WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jul 5, 2016 – 09:06 PM EDT

PDB ID	:	5K8F
Title	:	Crystal structure of Acetyl-CoA Synthetase in complex with ATP and Acetyl-AMP from Cryptococcus neoformans H99
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID); Fox III, D.; Delker, S.L.; Potts, K.T.; Lorimer, D.D.; Edwards, T.E.; Mutz, M.W.; SSGCID
Deposited on	:	2016-05-30
Resolution	:	2.45 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
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)	:	rb-20027790
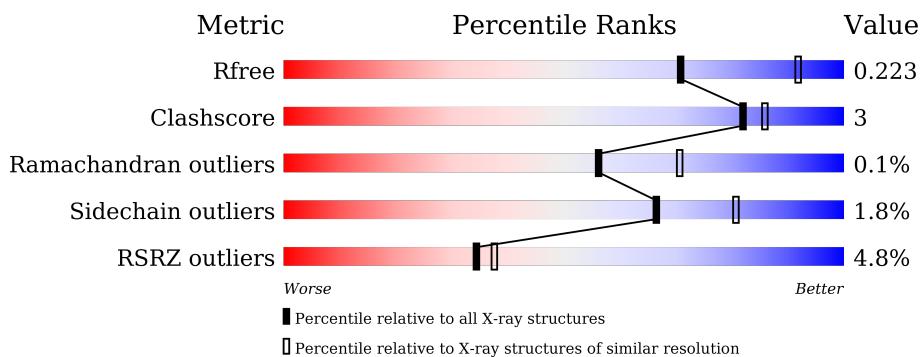
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
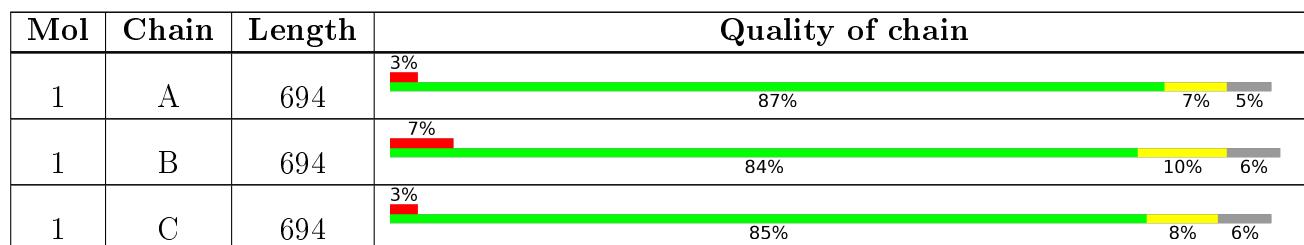
The reported resolution of this entry is 2.45 Å.

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	Percentile Ranks	Value
Rfree		0.223
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		1.8%
RSRZ outliers		4.8%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 <=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	694	3% · 87% · 7% · 5%
1	B	694	7% · 84% · 10% · 6%
1	C	694	3% · 85% · 8% · 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	705	-	-	-	X
5	EDO	A	706	-	-	-	X
5	EDO	B	705	-	-	-	X
5	EDO	B	706	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15669 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 Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	15	0
			5109	3250	875	957	27			
1	B	655	Total	C	N	O	S	0	5	0
			4978	3180	854	918	26			
1	C	651	Total	C	N	O	S	0	7	0
			4988	3193	851	917	27			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression tag	UNP J9VFT1
A	-6	HIS	-	expression tag	UNP J9VFT1
A	-5	HIS	-	expression tag	UNP J9VFT1
A	-4	GLU	-	expression tag	UNP J9VFT1
A	-3	ASN	-	expression tag	UNP J9VFT1
A	-2	LEU	-	expression tag	UNP J9VFT1
A	-1	TYR	-	expression tag	UNP J9VFT1
A	0	PHE	-	expression tag	UNP J9VFT1
A	1	GLN	-	expression tag	UNP J9VFT1
B	-13	MET	-	initiating methionine	UNP J9VFT1
B	-12	HIS	-	expression tag	UNP J9VFT1
B	-11	HIS	-	expression tag	UNP J9VFT1
B	-10	HIS	-	expression tag	UNP J9VFT1
B	-9	HIS	-	expression tag	UNP J9VFT1
B	-8	HIS	-	expression tag	UNP J9VFT1
B	-7	HIS	-	expression tag	UNP J9VFT1
B	-6	HIS	-	expression tag	UNP J9VFT1

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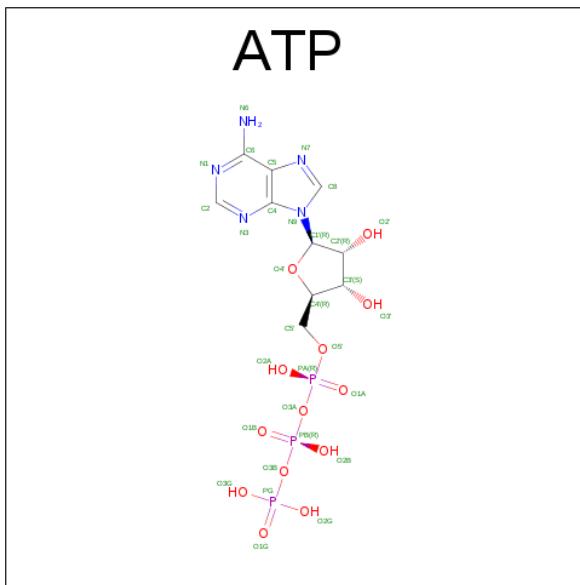
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
C	-13	MET	-	initiating methionine	UNP J9VFT1
C	-12	HIS	-	expression tag	UNP J9VFT1
C	-11	HIS	-	expression tag	UNP J9VFT1
C	-10	HIS	-	expression tag	UNP J9VFT1
C	-9	HIS	-	expression tag	UNP J9VFT1
C	-8	HIS	-	expression tag	UNP J9VFT1
C	-7	HIS	-	expression tag	UNP J9VFT1
C	-6	HIS	-	expression tag	UNP J9VFT1
C	-5	HIS	-	expression tag	UNP J9VFT1
C	-4	GLU	-	expression tag	UNP J9VFT1
C	-3	ASN	-	expression tag	UNP J9VFT1
C	-2	LEU	-	expression tag	UNP J9VFT1
C	-1	TYR	-	expression tag	UNP J9VFT1
C	0	PHE	-	expression tag	UNP J9VFT1
C	1	GLN	-	expression tag	UNP J9VFT1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).
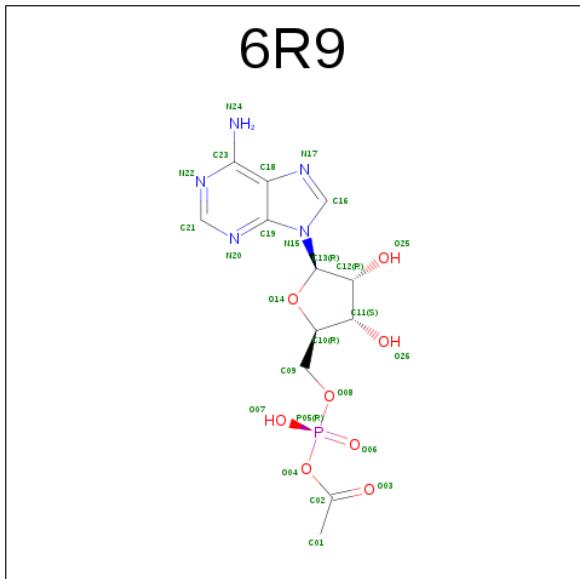
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	2
2	A	2	Total 2	Mg 2	0	2
2	C	3	Total 3	Mg 3	0	2

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
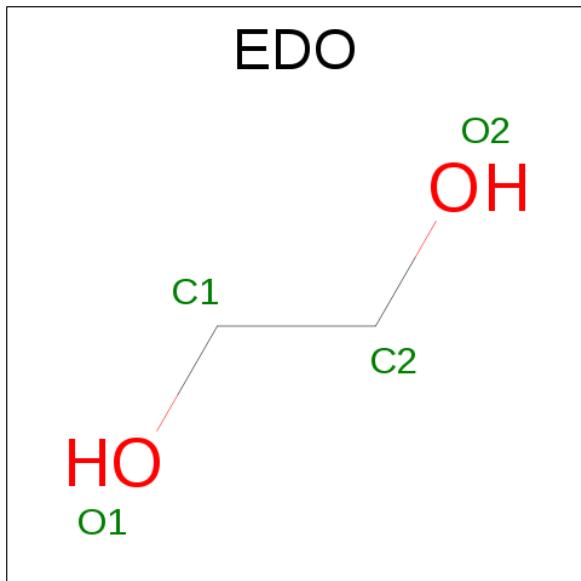
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	1
			31	10	5	13	3		

- Molecule 4 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] ethanoate (three-letter code: 6R9) (formula: $C_{12}H_{16}N_5O_8P$).
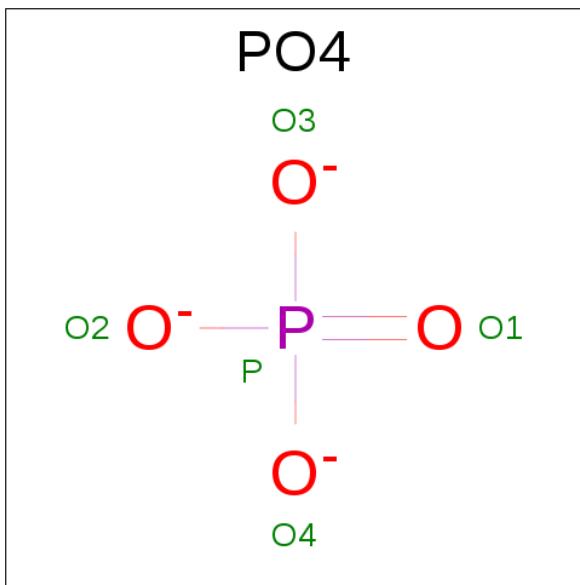
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			26	12	5	8	1		
4	B	1	Total	C	N	O	P	0	1
			26	12	5	8	1		
4	C	1	Total	C	N	O	P	0	1
			26	12	5	8	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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

• Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 5	O 4	P 1	0	0
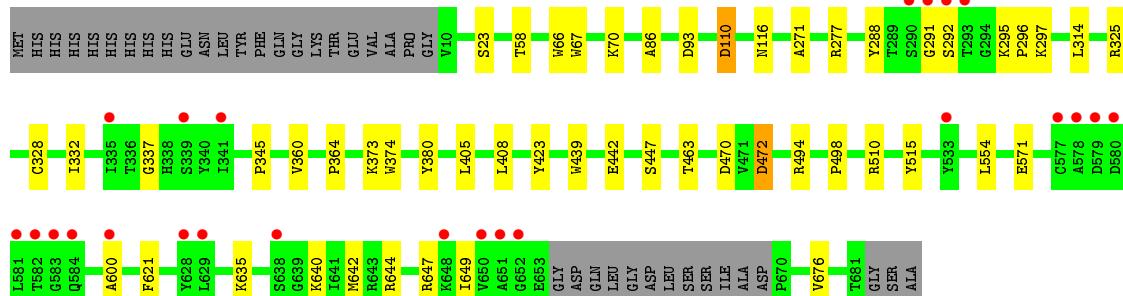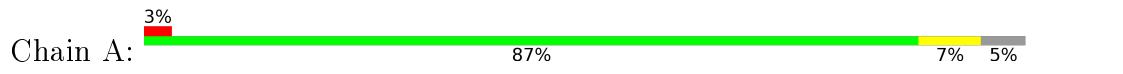
• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total 188	O 188	0	3
7	B	84	Total 86	O 86	0	2
7	C	99	Total 101	O 101	0	2
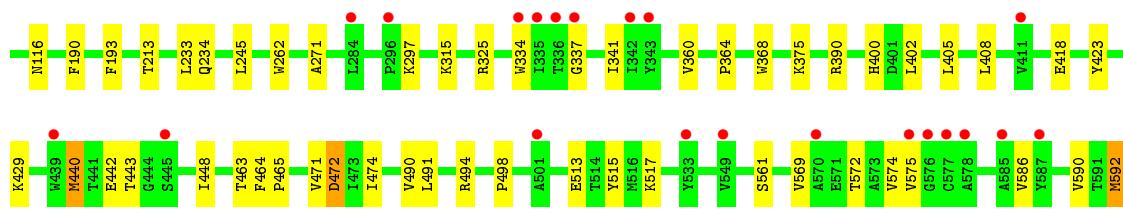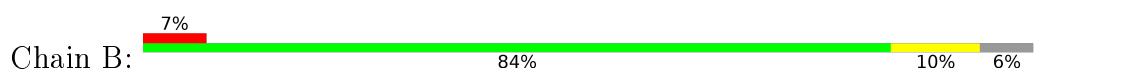
3 Residue-property plots ⓘ

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.
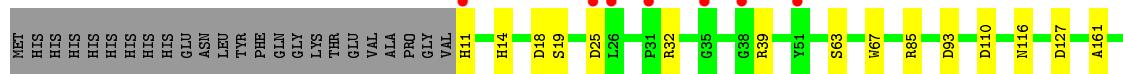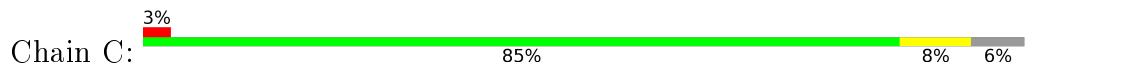
- Molecule 1: Acetyl-coenzyme A synthetase
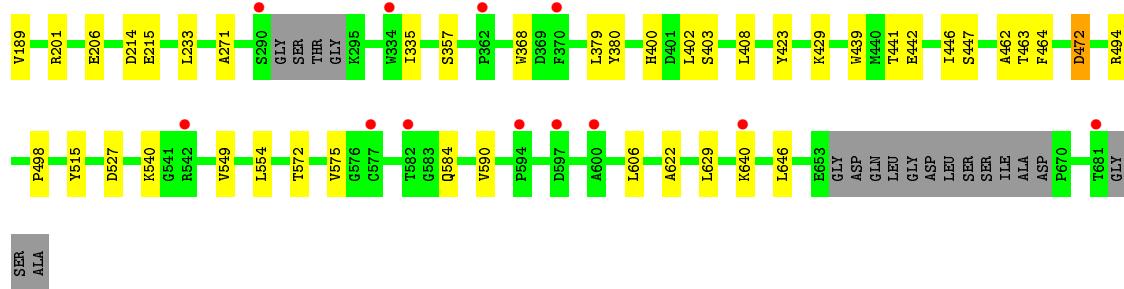
- Molecule 1: Acetyl-coenzyme A synthetase

- Molecule 1: Acetyl-coenzyme A synthetase

4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.37Å　　83.92Å　　101.57Å 110.06°　　105.24°　　87.65°	Depositor
Resolution (Å)	26.62　–　2.45 47.48　–　2.45	Depositor EDS
% Data completeness (in resolution range)	98.6 (26.62-2.45) 87.8 (47.48-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.71 (at 2.45Å)	Xtriage
Refinement program	PHENIX (DEV_2415: ???)	Depositor
R, R_{free}	0.178　,　0.223 0.177　,　0.223	Depositor DCC
R_{free} test set	1999 reflections (2.59%)	DCC
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.7	EDS
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15669	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: MG, 6R9, PO4, ATP, EDO

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	0.25	0/5258	0.46	0/7177
1	B	0.25	0/5128	0.44	0/7011
1	C	0.25	0/5144	0.44	0/7029
All	All	0.25	0/15530	0.45	0/21217

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292[A]	SER	Peptide

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	5109	0	4822	28	0
1	B	4978	0	4636	36	0
1	C	4988	0	4687	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
4	A	26	0	0	0	0
4	B	26	0	0	0	0
4	C	26	0	0	1	0
5	A	16	0	24	0	0
5	B	12	0	18	2	0
5	C	8	0	12	3	0
6	C	5	0	0	0	0
7	A	188	0	0	1	0
7	B	86	0	0	0	0
7	C	101	0	0	0	0
All	All	15669	0	14235	93	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 3.

All (93) 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:C:554:LEU:HD11	1:C:622:ALA:HA	1.80	0.63
1:B:472:ASP:OD2	1:B:494:ARG:NH2	2.32	0.62
1:B:513:GLU:HA	1:B:517:LYS:HG3	1.80	0.62
1:C:540:LYS:HG2	5:C:708:EDO:H21	1.83	0.59
1:C:606:LEU:HD23	1:C:629:LEU:HD21	1.86	0.57
1:B:572:THR:HG22	1:B:590:VAL:HG13	1.87	0.57
1:C:527:ASP:OD1	3:C:703[B]:ATP:O2'	2.20	0.56
1:A:271:ALA:HB3	1:C:93:ASP:HB3	1.86	0.56
1:A:291[A]:GLY:O	1:A:644:ARG:NH1	2.39	0.55
1:C:527:ASP:OD1	4:C:704[A]:6R9:O25	2.24	0.54
1:A:86:ALA:HA	5:B:706:EDO:H22	1.89	0.54
1:A:405:LEU:HD13	1:A:408:LEU:HD21	1.89	0.53
1:B:440:MET:HG3	1:B:443:THR:HG23	1.90	0.53
1:A:600:ALA:O	7:A:801:HOH:O	2.18	0.53
1:C:400:HIS:O	1:C:429:LYS:NZ	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ARG:HD3	1:C:39:ARG:HE	1.73	0.52
1:A:373:LYS:HD2	1:A:374:TRP:CE2	2.45	0.51
1:C:472:ASP:OD2	1:C:494:ARG:NH1	2.43	0.51
1:B:54:GLU:OE1	1:B:57:LYS:NZ	2.43	0.51
1:B:440:MET:HB3	3:B:703[A]:ATP:H5'1	1.93	0.51
1:C:549:VAL:HG12	1:C:584:GLN:O	2.11	0.51
1:B:400:HIS:O	1:B:429:LYS:NZ	2.35	0.50
1:C:214:ASP:OD1	1:C:215:GLU:N	2.42	0.50
1:A:649:ILE:HG21	1:A:676:VAL:HG12	1.93	0.49
1:B:569:VAL:HA	1:B:592:MET:HG3	1.94	0.49
1:B:11:HIS:O	1:B:14:HIS:NE2	2.45	0.49
1:C:335:ILE:HG12	1:C:441:THR:HA	1.95	0.48
1:A:644:ARG:HA	1:A:647:ARG:NH1	2.29	0.48
1:A:472:ASP:OD2	1:A:494:ARG:NH1	2.44	0.48
1:A:442:GLU:HG2	1:A:515:TYR:CZ	2.49	0.48
1:A:295[B]:LYS:O	1:A:510:ARG:NH2	2.45	0.48
1:B:58:THR:HG22	1:B:66:TRP:CD2	2.49	0.48
1:A:58:THR:HG22	1:A:66:TRP:CD2	2.49	0.47
1:A:314:LEU:HD22	1:A:345:PRO:HA	1.96	0.47
1:C:67:TRP:CZ3	1:C:498:PRO:HG2	2.48	0.47
1:C:439:TRP:HB3	1:C:447:SER:H	1.78	0.47
1:B:190[B]:PHE:CZ	1:B:334[B]:TRP:HB2	2.49	0.47
1:A:328:CYS:HA	1:A:380:TYR:HB3	1.96	0.47
1:C:442:GLU:HG2	1:C:515:TYR:CZ	2.50	0.46
1:A:554:LEU:HD21	1:A:621:PHE:HE2	1.81	0.46
1:C:463:THR:OG1	1:C:464:PHE:N	2.48	0.46
1:A:110:ASP:N	1:A:110:ASP:OD1	2.49	0.46
1:B:471:VAL:HB	1:B:491:LEU:HD11	1.98	0.45
1:C:11:HIS:O	1:C:14:HIS:NE2	2.49	0.45
1:A:93:ASP:HB3	1:B:271:ALA:HB3	1.98	0.45
1:B:390:ARG:NH2	1:B:418:GLU:OE2	2.50	0.45
1:B:190[B]:PHE:HZ	1:B:334[B]:TRP:HB2	1.80	0.45
1:A:332:ILE:HA	1:A:337:GLY:HA3	1.99	0.45
1:B:17:PRO:HD2	1:B:561:SER:HB2	1.99	0.44
1:B:93:ASP:HB3	1:C:271:ALA:HB3	2.00	0.44
1:C:379:LEU:HB3	1:C:408:LEU:HD23	1.99	0.44
1:C:575:VAL:HG11	1:C:646:LEU:HB2	1.99	0.44
1:A:439:TRP:HB3	1:A:447:SER:H	1.83	0.44
1:B:360:VAL:HA	1:B:364:PRO:HA	2.00	0.44
1:C:39:ARG:NH2	1:C:403:SER:O	2.51	0.44
1:B:67:TRP:CZ3	1:B:498:PRO:HG2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:VAL:HG12	1:B:643:ARG:HB3	2.00	0.43
1:A:360:VAL:HA	1:A:364:PRO:HA	2.00	0.43
1:C:439:TRP:HB3	1:C:446:ILE:HA	2.01	0.43
1:B:30:PRO:O	1:B:34:GLN:HG3	2.18	0.43
1:B:325:ARG:NH2	1:B:375:LYS:O	2.50	0.43
1:B:337:GLY:HA2	1:B:341:ILE:HD12	2.01	0.42
1:A:373:LYS:HD2	1:A:374:TRP:NE1	2.33	0.42
1:B:233:LEU:HA	1:B:233:LEU:HD23	1.87	0.42
1:A:67:TRP:CZ3	1:A:498:PRO:HG2	2.55	0.42
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.55	0.42
1:B:83:THR:O	1:B:98:PRO:HD2	2.20	0.42
1:C:368:TRP:HB3	1:C:402:LEU:HD21	2.01	0.42
1:B:190[A]:PHE:HB3	1:B:193:PHE:CD1	2.54	0.42
1:B:213:THR:HG22	1:B:245:LEU:HB3	2.02	0.42
1:A:470:ASP:OD2	1:A:494:ARG:HD3	2.19	0.42
1:A:288:TYR:CD2	1:A:296[A]:PRO:HB2	2.55	0.41
1:A:297[B]:LYS:HG2	1:A:297[B]:LYS:H	1.69	0.41
1:B:474:ILE:O	1:B:490:VAL:HG22	2.20	0.41
1:B:55:TRP:CH2	1:B:59:VAL:HG21	2.55	0.41
1:C:572:THR:HG22	1:C:590:VAL:HG22	2.01	0.41
1:B:463:THR:OG1	1:B:464:PHE:N	2.52	0.41
1:C:161:ALA:H	5:C:707:EDO:H11	1.86	0.41
1:B:574:VAL:HG13	1:B:586:VAL:HG13	2.01	0.41
1:A:66:TRP:CH2	1:A:70:LYS:HG3	2.56	0.41
1:B:368:TRP:HB3	1:B:402:LEU:HD21	2.02	0.41
1:C:127:ASP:HA	1:C:357:SER:HB2	2.02	0.41
1:A:554:LEU:HD21	1:A:621:PHE:CE2	2.55	0.40
1:A:571:GLU:CD	1:A:635:LYS:HZ1	2.23	0.40
1:B:405:LEU:HD13	1:B:408:LEU:HD21	2.02	0.40
1:B:448:ILE:HA	1:B:465:PRO:HA	2.02	0.40
1:C:462:ALA:O	1:C:463:THR:OG1	2.36	0.40
1:C:206:GLU:O	5:C:707:EDO:H12	2.22	0.40
1:C:18:ASP:OD1	1:C:19:SER:N	2.53	0.40
1:C:189:VAL:HG22	1:C:201:ARG:HD3	2.02	0.40
1:B:315:LYS:NZ	5:B:707:EDO:H12	2.37	0.40
1:C:233:LEU:HA	1:C:233:LEU:HD23	1.91	0.40
1:C:63:SER:OG	1:C:85:ARG:NH2	2.48	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	667/694 (96%)	643 (96%)	23 (3%)	1 (0%)	56	71
1	B	655/694 (94%)	634 (97%)	21 (3%)	0	100	100
1	C	652/694 (94%)	633 (97%)	19 (3%)	0	100	100
All	All	1974/2082 (95%)	1910 (97%)	63 (3%)	1 (0%)	56	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	THR

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	515/576 (89%)	504 (98%)	11 (2%)	61	77
1	B	485/576 (84%)	474 (98%)	11 (2%)	58	74
1	C	494/576 (86%)	486 (98%)	8 (2%)	70	83
All	All	1494/1728 (86%)	1464 (98%)	30 (2%)	66	78

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	110	ASP

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Mol	Chain	Res	Type
1	A	116	ASN
1	A	277[A]	ARG
1	A	277[B]	ARG
1	A	325[A]	ARG
1	A	325[B]	ARG
1	A	423	TYR
1	A	472	ASP
1	A	640	LYS
1	A	642	MET
1	B	25	ASP
1	B	110	ASP
1	B	116	ASN
1	B	234	GLN
1	B	262	TRP
1	B	297	LYS
1	B	423	TYR
1	B	440	MET
1	B	472	ASP
1	B	592	MET
1	B	640	LYS
1	C	25	ASP
1	C	110	ASP
1	C	116	ASN
1	C	380	TYR
1	C	423	TYR
1	C	472	ASP
1	C	640[A]	LYS
1	C	640[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 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	#$|Z| > 2$
3	ATP	A	703[B]	2	26,33,33	0.96	1 (3%)	26,52,52	1.68	2 (7%)
4	6R9	A	704[A]	-	25,28,28	4.19	6 (24%)	24,42,42	2.33	4 (16%)
5	EDO	A	705	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	A	706	-	3,3,3	0.45	0	2,2,2	0.41	0
5	EDO	A	707	-	3,3,3	0.44	0	2,2,2	0.42	0
5	EDO	A	708	-	3,3,3	0.49	0	2,2,2	0.25	0
3	ATP	B	703[A]	-	26,33,33	0.94	1 (3%)	26,52,52	1.70	3 (11%)
4	6R9	B	704[B]	2	25,28,28	4.17	6 (24%)	24,42,42	2.38	7 (29%)
5	EDO	B	705	-	3,3,3	0.42	0	2,2,2	0.51	0
5	EDO	B	706	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	B	707	-	3,3,3	0.44	0	2,2,2	0.44	0
3	ATP	C	703[B]	2	26,33,33	0.95	1 (3%)	26,52,52	1.67	1 (3%)
4	6R9	C	704[A]	-	25,28,28	4.19	6 (24%)	24,42,42	2.28	5 (20%)
6	PO4	C	706	-	4,4,4	0.66	0	6,6,6	0.23	0
5	EDO	C	707	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	C	708	-	3,3,3	0.44	0	2,2,2	0.47	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
3	ATP	A	703[B]	2	-	0/18/38/38	0/3/3/3
4	6R9	A	704[A]	-	-	0/9/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	705	-	-	0/1/1/1	0/0/0/0
5	EDO	A	706	-	-	0/1/1/1	0/0/0/0
5	EDO	A	707	-	-	0/1/1/1	0/0/0/0
5	EDO	A	708	-	-	0/1/1/1	0/0/0/0
3	ATP	B	703[A]	-	-	0/18/38/38	0/3/3/3
4	6R9	B	704[B]	2	-	0/9/31/31	0/3/3/3
5	EDO	B	705	-	-	0/1/1/1	0/0/0/0
5	EDO	B	706	-	-	0/1/1/1	0/0/0/0
5	EDO	B	707	-	-	0/1/1/1	0/0/0/0
3	ATP	C	703[B]	2	-	0/18/38/38	0/3/3/3
4	6R9	C	704[A]	-	-	0/9/31/31	0/3/3/3
6	PO4	C	706	-	-	0/0/0/0	0/0/0/0
5	EDO	C	707	-	-	0/1/1/1	0/0/0/0
5	EDO	C	708	-	-	0/1/1/1	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	704[A]	6R9	C12-C13	-12.09	1.34	1.53
4	A	704[A]	6R9	C12-C13	-12.07	1.34	1.53
4	B	704[B]	6R9	C12-C13	-11.85	1.34	1.53
4	B	704[B]	6R9	O14-C10	-6.27	1.30	1.45
4	C	704[A]	6R9	O14-C10	-6.15	1.30	1.45
4	A	704[A]	6R9	O14-C10	-6.14	1.31	1.45
4	A	704[A]	6R9	P05-O04	2.43	1.65	1.60
4	C	704[A]	6R9	P05-O04	2.51	1.65	1.60
4	B	704[B]	6R9	P05-O04	2.63	1.66	1.60
4	A	704[A]	6R9	C23-N24	2.66	1.45	1.34
4	C	704[A]	6R9	C23-N24	2.66	1.45	1.34
4	B	704[B]	6R9	C23-N24	2.67	1.45	1.34
3	A	703[B]	ATP	C5-C4	3.04	1.47	1.40
3	C	703[B]	ATP	C5-C4	3.06	1.47	1.40
3	B	703[A]	ATP	C5-C4	3.07	1.47	1.40
4	B	704[B]	6R9	O04-C02	3.21	1.41	1.37
4	C	704[A]	6R9	O04-C02	3.23	1.41	1.37
4	A	704[A]	6R9	O04-C02	3.27	1.41	1.37
4	B	704[B]	6R9	O14-C13	14.59	1.62	1.41
4	C	704[A]	6R9	O14-C13	14.61	1.62	1.41
4	A	704[A]	6R9	O14-C13	14.63	1.62	1.41

All (22) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	704[B]	6R9	N20-C21-N22	-8.68	122.05	128.87
4	C	704[A]	6R9	N20-C21-N22	-8.58	122.13	128.87
4	A	704[A]	6R9	N20-C21-N22	-8.45	122.23	128.87
3	A	703[B]	ATP	N3-C2-N1	-6.70	123.61	128.87
3	C	703[B]	ATP	N3-C2-N1	-6.66	123.64	128.87
3	B	703[A]	ATP	N3-C2-N1	-6.63	123.66	128.87
4	A	704[A]	6R9	O14-C13-N15	-4.34	99.91	108.11
4	C	704[A]	6R9	O14-C13-N15	-3.90	100.74	108.11
4	B	704[B]	6R9	O14-C13-N15	-3.86	100.81	108.11
4	B	704[B]	6R9	C10-O14-C13	-3.29	106.15	109.64
4	A	704[A]	6R9	C10-O14-C13	-3.06	106.40	109.64
4	C	704[A]	6R9	C10-O14-C13	-2.79	106.69	109.64
4	B	704[B]	6R9	C13-N15-C19	-2.77	123.72	126.81
3	B	703[A]	ATP	C2'-C1'-N9	-2.42	107.00	113.47
4	B	704[B]	6R9	O04-C02-O03	-2.33	120.32	122.07
3	A	703[B]	ATP	C2'-C1'-N9	-2.25	107.44	113.47
3	B	703[A]	ATP	C1'-N9-C4	-2.23	124.32	126.81
4	B	704[B]	6R9	O04-P05-O08	2.03	108.71	102.98
4	C	704[A]	6R9	O04-P05-O08	2.07	108.81	102.98
4	B	704[B]	6R9	C12-C13-N15	2.51	120.19	113.47
4	C	704[A]	6R9	C12-C13-N15	2.63	120.51	113.47
4	A	704[A]	6R9	C12-C13-N15	3.14	121.88	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703[A]	ATP	1	0
5	B	706	EDO	1	0
5	B	707	EDO	1	0
3	C	703[B]	ATP	1	0
4	C	704[A]	6R9	1	0
5	C	707	EDO	2	0
5	C	708	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	656/694 (94%)	-0.17	24 (3%)	45	49	22, 41, 89, 122	0
1	B	655/694 (94%)	0.22	52 (7%)	15	16	25, 58, 100, 124	0
1	C	651/694 (93%)	-0.05	19 (2%)	55	58	27, 55, 94, 130	0
All	All	1962/2082 (94%)	-0.00	95 (4%)	34	37	22, 50, 96, 130	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	ALA	6.7
1	B	676	VAL	6.2
1	A	291[A]	GLY	5.8
1	A	578	ALA	5.7
1	A	577	CYS	4.7
1	A	652	GLY	4.4
1	B	681	THR	4.3
1	B	578	ALA	4.3
1	B	673	VAL	4.2
1	C	38	GLY	4.2
1	B	334[A]	TRP	4.1
1	C	334[A]	TRP	4.1
1	A	579	ASP	4.1
1	B	652	GLY	4.0
1	A	581	LEU	3.9
1	C	640[A]	LYS	3.9
1	B	628	TYR	3.9
1	B	577	CYS	3.8
1	C	582	THR	3.8
1	A	293[A]	THR	3.7
1	B	650	VAL	3.6
1	B	604	ALA	3.6
1	A	292[A]	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	51	TYR	3.5
1	B	634	PRO	3.5
1	B	335	ILE	3.4
1	B	649	ILE	3.3
1	A	628	TYR	3.3
1	B	576	GLY	3.2
1	B	675	GLU	3.1
1	B	645	VAL	3.1
1	C	597	ASP	3.0
1	B	679	LYS	3.0
1	B	575	VAL	2.9
1	B	680	VAL	2.9
1	B	605	ASP	2.9
1	C	31	PRO	2.9
1	C	600	ALA	2.9
1	B	638	SER	2.8
1	B	677	LYS	2.8
1	B	587	TYR	2.8
1	A	629	LEU	2.8
1	C	290	SER	2.8
1	B	533	TYR	2.8
1	B	549	VAL	2.7
1	B	646	LEU	2.7
1	A	533	TYR	2.6
1	B	38	GLY	2.6
1	B	439	TRP	2.6
1	B	653	GLU	2.6
1	A	580	ASP	2.5
1	B	633	LEU	2.5
1	A	648	LYS	2.5
1	B	28	ALA	2.5
1	A	650	VAL	2.5
1	A	600	ALA	2.4
1	B	632	ASP	2.4
1	B	343	TYR	2.4
1	B	337	GLY	2.4
1	B	595	GLU	2.4
1	A	290[A]	SER	2.4
1	C	51	TYR	2.4
1	B	296	PRO	2.4
1	B	618	ILE	2.4
1	C	542[A]	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	336	THR	2.4
1	C	35	GLY	2.3
1	B	651	ALA	2.3
1	A	583	GLY	2.3
1	B	411	VAL	2.3
1	B	585	ALA	2.3
1	C	681	THR	2.3
1	A	584	GLN	2.3
1	A	651	ALA	2.3
1	B	445	SER	2.3
1	C	26	LEU	2.2
1	C	577	CYS	2.2
1	B	570	ALA	2.2
1	C	25	ASP	2.2
1	A	339	SER	2.2
1	C	594	PRO	2.2
1	A	335	ILE	2.1
1	A	582	THR	2.1
1	B	612	ILE	2.1
1	C	362	PRO	2.1
1	B	342	ILE	2.1
1	B	672	ILE	2.1
1	B	629	LEU	2.1
1	A	638	SER	2.1
1	C	11	HIS	2.1
1	A	341	ILE	2.1
1	B	284	LEU	2.1
1	B	501	ALA	2.0
1	B	37	GLU	2.0
1	C	370	PHE	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
5	EDO	B	706	4/4	0.95	0.26	13.87	51,51,52,52	0
5	EDO	A	705	4/4	0.96	0.20	4.36	45,45,46,46	0
5	EDO	A	706	4/4	0.90	0.20	3.69	65,68,70,72	0
5	EDO	B	705	4/4	0.95	0.16	2.68	47,47,50,50	0
5	EDO	A	707	4/4	0.95	0.17	1.65	34,34,35,37	0
5	EDO	A	708	4/4	0.89	0.18	1.36	47,47,48,49	0
5	EDO	C	707	4/4	0.94	0.15	1.31	50,51,51,52	0
5	EDO	C	708	4/4	0.92	0.16	0.40	54,56,57,58	0
4	6R9	C	704[A]	26/26	0.95	0.24	-0.12	39,45,47,47	26
4	6R9	A	704[A]	26/26	0.96	0.17	-0.40	23,32,34,35	26
3	ATP	C	703[B]	31/31	0.95	0.20	-0.57	39,45,54,55	31
3	ATP	A	703[B]	31/31	0.97	0.14	-0.88	31,33,50,55	31
4	6R9	B	704[B]	26/26	0.90	0.16	-0.93	64,72,76,76	26
3	ATP	B	703[A]	31/31	0.93	0.13	-1.45	61,72,76,76	31
5	EDO	B	707	4/4	0.96	0.10	-	49,51,53,54	0
2	MG	C	705	1/1	0.80	0.17	-	74,74,74,74	0
2	MG	C	702[B]	1/1	0.86	0.39	-	48,48,48,48	1
2	MG	A	701[B]	1/1	0.98	0.26	-	41,41,41,41	1
2	MG	C	701[B]	1/1	0.95	0.35	-	38,38,38,38	1
6	PO4	C	706	5/5	0.91	0.14	-	78,80,81,81	0
2	MG	B	702[B]	1/1	0.87	0.62	-	66,66,66,66	1
2	MG	A	702[B]	1/1	0.76	0.15	-	49,49,49,49	1
2	MG	B	701[B]	1/1	0.95	0.38	-	34,34,34,34	1

6.5 Other polymers (i)

There are no such residues in this entry.