



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MOE
Title : The structure of rat cytosolic PEPCK mutant A467G in complex with Beta-Sulfo-pyruvate and GTP
Authors : Johnson, T.A.; Holyoak, T.
Deposited on : 2010-04-22
Resolution : 1.25 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 (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

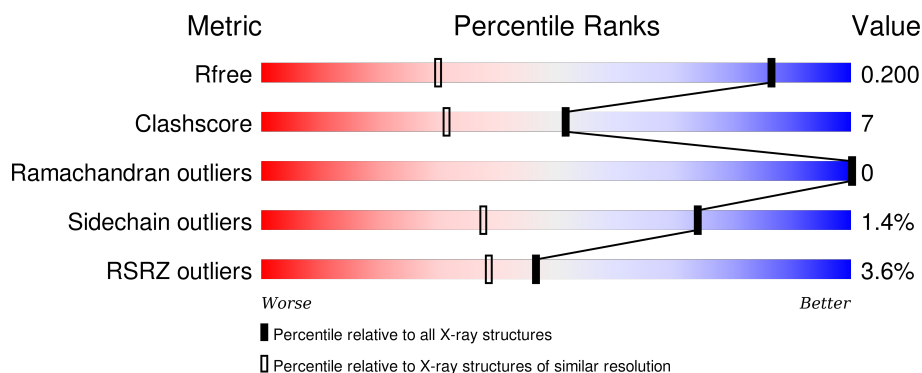
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.25 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	1442 (1.30-1.22)
Clashscore	102246	1530 (1.30-1.22)
Ramachandran outliers	100387	1467 (1.30-1.22)
Sidechain outliers	100360	1465 (1.30-1.22)
RSRZ outliers	91569	1442 (1.30-1.22)

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	

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
6	1PE	A	1300	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1PE	A	1301	-	-	-	X
7	EDO	A	1401	-	-	X	X
7	EDO	A	1403	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5758 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.

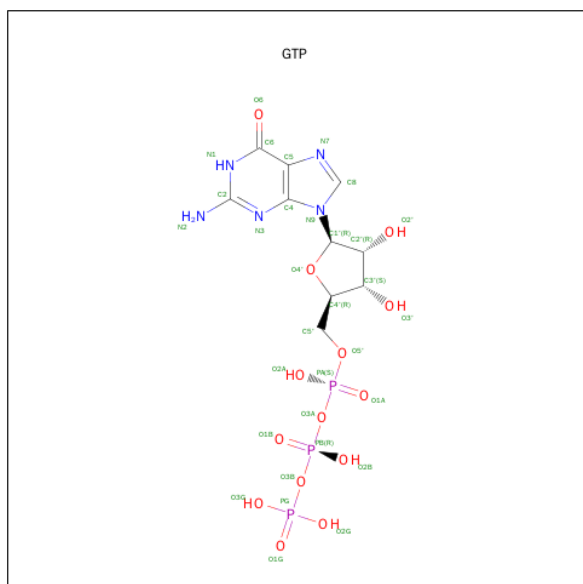
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	618	5051	3248	858	910	35	0	33	0

There are 3 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

- 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
			Total	C	N	O	P		
2	A	1	32	10	5	14	3	0	0

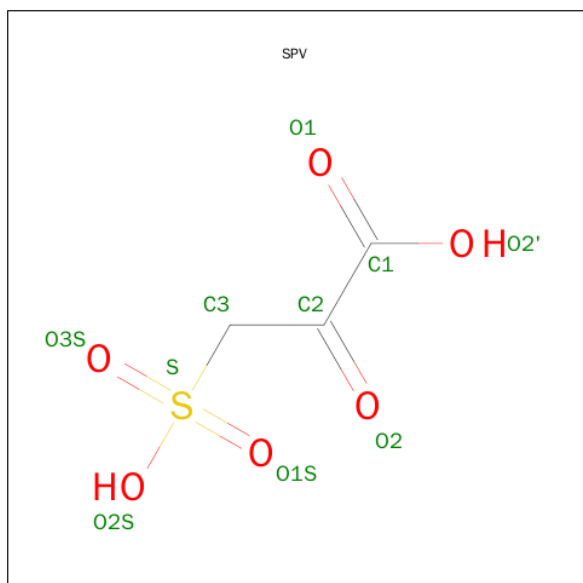
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is SULFOPYRUVATE (three-letter code: SPV) (formula: C₃H₄O₆S).



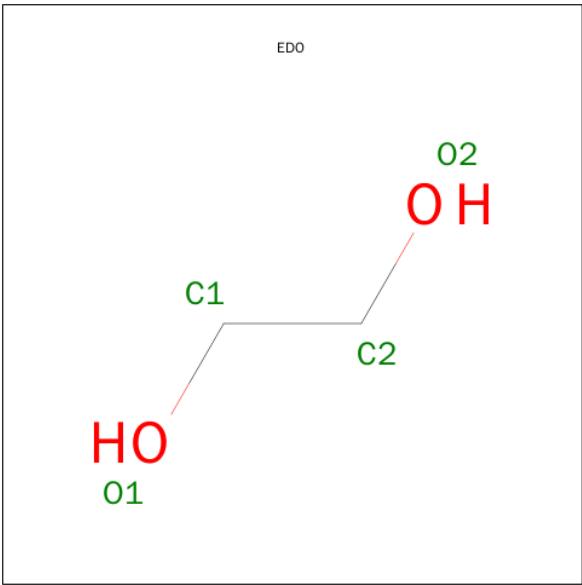
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			10	3	6	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	A	1	Total	C	O	0	0
			5	3	2		
6	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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		

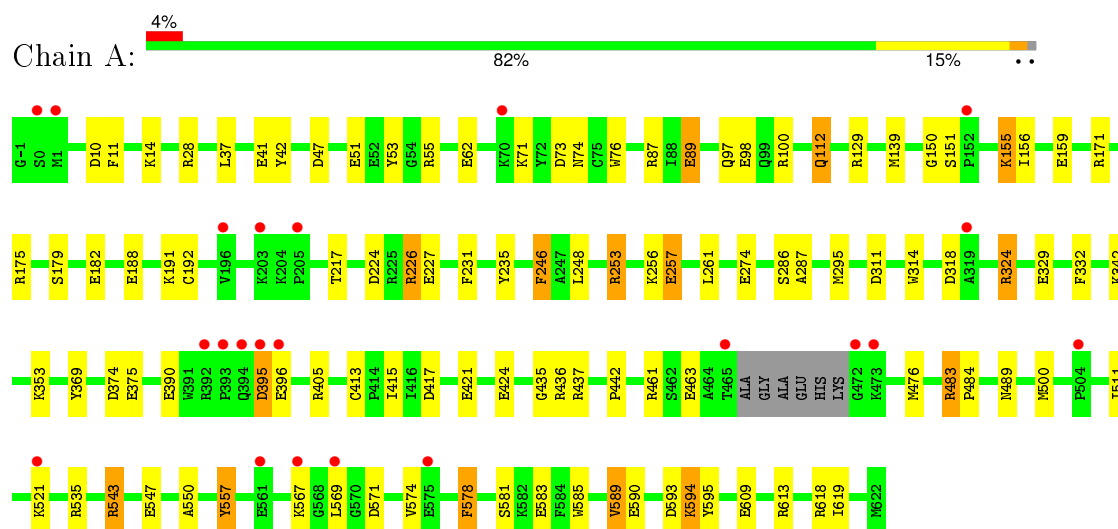
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	620	Total	O	0	0
			620	620		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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	44.32Å 119.12Å 60.05Å 90.00° 111.19° 90.00°	Depositor
Resolution (Å)	20.57 – 1.25 20.57 – 1.25	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.57-1.25) 94.8 (20.57-1.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.148 , 0.174 0.175 , 0.200	Depositor DCC
R_{free} test set	7650 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.7	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 151977 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5758	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	1.45	30/5275 (0.6%)	1.38	57/7133 (0.8%)

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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	CYS	CB-SG	-11.79	1.62	1.82
1	A	594	LYS	CE-NZ	7.68	1.68	1.49
1	A	557	TYR	CD2-CE2	7.58	1.50	1.39
1	A	274	GLU	CG-CD	-7.42	1.40	1.51
1	A	151	SER	CB-OG	7.17	1.51	1.42
1	A	375	GLU	CD-OE2	6.95	1.33	1.25
1	A	547	GLU	CB-CG	-6.53	1.39	1.52
1	A	353	LYS	CB-CG	-6.24	1.35	1.52
1	A	589[A]	VAL	CB-CG2	-6.04	1.40	1.52
1	A	589[B]	VAL	CB-CG2	-6.04	1.40	1.52
1	A	590	GLU	CD-OE2	6.00	1.32	1.25
1	A	595	TYR	CD1-CE1	6.00	1.48	1.39
1	A	435	GLY	N-CA	5.84	1.54	1.46
1	A	175	ARG	CG-CD	-5.81	1.37	1.51
1	A	424	GLU	CB-CG	5.66	1.62	1.52
1	A	257[A]	GLU	CG-CD	5.56	1.60	1.51
1	A	257[B]	GLU	CG-CD	5.56	1.60	1.51
1	A	332	PHE	CD2-CE2	5.50	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	GLU	CB-CG	-5.50	1.41	1.52
1	A	369	TYR	CD2-CE2	5.49	1.47	1.39
1	A	463	GLU	CD-OE1	-5.45	1.19	1.25
1	A	324	ARG	CG-CD	5.37	1.65	1.51
1	A	583	GLU	CB-CG	-5.36	1.42	1.52
1	A	314	TRP	CE3-CZ3	5.34	1.47	1.38
1	A	369	TYR	CE1-CZ	-5.30	1.31	1.38
1	A	581	SER	CB-OG	-5.30	1.35	1.42
1	A	62	GLU	CD-OE1	-5.16	1.20	1.25
1	A	53	TYR	CB-CG	-5.08	1.44	1.51
1	A	179	SER	CB-OG	-5.07	1.35	1.42
1	A	139	MET	SD-CE	-5.03	1.49	1.77

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ARG	NE-CZ-NH1	12.79	126.70	120.30
1	A	28	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	235	TYR	CB-CG-CD1	-10.18	114.89	121.00
1	A	274	GLU	OE1-CD-OE2	-9.66	111.71	123.30
1	A	483[A]	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	483[B]	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	324	ARG	NE-CZ-NH1	-9.26	115.67	120.30
1	A	155[A]	LYS	CD-CE-NZ	8.47	131.17	111.70
1	A	155[B]	LYS	CD-CE-NZ	8.47	131.17	111.70
1	A	47	ASP	CB-CG-OD1	8.18	125.66	118.30
1	A	535	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	139	MET	CG-SD-CE	-7.67	87.92	100.20
1	A	436	ARG	NE-CZ-NH2	7.65	124.12	120.30
1	A	543[A]	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	543[B]	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	578[A]	PHE	CB-CG-CD2	-7.50	115.55	120.80
1	A	578[B]	PHE	CB-CG-CD2	-7.50	115.55	120.80
1	A	461	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	593	ASP	CB-CG-OD1	7.34	124.90	118.30
1	A	374	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	A	87	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	226	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	311	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	89	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	A	246	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	A	483[A]	ARG	NE-CZ-NH2	-6.75	116.93	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483[B]	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	595	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	A	618	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	A	235	TYR	CB-CG-CD2	6.63	124.98	121.00
1	A	417	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	405	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	618	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	A	569	LEU	CB-CG-CD2	6.08	121.33	111.00
1	A	226	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	112[A]	GLN	CA-CB-CG	5.86	126.30	113.40
1	A	112[B]	GLN	CA-CB-CG	5.86	126.30	113.40
1	A	171	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	318	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	253	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	129	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	436	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	557	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	329	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	73	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	10	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	37	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	A	489	ASN	N-CA-CB	-5.26	101.13	110.60
1	A	463	GLU	OE1-CD-OE2	5.22	129.57	123.30
1	A	71	LYS	CD-CE-NZ	-5.21	99.70	111.70
1	A	476[A]	MET	CG-SD-CE	5.21	108.54	100.20
1	A	476[B]	MET	CG-SD-CE	5.21	108.54	100.20
1	A	421	GLU	CB-CA-C	-5.16	100.07	110.40
1	A	11	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	A	567	LYS	CD-CE-NZ	5.13	123.49	111.70
1	A	311	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	442	PRO	N-CD-CG	-5.03	95.66	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150[A]	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5051	0	5097	67	1
2	A	32	0	12	1	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	10	0	2	0	0
6	A	26	0	32	10	0
7	A	16	0	24	9	0
8	A	620	0	0	18	2
All	All	5758	0	5167	70	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 7.

All (70) 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:594:LYS:CE	1:A:594:LYS:NZ	1.68	1.51
1:A:342:LYS:HG3	8:A:1163:HOH:O	1.30	1.24
1:A:578[A]:PHE:HD1	8:A:1223:HOH:O	1.12	1.23
1:A:42[B]:TYR:HE2	8:A:1243:HOH:O	1.32	1.12
1:A:578[A]:PHE:CD1	8:A:1223:HOH:O	1.90	1.11
1:A:256:LYS:HE2	8:A:1012:HOH:O	1.62	0.97
1:A:286[A]:SER:OG	8:A:1176:HOH:O	1.81	0.95
1:A:574:VAL:HG13	1:A:578[B]:PHE:CD2	2.01	0.95
1:A:42[B]:TYR:OH	8:A:1224:HOH:O	1.83	0.91
6:A:1301:1PE:H121	8:A:1105:HOH:O	1.73	0.89
1:A:585:TRP:O	1:A:589[B]:VAL:HG23	1.78	0.83
1:A:100[B]:ARG:HG2	1:A:100[B]:ARG:HH11	1.51	0.75
1:A:609:GLU:OE2	1:A:613[B]:ARG:NH2	2.19	0.74
1:A:156:ILE:H	7:A:1401:EDO:H22	1.52	0.73
1:A:589[B]:VAL:HG21	1:A:619[B]:ILE:CD1	2.20	0.72
1:A:437:ARG:HH21	7:A:1403:EDO:H22	1.55	0.72
1:A:390:GLU:HG3	8:A:1169:HOH:O	1.89	0.71
1:A:574:VAL:HG13	1:A:578[B]:PHE:HD2	1.56	0.70
1:A:589[B]:VAL:HG21	1:A:619[B]:ILE:HD12	1.72	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:HG13	1:A:578[B]:PHE:CE2	2.29	0.68
1:A:100[B]:ARG:HG2	1:A:100[B]:ARG:NH1	2.09	0.67
1:A:55[A]:ARG:NH2	8:A:1064:HOH:O	2.29	0.64
1:A:543[A]:ARG:HH22	7:A:1400:EDO:H21	1.61	0.64
1:A:511:ILE:H	6:A:1301:1PE:C23	2.11	0.63
1:A:155[B]:LYS:HA	7:A:1401:EDO:H11	1.80	0.63
1:A:42[B]:TYR:CE2	8:A:1243:HOH:O	2.20	0.62
1:A:14[A]:LYS:NZ	6:A:1300:1PE:H242	2.15	0.61
1:A:574:VAL:CG1	1:A:578[B]:PHE:CD2	2.82	0.60
1:A:14[B]:LYS:HE2	6:A:1300:1PE:H242	1.83	0.60
1:A:188:GLU:O	7:A:1401:EDO:H21	2.01	0.60
1:A:589[B]:VAL:CG2	1:A:619[B]:ILE:CD1	2.80	0.59
1:A:437:ARG:HH21	7:A:1403:EDO:C2	2.15	0.58
1:A:226:ARG:HB2	8:A:1207:HOH:O	2.03	0.58
1:A:156:ILE:H	7:A:1401:EDO:C2	2.15	0.57
1:A:224:ASP:OD1	1:A:253:ARG:NH2	2.37	0.57
1:A:287:ALA:HA	2:A:1100:GTP:O2A	2.04	0.57
1:A:14[B]:LYS:HE2	6:A:1300:1PE:H251	1.86	0.56
1:A:483[B]:ARG:HB3	1:A:484:PRO:HD3	1.87	0.56
1:A:14[A]:LYS:HZ2	6:A:1300:1PE:H242	1.70	0.55
1:A:155[A]:LYS:HA	7:A:1401:EDO:H11	1.89	0.53
1:A:574:VAL:CG1	1:A:578[B]:PHE:HD2	2.20	0.52
1:A:550:ALA:HB1	1:A:557:TYR:HB3	1.92	0.52
1:A:191:LYS:HB2	1:A:227[A]:GLU:HG2	1.95	0.49
1:A:182:GLU:OE1	8:A:981:HOH:O	2.20	0.49
1:A:14[A]:LYS:NZ	6:A:1300:1PE:H251	2.28	0.48
1:A:74:ASN:ND2	1:A:76:TRP:HE1	2.12	0.48
1:A:609:GLU:O	1:A:613[A]:ARG:HG3	2.14	0.47
1:A:613[B]:ARG:CZ	8:A:1208:HOH:O	2.63	0.46
1:A:543[A]:ARG:HH22	7:A:1400:EDO:C2	2.28	0.46
1:A:159:GLU:HA	1:A:192:CYS:HB2	1.99	0.44
1:A:217:THR:HA	1:A:231:PHE:O	2.17	0.44
1:A:543[A]:ARG:HD2	1:A:543[A]:ARG:HA	1.82	0.43
1:A:100[B]:ARG:CG	1:A:100[B]:ARG:NH1	2.70	0.42
1:A:609:GLU:OE2	1:A:613[B]:ARG:CZ	2.67	0.42
1:A:395:ASP:N	1:A:395:ASP:OD1	2.52	0.42
1:A:594:LYS:CD	1:A:594:LYS:NZ	2.68	0.42
1:A:14[A]:LYS:HE2	8:A:1152:HOH:O	2.20	0.41
1:A:257[A]:GLU:OE2	8:A:1080:HOH:O	2.21	0.41
1:A:324:ARG:HH11	1:A:324:ARG:HD3	1.59	0.41
6:A:1300:1PE:H242	6:A:1300:1PE:H251	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1300:1PE:H122	8:A:1179:HOH:O	2.20	0.41
1:A:97[B]:GLN:OE1	1:A:98[B]:GLU:HG2	2.21	0.41
1:A:261:LEU:HD11	1:A:500[A]:MET:SD	2.61	0.41
1:A:295:MET:HA	1:A:415:ILE:HD11	2.02	0.40
1:A:248:LEU:HA	1:A:248:LEU:HD23	1.93	0.40
1:A:41[B]:GLU:OE2	8:A:1171:HOH:O	2.22	0.40
1:A:589[B]:VAL:CG2	1:A:619[B]:ILE:HD13	2.51	0.40
1:A:89:GLU:OE2	1:A:483[B]:ARG:NH1	2.46	0.40
1:A:14[B]:LYS:NZ	6:A:1300:1PE:H131	2.36	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)
1:A:41[A]:GLU:OE2	8:A:1206:HOH:O[2_545]	2.08	0.12
8:A:1206:HOH:O	8:A:1224:HOH:O[2_555]	2.11	0.09

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	647/624 (104%)	628 (97%)	19 (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	549/520 (106%)	541 (98%)	8 (2%)	72	34

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	112[A]	GLN
1	A	112[B]	GLN
1	A	246	PHE
1	A	395	ASP
1	A	396	GLU
1	A	521	LYS
1	A	571	ASP

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	74	ASN
1	A	502	HIS

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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	GTP	A	1100	3	25,34,34	1.93	7 (28%)	34,54,54	2.85	6 (17%)
5	SPV	A	1200	3	5,9,9	2.19	2 (40%)	7,13,13	0.97	0
6	1PE	A	1300	-	15,15,15	0.92	0	14,14,14	1.33	1 (7%)
6	1PE	A	1301	-	4,4,15	0.83	0	3,3,14	1.49	0
6	1PE	A	1302	-	4,4,15	0.84	0	3,3,14	0.50	0
7	EDO	A	1400	-	3,3,3	0.37	0	2,2,2	1.19	0
7	EDO	A	1401	-	3,3,3	0.56	0	2,2,2	1.23	0
7	EDO	A	1402	-	3,3,3	0.30	0	2,2,2	0.94	0
7	EDO	A	1403	-	3,3,3	0.62	0	2,2,2	0.58	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	GTP	A	1100	3	-	0/18/38/38	0/3/3/3
5	SPV	A	1200	3	-	0/5/9/9	0/0/0/0
6	1PE	A	1300	-	-	0/13/13/13	0/0/0/0
6	1PE	A	1301	-	-	0/2/2/13	0/0/0/0
6	1PE	A	1302	-	-	0/2/2/13	0/0/0/0
7	EDO	A	1400	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1401	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1402	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1403	-	-	0/1/1/1	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1100	GTP	PA-O2A	-3.01	1.42	1.54
2	A	1100	GTP	C2-N1	-2.87	1.30	1.35
2	A	1100	GTP	C8-N7	-2.47	1.29	1.34
2	A	1100	GTP	PG-O3G	-2.24	1.46	1.54
2	A	1100	GTP	C2-N2	2.54	1.39	1.34
5	A	1200	SPV	O2-C2	2.95	1.27	1.22
5	A	1200	SPV	C3-C2	3.63	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1100	GTP	O4'-C1'	4.06	1.46	1.41
2	A	1100	GTP	C6-N1	4.12	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1100	GTP	C5-C6-N1	-10.74	108.91	123.59
2	A	1100	GTP	C4-C5-N7	-4.73	105.13	109.48
2	A	1100	GTP	O3A-PA-O5'	-3.79	92.89	102.94
2	A	1100	GTP	N3-C2-N1	-2.97	122.92	127.44
2	A	1100	GTP	C2'-C3'-C4'	-2.25	97.98	102.61
6	A	1300	1PE	OH5-C25-C15	3.13	124.27	110.36
2	A	1100	GTP	C6-N1-C2	9.04	128.48	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	GTP	1	0
6	A	1300	1PE	8	0
6	A	1301	1PE	2	0
7	A	1400	EDO	2	0
7	A	1401	EDO	5	0
7	A	1403	EDO	2	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	618/624 (99%)	0.17	22 (3%)	46 38	3, 7, 21, 52	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLN	7.8
1	A	504	PRO	6.8
1	A	393	PRO	5.8
1	A	472	GLY	5.4
1	A	465	THR	5.4
1	A	392	ARG	5.1
1	A	395	ASP	4.5
1	A	473	LYS	4.5
1	A	521	LYS	4.3
1	A	205	PRO	4.2
1	A	396	GLU	3.8
1	A	569	LEU	3.7
1	A	575	GLU	3.2
1	A	0	SER	3.1
1	A	203	LYS	2.9
1	A	561	GLU	2.9
1	A	152	PRO	2.6
1	A	196	VAL	2.4
1	A	567	LYS	2.4
1	A	319	ALA	2.4
1	A	1	MET	2.2
1	A	70	LYS	2.0

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

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(\AA^2)	Q<0.9
7	EDO	A	1401	4/4	0.93	0.21	3.24	29,30,32,32	0
6	1PE	A	1301	5/16	0.90	0.10	2.69	11,22,25,36	0
7	EDO	A	1403	4/4	0.95	0.11	2.55	18,26,28,36	0
6	1PE	A	1300	16/16	0.81	0.14	2.44	24,44,58,62	0
4	NA	A	800	1/1	0.93	0.08	-0.26	22,22,22,22	1
7	EDO	A	1400	4/4	0.89	0.08	-0.32	37,39,40,42	0
2	GTP	A	1100	32/32	0.99	0.06	-1.09	9,10,13,14	0
3	MN	A	700	1/1	1.00	0.06	-1.45	10,10,10,10	0
3	MN	A	701	1/1	1.00	0.07	-1.55	10,10,10,10	0
5	SPV	A	1200	10/10	0.99	0.05	-1.72	10,11,11,12	0
7	EDO	A	1402	4/4	0.92	0.08	-	42,43,43,45	0
6	1PE	A	1302	5/16	0.68	0.12	-	42,46,49,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.