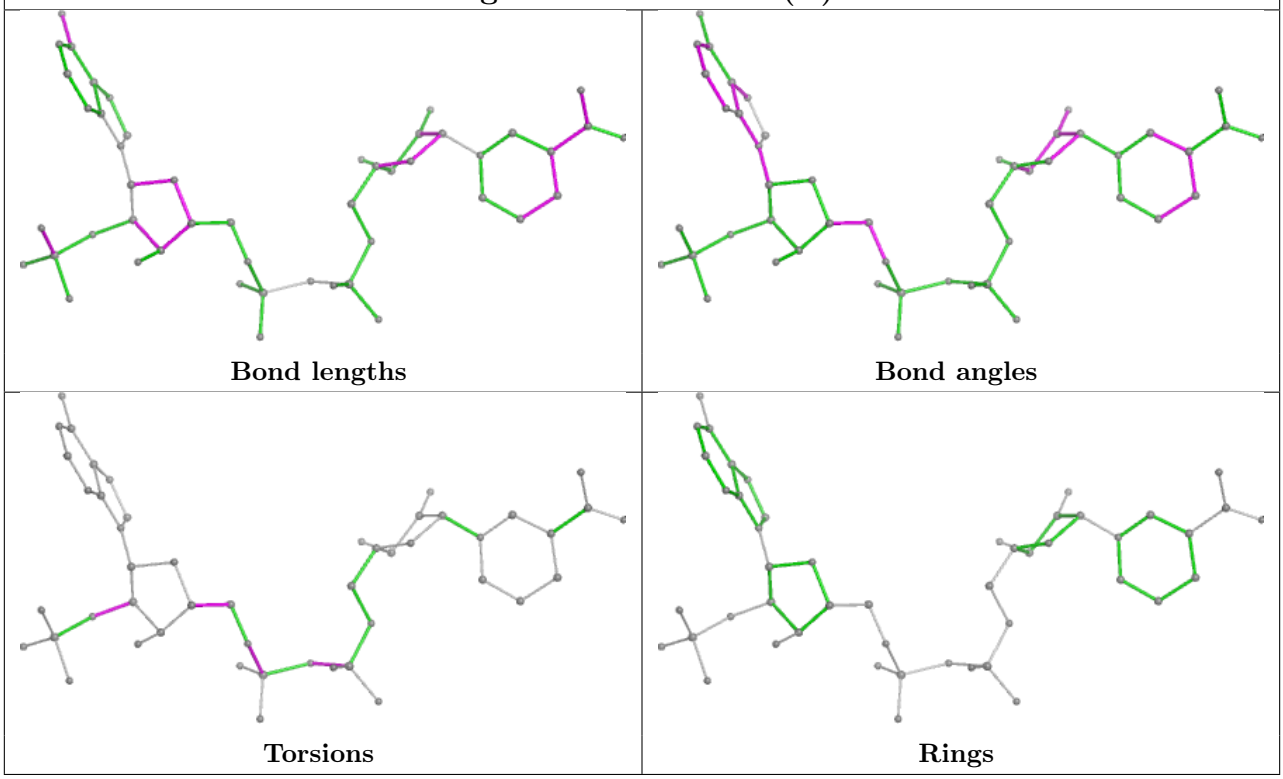
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1359	1PE	11	0
4	A	1339	1PE	1	0
3	A	1356	GLV	2	0
4	A	1343	1PE	24	0
2	A	1335[A]	NAP	2	0
4	A	1344	1PE	1	0
3	A	1336	GLV	1	0
4	A	1347	1PE	9	0
4	A	1340	1PE	2	0
4	A	1345	1PE	2	0
4	A	1348	1PE	5	0
4	A	1341	1PE	1	0
4	A	1349	1PE	14	0
4	A	1338	1PE	5	0

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 NAP A 1335 (A)



Ligand NAP A 1335 (B)



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	334/336 (99%)	-0.48	3 (0%) 84 82	16, 23, 40, 78	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ASN	5.3
1	A	1	MET	5.1
1	A	330	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1351	4/4	0.70	0.16	59,71,78,79	0
4	1PE	A	1344	10/16	0.72	0.23	39,63,69,70	0
5	EDO	A	1354	4/4	0.74	0.24	68,82,95,114	0
5	EDO	A	1352	4/4	0.75	0.25	66,79,92,92	0

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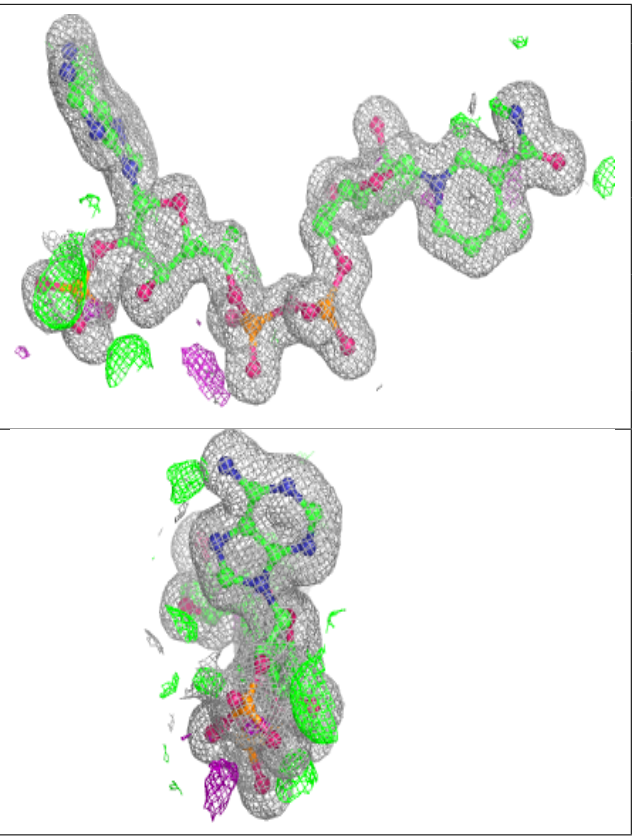
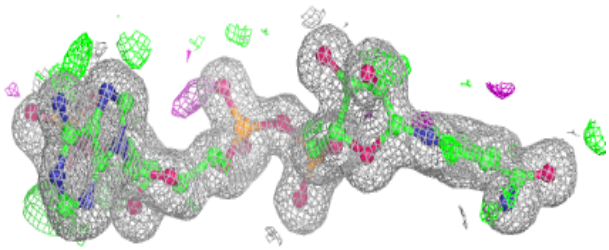
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1PE	A	1359	13/16	0.76	0.28	20,39,58,64	13
4	1PE	A	1355	7/16	0.78	0.19	75,78,87,99	0
4	1PE	A	1341	7/16	0.83	0.09	64,69,75,79	0
4	1PE	A	1345	10/16	0.84	0.10	38,47,67,73	0
4	1PE	A	1346	10/16	0.85	0.15	37,71,78,82	0
5	EDO	A	1353	4/4	0.85	0.35	47,70,87,95	0
4	1PE	A	1343	10/16	0.85	0.19	28,47,68,73	0
4	1PE	A	1348	16/16	0.87	0.15	34,53,75,77	0
6	ACY	A	1357	4/4	0.87	0.12	25,31,33,37	0
4	1PE	A	1340	7/16	0.89	0.18	46,55,78,82	0
4	1PE	A	1338	7/16	0.90	0.10	52,58,78,79	0
5	EDO	A	1350	4/4	0.91	0.09	49,60,72,83	0
4	1PE	A	1349	16/16	0.93	0.11	30,48,82,87	0
4	1PE	A	1347	13/16	0.93	0.11	30,46,66,87	0
3	GLV	A	1356	5/5	0.93	0.31	19,21,36,50	5
6	ACY	A	1358	4/4	0.93	0.09	30,36,44,53	0
4	1PE	A	1337	7/16	0.94	0.07	31,33,44,52	0
4	1PE	A	1342	7/16	0.94	0.08	41,51,77,81	0
4	1PE	A	1339	7/16	0.95	0.09	49,56,77,88	0
3	GLV	A	1336	5/5	0.98	0.06	15,24,26,29	0
2	NAP	A	1335[A]	48/48	0.98	0.09	13,18,29,31	48
2	NAP	A	1335[B]	48/48	0.98	0.09	14,17,22,26	48

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 NAP A 1335 (A):

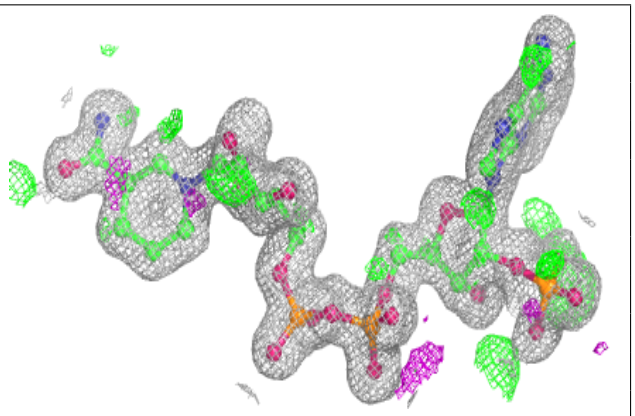
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

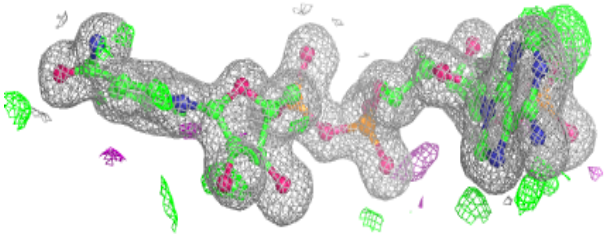


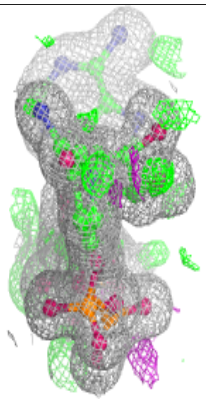


Electron density around NAP A 1335 (B):

$2mF_o$-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.