



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MOF  
Title : The structure of rat cytosolic PEPCK mutant A467G in complex with oxalate and GTP  
Authors : Johnson, T.A.; Holyoak, T.  
Deposited on : 2010-04-22  
Resolution : 1.75 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](mailto: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 (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

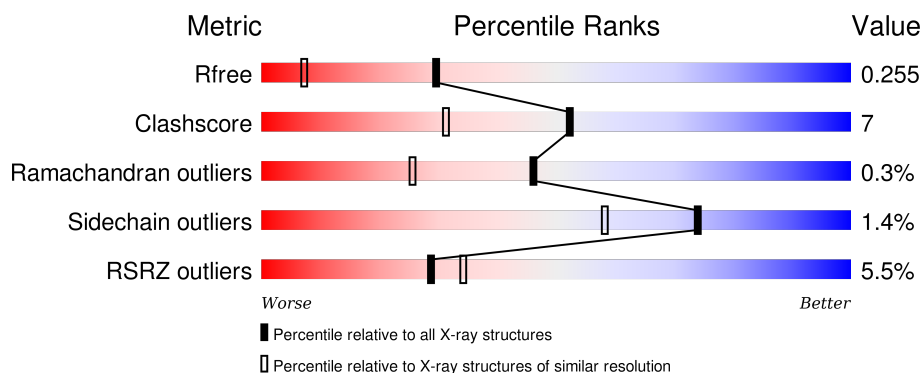
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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  $\geq 3$ , 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>5%</div> <div>89%</div> <div>10%</div> </div>
1	B	624	<div> <div>5%</div> <div>89%</div> <div>10%</div> </div>

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	GTP	A	900[B]	-	-	X	-
7	EDO	B	3000	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11021 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.

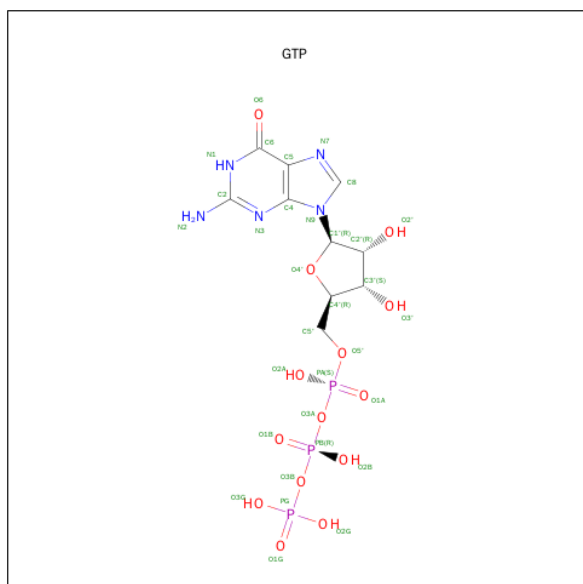
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	21	0
			5009	3215	847	912	35			
1	B	616	Total	C	N	O	S	0	14	0
			4920	3155	836	895	34			

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'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

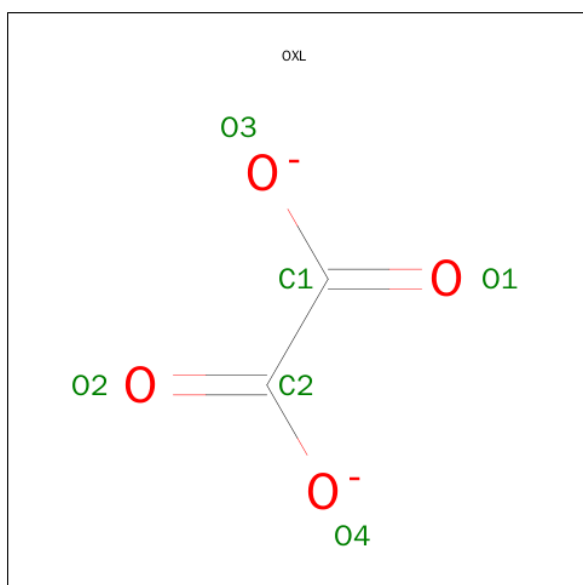


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- 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	1
			3	3		

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).



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

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

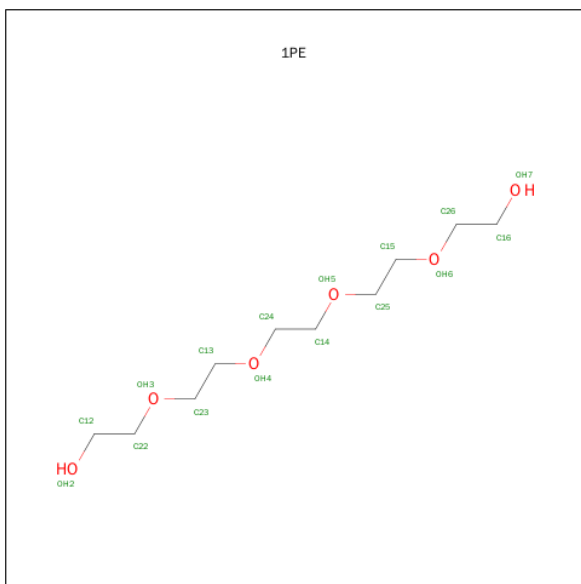
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

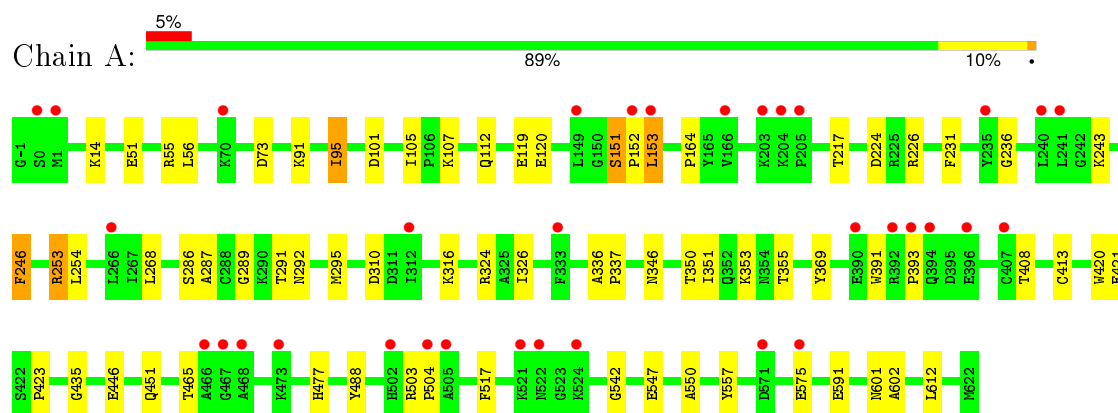
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	457	Total	O	0	0
			457	457		
8	B	456	Total	O	0	0
			456	456		

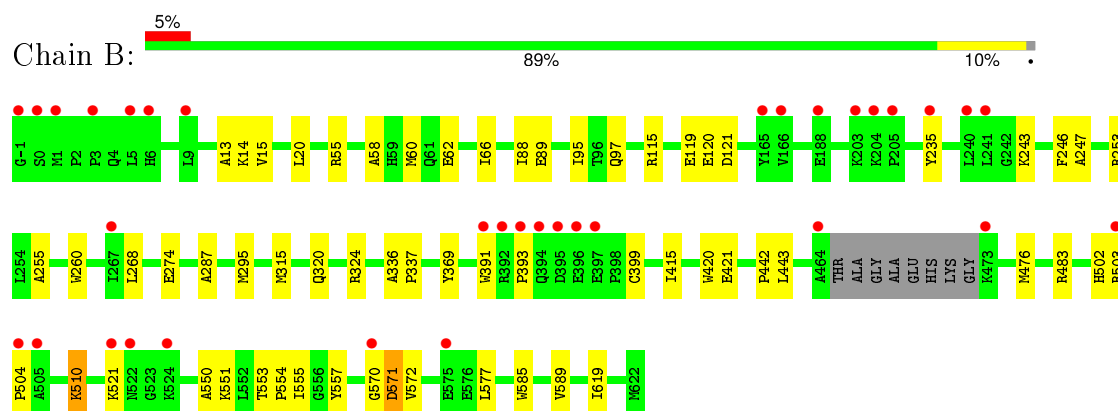
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	61.98 Å 119.60 Å 87.07 Å 90.00° 106.87° 90.00°	Depositor
Resolution (Å)	33.24 – 1.75 33.24 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.6 (33.24-1.75) 96.6 (33.24-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.75 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.179 , 0.228 0.206 , 0.255	Depositor DCC
$R_{free}$ test set	5913 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 118250 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	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 70.48 % 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 3.0993e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, NA, MN, EDO, 1PE, OXL

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	0.74	0/5205	0.74	2/7048 (0.0%)
1	B	0.73	0/5091	0.72	0/6888
All	All	0.74	0/10296	0.73	2/13936 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	A	95	ILE	CG1-CB-CG2	-5.18	100.00	111.40

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	5009	0	5005	77	1
1	B	4920	0	4911	55	0
2	A	64	0	24	13	0
2	B	32	0	12	1	0
3	A	3	0	0	1	0
3	B	2	0	0	0	0
4	A	6	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	24	0	30	5	0
6	B	16	0	22	2	0
7	A	12	0	18	0	0
7	B	12	0	18	1	0
8	A	457	0	0	13	0
8	B	456	0	0	13	1
All	All	11021	0	10040	135	1

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 7.

All (135) 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)
2:A:900[B]:GTP:H1'	8:A:965:HOH:O	1.54	1.07
1:A:351:ILE:HG22	1:A:408[B]:THR:HG21	1.29	1.05
1:A:350[B]:THR:HG22	1:A:413:CYS:HA	1.50	0.91
1:A:152:PRO:HB2	1:A:153:LEU:HD13	1.50	0.90
1:A:153:LEU:HD23	1:A:326:ILE:HG21	1.54	0.90
1:A:151:SER:OG	1:A:153:LEU:HD22	1.76	0.84
1:A:292[A]:ASN:OD1	2:A:900[A]:GTP:C8	2.31	0.83
1:A:112:GLN:NE2	8:A:857:HOH:O	2.11	0.82
1:A:292[A]:ASN:OD1	2:A:900[A]:GTP:H8	1.62	0.82
1:B:589[A]:VAL:HG11	1:B:619[A]:ILE:HD12	1.62	0.80
1:A:153:LEU:HG	6:A:1200:1PE:OH3	1.82	0.79
1:B:89:GLU:OE1	1:B:483:ARG:NH1	2.15	0.79
1:B:55:ARG:HG2	1:B:55:ARG:HH11	1.47	0.79
3:A:700[B]:MN:MN	8:A:794:HOH:O	1.42	0.75
1:A:287:ALA:HA	2:A:900[B]:GTP:O3A	1.87	0.74
1:A:153:LEU:HD23	1:A:326:ILE:CG2	2.19	0.73
1:B:585:TRP:HB3	1:B:619[A]:ILE:HD13	1.72	0.72
1:B:503:ARG:HG2	1:B:504:PRO:HD2	1.72	0.71
1:A:56:LEU:HD11	1:A:164:PRO:HB3	1.71	0.71
1:A:224:ASP:HB3	8:A:909:HOH:O	1.90	0.70
1:B:89:GLU:CD	1:B:483:ARG:HH12	1.95	0.70
1:A:355:THR:OG1	1:A:408[B]:THR:HG22	1.93	0.69
1:B:476[A]:MET:CE	8:B:999:HOH:O	2.40	0.68
1:B:89:GLU:HG2	1:B:115[A]:ARG:HH11	1.58	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510[B]:LYS:HE2	8:B:911:HOH:O	1.94	0.67
1:B:13:ALA:HB3	6:B:1300:1PE:H131	1.76	0.67
1:A:55:ARG:HG2	1:A:55:ARG:HH11	1.61	0.66
1:A:346:ASN:O	1:A:350[B]:THR:HG23	1.97	0.65
1:A:153:LEU:HB3	6:A:1200:1PE:H131	1.80	0.64
1:A:503:ARG:HB2	1:A:504:PRO:CD	2.28	0.63
1:A:351:ILE:HG22	1:A:408[B]:THR:CG2	2.18	0.63
1:B:570:GLY:O	1:B:572:VAL:N	2.29	0.63
1:A:503:ARG:HB2	1:A:504:PRO:HD3	1.79	0.62
1:B:89:GLU:HG2	1:B:115[A]:ARG:NH1	2.15	0.62
1:A:14:LYS:HZ2	6:A:1201:1PE:H232	1.62	0.62
1:A:105:ILE:O	1:A:601[B]:ASN:ND2	2.31	0.62
1:B:510[B]:LYS:HG2	8:B:911:HOH:O	2.00	0.62
1:A:153:LEU:HD13	1:A:153:LEU:N	2.15	0.61
1:A:503:ARG:NH2	8:A:874:HOH:O	2.34	0.61
1:B:476[A]:MET:HE3	8:B:999:HOH:O	1.99	0.60
1:A:287:ALA:HA	2:A:900[B]:GTP:PA	2.42	0.60
1:A:95:ILE:CG2	1:A:119[A]:GLU:HG3	2.31	0.60
1:B:571:ASP:N	1:B:571:ASP:OD1	2.33	0.59
1:B:420:TRP:CE2	1:B:421:GLU:HG3	2.39	0.58
1:A:152:PRO:HA	8:A:1054:HOH:O	2.04	0.57
1:B:557:TYR:CZ	7:B:3001:EDO:H11	2.40	0.57
1:A:152:PRO:HB2	1:A:153:LEU:CD1	2.32	0.55
1:B:60:MET:HB3	1:B:66:ILE:HG12	1.86	0.55
1:A:292[A]:ASN:OD1	2:A:900[A]:GTP:H2'	2.06	0.55
1:B:476[A]:MET:HE2	8:B:999:HOH:O	2.05	0.54
1:B:589[A]:VAL:CG1	1:B:619[A]:ILE:HD12	2.36	0.53
1:B:570:GLY:O	1:B:572:VAL:HG22	2.08	0.53
1:A:391:TRP:CH2	1:A:393:PRO:HA	2.44	0.53
1:A:153:LEU:HG	6:A:1200:1PE:C22	2.38	0.52
1:B:55:ARG:HG2	1:B:55:ARG:NH1	2.22	0.52
1:B:589[A]:VAL:HG23	8:B:1028:HOH:O	2.10	0.52
1:A:153:LEU:CG	6:A:1200:1PE:OH3	2.58	0.51
1:A:287:ALA:HA	2:A:900[B]:GTP:O2A	2.10	0.51
1:A:550:ALA:HB1	1:A:557:TYR:HB3	1.91	0.51
1:A:575:GLU:OE2	1:A:575:GLU:HA	2.10	0.50
1:A:55:ARG:NH2	8:A:632:HOH:O	2.44	0.50
2:A:900[B]:GTP:O1G	8:A:794:HOH:O	2.20	0.50
1:A:152:PRO:HD2	1:A:423:PRO:O	2.12	0.49
1:A:101:ASP:OD2	8:A:625:HOH:O	2.20	0.49
1:A:151:SER:OG	1:A:153:LEU:CD2	2.56	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.95	0.49
1:A:95:ILE:HG21	1:A:119[A]:GLU:HG3	1.94	0.48
1:A:316:LYS:HD3	8:A:812:HOH:O	2.12	0.48
1:A:286[B]:SER:HG	4:A:1000:OXL:C2	2.26	0.48
1:B:243:LYS:O	1:B:247:ALA:HB3	2.13	0.48
1:B:589[A]:VAL:CG2	8:B:1028:HOH:O	2.61	0.48
1:A:217:THR:HA	1:A:231:PHE:O	2.15	0.47
1:B:62[B]:GLU:HA	1:B:62[B]:GLU:OE1	2.14	0.47
1:A:289:GLY:HA2	2:A:900[A]:GTP:C8	2.50	0.47
1:A:542:GLY:O	1:A:547:GLU:HB2	2.15	0.46
1:A:355:THR:HG23	1:A:408[B]:THR:CG2	2.46	0.46
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.98	0.46
1:B:391:TRP:CH2	1:B:393:PRO:HA	2.50	0.46
1:B:97[B]:GLN:NE2	8:B:844:HOH:O	1.57	0.46
1:B:502:HIS:CD2	8:B:839:HOH:O	2.69	0.46
1:A:355:THR:CG2	1:A:408[B]:THR:HG22	2.45	0.46
1:B:89:GLU:HG3	8:B:698:HOH:O	2.16	0.46
1:B:120:GLU:HG2	1:B:121:ASP:N	2.30	0.45
1:A:435:GLY:CA	8:A:809:HOH:O	2.65	0.45
1:A:226:ARG:HD3	8:A:881:HOH:O	2.16	0.45
1:B:14:LYS:HZ2	6:B:1300:1PE:H142	1.82	0.45
1:A:73:ASP:O	1:A:353:LYS:HA	2.17	0.45
1:B:255:ALA:HB1	1:B:260:TRP:O	2.17	0.45
1:B:95:ILE:CG2	1:B:119:GLU:HG2	2.47	0.45
1:B:115[A]:ARG:NH2	8:B:940:HOH:O	2.50	0.44
1:A:268:LEU:HD12	1:A:268:LEU:C	2.38	0.44
1:B:315:MET:HA	1:B:324:ARG:O	2.18	0.44
1:B:287:ALA:HA	2:B:1000:GTP:O1A	2.17	0.44
1:A:291:THR:O	1:A:295:MET:HG2	2.18	0.44
1:A:291:THR:OG1	1:A:310:ASP:OD2	2.35	0.44
1:A:446:GLU:HB3	1:A:557:TYR:HB2	2.00	0.44
1:B:553:THR:HB	1:B:554:PRO:HD2	2.00	0.44
1:B:585:TRP:O	1:B:589[A]:VAL:HG13	2.18	0.43
1:B:391:TRP:CE2	1:B:399:CYS:HB3	2.53	0.43
1:B:521:LYS:HG2	8:B:765:HOH:O	2.17	0.43
1:B:585:TRP:HB3	1:B:619[A]:ILE:CD1	2.46	0.43
1:A:517:PHE:CE1	2:A:900[B]:GTP:N3	2.87	0.43
1:A:350[B]:THR:CG2	1:A:413:CYS:HA	2.35	0.43
1:A:107:LYS:HE3	1:A:601[A]:ASN:OD1	2.19	0.43
1:B:550:ALA:HB1	1:B:557:TYR:HB3	1.99	0.43
1:A:420:TRP:CE2	1:A:421:GLU:HG3	2.54	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:PRO:HG2	1:B:555:ILE:HD11	2.00	0.42
1:A:287:ALA:HB3	1:A:465:THR:CB	2.49	0.42
1:A:287:ALA:N	2:A:900[B]:GTP:O3B	2.46	0.42
1:A:153:LEU:CD1	1:A:153:LEU:N	2.83	0.42
1:B:58:ALA:O	1:B:62[A]:GLU:HG3	2.19	0.42
1:A:91:LYS:HD3	1:A:217:THR:O	2.20	0.42
1:B:268:LEU:HD12	1:B:268:LEU:C	2.40	0.42
1:A:253:ARG:HG2	1:A:488:TYR:HB3	2.02	0.42
1:A:287:ALA:HB3	1:A:465:THR:HB	2.01	0.41
1:B:295:MET:HA	1:B:415:ILE:HD11	2.01	0.41
1:A:601[B]:ASN:OD1	1:A:602:ALA:N	2.44	0.41
1:B:62[B]:GLU:HG3	8:B:1066:HOH:O	2.20	0.41
1:A:151:SER:C	1:A:153:LEU:N	2.74	0.41
1:A:517:PHE:CE1	2:A:900[B]:GTP:C4	3.08	0.41
1:B:255:ALA:HB1	1:B:260:TRP:C	2.40	0.41
1:B:443:LEU:HB2	1:B:577:LEU:HG	2.03	0.41
1:A:451[A]:GLN:CD	1:A:451[A]:GLN:H	2.23	0.41
1:A:287:ALA:CA	2:A:900[B]:GTP:O3A	2.63	0.41
1:A:355:THR:CG2	1:A:408[B]:THR:CG2	2.99	0.41
1:A:152:PRO:C	1:A:153:LEU:HD13	2.42	0.41
1:B:15:VAL:HG21	1:B:20:LEU:HG	2.03	0.41
1:A:477:HIS:NE2	1:A:591:GLU:OE2	2.52	0.41
1:A:601[A]:ASN:HB3	8:A:808:HOH:O	2.20	0.40
1:A:226:ARG:HH21	1:A:254:LEU:CD2	2.35	0.40
1:B:589[A]:VAL:CG1	1:B:619[A]:ILE:CD1	3.00	0.40

All (1) 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)
1:A:324:ARG:NH2	8:B:624:HOH:O[1_656]	1.97	0.23

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	643/624 (103%)	620 (96%)	20 (3%)	3 (0%)	34	14
1	B	626/624 (100%)	606 (97%)	19 (3%)	1 (0%)	52	32
All	All	1269/1248 (102%)	1226 (97%)	39 (3%)	4 (0%)	46	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	571	ASP
1	A	236	GLY
1	A	243	LYS
1	A	151	SER

### 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	541/520 (104%)	534 (99%)	7 (1%)	76	60
1	B	530/520 (102%)	521 (98%)	9 (2%)	68	49
All	All	1071/1040 (103%)	1055 (98%)	16 (2%)	74	55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	120	GLU
1	A	153	LEU
1	A	246[A]	PHE
1	A	246[B]	PHE
1	A	253	ARG
1	A	369	TYR
1	B	88	ILE
1	B	246	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	253	ARG
1	B	274	GLU
1	B	320	GLN
1	B	369	TYR
1	B	510[A]	LYS
1	B	510[B]	LYS
1	B	551	LYS

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

Mol	Chain	Res	Type
1	B	297	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	OXL	A	1000	3	0,5,5	0.00	-	0,6,6	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	1PE	A	1200	-	7,7,15	0.54	0	6,6,14	0.32	0
6	1PE	A	1201	-	15,15,15	0.46	0	14,14,14	0.40	0
7	EDO	A	3001	-	3,3,3	0.63	0	2,2,2	0.32	0
7	EDO	A	3002	-	3,3,3	0.39	0	2,2,2	0.71	0
7	EDO	A	3003	-	3,3,3	0.46	0	2,2,2	0.40	0
2	GTP	A	900[A]	3	25,34,34	0.94	1 (4%)	34,54,54	1.66	6 (17%)
2	GTP	A	900[B]	3	25,34,34	0.95	2 (8%)	34,54,54	1.71	7 (20%)
2	GTP	B	1000	3	25,34,34	1.04	2 (8%)	34,54,54	1.79	9 (26%)
4	OXL	B	1200	3	0,5,5	0.00	-	0,6,6	0.00	-
6	1PE	B	1300	-	15,15,15	0.58	0	14,14,14	0.33	0
7	EDO	B	3000	-	3,3,3	0.91	0	2,2,2	0.36	0
7	EDO	B	3001	-	3,3,3	0.44	0	2,2,2	0.14	0
7	EDO	B	3002	-	3,3,3	0.55	0	2,2,2	0.41	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	OXL	A	1000	3	-	0/0/4/4	0/0/0/0
6	1PE	A	1200	-	-	0/5/5/13	0/0/0/0
6	1PE	A	1201	-	-	0/13/13/13	0/0/0/0
7	EDO	A	3001	-	-	0/1/1/1	0/0/0/0
7	EDO	A	3002	-	-	0/1/1/1	0/0/0/0
7	EDO	A	3003	-	-	0/1/1/1	0/0/0/0
2	GTP	A	900[A]	3	-	0/18/38/38	0/3/3/3
2	GTP	A	900[B]	3	-	0/18/38/38	0/3/3/3
2	GTP	B	1000	3	-	0/18/38/38	0/3/3/3
4	OXL	B	1200	3	-	0/0/4/4	0/0/0/0
6	1PE	B	1300	-	-	0/13/13/13	0/0/0/0
7	EDO	B	3000	-	-	0/1/1/1	0/0/0/0
7	EDO	B	3001	-	-	0/1/1/1	0/0/0/0
7	EDO	B	3002	-	-	0/1/1/1	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900[B]	GTP	C2-N1	2.05	1.39	1.35
2	A	900[B]	GTP	C6-N1	2.36	1.37	1.33
2	B	1000	GTP	C2-N1	2.37	1.39	1.35
2	A	900[A]	GTP	C6-N1	2.89	1.38	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	GTP	C6-N1	2.95	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900[A]	GTP	N3-C2-N1	-5.20	119.53	127.44
2	B	1000	GTP	N3-C2-N1	-4.86	120.04	127.44
2	A	900[B]	GTP	N3-C2-N1	-4.16	121.11	127.44
2	B	1000	GTP	C5-C6-N1	-4.00	118.12	123.59
2	A	900[B]	GTP	PB-O3B-PG	-3.71	120.21	132.67
2	A	900[B]	GTP	O3A-PA-O5'	-3.47	93.73	102.94
2	B	1000	GTP	C4-C5-N7	-3.26	106.48	109.48
2	A	900[B]	GTP	C5-C6-N1	-3.05	119.41	123.59
2	A	900[A]	GTP	C5-C6-N1	-3.02	119.46	123.59
2	A	900[B]	GTP	C2'-C1'-N9	-2.96	109.77	114.29
2	B	1000	GTP	O3A-PA-O5'	-2.90	95.25	102.94
2	A	900[B]	GTP	PA-O3A-PB	-2.70	125.15	132.73
2	B	1000	GTP	O2B-PB-O3B	2.01	114.19	105.09
2	A	900[A]	GTP	O3G-PG-O2G	2.03	115.11	107.38
2	B	1000	GTP	O2A-PA-O3A	2.16	114.88	105.09
2	A	900[A]	GTP	N2-C2-N3	2.19	122.01	117.80
2	A	900[A]	GTP	O2B-PB-O3B	2.25	115.31	105.09
2	B	1000	GTP	O3G-PG-O2G	2.32	116.21	107.38
2	B	1000	GTP	N2-C2-N1	2.51	121.35	117.20
2	A	900[B]	GTP	C6-N1-C2	2.55	119.48	115.94
2	A	900[A]	GTP	C6-N1-C2	3.67	121.04	115.94
2	B	1000	GTP	C6-N1-C2	4.23	121.81	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	OXL	1	0
6	A	1200	1PE	4	0
6	A	1201	1PE	1	0
2	A	900[A]	GTP	4	0
2	A	900[B]	GTP	9	0
2	B	1000	GTP	1	0
6	B	1300	1PE	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3001	EDO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	624/624 (100%)	0.28	34 (5%) 29 35	3, 8, 21, 29	14 (2%)
1	B	616/624 (98%)	0.25	34 (5%) 29 34	2, 8, 21, 35	1 (0%)
All	All	1240/1248 (99%)	0.26	68 (5%) 29 34	2, 8, 21, 35	15 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	PRO	6.7
1	B	504	PRO	6.6
1	A	504	PRO	6.1
1	A	394	GLN	6.0
1	B	396	GLU	5.7
1	B	393	PRO	5.7
1	B	1	MET	5.7
1	B	394	GLN	5.5
1	A	152	PRO	5.4
1	B	205	PRO	5.1
1	A	153	LEU	4.9
1	A	205	PRO	4.6
1	B	570	GLY	4.4
1	A	396	GLU	4.4
1	A	505	ALA	4.2
1	A	149	LEU	4.2
1	B	392	ARG	4.1
1	A	392	ARG	4.1
1	A	235[A]	TYR	4.1
1	B	5	LEU	4.1
1	B	395	ASP	4.0
1	B	3	PRO	4.0
1	A	473	LYS	3.9
1	A	521	LYS	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	3.7
1	A	571	ASP	3.2
1	B	575	GLU	3.0
1	B	203	LYS	3.0
1	B	505	ALA	3.0
1	B	166	VAL	2.9
1	A	203	LYS	2.9
1	A	204	LYS	2.9
1	A	575	GLU	2.8
1	A	522	ASN	2.8
1	A	166	VAL	2.8
1	A	240	LEU	2.7
1	B	521	LYS	2.7
1	B	235[A]	TYR	2.7
1	B	522	ASN	2.7
1	B	204	LYS	2.7
1	B	464	ALA	2.6
1	B	503	ARG	2.6
1	A	0	SER	2.5
1	A	524	LYS	2.5
1	B	524	LYS	2.5
1	B	165	TYR	2.5
1	A	333	PHE	2.5
1	A	466	ALA	2.4
1	B	391	TRP	2.4
1	B	473	LYS	2.4
1	B	397	GLU	2.3
1	B	0	SER	2.3
1	A	266	LEU	2.3
1	B	6	HIS	2.3
1	A	390	GLU	2.2
1	B	241	LEU	2.2
1	A	1	MET	2.2
1	B	267	ILE	2.2
1	A	468	ALA	2.2
1	A	502	HIS	2.2
1	B	240	LEU	2.1
1	B	9	LEU	2.1
1	B	188	GLU	2.1
1	A	312[A]	ILE	2.1
1	A	241	LEU	2.1
1	A	70	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	467	GLY	2.0
1	A	407	CYS	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	EDO	B	3000	4/4	0.83	0.16	3.94	20,25,28,31	0
6	1PE	B	1300	16/16	0.71	0.17	1.87	55,57,58,59	0
6	1PE	A	1201	16/16	0.90	0.15	1.83	43,44,48,51	0
7	EDO	A	3003	4/4	0.81	0.12	1.06	47,48,50,50	0
6	1PE	A	1200	8/16	0.85	0.22	0.80	48,49,50,50	0
7	EDO	B	3001	4/4	0.85	0.10	0.44	39,40,40,41	0
7	EDO	A	3001	4/4	0.94	0.10	0.05	18,20,22,30	0
3	MN	B	701	1/1	0.99	0.12	-0.14	13,13,13,13	1
2	GTP	A	900[B]	32/32	0.97	0.11	-0.19	9,12,18,20	32
2	GTP	A	900[A]	32/32	0.97	0.11	-0.30	9,19,23,23	32
3	MN	A	700[B]	1/1	0.99	0.11	-1.11	18,18,18,18	1
4	OXL	A	1000	6/6	0.97	0.10	-1.35	11,16,19,19	0
2	GTP	B	1000	32/32	0.98	0.07	-1.50	13,19,23,25	0
3	MN	A	700[A]	1/1	0.99	0.11	-1.58	16,16,16,16	1
5	NA	A	1100	1/1	0.98	0.04	-1.81	30,30,30,30	0
5	NA	B	1100	1/1	0.97	0.06	-2.03	24,24,24,24	0
3	MN	A	800	1/1	1.00	0.10	-2.08	14,14,14,14	0
4	OXL	B	1200	6/6	0.96	0.06	-2.42	12,20,22,22	0
3	MN	B	700	1/1	1.00	0.09	-	14,14,14,14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	B	3002	4/4	0.75	0.18	-	41,45,45,47	0
7	EDO	A	3002	4/4	0.89	0.12	-	44,44,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.