Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 12:03 PM EST

PDB ID	:	6ENL
Title	:	INHIBITION OF ENOLASE: THE CRYSTAL STRUCTURES OF ENOLASE-CA2+-PHOSPHOGLYCERATE AND ENOLASE-ZN2+-PHOSPHOGLYCOLATE COMPLEXES AT 2.2-ANGSTROMS RESOLUTION
Authors	:	Lebioda, L.; Stec, B.
Deposited on	:	1990-11-13
Resolution	:	2.20 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:

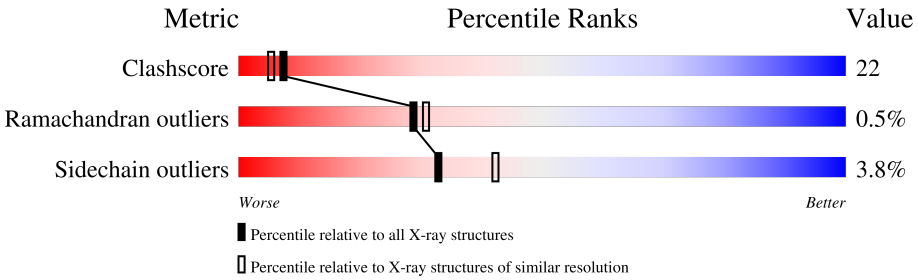
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	61% 32% 6% •

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	PGA	A	442	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3643 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.

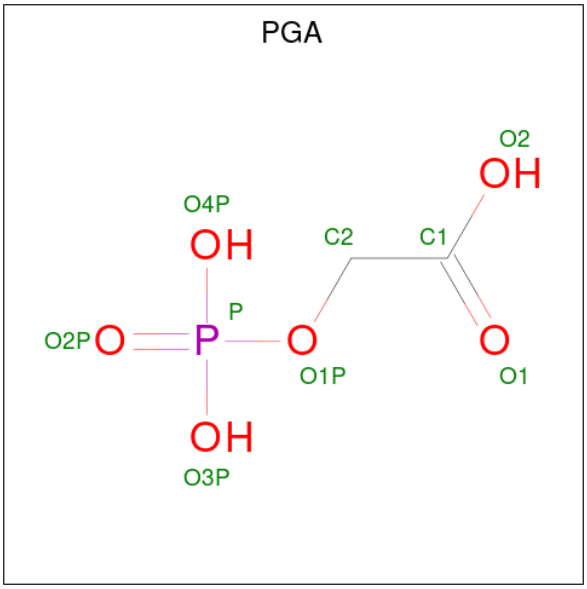
- Molecule 1 is a protein called ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3289	2076	569	638	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	SER	LYS	conflict	UNP P00924

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	9	2	6	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	344	Total O 344 344	0	0

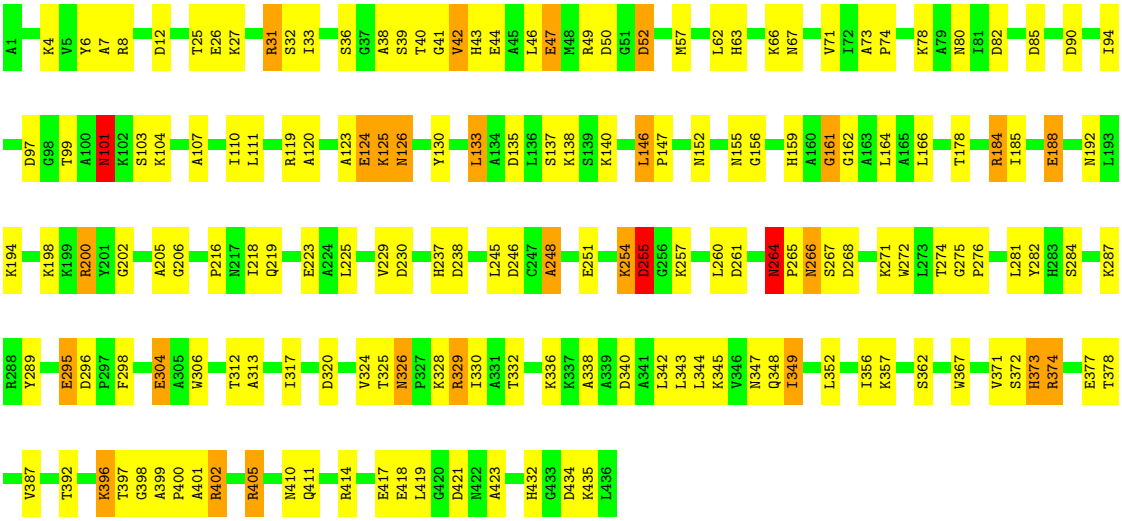
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: ENOLASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.10Å 124.10Å 66.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3643	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PGA

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	0.88	0/3349	1.86	77/4531 (1.7%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	ARG	NE-CZ-NH1	-18.91	110.84	120.30
1	A	414	ARG	NE-CZ-NH1	16.52	128.56	120.30
1	A	8	ARG	NE-CZ-NH1	15.97	128.28	120.30
1	A	340	ASP	CB-CG-OD1	12.20	129.28	118.30
1	A	304	GLU	OE1-CD-OE2	12.15	137.88	123.30
1	A	405	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	A	8	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	A	184	ARG	NH1-CZ-NH2	10.69	131.16	119.40
1	A	119	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	A	405	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	421	ASP	CB-CG-OD2	-9.39	109.85	118.30
1	A	374	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	414	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	A	329	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	A	184	ARG	CD-NE-CZ	-8.24	112.06	123.60
1	A	434	ASP	CB-CG-OD1	8.17	125.66	118.30
1	A	52	ASP	CB-CG-OD1	-8.15	110.96	118.30
1	A	7	ALA	N-CA-CB	8.11	121.45	110.10
1	A	329	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	A	200	ARG	CD-NE-CZ	8.08	134.92	123.60
1	A	246	ASP	N-CA-CB	8.07	125.13	110.60
1	A	421	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	49	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	146	LEU	CB-CA-C	7.73	124.88	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	GLU	OE1-CD-OE2	7.70	132.53	123.30
1	A	31	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	178	THR	O-C-N	6.99	133.88	122.70
1	A	402	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	229	VAL	CB-CA-C	6.78	124.28	111.40
1	A	402	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	255	ASP	CA-C-O	-6.66	106.12	120.10
1	A	348	GLN	N-CA-CB	6.48	122.26	110.60
1	A	245	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	36	SER	CB-CA-C	6.21	121.91	110.10
1	A	296	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	A	397	THR	C-N-CA	6.18	135.28	122.30
1	A	251	GLU	CG-CD-OE1	-6.10	106.10	118.30
1	A	387	VAL	CA-CB-CG1	6.03	119.94	110.90
1	A	246	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	372	SER	N-CA-CB	-5.82	101.78	110.50
1	A	417	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	120	ALA	CB-CA-C	5.78	118.78	110.10
1	A	230	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	125	LYS	CA-CB-CG	5.76	126.06	113.40
1	A	320	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	349	ILE	CB-CA-C	5.68	122.97	111.60
1	A	166	LEU	CB-CA-C	5.67	120.97	110.20
1	A	251	GLU	CG-CD-OE2	5.67	129.64	118.30
1	A	140	LYS	CA-CB-CG	5.64	125.81	113.40
1	A	264	ASN	CA-CB-CG	-5.60	101.08	113.40
1	A	282	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	A	282	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	255	ASP	O-C-N	5.49	132.53	123.20
1	A	40	THR	N-CA-CB	5.42	120.59	110.30
1	A	295	GLU	CA-CB-CG	5.41	125.31	113.40
1	A	411	GLN	CG-CD-OE1	5.41	132.41	121.60
1	A	6	TYR	N-CA-CB	-5.35	100.97	110.60
1	A	248	ALA	N-CA-CB	5.33	117.56	110.10
1	A	101	ASN	O-C-N	5.26	131.12	122.70
1	A	188	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	A	304	GLU	CB-CA-C	-5.22	99.95	110.40
1	A	410	ASN	N-CA-CB	5.22	120.00	110.60
1	A	200	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	396	LYS	CA-CB-CG	5.21	124.86	113.40
1	A	12	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	124	GLU	CG-CD-OE1	-5.18	107.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	GLU	CG-CD-OE1	-5.13	108.03	118.30
1	A	42	VAL	CA-CB-CG1	5.13	118.59	110.90
1	A	324	VAL	CA-CB-CG1	5.08	118.52	110.90
1	A	223	GLU	CG-CD-OE2	-5.06	108.19	118.30
1	A	304	GLU	CA-CB-CG	5.04	124.48	113.40
1	A	419	LEU	CB-CG-CD2	-5.03	102.46	111.00
1	A	25	THR	N-CA-CB	5.02	119.84	110.30
1	A	340	ASP	OD1-CG-OD2	-5.02	113.77	123.30
1	A	200	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	32	SER	N-CA-CB	5.00	118.00	110.50
1	A	161	GLY	N-CA-C	-5.00	100.59	113.10

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	3289	0	3293	146	1
2	A	9	0	2	1	0
3	A	1	0	0	0	0
4	A	344	0	0	60	2
All	All	3643	0	3295	147	3

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 22.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:ND2	1:A:267:SER:HA	1.44	1.27
1:A:85:ASP:HB3	4:A:715:HOH:O	1.42	1.18
1:A:268:ASP:HB3	1:A:271:LYS:HD2	1.24	1.12
1:A:435:LYS:HE3	4:A:693:HOH:O	1.60	0.99
1:A:264:ASN:ND2	1:A:267:SER:CA	2.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HE3	4:A:570:HOH:O	1.74	0.87
1:A:200:ARG:HB3	4:A:765:HOH:O	1.76	0.86
1:A:264:ASN:HD22	1:A:267:SER:HA	1.43	0.84
1:A:41:GLY:N	1:A:46:LEU:HD21	1.96	0.81
1:A:152:ASN:HB2	4:A:753:HOH:O	1.80	0.81
1:A:268:ASP:HB3	1:A:271:LYS:CD	2.07	0.81
1:A:41:GLY:CA	1:A:46:LEU:HD21	2.11	0.81
1:A:254:LYS:HE3	4:A:702:HOH:O	1.81	0.79
1:A:101:ASN:ND2	1:A:103:SER:HB3	1.98	0.78
1:A:4:LYS:HE2	4:A:599:HOH:O	1.83	0.78
1:A:138:LYS:HE2	4:A:770:HOH:O	1.83	0.78
1:A:57:MET:SD	4:A:691:HOH:O	2.43	0.75
1:A:42:VAL:HG23	4:A:726:HOH:O	1.86	0.75
1:A:152:ASN:O	1:A:399:ALA:HB2	1.86	0.75
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.70	0.74
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.17	0.74
1:A:194:LYS:HE3	1:A:206:GLY:O	1.88	0.73
1:A:432:HIS:HD2	4:A:670:HOH:O	1.72	0.73
1:A:161:GLY:O	4:A:701:HOH:O	2.06	0.71
1:A:126:ASN:ND2	4:A:663:HOH:O	2.25	0.70
1:A:264:ASN:HD22	1:A:267:SER:CB	2.05	0.69
1:A:287:LYS:HE2	4:A:747:HOH:O	1.91	0.69
1:A:326:ASN:C	1:A:326:ASN:HD22	1.95	0.69
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.74	0.68
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.75	0.68
1:A:130:TYR:OH	1:A:418:GLU:OE2	2.07	0.67
1:A:261:ASP:OD2	1:A:264:ASN:ND2	2.27	0.66
1:A:156:GLY:HA2	4:A:758:HOH:O	1.95	0.66
1:A:264:ASN:HB2	1:A:267:SER:HB2	1.78	0.66
1:A:254:LYS:CE	4:A:702:HOH:O	2.43	0.64
1:A:52:ASP:OD1	1:A:52:ASP:C	2.36	0.64
1:A:432:HIS:CD2	4:A:670:HOH:O	2.50	0.64
1:A:57:MET:CB	4:A:691:HOH:O	2.47	0.63
1:A:343:LEU:HD23	1:A:345:LYS:HE3	1.80	0.63
1:A:216:PRO:HG2	1:A:218:ILE:CD1	2.29	0.62
1:A:205:ALA:O	4:A:510:HOH:O	2.15	0.62
1:A:41:GLY:HA3	1:A:46:LEU:HD21	1.81	0.62
1:A:66:LYS:HG2	4:A:684:HOH:O	1.99	0.62
1:A:264:ASN:CG	1:A:267:SER:HA	2.16	0.61
1:A:373:HIS:ND1	1:A:405:ARG:NH1	2.49	0.61
1:A:399:ALA:HB1	1:A:400:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:CD1	1:A:423:ALA:HB1	2.30	0.60
1:A:401:ALA:HB1	4:A:775:HOH:O	2.01	0.60
1:A:104:LYS:HG2	4:A:679:HOH:O	2.02	0.59
2:A:442:PGA:O1P	4:A:611:HOH:O	2.17	0.59
1:A:42:VAL:HA	4:A:726:HOH:O	2.02	0.59
1:A:41:GLY:N	1:A:46:LEU:CD2	2.66	0.58
1:A:138:LYS:HG3	4:A:770:HOH:O	2.02	0.58
1:A:347:ASN:OD1	1:A:374:ARG:NH1	2.31	0.57
1:A:194:LYS:O	1:A:198:LYS:HG3	2.03	0.57
1:A:332:THR:O	1:A:336:LYS:HG3	2.04	0.57
1:A:264:ASN:HB3	1:A:266:ASN:N	2.20	0.56
1:A:264:ASN:HD22	1:A:267:SER:CA	2.07	0.55
1:A:57:MET:CG	4:A:691:HOH:O	2.53	0.55
1:A:260:LEU:HD11	1:A:281:LEU:HD23	1.88	0.54
1:A:264:ASN:HB3	1:A:265:PRO:CA	2.37	0.54
1:A:107:ALA:HB1	4:A:754:HOH:O	2.06	0.54
1:A:216:PRO:HG2	1:A:218:ILE:HD12	1.89	0.54
1:A:298:PHE:HB2	1:A:306:TRP:CD1	2.43	0.54
1:A:399:ALA:HB1	1:A:400:PRO:CD	2.38	0.54
1:A:66:LYS:CG	4:A:684:HOH:O	2.55	0.53
1:A:164:LEU:HD23	4:A:758:HOH:O	2.09	0.53
1:A:313:ALA:HB3	1:A:317:ILE:HD11	1.89	0.53
1:A:101:ASN:HD21	1:A:103:SER:HB3	1.71	0.52
1:A:326:ASN:OD1	1:A:328:LYS:HE3	2.10	0.52
1:A:325:THR:O	1:A:349:ILE:HD12	2.10	0.51
1:A:66:LYS:HG3	4:A:674:HOH:O	2.10	0.51
1:A:357:LYS:NZ	4:A:648:HOH:O	2.44	0.51
1:A:42:VAL:CG2	4:A:726:HOH:O	2.52	0.51
1:A:374:ARG:O	1:A:377:GLU:HG2	2.10	0.51
1:A:33:ILE:CG2	1:A:378:THR:HG21	2.39	0.50
1:A:255:ASP:N	4:A:705:HOH:O	2.45	0.50
1:A:80:ASN:O	1:A:80:ASN:ND2	2.45	0.50
1:A:123:ALA:HB1	4:A:662:HOH:O	2.12	0.49
1:A:275:GLY:N	1:A:276:PRO:CD	2.75	0.49
1:A:63:HIS:NE2	4:A:687:HOH:O	2.35	0.49
1:A:312:THR:CG2	4:A:622:HOH:O	2.60	0.49
1:A:125:LYS:NZ	1:A:135:ASP:OD2	2.45	0.49
1:A:99:THR:HG21	1:A:104:LYS:HB2	1.94	0.48
1:A:111:LEU:HD22	1:A:347:ASN:HA	1.94	0.48
1:A:254:LYS:HD3	1:A:272:TRP:CH2	2.48	0.48
1:A:42:VAL:HG22	1:A:43:HIS:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LYS:HE3	4:A:672:HOH:O	2.14	0.48
1:A:90:ASP:O	1:A:94:ILE:HG13	2.14	0.48
1:A:184:ARG:NH1	4:A:536:HOH:O	2.44	0.48
1:A:26:GLU:HG2	1:A:27:LYS:N	2.26	0.47
1:A:74:PRO:O	1:A:78:LYS:HD2	2.14	0.47
1:A:138:LYS:HE3	4:A:771:HOH:O	2.14	0.47
1:A:162:GLY:HA2	1:A:219:GLN:HE22	1.80	0.47
1:A:328:LYS:NZ	4:A:710:HOH:O	2.13	0.46
1:A:295:GLU:OE1	1:A:396:LYS:NZ	2.45	0.46
1:A:137:SER:HB3	1:A:356:ILE:HG23	1.96	0.46
1:A:330:ILE:HG12	1:A:342:LEU:HD13	1.97	0.46
1:A:82:ASP:O	4:A:715:HOH:O	2.20	0.45
1:A:264:ASN:CG	1:A:267:SER:CA	2.82	0.45
1:A:31:ARG:NH1	4:A:509:HOH:O	2.44	0.45
1:A:73:ALA:HB3	1:A:74:PRO:CD	2.44	0.45
1:A:159:HIS:CE1	4:A:589:HOH:O	2.70	0.45
1:A:57:MET:HB2	4:A:691:HOH:O	2.16	0.45
1:A:344:LEU:HD23	1:A:371:VAL:HG22	1.99	0.45
1:A:156:GLY:CA	4:A:758:HOH:O	2.58	0.45
1:A:185:ILE:HD13	1:A:185:ILE:HG21	1.70	0.45
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.97	0.45
1:A:343:LEU:CD2	1:A:345:LYS:HE3	2.47	0.45
1:A:50:ASP:OD2	1:A:62:LEU:HB2	2.17	0.44
1:A:260:LEU:HD11	1:A:281:LEU:CD2	2.48	0.44
1:A:257:LYS:HG3	4:A:613:HOH:O	2.16	0.44
1:A:101:ASN:ND2	1:A:103:SER:CB	2.75	0.44
1:A:67:ASN:O	1:A:71:VAL:HB	2.18	0.44
1:A:357:LYS:HE2	4:A:648:HOH:O	2.16	0.44
1:A:312:THR:HG23	4:A:622:HOH:O	2.17	0.44
1:A:264:ASN:ND2	1:A:267:SER:CB	2.74	0.44
1:A:260:LEU:CD1	1:A:281:LEU:CD2	2.96	0.44
1:A:398:GLY:HA3	1:A:405:ARG:HD2	2.00	0.44
1:A:152:ASN:O	1:A:399:ALA:CB	2.62	0.43
1:A:200:ARG:HD3	4:A:742:HOH:O	2.18	0.43
1:A:27:LYS:HD2	1:A:124:GLU:HA	2.00	0.43
1:A:268:ASP:OD1	1:A:268:ASP:C	2.56	0.43
1:A:99:THR:CG2	1:A:104:LYS:HB2	2.47	0.43
1:A:328:LYS:HD2	4:A:525:HOH:O	2.17	0.43
1:A:94:ILE:HG23	4:A:683:HOH:O	2.18	0.43
1:A:238:ASP:HB2	4:A:694:HOH:O	2.18	0.43
1:A:94:ILE:HA	4:A:683:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:O	1:A:367:TRP:HB2	2.19	0.43
1:A:328:LYS:HG2	1:A:329:ARG:N	2.34	0.42
1:A:264:ASN:HD22	1:A:267:SER:HB2	1.83	0.42
1:A:97:ASP:OD2	1:A:99:THR:OG1	2.29	0.42
1:A:133:LEU:HD11	1:A:352:LEU:HD21	2.02	0.42
1:A:4:LYS:NZ	4:A:764:HOH:O	2.53	0.42
1:A:188:GLU:OE1	1:A:237:HIS:NE2	2.39	0.42
1:A:202:GLY:O	1:A:205:ALA:HB3	2.19	0.41
1:A:306:TRP:HB3	1:A:338:ALA:HB1	2.02	0.41
1:A:63:HIS:CD2	4:A:687:HOH:O	2.74	0.41
1:A:80:ASN:HA	4:A:556:HOH:O	2.19	0.41
1:A:274:THR:HG23	4:A:614:HOH:O	2.20	0.41
1:A:357:LYS:CE	4:A:648:HOH:O	2.67	0.41
1:A:248:ALA:HB1	4:A:751:HOH:O	2.20	0.41
1:A:261:ASP:C	4:A:574:HOH:O	2.59	0.40
1:A:39:SER:HA	1:A:47:GLU:O	2.21	0.40
1:A:38:ALA:O	1:A:47:GLU:HG2	2.21	0.40
1:A:97:ASP:HB2	1:A:110:ILE:HD11	2.04	0.40
1:A:225:LEU:HD13	1:A:289:TYR:CD2	2.56	0.40

All (3) 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)
4:A:704:HOH:O	4:A:763:HOH:O[5_655]	1.75	0.45
4:A:725:HOH:O	4:A:725:HOH:O[8_666]	2.08	0.12
1:A:57:MET:CE	1:A:192:ASN:ND2[8_666]	2.19	0.01

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	434/436 (100%)	412 (95%)	20 (5%)	2 (0%)	29 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	402	ARG

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	344/344 (100%)	331 (96%)	13 (4%)	33 42

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	126	ASN
1	A	133	LEU
1	A	147	PRO
1	A	155	ASN
1	A	254	LYS
1	A	255	ASP
1	A	266	ASN
1	A	284	SER
1	A	304	GLU
1	A	326	ASN
1	A	373	HIS
1	A	392	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	101	ASN
1	A	152	ASN
1	A	155	ASN
1	A	219	GLN
1	A	264	ASN
1	A	326	ASN
1	A	348	GLN

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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	PGA	A	442	3	8,8,8	2.85	3 (37%)	10,11,11	3.32	6 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGA	A	442	3	-	3/6/6/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	442	PGA	O1P-C2	-6.00	1.39	1.43
2	A	442	PGA	P-O3P	4.09	1.70	1.54
2	A	442	PGA	P-O2P	2.67	1.59	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	442	PGA	O1P-P-O2P	7.48	127.45	106.47
2	A	442	PGA	O1P-C2-C1	4.36	117.12	110.54
2	A	442	PGA	O2-C1-O1	-3.33	115.01	123.30
2	A	442	PGA	O3P-P-O1P	2.92	114.51	106.73
2	A	442	PGA	O4P-P-O3P	-2.11	99.58	107.64
2	A	442	PGA	O4P-P-O1P	-2.08	101.20	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	442	PGA	C2-O1P-P-O3P
2	A	442	PGA	O2-C1-C2-O1P
2	A	442	PGA	C2-O1P-P-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	442	PGA	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.