



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 01:59 AM EDT

PDB ID : 3MOH
Title : The structure of rat cytosolic PEPCK mutant A467G in complex with phosphoglycolate and GDP
Authors : Johnson, T.A.; Holyoak, T.
Deposited on : unknown
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

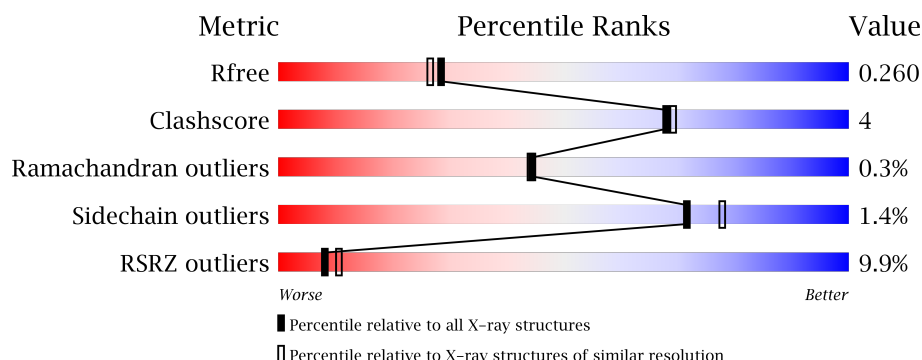
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	624	<div> <div>9%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	B	624	<div> <div>10%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10430 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.

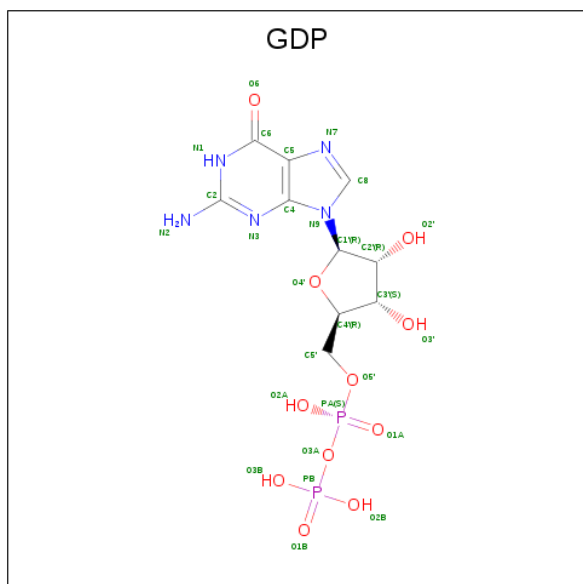
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	10	0
			4811	3079	820	881	31			
1	B	613	Total	C	N	O	S	0	6	0
			4852	3104	828	887	33			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P07379
A	0	SER	-	EXPRESSION TAG	UNP P07379
A	467	GLY	ALA	ENGINEERED	UNP P07379
B	-1	GLY	-	EXPRESSION TAG	UNP P07379
B	0	SER	-	EXPRESSION TAG	UNP P07379
B	467	GLY	ALA	ENGINEERED	UNP P07379

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

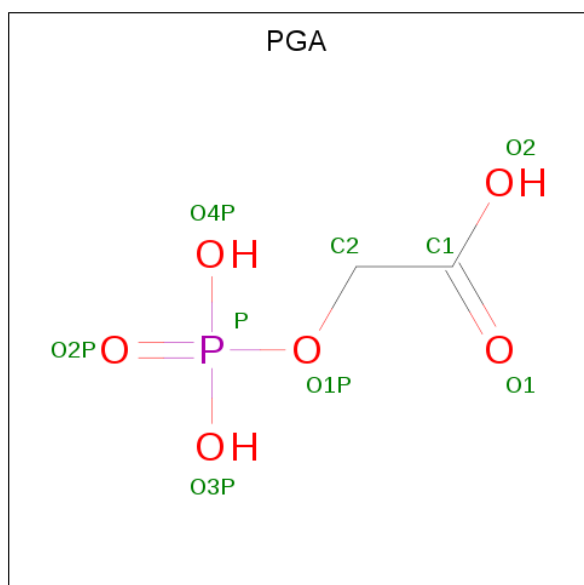


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: C₂H₅O₆P).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

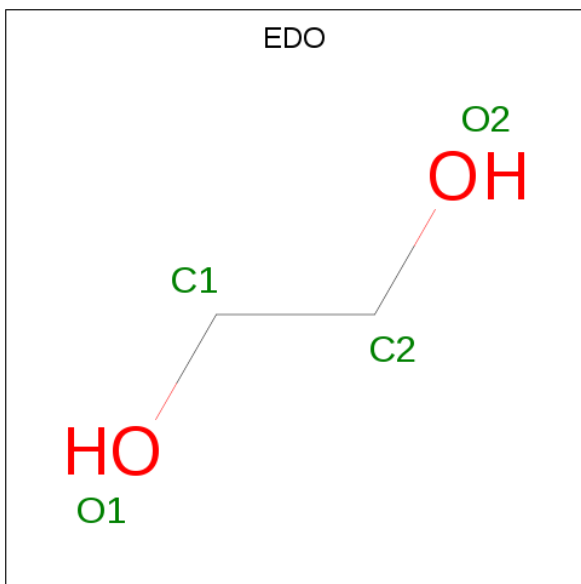
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

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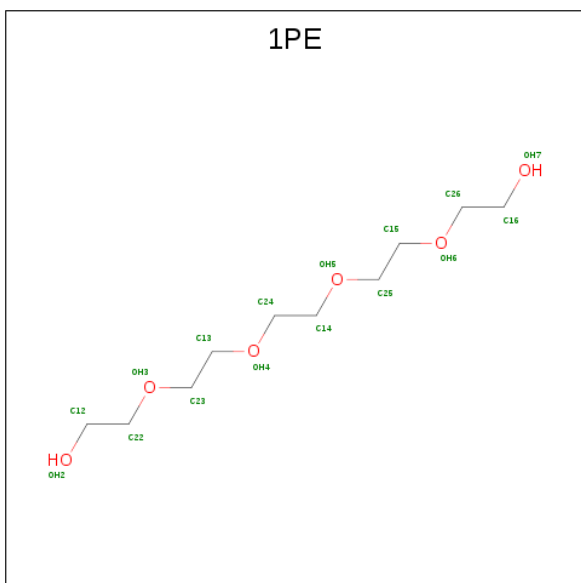
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		
7	B	1	Total	C	O	0	0
			10	6	4		

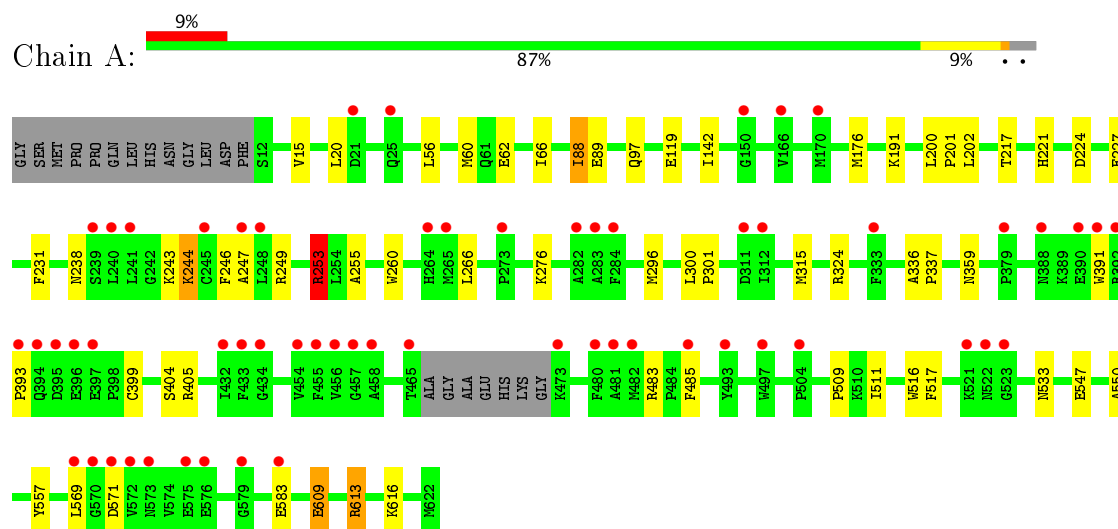
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	370	Total	O	0	0
			370	370		
8	B	298	Total	O	0	0
			298	298		

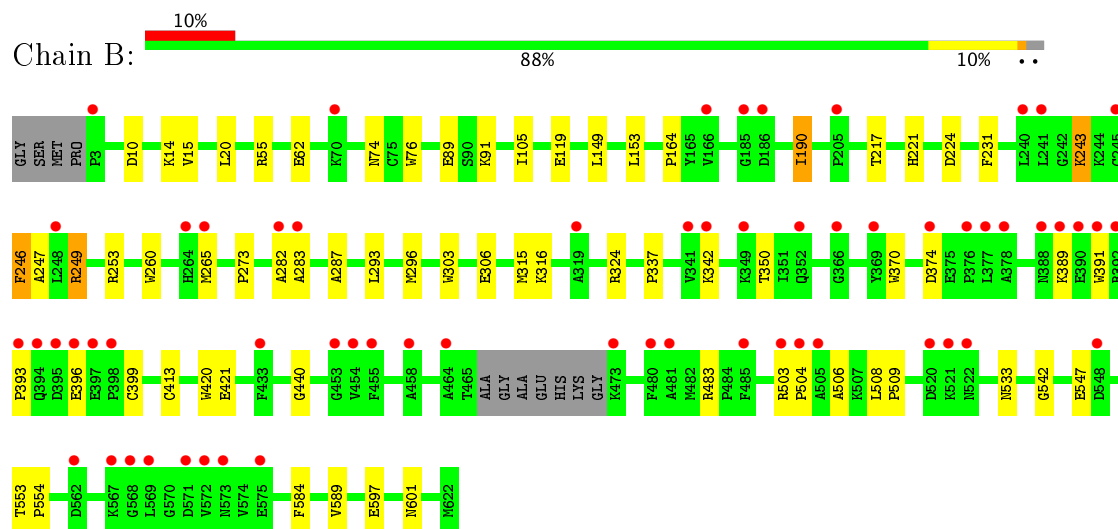
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]



- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.08 Å 119.52 Å 87.02 Å 90.00° 107.15° 90.00°	Depositor
Resolution (Å)	35.93 – 2.10 35.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (35.93-2.10) 96.8 (35.93-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.10 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.247 0.205 , 0.260	Depositor DCC
R_{free} test set	3477 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10430	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1384e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, PGA, NA, MN, EDO, 1PE

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	0.70	0/4965	0.71	3/6717 (0.0%)
1	B	0.68	0/4997	0.71	3/6765 (0.0%)
All	All	0.69	0/9962	0.71	6/13482 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	B	249	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	613	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	613	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	253	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	10	ASP	CB-CG-OD1	5.03	122.83	118.30

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	4811	0	4787	42	0
1	B	4852	0	4812	40	0
2	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	12	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	2	1	0
4	B	9	0	2	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	6	0	0
7	A	5	0	5	2	0
7	B	10	0	13	1	0
8	A	370	0	0	5	0
8	B	298	0	0	8	0
All	All	10430	0	9651	85	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 4.

All (85) 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:296:MET:HE2	1:A:533:ASN:HB2	1.59	0.83
1:A:119[B]:GLU:HG3	8:A:916:HOH:O	1.86	0.74
2:B:1000:GDP:O1B	8:B:746:HOH:O	2.11	0.69
1:B:89:GLU:OE2	1:B:483:ARG:NH1	2.28	0.66
1:B:224:ASP:OD2	8:B:626:HOH:O	2.14	0.65
1:B:190:ILE:HG21	1:B:246:PHE:CE2	2.36	0.60
1:B:287:ALA:HA	2:B:1000:GDP:H5'	1.83	0.60
1:A:509:PRO:O	7:A:1300:1PE:H122	2.02	0.60
1:A:511:ILE:H	7:A:1300:1PE:C23	2.14	0.59
1:A:62[B]:GLU:OE1	1:A:62[B]:GLU:HA	2.03	0.58
1:B:91:LYS:HD3	1:B:217:THR:O	2.03	0.58
1:A:217:THR:HA	1:A:231:PHE:O	2.04	0.58
1:B:14:LYS:NZ	7:B:1300:1PE:H122	2.20	0.57
1:A:315:MET:HA	1:A:324:ARG:O	2.05	0.57
1:B:62[B]:GLU:HG2	8:B:796:HOH:O	2.05	0.56
1:A:89:GLU:OE1	1:A:483:ARG:NH2	2.28	0.56
1:B:224:ASP:OD1	1:B:253:ARG:NH2	2.39	0.56
1:A:243:LYS:HG2	1:A:244:LYS:HD2	1.89	0.55
1:B:55:ARG:NH2	8:B:665:HOH:O	2.39	0.55
1:A:97[B]:GLN:OE1	1:A:119[B]:GLU:OE1	2.25	0.55
1:A:224:ASP:OD1	1:A:253:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TRP:CE2	1:B:421:GLU:HG3	2.42	0.54
1:A:62[B]:GLU:HG2	8:A:664:HOH:O	2.08	0.54
1:A:244:LYS:HE2	1:A:485:PHE:CZ	2.44	0.53
1:A:296:MET:CE	1:A:533:ASN:HB2	2.35	0.53
1:A:255:ALA:HB1	1:A:260:TRP:O	2.10	0.52
1:B:503:ARG:HG2	1:B:506:ALA:HB2	1.91	0.52
1:A:244:LYS:HE2	1:A:485:PHE:CE1	2.44	0.52
1:B:217:THR:HA	1:B:231:PHE:O	2.10	0.51
1:A:609:GLU:OE1	1:A:613:ARG:HD2	2.10	0.51
1:B:243:LYS:O	1:B:247:ALA:HB3	2.11	0.51
1:B:153:LEU:HD11	1:B:316:LYS:HD3	1.93	0.51
1:B:391:TRP:CD2	1:B:399:CYS:HB3	2.46	0.51
1:A:391:TRP:CD2	1:A:399:CYS:HB3	2.47	0.50
1:B:164:PRO:HD2	8:B:705:HOH:O	2.12	0.49
1:B:293:LEU:HD12	1:B:296:MET:HE2	1.94	0.49
1:A:391:TRP:CE2	1:A:399:CYS:HB3	2.47	0.49
1:B:105:ILE:O	1:B:601[B]:ASN:ND2	2.46	0.47
1:A:276:LYS:HE3	8:B:658:HOH:O	2.14	0.47
1:A:266:LEU:C	1:A:266:LEU:HD12	2.35	0.47
2:B:1000:GDP:PB	8:B:746:HOH:O	2.73	0.47
1:B:15:VAL:HG21	1:B:20:LEU:HG	1.97	0.47
1:B:350:THR:OG1	1:B:413:CYS:HA	2.15	0.47
1:A:202:LEU:HD22	8:A:682:HOH:O	2.15	0.47
1:B:89:GLU:CD	1:B:483:ARG:HH12	2.19	0.46
1:A:88:ILE:H	1:A:238:ASN:HD21	1.63	0.46
1:B:553:THR:HB	1:B:554:PRO:HD2	1.98	0.46
1:A:15:VAL:HG21	1:A:20:LEU:HG	1.98	0.46
1:B:265:MET:HA	1:B:282:ALA:O	2.16	0.45
1:A:244:LYS:HG3	1:A:485:PHE:CE1	2.51	0.45
1:B:342:LYS:HE2	1:B:374:ASP:OD2	2.16	0.45
1:B:391:TRP:CE2	1:B:399:CYS:HB3	2.52	0.44
1:B:508:LEU:HA	1:B:509:PRO:HD2	1.88	0.44
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.98	0.44
1:A:547[A]:GLU:OE1	8:A:890:HOH:O	2.21	0.44
1:B:273:PRO:HD3	1:B:303:TRP:CE2	2.52	0.44
1:A:191:LYS:HB2	1:A:227:GLU:HG2	2.00	0.44
1:B:74:ASN:ND2	1:B:76:TRP:HE1	2.16	0.44
4:B:900:PGA:P	8:B:845:HOH:O	2.76	0.44
1:A:516:TRP:HB2	1:A:517:PHE:CE2	2.53	0.43
1:B:389:LYS:HA	1:B:389:LYS:HD3	1.84	0.43
1:B:296:MET:HE1	1:B:533:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:TRP:HB3	1:B:316:LYS:HD2	1.99	0.43
1:A:200:LEU:HA	1:A:201:PRO:C	2.38	0.43
1:B:260:TRP:HB2	1:B:315:MET:O	2.19	0.43
1:A:89:GLU:OE2	1:A:483:ARG:NH1	2.40	0.42
1:A:221:HIS:CE1	1:A:249:ARG:HD2	2.55	0.42
1:B:503:ARG:HA	1:B:504:PRO:HD3	1.78	0.42
1:A:300:LEU:HA	1:A:301:PRO:HD3	1.95	0.42
1:A:616:LYS:HE3	1:A:616:LYS:HB2	1.79	0.42
1:A:89:GLU:HB2	8:A:862:HOH:O	2.18	0.42
1:A:550:ALA:HB1	1:A:557:TYR:HB3	2.02	0.42
1:B:315:MET:HA	1:B:324:ARG:O	2.20	0.42
1:B:221:HIS:CE1	1:B:249:ARG:HE	2.37	0.42
1:B:597:GLU:O	1:B:601[B]:ASN:HB3	2.20	0.41
1:A:359:ASN:O	1:A:404:SER:HB3	2.21	0.41
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.89	0.41
1:B:265:MET:HG2	1:B:283:ALA:HB2	2.03	0.41
1:A:405:ARG:NH1	4:A:900:PGA:O2P	2.40	0.41
1:B:542:GLY:O	1:B:547:GLU:HB2	2.21	0.41
1:A:142:ILE:HG23	1:A:176:MET:CG	2.51	0.40
1:B:440:GLY:HA3	1:B:584:PHE:CZ	2.57	0.40
1:B:337:PRO:HA	1:B:370:TRP:CD1	2.56	0.40
1:A:243:LYS:O	1:A:247:ALA:HB3	2.22	0.40
1:A:60:MET:HB3	1:A:66:ILE:HG12	2.02	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	610/624 (98%)	590 (97%)	19 (3%)	1 (0%)	51	52
1	B	615/624 (99%)	587 (95%)	25 (4%)	3 (0%)	32	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1225/1248 (98%)	1177 (96%)	44 (4%)	4 (0%)	44	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	LEU
1	B	243	LYS
1	B	393	PRO
1	A	393	PRO

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	516/520 (99%)	508 (98%)	8 (2%)	68	74
1	B	520/520 (100%)	514 (99%)	6 (1%)	75	81
All	All	1036/1040 (100%)	1022 (99%)	14 (1%)	71	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ILE
1	A	244	LYS
1	A	246	PHE
1	A	253	ARG
1	A	569	LEU
1	A	571	ASP
1	A	583	GLU
1	A	609	GLU
1	B	119	GLU
1	B	190	ILE
1	B	246	PHE
1	B	306	GLU
1	B	396	GLU
1	B	589	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	B	74	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	GDP	A	1000	3	25,30,30	1.21	2 (8%)	26,47,47	1.96	7 (26%)
6	EDO	A	1200	-	3,3,3	0.91	0	2,2,2	0.41	0
7	1PE	A	1300	-	4,4,15	0.63	0	3,3,14	0.66	0
4	PGA	A	900	3	5,8,8	0.72	0	6,11,11	1.11	0
2	GDP	B	1000	3	25,30,30	1.38	4 (16%)	26,47,47	1.70	6 (23%)
7	1PE	B	1300	-	9,9,15	0.70	0	8,8,14	0.59	0
4	PGA	B	900	3	5,8,8	0.78	0	6,11,11	1.02	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
2	GDP	A	1000	3	-	0/12/32/32	0/3/3/3
6	EDO	A	1200	-	-	0/1/1/1	0/0/0/0
7	1PE	A	1300	-	-	0/2/2/13	0/0/0/0
4	PGA	A	900	3	-	0/4/6/6	0/0/0/0
2	GDP	B	1000	3	-	0/12/32/32	0/3/3/3
7	1PE	B	1300	-	-	0/7/7/13	0/0/0/0
4	PGA	B	900	3	-	0/4/6/6	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	GDP	O4'-C1'	2.00	1.44	1.41
2	B	1000	GDP	C6-N1	2.03	1.36	1.33
2	A	1000	GDP	C5-C4	2.48	1.46	1.40
2	B	1000	GDP	C6-C5	3.10	1.47	1.41
2	A	1000	GDP	C6-C5	3.57	1.48	1.41
2	B	1000	GDP	C5-C4	3.84	1.49	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	GDP	C5-C6-N1	-3.70	118.21	123.48
2	A	1000	GDP	C5-C6-N1	-3.61	118.34	123.48
2	A	1000	GDP	C6-C5-C4	-3.46	117.40	120.84
2	A	1000	GDP	N3-C2-N1	-3.06	122.99	127.46
2	B	1000	GDP	C6-C5-C4	-2.73	118.13	120.84
2	B	1000	GDP	N3-C2-N1	-2.64	123.61	127.46
2	B	1000	GDP	O3'-C3'-C2'	-2.55	103.67	111.83
2	A	1000	GDP	C4-C5-N7	-2.38	107.11	109.41
2	A	1000	GDP	N2-C2-N1	2.41	121.09	117.24
2	A	1000	GDP	C6-N1-C2	3.49	121.08	116.06
2	B	1000	GDP	C6-N1-C2	3.70	121.39	116.06
2	B	1000	GDP	C2-N3-C4	3.97	119.80	115.16
2	A	1000	GDP	C2-N3-C4	4.98	120.97	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1300	1PE	2	0
4	A	900	PGA	1	0
2	B	1000	GDP	3	0
7	B	1300	1PE	1	0
4	B	900	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

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	604/624 (96%)	0.48	59 (9%) 8 11	6, 12, 16, 21	0
1	B	613/624 (98%)	0.51	61 (9%) 8 10	7, 13, 17, 21	0
All	All	1217/1248 (97%)	0.50	120 (9%) 8 10	6, 12, 17, 21	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLN	8.7
1	B	394	GLN	6.6
1	A	396	GLU	6.5
1	A	504	PRO	5.9
1	A	395	ASP	5.6
1	A	392	ARG	5.5
1	A	571	ASP	5.5
1	B	396	GLU	5.4
1	B	392	ARG	5.2
1	B	393	PRO	4.8
1	B	572	VAL	4.7
1	B	395	ASP	4.6
1	A	393	PRO	4.3
1	A	569	LEU	4.1
1	B	504	PRO	4.0
1	B	391	TRP	4.0
1	B	473	LYS	4.0
1	B	341	VAL	3.9
1	A	248	LEU	3.8
1	A	391	TRP	3.8
1	B	505	ALA	3.8
1	B	390	GLU	3.7
1	A	397	GLU	3.6
1	A	480	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	575	GLU	3.5
1	A	570	GLY	3.5
1	A	240	LEU	3.5
1	A	312	ILE	3.4
1	B	481	ALA	3.4
1	A	273	PRO	3.3
1	A	481	ALA	3.3
1	A	521	LYS	3.3
1	A	575	GLU	3.3
1	B	398	PRO	3.3
1	A	241	LEU	3.3
1	B	366	GLY	3.2
1	A	283	ALA	3.1
1	B	397	GLU	3.1
1	A	433	PHE	3.1
1	B	522	ASN	3.0
1	A	465	THR	3.0
1	B	568	GLY	3.0
1	B	571	ASP	3.0
1	A	522	ASN	3.0
1	B	186	ASP	2.9
1	B	248	LEU	2.9
1	B	377	LEU	2.9
1	B	388	ASN	2.9
1	B	567	LYS	2.8
1	B	70	LYS	2.8
1	A	432	ILE	2.8
1	A	482	MET	2.8
1	B	548	ASP	2.8
1	A	523	GLY	2.8
1	B	240	LEU	2.8
1	B	569	LEU	2.8
1	A	284	PHE	2.7
1	B	264	HIS	2.7
1	A	245	CYS	2.6
1	B	520	ASP	2.6
1	A	282	ALA	2.6
1	B	3	PRO	2.6
1	B	521	LYS	2.6
1	A	388	ASN	2.5
1	B	389	LYS	2.5
1	A	390	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	319	ALA	2.5
1	A	265	MET	2.5
1	B	205	PRO	2.4
1	B	433	PHE	2.4
1	B	480	PHE	2.4
1	B	573	ASN	2.4
1	A	434	GLY	2.4
1	A	485	PHE	2.4
1	A	264	HIS	2.4
1	B	369	TYR	2.3
1	A	473	LYS	2.3
1	B	241	LEU	2.3
1	A	583	GLU	2.3
1	B	455	PHE	2.3
1	B	374	ASP	2.3
1	B	453	GLY	2.3
1	B	464	ALA	2.3
1	B	485	PHE	2.3
1	B	245	CYS	2.3
1	A	25	GLN	2.3
1	A	166	VAL	2.2
1	A	379	PRO	2.2
1	A	247	ALA	2.2
1	A	170	MET	2.2
1	B	458	ALA	2.2
1	B	342	LYS	2.2
1	A	239	SER	2.2
1	B	376	PRO	2.2
1	A	150	GLY	2.2
1	A	457	GLY	2.2
1	A	497	TRP	2.1
1	A	333	PHE	2.1
1	A	573	ASN	2.1
1	A	311	ASP	2.1
1	B	503	ARG	2.1
1	A	576	GLU	2.1
1	A	454	VAL	2.1
1	A	458	ALA	2.1
1	A	579	GLY	2.1
1	B	283	ALA	2.1
1	B	352	GLN	2.1
1	B	378	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	349	LYS	2.1
1	B	265	MET	2.0
1	A	456	VAL	2.0
1	A	572	VAL	2.0
1	A	455	PHE	2.0
1	A	493	TYR	2.0
1	B	185	GLY	2.0
1	B	166	VAL	2.0
1	B	454	VAL	2.0
1	A	21	ASP	2.0
1	B	282	ALA	2.0
1	B	562	ASP	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, 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	LLDF	B-factors(Å ²)	Q<0.9
7	1PE	A	1300	5/16	0.88	0.21	1.92	17,20,24,25	0
7	1PE	B	1300	10/16	0.83	0.17	0.34	23,28,29,30	0
5	NA	A	1100	1/1	0.87	0.12	-0.28	22,22,22,22	0
2	GDP	A	1000	28/28	0.97	0.13	-0.43	14,17,19,23	0
2	GDP	B	1000	28/28	0.94	0.12	-0.59	15,18,21,22	0
4	PGA	A	900	9/9	0.96	0.18	-0.79	15,16,18,18	0
4	PGA	B	900	9/9	0.96	0.13	-0.83	19,20,21,21	0
5	NA	B	1100	1/1	0.92	0.08	-1.87	24,24,24,24	0
3	MN	A	701	1/1	0.99	0.13	-2.68	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MN	B	701	1/1	0.99	0.08	-2.88	20,20,20,20	0
3	MN	B	700	1/1	0.99	0.11	-3.52	19,19,19,19	0
3	MN	A	700	1/1	0.99	0.13	-4.27	18,18,18,18	0
6	EDO	A	1200	4/4	0.83	0.12	-	25,27,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.