



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:13 AM GMT

PDB ID : 3DT7
Title : The structure of rat cytosolic PEPCK in complex with beta-sulfoxyruvate and GTP
Authors : Sullivan, S.M.; Holyoak, T.
Deposited on : 2008-07-14
Resolution : 1.50 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

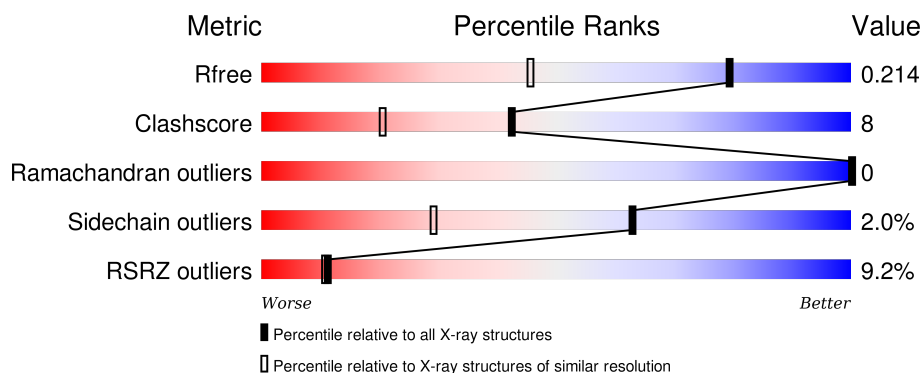
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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>12%</div> <div>.</div> </div>
1	B	624	<div> <div>9%</div> <div>87%</div> <div>9%</div> <div>..</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
7	ETX	B	3430	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11144 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	31	0
			5068	3255	858	920	35			
1	B	611	Total	C	N	O	S	0	27	0
			4964	3184	842	905	33			

There are 4 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
B	-1	GLY	-	EXPRESSION TAG	UNP P07379
B	0	SER	-	EXPRESSION TAG	UNP P07379

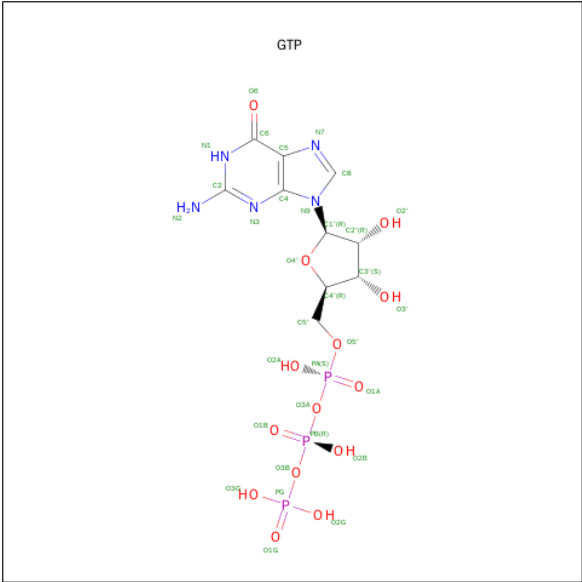
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

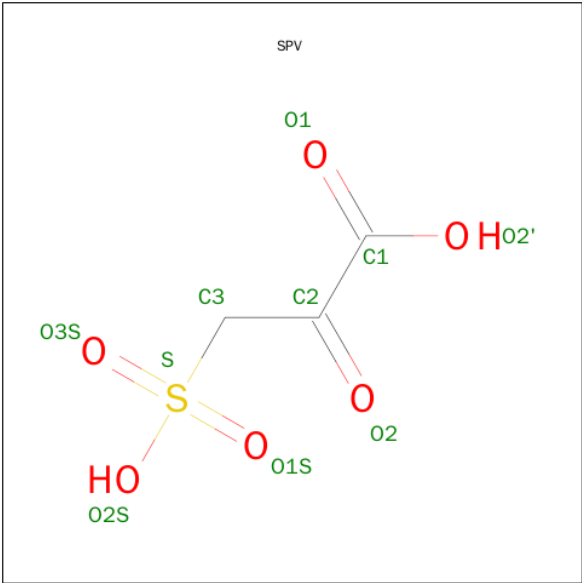
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



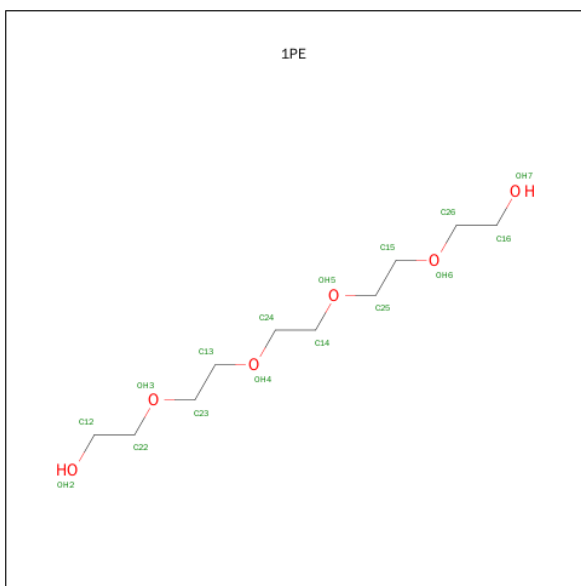
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	B	1	Total 32	C 10	N 5	O 14	P 3	0	0

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



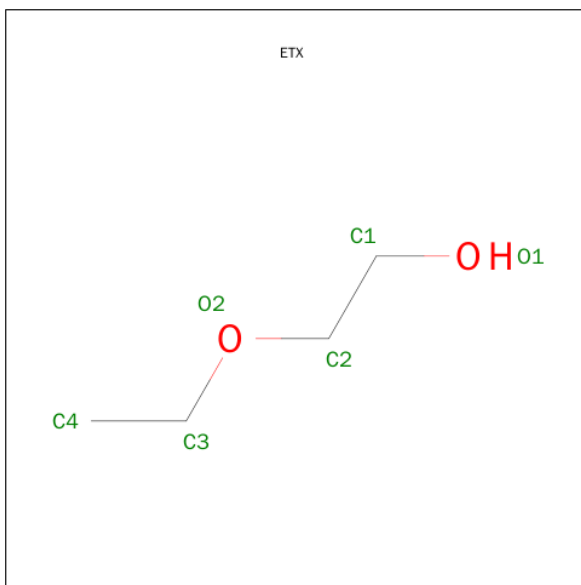
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			10	3	6	1		
5	B	1	Total	C	O	S	0	0
			10	3	6	1		

- 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
			10	6	4		

- Molecule 7 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: $C_4H_{10}O_2$).



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

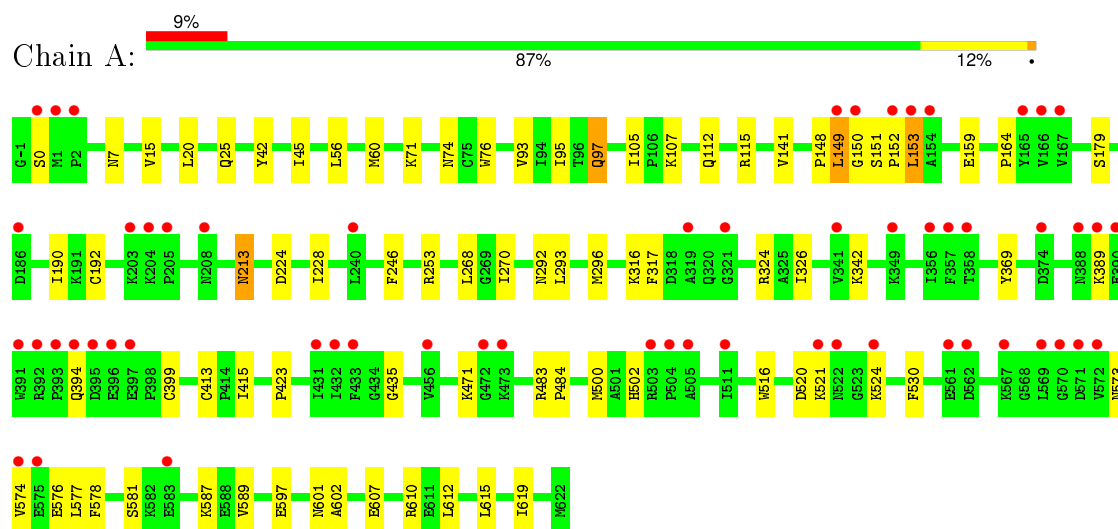
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	502	Total 502	O 502	0	0
8	B	497	Total 497	O 497	0	0

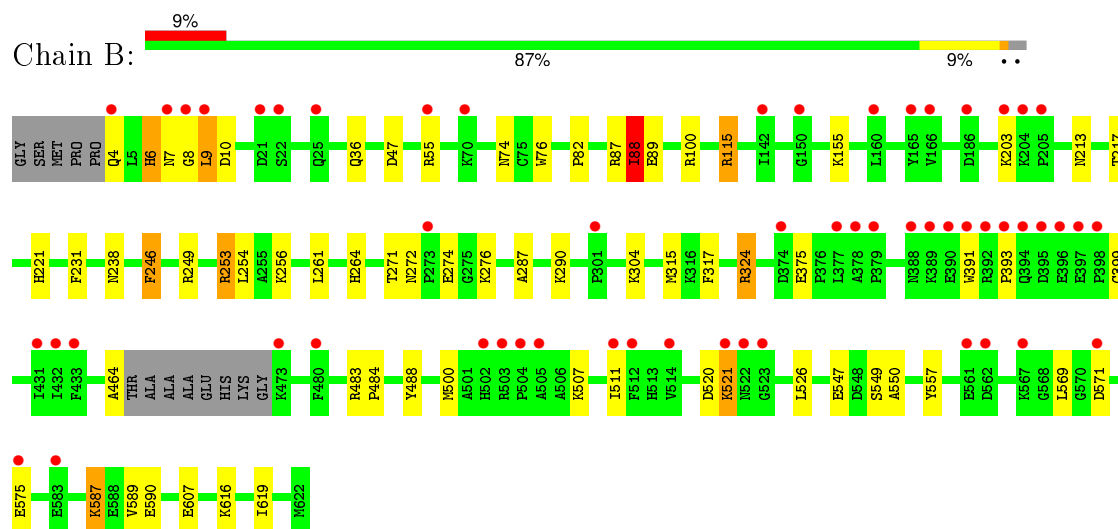
3 Residue-property plots

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 ($RSRZ > 2$). 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]



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.02Å 119.50Å 87.28Å 90.00° 107.07° 90.00°	Depositor
Resolution (Å)	29.15 – 1.50 29.15 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.15-1.50) 97.3 (29.15-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.174 , 0.209 0.182 , 0.214	Depositor DCC
R_{free} test set	9440 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 187706 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å ²)	8.0	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 67.64 % 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 4.9764e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, ETX, MN, 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	0.90	2/5290 (0.0%)	0.85	2/7157 (0.0%)
1	B	0.89	0/5172	0.86	5/6996 (0.1%)
All	All	0.90	2/10462 (0.0%)	0.85	7/14153 (0.0%)

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
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	CYS	CB-SG	-5.41	1.73	1.81
1	A	516	TRP	CE3-CZ3	5.14	1.47	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	150	GLY	N-CA-C	-6.96	95.69	113.10
1	B	47	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	324	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	88	ILE	CB-CA-C	-5.55	100.51	111.60
1	B	246	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	B	87	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	612	LEU	CB-CG-CD2	-5.10	102.33	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	LEU	Peptide
1	B	6	HIS	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	5068	0	5099	91	0
1	B	4964	0	4977	76	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	12	4	0
4	B	32	0	12	1	0
5	A	10	0	2	0	0
5	B	10	0	2	0	0
6	A	10	0	13	5	0
7	A	6	0	10	1	0
7	B	6	0	10	3	0
8	A	502	0	0	23	1
8	B	497	0	0	21	0
All	All	11144	0	10137	168	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 8.

All (168) 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:B:7:ASN:OD1	1:B:8:GLY:HA3	1.19	1.30
1:B:115[A]:ARG:NH1	1:B:115[A]:ARG:HB3	1.49	1.28
1:A:324:ARG:NH2	8:A:3913:HOH:O	1.75	1.15
1:A:601[B]:ASN:OD1	8:A:3457:HOH:O	1.64	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190[B]:ILE:HG21	1:A:246:PHE:CE1	1.83	1.14
1:B:511:ILE:H	7:B:3430:ETX:H11	1.10	1.11
1:B:115[A]:ARG:HH11	1:B:115[A]:ARG:CG	1.63	1.10
1:A:153:LEU:HA	8:A:3817:HOH:O	1.52	1.08
1:B:115[A]:ARG:HH11	1:B:115[A]:ARG:CB	1.68	1.06
1:B:115[A]:ARG:NH1	1:B:115[A]:ARG:CB	2.19	1.06
1:B:7:ASN:CG	1:B:8:GLY:HA3	1.76	1.04
1:A:93:VAL:HG12	1:A:115[B]:ARG:HG2	1.41	1.02
1:B:7:ASN:OD1	1:B:8:GLY:CA	2.06	1.02
1:B:375[A]:GLU:CG	8:B:4189:HOH:O	2.08	1.00
1:B:115[A]:ARG:HH11	1:B:115[A]:ARG:HG2	1.28	0.97
1:B:375[A]:GLU:HG3	8:B:4189:HOH:O	1.63	0.96
1:A:578[B]:PHE:HD1	8:A:3918:HOH:O	1.48	0.95
1:A:316:LYS:HZ3	6:A:1000:1PE:H231	1.31	0.95
1:B:256[B]:LYS:HE3	8:B:4240:HOH:O	1.68	0.92
1:B:274:GLU:HG3	8:B:3983:HOH:O	1.71	0.90
1:A:112[B]:GLN:NE2	8:A:3776:HOH:O	2.03	0.90
1:B:590[A]:GLU:CD	8:B:3953:HOH:O	2.14	0.87
1:B:511:ILE:N	7:B:3430:ETX:H11	1.91	0.86
1:A:268:LEU:HD13	1:A:270[B]:ILE:HG22	1.59	0.85
1:B:82[B]:PRO:HG3	8:B:4053:HOH:O	1.77	0.83
1:A:42:TYR:CE2	8:A:3743:HOH:O	2.30	0.83
1:A:42:TYR:HE2	8:A:3743:HOH:O	1.60	0.82
1:A:292[B]:ASN:OD1	4:A:800:GTP:H8	1.63	0.81
1:B:9:LEU:HG	1:B:36:GLN:NE2	1.98	0.79
1:A:292[B]:ASN:OD1	4:A:800:GTP:C8	2.37	0.78
1:A:224[B]:ASP:OD2	8:A:3906:HOH:O	2.02	0.77
1:A:253:ARG:NH1	8:A:3800:HOH:O	2.16	0.76
1:A:268:LEU:HD13	1:A:270[B]:ILE:CG2	2.16	0.75
1:A:574:VAL:O	1:A:578[A]:PHE:HD2	1.69	0.75
1:B:375[A]:GLU:HG2	8:B:4189:HOH:O	1.76	0.75
1:A:317:PHE:HE2	1:A:500[B]:MET:CE	2.01	0.73
1:A:152:PRO:HG2	1:A:153:LEU:HD13	1.71	0.73
1:A:0:SER:H	1:A:25:GLN:HE22	1.34	0.73
1:B:7:ASN:CG	1:B:8:GLY:CA	2.56	0.72
1:A:316:LYS:NZ	6:A:1000:1PE:H122	2.04	0.72
1:B:375[B]:GLU:OE2	8:B:4008:HOH:O	2.07	0.71
1:B:464:ALA:HB3	8:B:4049:HOH:O	1.89	0.70
1:A:153:LEU:CD2	8:A:3813:HOH:O	2.39	0.70
1:A:268:LEU:CD1	1:A:270[B]:ILE:CG2	2.69	0.70
1:A:152:PRO:HG2	1:A:153:LEU:CD1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:HG2	8:A:3662:HOH:O	1.92	0.68
1:A:413:CYS:SG	1:A:415[B]:ILE:HD13	2.34	0.68
1:A:224[B]:ASP:OD1	1:A:253:ARG:NH2	2.27	0.68
1:A:190[B]:ILE:CG2	1:A:246:PHE:CE1	2.71	0.66
1:B:115[A]:ARG:NH1	1:B:115[A]:ARG:HG2	2.03	0.66
1:A:153:LEU:HD22	8:A:3813:HOH:O	1.95	0.66
1:A:151:SER:OG	1:A:153:LEU:HD22	1.97	0.64
1:B:7:ASN:HD21	1:B:10:ASP:H	1.44	0.64
1:B:256[B]:LYS:HE2	8:B:4218:HOH:O	1.96	0.64
1:A:578[B]:PHE:CD1	8:A:3918:HOH:O	2.33	0.63
1:A:520:ASP:OD1	1:A:524:LYS:HG2	1.99	0.63
1:A:317:PHE:HE2	1:A:500[B]:MET:HE3	1.63	0.62
1:B:547[A]:GLU:HG2	1:B:549:SER:HB3	1.80	0.62
1:B:7:ASN:ND2	1:B:10:ASP:H	1.96	0.62
1:B:607:GLU:HG3	8:B:4007:HOH:O	1.98	0.62
1:A:74:ASN:ND2	1:A:76:TRP:HE1	1.98	0.61
1:B:55[A]:ARG:NH2	8:B:4227:HOH:O	2.32	0.61
1:B:6:HIS:O	1:B:7:ASN:HB2	2.01	0.61
1:B:115[A]:ARG:HD3	8:B:3913:HOH:O	1.99	0.61
1:A:7:ASN:HB3	8:A:3814:HOH:O	2.00	0.61
1:B:587:LYS:HD3	1:B:587:LYS:O	2.00	0.60
7:B:3430:ETX:H32	8:B:4330:HOH:O	2.02	0.59
1:B:520:ASP:HB3	1:B:526[B]:LEU:HD11	1.84	0.59
1:A:268:LEU:CD1	1:A:270[B]:ILE:HG23	2.32	0.59
1:A:317:PHE:CE2	1:A:500[B]:MET:CE	2.84	0.59
1:B:155:LYS:HE2	1:B:254:LEU:CD1	2.33	0.59
1:A:293:LEU:HD12	1:A:296:MET:HE3	1.84	0.58
1:B:203:LYS:HE3	8:B:3957:HOH:O	2.02	0.58
1:A:601[B]:ASN:OD1	1:A:602:ALA:N	2.30	0.58
1:B:115[A]:ARG:CB	1:B:115[A]:ARG:CZ	2.81	0.58
1:A:153:LEU:HD13	1:A:153:LEU:N	2.21	0.56
1:A:105:ILE:O	1:A:601[B]:ASN:ND2	2.39	0.56
1:A:573:ASN:ND2	1:A:576:GLU:HB2	2.20	0.56
1:A:317:PHE:HE2	1:A:500[B]:MET:HE2	1.71	0.55
1:B:115[A]:ARG:HB3	1:B:115[A]:ARG:CZ	2.30	0.55
1:A:292[B]:ASN:CG	4:A:800:GTP:C8	2.80	0.55
1:A:317:PHE:CE2	1:A:500[B]:MET:HE3	2.41	0.55
1:B:272:ASN:HD21	1:B:276:LYS:NZ	2.05	0.54
1:B:88:ILE:H	1:B:238:ASN:HD21	1.54	0.54
1:B:89:GLU:OE1	1:B:483[B]:ARG:NH1	2.40	0.54
1:B:587:LYS:HD3	1:B:587:LYS:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:ND2	1:B:76:TRP:HE1	2.05	0.54
1:A:574:VAL:O	1:A:578[A]:PHE:CD2	2.56	0.54
8:A:3836:HOH:O	1:B:276:LYS:HE2	2.08	0.54
1:A:317:PHE:CE2	1:A:500[B]:MET:HE2	2.43	0.53
7:A:3430:ETX:H31	8:A:3929:HOH:O	2.07	0.53
1:B:589:VAL:HG11	1:B:619[A]:ILE:HD12	1.90	0.53
1:A:316:LYS:HZ3	6:A:1000:1PE:H122	1.74	0.53
1:A:316:LYS:HZ1	6:A:1000:1PE:H122	1.74	0.53
1:A:149:LEU:HD21	1:A:179[A]:SER:HB2	1.90	0.53
1:B:375[B]:GLU:HG2	8:B:4189:HOH:O	2.09	0.51
1:A:292[B]:ASN:OD1	4:A:800:GTP:H2'	2.10	0.51
1:A:316:LYS:NZ	6:A:1000:1PE:H242	2.26	0.51
1:B:317:PHE:CE2	1:B:500[B]:MET:HE3	2.45	0.51
1:A:107:LYS:O	1:B:507:LYS:NZ	2.44	0.50
1:A:153:LEU:HD23	1:A:326:ILE:HD12	1.93	0.50
1:B:590[A]:GLU:CG	8:B:3953:HOH:O	2.57	0.50
1:B:155:LYS:HE2	1:B:254:LEU:HD13	1.94	0.50
1:A:149:LEU:HD21	1:A:179[B]:SER:HB3	1.92	0.50
1:A:435:GLY:CA	8:A:3702:HOH:O	2.60	0.50
1:B:88:ILE:HD11	1:B:217:THR:HG21	1.94	0.50
1:A:153:LEU:HD21	1:A:423[A]:PRO:HA	1.92	0.50
1:A:190[B]:ILE:HG21	1:A:246:PHE:CZ	2.41	0.50
1:B:317:PHE:CE2	1:B:500[B]:MET:CE	2.96	0.49
1:B:55[A]:ARG:HG2	1:B:55[A]:ARG:HH11	1.77	0.49
1:B:7:ASN:OD1	1:B:9:LEU:N	2.45	0.49
1:B:317:PHE:HE2	1:B:500[B]:MET:CE	2.25	0.49
1:A:190[B]:ILE:CG2	1:A:246:PHE:CZ	2.95	0.49
1:A:151:SER:HG	1:A:153:LEU:HD22	1.76	0.48
1:B:253:ARG:HG2	1:B:488:TYR:HB3	1.94	0.48
1:A:415[B]:ILE:HD13	1:A:415[B]:ILE:H	1.78	0.48
1:B:9:LEU:HG	1:B:36:GLN:CD	2.34	0.48
1:A:292[B]:ASN:ND2	1:A:530:PHE:CE1	2.82	0.47
1:A:107:LYS:NZ	1:A:597[B]:GLU:OE1	2.42	0.47
1:B:521:LYS:HD2	8:B:4020:HOH:O	2.15	0.47
1:A:607[A]:GLU:HG2	1:A:610:ARG:NH2	2.29	0.47
1:A:153:LEU:HD21	1:A:423[B]:PRO:HA	1.96	0.47
1:A:435:GLY:N	8:A:3702:HOH:O	2.48	0.47
1:B:391:TRP:CH2	1:B:393:PRO:HA	2.50	0.47
1:B:483[A]:ARG:HB3	1:B:484:PRO:HD3	1.97	0.46
1:A:71[A]:LYS:NZ	8:A:3796:HOH:O	2.47	0.46
1:B:483[B]:ARG:CD	8:B:3911:HOH:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ALA:HA	4:B:800:GTP:O2A	2.15	0.46
1:B:317:PHE:HE2	1:B:500[B]:MET:HE3	1.81	0.46
1:A:483:ARG:HB3	1:A:484:PRO:HD3	1.98	0.46
1:B:271:THR:HB	1:B:304:LYS:HD3	1.98	0.46
1:A:97[A]:GLN:HB2	1:A:97[A]:GLN:HE21	1.56	0.45
1:A:342:LYS:HE3	8:A:3662:HOH:O	2.15	0.45
1:A:56:LEU:O	1:A:60[B]:MET:HG3	2.17	0.45
1:A:589[B]:VAL:HG11	1:A:615:LEU:HG	1.99	0.45
1:A:520:ASP:HB2	8:A:3740:HOH:O	2.18	0.44
1:A:159:GLU:HA	1:A:192:CYS:HB2	1.99	0.44
1:A:148:PRO:HD2	8:A:3813:HOH:O	2.17	0.44
1:B:616[B]:LYS:HD2	8:B:4329:HOH:O	2.15	0.44
1:B:315:MET:HA	1:B:324:ARG:O	2.18	0.44
1:A:292[B]:ASN:ND2	1:A:530:PHE:HE1	2.16	0.44
1:A:15:VAL:HG21	1:A:20:LEU:HG	2.01	0.43
1:B:203:LYS:HD2	8:B:4086:HOH:O	2.18	0.43
1:B:272:ASN:HD21	1:B:276:LYS:HZ1	1.66	0.43
1:A:45[B]:ILE:CD1	1:A:141:VAL:HG21	2.48	0.43
1:A:502:HIS:CD2	8:A:3673:HOH:O	2.71	0.42
1:B:7:ASN:HD22	1:B:10:ASP:HB3	1.83	0.42
1:A:60[B]:MET:HE2	1:A:60[B]:MET:HB3	1.80	0.42
1:B:261:LEU:HD11	1:B:500[B]:MET:SD	2.60	0.41
1:A:190[B]:ILE:HD11	1:A:228:ILE:HG13	2.01	0.41
1:A:589[B]:VAL:HG11	1:A:619:ILE:HD12	2.02	0.41
1:B:217:THR:HA	1:B:231:PHE:O	2.20	0.41
1:A:56:LEU:HD11	1:A:164:PRO:HB3	2.02	0.41
1:A:45[B]:ILE:HD13	1:A:141:VAL:CG2	2.50	0.41
1:B:391:TRP:CD2	1:B:399:CYS:HB3	2.55	0.41
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.81	0.41
1:B:520:ASP:HB3	1:B:526[B]:LEU:CD1	2.50	0.41
1:B:221:HIS:CE1	1:B:249:ARG:HD2	2.56	0.41
1:B:264:HIS:CD2	1:B:290:LYS:HE3	2.56	0.41
1:A:268:LEU:HD12	1:A:268:LEU:C	2.41	0.41
1:A:0:SER:N	1:A:25:GLN:HE22	2.12	0.40
1:B:550:ALA:HB1	1:B:557:TYR:HB3	2.02	0.40
1:A:389:LYS:HA	1:A:389:LYS:HE2	2.03	0.40
1:A:95:ILE:N	1:A:95:ILE:HD12	2.36	0.40
1:A:413:CYS:SG	1:A:415[B]:ILE:CD1	3.09	0.40
1:A:213:ASN:C	1:A:213:ASN:HD22	2.24	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)
8:A:3626:HOH:O	8:A:3743:HOH:O[2_645]	2.14	0.06

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	653/624 (105%)	631 (97%)	22 (3%)	0	100	100
1	B	634/624 (102%)	616 (97%)	18 (3%)	0	100	100
All	All	1287/1248 (103%)	1247 (97%)	40 (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	551/520 (106%)	540 (98%)	11 (2%)	63	29
1	B	539/520 (104%)	527 (98%)	12 (2%)	60	25
All	All	1090/1040 (105%)	1067 (98%)	23 (2%)	63	27

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97[A]	GLN
1	A	97[B]	GLN
1	A	153	LEU

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Mol	Chain	Res	Type
1	A	213	ASN
1	A	369	TYR
1	A	394	GLN
1	A	471	LYS
1	A	521	LYS
1	A	577	LEU
1	A	581	SER
1	A	587	LYS
1	B	4	GLN
1	B	9	LEU
1	B	88	ILE
1	B	115[A]	ARG
1	B	115[B]	ARG
1	B	213	ASN
1	B	246	PHE
1	B	253	ARG
1	B	521	LYS
1	B	571	ASP
1	B	575	GLU
1	B	587	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	74	ASN
1	A	208	ASN
1	A	213	ASN
1	A	238	ASN
1	A	297	ASN
1	A	320	GLN
1	A	322	ASN
1	A	515	ASN
1	B	36	GLN
1	B	59	HIS
1	B	74	ASN
1	B	209	ASN
1	B	213	ASN
1	B	238	ASN
1	B	272	ASN
1	B	292	ASN
1	B	297	ASN

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Mol	Chain	Res	Type
1	B	502	HIS
1	B	515	ASN
1	B	522	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 14 ligands modelled in this entry, 7 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	$\# Z > 2$
6	1PE	A	1000	-	9,9,15	0.67	0	8,8,14	0.60	0
7	ETX	A	3430	-	5,5,5	0.58	0	4,4,4	0.58	0
4	GTP	A	800	2	25,34,34	1.21	2 (8%)	34,54,54	1.60	6 (17%)
5	SPV	A	900	2	5,9,9	0.72	0	7,13,13	0.94	0
7	ETX	B	3430	-	5,5,5	0.60	0	4,4,4	0.77	0
4	GTP	B	800	2	25,34,34	0.92	0	34,54,54	2.09	8 (23%)
5	SPV	B	900	2	5,9,9	1.18	1 (20%)	7,13,13	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
6	1PE	A	1000	-	-	0/7/7/13	0/0/0/0
7	ETX	A	3430	-	-	0/3/3/3	0/0/0/0
4	GTP	A	800	2	-	0/18/38/38	0/3/3/3
5	SPV	A	900	2	-	0/5/9/9	0/0/0/0
7	ETX	B	3430	-	-	0/3/3/3	0/0/0/0
4	GTP	B	800	2	-	0/18/38/38	0/3/3/3
5	SPV	B	900	2	-	0/5/9/9	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	GTP	PG-O2G	-2.66	1.45	1.54
4	A	800	GTP	O4'-C4'	-2.12	1.40	1.45
5	B	900	SPV	O2-C2	2.11	1.26	1.22

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	GTP	N3-C2-N1	-5.23	119.48	127.44
4	A	800	GTP	C4-C5-N7	-4.04	105.76	109.48
4	B	800	GTP	C5-C6-N1	-3.92	118.23	123.59
4	B	800	GTP	C6-C5-C4	-3.90	116.24	120.90
4	A	800	GTP	N3-C2-N1	-3.53	122.07	127.44
4	B	800	GTP	C1'-N9-C4	-2.88	122.59	126.94
4	B	800	GTP	O3A-PA-O5'	-2.57	96.13	102.94
4	A	800	GTP	C5-C6-N1	-2.54	120.12	123.59
4	A	800	GTP	O2B-PB-O3B	2.01	114.23	105.09
4	B	800	GTP	O2G-PG-O1G	2.26	117.86	110.58
4	A	800	GTP	N2-C2-N1	2.32	121.04	117.20
4	A	800	GTP	C6-N1-C2	2.32	119.17	115.94
4	B	800	GTP	N2-C2-N1	2.86	121.94	117.20
4	B	800	GTP	C6-N1-C2	6.07	124.37	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1000	1PE	5	0
7	A	3430	ETX	1	0
4	A	800	GTP	4	0
7	B	3430	ETX	3	0
4	B	800	GTP	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	624/624 (100%)	0.48	58 (9%)	11 10	2, 6, 18, 35	11 (1%)
1	B	611/624 (97%)	0.51	56 (9%)	11 11	2, 6, 19, 34	2 (0%)
All	All	1235/1248 (98%)	0.49	114 (9%)	11 11	2, 6, 19, 35	13 (1%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASN	7.2
1	A	504	PRO	7.2
1	A	394	GLN	7.1
1	B	394	GLN	6.9
1	B	396	GLU	6.8
1	A	393	PRO	6.6
1	B	8	GLY	6.4
1	B	504	PRO	6.1
1	A	149	LEU	5.8
1	B	395	ASP	5.6
1	B	393	PRO	5.5
1	A	150	GLY	5.5
1	A	396	GLU	5.5
1	A	392	ARG	5.5
1	A	152	PRO	5.2
1	B	392	ARG	4.8
1	A	153	LEU	4.6
1	B	521	LYS	4.3
1	B	575	GLU	4.3
1	A	574	VAL	4.1
1	B	205	PRO	4.1
1	A	341	VAL	4.0
1	A	395	ASP	3.9
1	A	205	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	150	GLY	3.9
1	B	9	LEU	3.8
1	A	397	GLU	3.8
1	A	319	ALA	3.8
1	A	0	SER	3.7
1	A	575	GLU	3.7
1	B	473	LYS	3.7
1	B	432	ILE	3.5
1	B	379	PRO	3.5
1	A	432	ILE	3.4
1	A	473	LYS	3.4
1	B	583	GLU	3.3
1	A	522	ASN	3.3
1	B	4	GLN	3.3
1	B	203	LYS	3.2
1	A	389	LYS	3.2
1	A	1	MET	3.1
1	B	391	TRP	3.1
1	B	480	PHE	3.1
1	B	389	LYS	3.1
1	B	21	ASP	3.1
1	B	571	ASP	3.1
1	A	391	TRP	3.0
1	B	204	LYS	3.0
1	B	431	ILE	3.0
1	A	572	VAL	3.0
1	B	505	ALA	2.9
1	A	166	VAL	2.9
1	A	472	GLY	2.9
1	A	186	ASP	2.9
1	A	203	LYS	2.9
1	A	505	ALA	2.9
1	A	562	ASP	2.8
1	B	502	HIS	2.8
1	A	2	PRO	2.7
1	A	433	PHE	2.7
1	B	377	LEU	2.7
1	B	390	GLU	2.7
1	B	397[A]	GLU	2.7
1	A	204	LYS	2.7
1	A	357	PHE	2.6
1	B	378	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	186[A]	ASP	2.6
1	B	166	VAL	2.6
1	A	356	ILE	2.5
1	A	154	ALA	2.5
1	B	561	GLU	2.5
1	A	390	GLU	2.5
1	B	165	TYR	2.5
1	B	522	ASN	2.5
1	B	25	GLN	2.5
1	B	273	PRO	2.5
1	A	521	LYS	2.4
1	A	431	ILE	2.4
1	B	160	LEU	2.4
1	B	562	ASP	2.4
1	A	524	LYS	2.4
1	B	523	GLY	2.3
1	A	570	GLY	2.3
1	B	433	PHE	2.3
1	A	358	THR	2.3
1	B	514	VAL	2.3
1	A	569	LEU	2.3
1	B	374[A]	ASP	2.3
1	B	398	PRO	2.2
1	A	349	LYS	2.2
1	B	512	PHE	2.2
1	B	301	PRO	2.2
1	A	561	GLU	2.2
1	A	456	VAL	2.2
1	B	503	ARG	2.2
1	A	374	ASP	2.2
1	A	511	ILE	2.2
1	B	22[A]	SER	2.2
1	A	567	LYS	2.1
1	A	165	TYR	2.1
1	A	571	ASP	2.1
1	A	503	ARG	2.1
1	B	142	ILE	2.1
1	B	70	LYS	2.1
1	B	567	LYS	2.1
1	B	511	ILE	2.1
1	A	208	ASN	2.1
1	A	240	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	55[A]	ARG	2.0
1	A	167	VAL	2.0
1	A	321	GLY	2.0
1	A	388	ASN	2.0
1	B	388	ASN	2.0
1	A	583	GLU	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	ETX	B	3430	6/6	0.86	0.17	2.89	4,16,18,25	0
7	ETX	A	3430	6/6	0.91	0.14	1.68	6,14,21,23	0
4	GTP	A	800	32/32	0.95	0.12	1.10	2,2,6,7	32
6	1PE	A	1000	10/16	0.84	0.14	0.55	13,19,24,26	0
5	SPV	A	900	10/10	0.98	0.11	0.26	2,4,7,7	0
2	MN	A	703	1/1	0.99	0.10	-0.06	2,2,2,2	1
2	MN	A	700	1/1	1.00	0.10	-0.25	3,3,3,3	0
2	MN	B	700	1/1	1.00	0.12	-0.29	4,4,4,4	0
5	SPV	B	900	10/10	0.99	0.11	-0.36	2,3,5,6	0
4	GTP	B	800	32/32	0.98	0.07	-1.21	2,4,6,7	0
2	MN	B	701	1/1	1.00	0.08	-1.74	4,4,4,4	0
3	NA	A	1100	1/1	0.98	0.07	-1.90	22,22,22,22	0
3	NA	B	1100	1/1	0.99	0.06	-2.85	16,16,16,16	0
2	MN	A	701	1/1	1.00	0.05	-3.45	2,2,2,2	1

6.5 Other polymers [i](#)

There are no such residues in this entry.