Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:27 AM GMT

PDB ID	:	2H92
Title	:	Crystal Structure of Staphylococcus aureus Cytidine Monophosphate Kinase in complex with cytidine-5'-monophosphate
Authors	:	Dhaliwal, B.
Deposited on	:	2006-06-08
Resolution	:	2.30 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 (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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
Clashscore		19
Ramachandran outliers		0.3%
Sidechain outliers		6.7%
RSRZ outliers		6.6%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
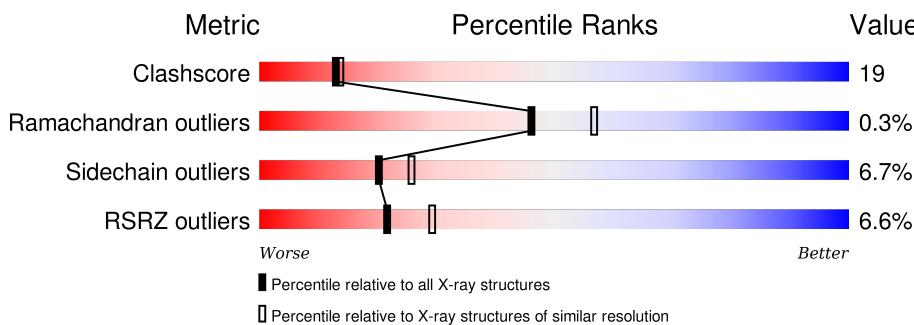
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	219	12%　　62%　　33%
1	B	219	2%　　71%　　25%
1	C	219	5%　　66%　　31%
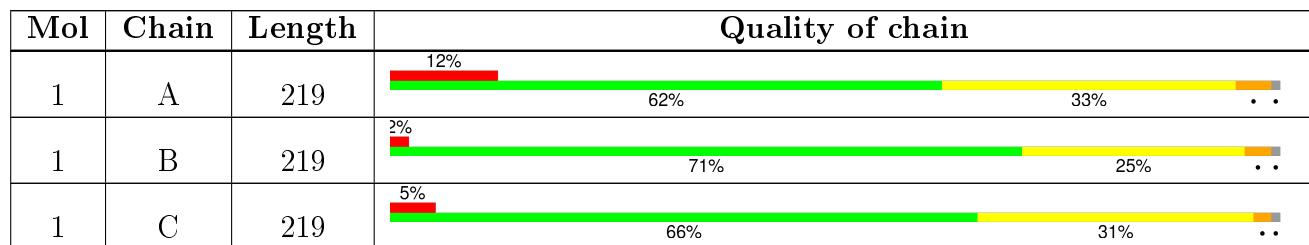
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PG4	B	1001	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5512 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 Cytidylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1696	1056	290	343	7			
1	B	216	Total	C	N	O	S	0	0	0
			1696	1056	290	343	7			
1	C	216	Total	C	N	O	S	0	0	0
			1696	1056	290	343	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
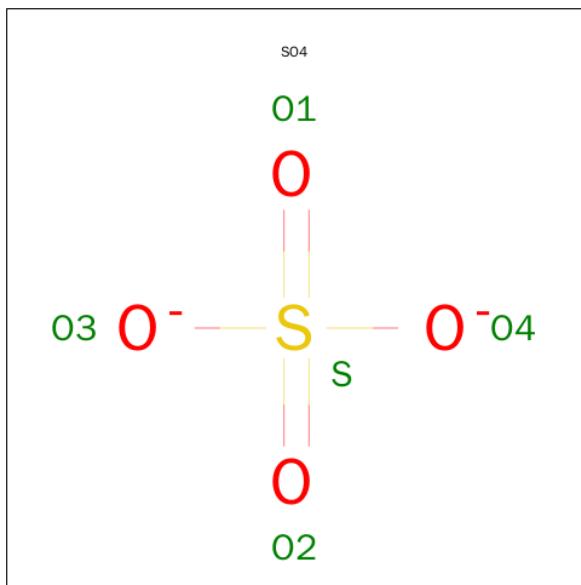
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$).
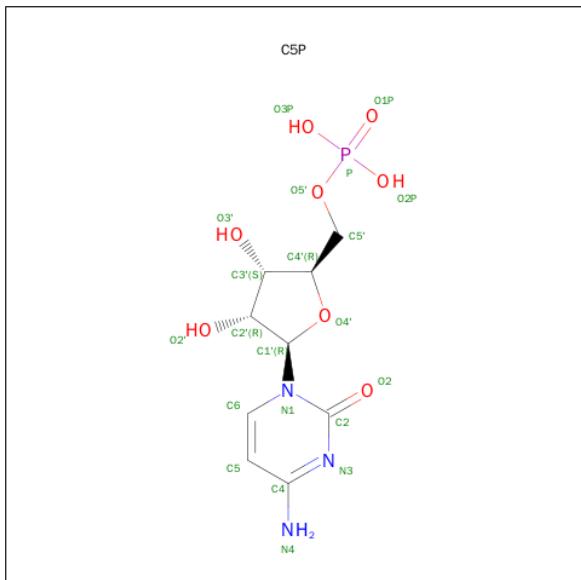
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
3	B	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
3	C	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
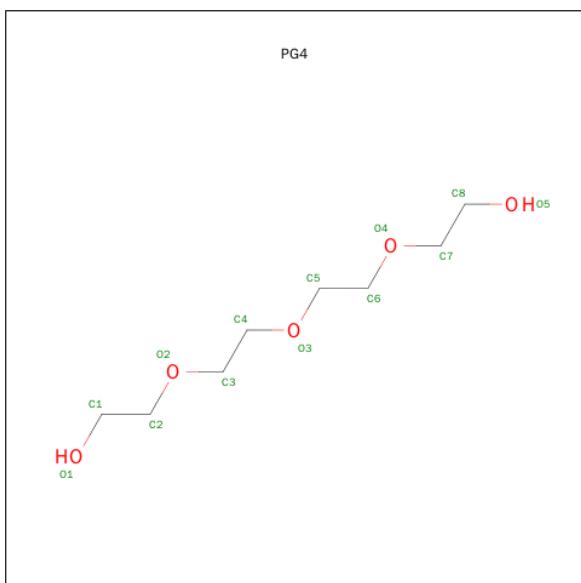
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 12	C 8	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total 92	O 92	0	0
5	B	122	Total 122	O 122	0	0
5	C	120	Total 120	O 120	0	0

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: Cytidylate kinase
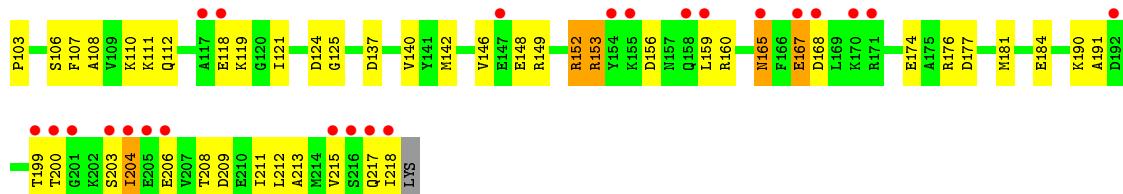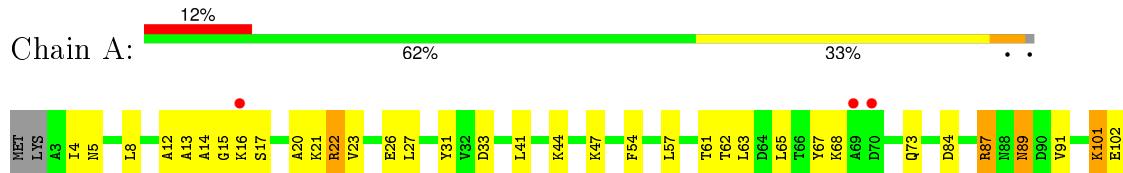
- Molecule 1: Cytidylate kinase
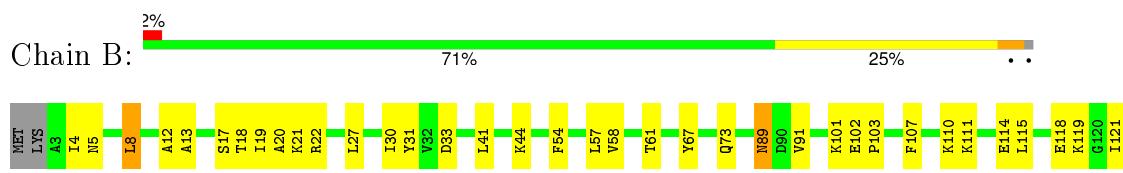
- Molecule 1: Cytidylate kinase
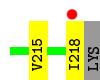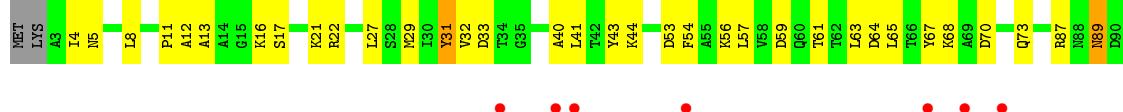
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	157.89Å 157.89Å 76.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.30) 100.0 (29.84-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.43 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.257 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 63.0	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 48267 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5512	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, 0.375 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: PG4, SO4, C5P

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	0.36	0/1713	0.61	0/2310
1	B	0.44	0/1713	0.69	0/2310
1	C	0.43	0/1713	0.66	0/2310
All	All	0.41	0/5139	0.65	0/6930

There are no bond length outliers.

There are no bond angle outliers.

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	1696	0	1709	83	0
1	B	1696	0	1709	62	0
1	C	1696	0	1709	52	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	21	0	12	1	0
3	B	21	0	12	0	0
3	C	21	0	12	1	0
4	B	12	0	15	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	92	0	0	7	0
5	B	122	0	0	2	0
5	C	120	0	0	3	0
All	All	5512	0	5178	198	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 19.

All (198) 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:22:ARG:HH12	1:C:205:GLU:HG2	1.14	1.07
1:A:149:ARG:HA	1:A:152:ARG:HD2	1.33	1.05
1:B:178:GLN:HE21	1:B:182:ASN:HD21	1.15	0.94
1:A:22:ARG:HB3	1:A:22:ARG:HH11	1.36	0.90
1:C:111:LYS:O	1:C:115:LEU:HD13	1.71	0.89
1:A:149:ARG:HA	1:A:152:ARG:CD	2.03	0.88
1:B:121:ILE:HD11	4:B:1001:PG4:H51	1.57	0.86
1:C:22:ARG:NH1	1:C:205:GLU:HG2	1.93	0.84
1:A:8:LEU:HD11	1:A:142:MET:SD	2.20	0.81
1:C:27:LEU:HD11	1:C:212:LEU:HD22	1.61	0.81
1:B:30:ILE:HD13	4:B:1001:PG4:H22	1.61	0.80
1:A:149:ARG:CA	1:A:152:ARG:HD2	2.13	0.78
1:B:30:ILE:HD12	4:B:1001:PG4:H71	1.66	0.77
1:C:198:ASP:OD2	1:C:200:THR:HG23	1.84	0.77
1:B:30:ILE:HD12	4:B:1001:PG4:H52	1.65	0.76
1:A:106:SER:O	1:A:110:LYS:HD3	1.85	0.76
1:C:203:SER:HB3	1:C:206:GLU:HG3	1.68	0.75
1:A:26:GLU:OE1	1:A:212:LEU:HD11	1.87	0.74
1:A:15:GLY:HA2	5:A:1478:HOH:O	1.87	0.74
1:B:4:ILE:HG13	1:B:137:ASP:HB2	1.70	0.73
1:B:30:ILE:HD13	4:B:1001:PG4:H41	1.69	0.73
1:B:54:PHE:CD2	1:B:101:LYS:HG2	2.26	0.71
1:C:211:ILE:O	1:C:215:VAL:HG23	1.92	0.70
1:A:176:ARG:HD3	5:A:1470:HOH:O	1.90	0.70
1:C:54:PHE:CD2	1:C:101:LYS:HG2	2.27	0.69
1:A:184:GLU:HB3	5:A:1452:HOH:O	1.92	0.69
1:C:17:SER:HB2	1:C:31:TYR:OH	1.92	0.68
1:A:4:ILE:HG13	1:A:137:ASP:HB2	1.74	0.68
1:C:33:ASP:H	1:C:73:GLN:HE22	1.40	0.68
1:A:142:MET:CE	1:A:199:THR:HG21	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HD11	1:B:212:LEU:CD2	2.24	0.68
1:B:198:ASP:OD2	1:B:200:THR:HG23	1.94	0.67
1:A:5:ASN:ND2	1:A:121:ILE:H	1.92	0.67
1:B:89:ASN:HD22	1:B:89:ASN:C	1.97	0.67
1:A:211:ILE:O	1:A:215:VAL:HG23	1.93	0.67
1:A:165:ASN:OD1	1:A:168:ASP:HB2	1.95	0.67
1:A:13:ALA:O	1:A:152:ARG:HD3	1.95	0.66
1:A:17:SER:O	1:A:21:LYS:HG3	1.95	0.66
1:C:4:ILE:HG13	1:C:137:ASP:HB2	1.78	0.66
1:B:198:ASP:OD1	1:B:200:THR:HG22	1.96	0.66
1:B:4:ILE:HG13	1:B:137:ASP:CB	2.27	0.65
1:A:22:ARG:HE	1:A:204:ILE:HD11	1.61	0.65
1:A:208:THR:O	1:A:212:LEU:HG	1.98	0.64
1:B:30:ILE:CD1	4:B:1001:PG4:H52	2.27	0.64
1:B:203:SER:HB3	1:B:206:GLU:HG3	1.80	0.64
1:A:87:ARG:HD2	5:A:1464:HOH:O	1.98	0.64
1:B:19:ILE:HG13	1:B:142:MET:HE1	1.80	0.63
1:C:27:LEU:HD11	1:C:212:LEU:CD2	2.29	0.63
1:B:198:ASP:OD1	1:B:200:THR:CG2	2.47	0.63
1:B:178:GLN:HE21	1:B:182:ASN:ND2	1.91	0.63
1:B:57:LEU:HD23	1:B:57:LEU:C	2.19	0.63
1:B:17:SER:HA	1:B:31:TYR:OH	2.00	0.61
1:B:121:ILE:CD1	4:B:1001:PG4:H51	2.28	0.61
1:C:203:SER:CB	1:C:206:GLU:HG3	2.31	0.61
1:B:143:ILE:HD11	1:B:196:THR:HG23	1.81	0.60
1:B:4:ILE:CG1	1:B:137:ASP:HB2	2.32	0.60
1:B:27:LEU:HD11	1:B:212:LEU:HD22	1.83	0.60
1:C:89:ASN:HD21	1:C:91:VAL:HB	1.67	0.60
1:C:12:ALA:O	1:C:149:ARG:HD2	2.02	0.60
1:B:30:ILE:CD1	4:B:1001:PG4:H22	2.31	0.59
1:C:31:TYR:CZ	1:C:33:ASP:HB2	2.37	0.59
1:A:22:ARG:CB	1:A:22:ARG:HH11	2.12	0.59
1:B:111:LYS:O	1:B:115:LEU:HD13	2.02	0.59
1:C:31:TYR:OH	1:C:33:ASP:HB2	2.02	0.59
1:B:30:ILE:CD1	4:B:1001:PG4:H41	2.32	0.58
1:C:33:ASP:H	1:C:73:GLN:NE2	2.01	0.58
1:B:17:SER:O	1:B:21:LYS:HG3	2.02	0.58
1:B:89:ASN:HD21	1:B:91:VAL:HB	1.68	0.58
1:A:142:MET:HE3	1:A:199:THR:HG21	1.85	0.58
1:C:68:LYS:HD2	5:C:1470:HOH:O	2.04	0.58
1:A:57:LEU:HD23	1:A:57:LEU:C	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ILE:HD13	1:C:204:ILE:O	2.04	0.57
1:C:5:ASN:ND2	1:C:119:LYS:HA	2.18	0.57
1:C:89:ASN:HD22	1:C:89:ASN:C	2.09	0.56
1:A:89:ASN:C	1:A:89:ASN:HD22	2.07	0.56
1:A:110:LYS:N	1:A:110:LYS:CD	2.68	0.56
1:B:200:THR:HG21	5:B:1507:HOH:O	2.06	0.56
1:C:5:ASN:HD21	1:C:119:LYS:HA	1.71	0.55
1:A:22:ARG:HD2	1:A:204:ILE:HG13	1.88	0.55
1:A:62:THR:HA	5:A:1418:HOH:O	2.07	0.55
1:B:89:ASN:ND2	1:B:91:VAL:H	2.04	0.55
4:B:1001:PG4:H82	5:B:1492:HOH:O	2.06	0.55
1:C:57:LEU:C	1:C:57:LEU:HD23	2.27	0.55
1:C:154:TYR:HE1	1:C:164:SER:O	1.90	0.54
1:A:4:ILE:HG13	1:A:137:ASP:CB	2.37	0.54
1:B:58:VAL:HG13	1:B:107:PHE:CD1	2.43	0.54
1:B:33:ASP:H	1:B:73:GLN:HE22	1.56	0.54
1:A:8:LEU:HD22	1:A:140:VAL:HB	1.90	0.54
1:B:110:LYS:O	1:B:114:GLU:HG3	2.08	0.53
1:A:27:LEU:HD11	1:A:212:LEU:CD2	2.39	0.53
1:A:27:LEU:HD11	1:A:212:LEU:HD22	1.91	0.53
1:A:89:ASN:HD21	1:A:91:VAL:HB	1.74	0.53
1:A:165:ASN:ND2	1:A:167:GLU:HG3	2.23	0.53
1:A:148:GLU:HG2	1:A:200:THR:HG22	1.91	0.52
1:C:4:ILE:HG13	1:C:137:ASP:CB	2.39	0.52
1:A:149:ARG:O	1:A:152:ARG:HD2	2.10	0.52
1:A:142:MET:HE2	1:A:199:THR:HG21	1.92	0.51
1:A:165:ASN:HD21	1:A:167:GLU:HG3	1.74	0.51
1:B:148:GLU:HG2	1:B:200:THR:HB	1.92	0.51
1:B:177:ASP:O	1:B:181:MET:HG3	2.11	0.51
1:C:108:ALA:O	1:C:112:GLN:HG3	2.11	0.51
1:C:169:LEU:O	1:C:173:ILE:HG13	2.12	0.50
1:C:59:ASP:HB2	5:C:1484:HOH:O	2.11	0.50
1:C:8:LEU:HD12	1:C:140:VAL:HB	1.94	0.50
1:B:178:GLN:NE2	1:B:182:ASN:HD21	1.97	0.50
1:B:13:ALA:HA	1:B:153:ARG:NH2	2.27	0.50
1:B:4:ILE:HG13	1:B:137:ASP:CG	2.31	0.50
1:C:44:LYS:NZ	1:C:61:THR:OG1	2.42	0.49
1:B:5:ASN:ND2	1:B:119:LYS:HA	2.27	0.49
1:A:54:PHE:CD2	1:A:101:LYS:HG2	2.48	0.49
1:A:209:ASP:HA	1:A:212:LEU:HD12	1.95	0.49
1:C:33:ASP:N	1:C:73:GLN:HE22	2.08	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:CG	1:B:200:THR:HG23	2.33	0.49
1:A:152:ARG:HG2	1:A:153:ARG:N	2.27	0.48
1:A:12:ALA:O	1:A:149:ARG:HD2	2.12	0.48
1:B:151:GLU:HA	1:B:166:PHE:HE1	1.78	0.48
1:C:156:ASP:OD2	1:C:160:ARG:HD3	2.13	0.48
1:A:27:LEU:N	1:A:27:LEU:HD12	2.29	0.48
1:B:44:LYS:NZ	1:B:61:THR:OG1	2.47	0.48
1:B:33:ASP:H	1:B:73:GLN:NE2	2.12	0.47
1:A:47:LYS:HE3	5:A:1423:HOH:O	2.14	0.47
1:A:8:LEU:O	1:A:124:ASP:HA	2.14	0.47
1:B:102:GLU:HB3	1:B:103:PRO:HD3	1.95	0.47
1:A:107:PHE:CZ	1:A:111:LYS:HE3	2.50	0.47
1:C:8:LEU:O	1:C:124:ASP:HA	2.14	0.47
1:A:20:ALA:HB1	1:A:31:TYR:CD1	2.50	0.47
1:B:8:LEU:O	1:B:124:ASP:HA	2.13	0.47
1:A:102:GLU:HB3	1:A:103:PRO:HD3	1.97	0.47
1:C:208:THR:O	1:C:212:LEU:HG	2.15	0.47
1:C:53:ASP:OD1	1:C:56:LYS:HE2	2.16	0.46
1:A:110:LYS:HD3	1:A:110:LYS:H	1.80	0.46
1:C:4:ILE:O	1:C:29:MET:HE3	2.16	0.46
1:A:14:ALA:C	1:A:152:ARG:HH12	2.19	0.46
1:B:4:ILE:HG12	1:B:5:ASN:N	2.30	0.46
1:A:165:ASN:HD21	1:A:167:GLU:CD	2.18	0.46
1:B:89:ASN:ND2	1:B:89:ASN:C	2.66	0.46
1:A:165:ASN:HD21	1:A:167:GLU:CG	2.28	0.46
1:C:5:ASN:ND2	1:C:121:ILE:H	2.14	0.45
1:B:107:PHE:CZ	1:B:111:LYS:HE2	2.52	0.45
1:B:154:TYR:O	1:B:158:GLN:HG2	2.16	0.45
1:B:5:ASN:HA	1:B:5:ASN:HD22	1.63	0.45
1:A:165:ASN:OD1	1:A:168:ASP:N	2.41	0.45
1:B:5:ASN:HD21	1:B:119:LYS:HA	1.82	0.45
1:B:20:ALA:HB3	1:B:31:TYR:CE1	2.51	0.45
1:A:84:ASP:OD2	1:A:84:ASP:O	2.35	0.45
1:A:27:LEU:N	1:A:27:LEU:CD1	2.80	0.45
1:A:26:GLU:OE1	1:A:212:LEU:CD1	2.63	0.45
1:A:142:MET:HE3	1:A:199:THR:CG2	2.46	0.45
1:C:13:ALA:O	1:C:149:ARG:HG2	2.16	0.45
1:A:203:SER:HB3	1:A:206:GLU:HG3	1.98	0.45
1:B:5:ASN:ND2	1:B:121:ILE:H	2.15	0.45
1:A:125:GLY:HA3	3:A:1300:C5P:HN42	1.81	0.45
1:C:4:ILE:CG1	1:C:137:ASP:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:HE	1:A:204:ILE:CD1	2.29	0.44
1:A:5:ASN:HA	1:A:5:ASN:HD22	1.56	0.44
1:A:14:ALA:C	1:A:152:ARG:NH1	2.71	0.44
1:B:18:THR:CG2	1:B:204:ILE:HD12	2.48	0.44
1:A:110:LYS:HD3	1:A:110:LYS:N	2.33	0.44
1:C:116:ALA:HA	1:C:121:ILE:HG13	2.00	0.44
1:C:63:LEU:HD23	1:C:64:ASP:N	2.32	0.44
1:B:197:LEU:C	1:B:197:LEU:HD23	2.38	0.44
1:A:165:ASN:ND2	1:A:167:GLU:OE2	2.43	0.43
1:A:31:TYR:CZ	1:A:33:ASP:HB2	2.54	0.43
1:A:149:ARG:C	1:A:152:ARG:HD2	2.38	0.43
1:A:108:ALA:O	1:A:112:GLN:HG3	2.18	0.43
1:C:21:LYS:HE3	1:C:21:LYS:HB2	1.80	0.43
1:A:17:SER:HA	1:A:31:TYR:OH	2.19	0.43
1:B:12:ALA:HB3	1:B:173:ILE:HG23	1.99	0.43
1:A:33:ASP:H	1:A:73:GLN:HE22	1.67	0.43
1:C:190:LYS:HG2	1:C:191:ALA:O	2.17	0.43
1:A:44:LYS:NZ	1:A:61:THR:OG1	2.49	0.43
1:A:67:TYR:CD1	1:A:67:TYR:N	2.86	0.43
1:A:26:GLU:C	1:A:27:LEU:HD12	2.39	0.42
1:A:4:ILE:HG12	1:A:5:ASN:N	2.34	0.42
1:C:27:LEU:CD1	1:C:27:LEU:N	2.82	0.42
1:A:146:VAL:HG21	1:A:174:GLU:OE2	2.19	0.42
1:A:68:LYS:HE2	5:A:1480:HOH:O	2.19	0.42
1:B:169:LEU:HD12	1:B:169:LEU:HA	1.91	0.42
1:A:22:ARG:HD3	1:A:208:THR:OG1	2.20	0.42
1:C:176:ARG:NH2	3:C:1302:C5P:O3P	2.51	0.42
1:A:213:ALA:O	1:A:217:GLN:HG3	2.20	0.42
1:C:87:ARG:NH1	5:C:1495:HOH:O	2.51	0.42
1:C:40:ALA:O	1:C:43:TYR:HB3	2.20	0.42
1:A:5:ASN:HD22	1:A:121:ILE:H	1.63	0.41
1:A:156:ASP:OD2	1:A:160:ARG:NH1	2.48	0.41
1:B:17:SER:HA	1:B:31:TYR:CZ	2.55	0.41
1:C:5:ASN:HA	1:C:5:ASN:HD22	1.67	0.41
1:A:5:ASN:ND2	1:A:119:LYS:HA	2.36	0.41
1:C:22:ARG:NH1	1:C:205:GLU:CG	2.76	0.41
1:C:32:VAL:HG22	1:C:67:TYR:OH	2.21	0.41
1:A:190:LYS:HG2	1:A:191:ALA:O	2.21	0.41
1:A:23:VAL:CG2	1:A:208:THR:HG23	2.51	0.41
1:B:27:LEU:CD1	1:B:212:LEU:CD2	2.97	0.41
1:A:33:ASP:H	1:A:73:GLN:NE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TYR:CD1	1:B:67:TYR:N	2.90	0.40
1:A:177:ASP:O	1:A:181:MET:HG3	2.21	0.40
1:B:22:ARG:HB3	1:B:22:ARG:HE	1.71	0.40
1:C:204:ILE:HD13	1:C:204:ILE:C	2.41	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)
4:B:1001:PG4:C1	4:B:1001:PG4:C1[4_675]	2.13	0.07

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	214/219 (98%)	205 (96%)	8 (4%)	1 (0%)	34	41
1	B	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
1	C	214/219 (98%)	206 (96%)	7 (3%)	1 (0%)	34	41
All	All	642/657 (98%)	618 (96%)	22 (3%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	16	LYS
1	A	16	LYS

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	185/188 (98%)	170 (92%)	15 (8%)	15	18
1	B	185/188 (98%)	176 (95%)	9 (5%)	31	41
1	C	185/188 (98%)	172 (93%)	13 (7%)	19	23
All	All	555/564 (98%)	518 (93%)	37 (7%)	20	26

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	41	LEU
1	A	63	LEU
1	A	65	LEU
1	A	87	ARG
1	A	89	ASN
1	A	101	LYS
1	A	118	GLU
1	A	152	ARG
1	A	153	ARG
1	A	159	LEU
1	A	165	ASN
1	A	167	GLU
1	A	204	ILE
1	A	218	ILE
1	B	8	LEU
1	B	41	LEU
1	B	89	ASN
1	B	118	GLU
1	B	143	ILE
1	B	189	ARG
1	B	200	THR
1	B	203	SER
1	B	204	ILE
1	C	11	PRO
1	C	31	TYR
1	C	41	LEU
1	C	65	LEU
1	C	70	ASP
1	C	89	ASN

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Mol	Chain	Res	Type
1	C	118	GLU
1	C	155	LYS
1	C	171	ARG
1	C	197	LEU
1	C	203	SER
1	C	204	ILE
1	C	218	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	60	GLN
1	A	73	GLN
1	A	89	ASN
1	A	93	GLN
1	A	157	ASN
1	A	158	GLN
1	A	182	ASN
1	A	217	GLN
1	B	5	ASN
1	B	73	GLN
1	B	79	ASN
1	B	89	ASN
1	B	93	GLN
1	B	157	ASN
1	B	158	GLN
1	B	165	ASN
1	B	182	ASN
1	C	5	ASN
1	C	73	GLN
1	C	79	ASN
1	C	89	ASN
1	C	93	GLN
1	C	157	ASN
1	C	158	GLN
1	C	165	ASN
1	C	178	GLN
1	C	182	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)

7 ligands are modelled in this entry.

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	C5P	A	1300	-	17,22,22	1.55	1 (5%)	22,33,33	1.24	1 (4%)
2	SO4	A	1400	-	4,4,4	0.24	0	6,6,6	0.12	0
4	PG4	B	1001	-	11,11,12	0.59	0	10,10,11	0.56	0
3	C5P	B	1301	-	17,22,22	1.64	2 (11%)	22,33,33	1.21	1 (4%)
2	SO4	B	1401	-	4,4,4	0.28	0	6,6,6	0.08	0
3	C5P	C	1302	-	17,22,22	1.56	2 (11%)	22,33,33	1.22	1 (4%)
2	SO4	C	1402	-	4,4,4	0.29	0	6,6,6	0.15	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	C5P	A	1300	-	-	0/6/26/26	0/2/2/2
2	SO4	A	1400	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	B	1001	-	-	0/9/9/10	0/0/0/0
3	C5P	B	1301	-	-	0/6/26/26	0/2/2/2
2	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
3	C5P	C	1302	-	-	0/6/26/26	0/2/2/2
2	SO4	C	1402	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	C5P	C5-C4	2.17	1.45	1.40
3	C	1302	C5P	C5-C4	2.22	1.46	1.40
3	A	1300	C5P	C6-N1	5.23	1.43	1.35
3	B	1301	C5P	C6-N1	5.41	1.43	1.35
3	C	1302	C5P	C6-N1	5.48	1.43	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1300	C5P	C2-N3-C4	4.08	121.37	115.61
3	B	1301	C5P	C2-N3-C4	4.23	121.58	115.61
3	C	1302	C5P	C2-N3-C4	4.63	122.14	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1300	C5P	1	0
4	B	1001	PG4	10	1
3	C	1302	C5P	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	216/219 (98%)	0.44	27 (12%)	5	8	17, 49, 102, 119	0
1	B	216/219 (98%)	-0.09	4 (1%)	70	76	13, 31, 64, 98	0
1	C	216/219 (98%)	0.10	12 (5%)	28	36	16, 32, 69, 93	0
All	All	648/657 (98%)	0.15	43 (6%)	22	29	13, 36, 84, 119	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	GLY	6.4
1	A	218	ILE	5.8
1	A	204	ILE	4.6
1	A	159	LEU	4.2
1	C	159	LEU	4.1
1	B	159	LEU	4.0
1	C	171	ARG	3.8
1	A	167	GLU	3.6
1	A	199	THR	3.4
1	C	160	ARG	3.4
1	B	218	ILE	3.3
1	A	216	SER	3.3
1	A	170	LYS	3.2
1	B	158	GLN	3.1
1	A	171	ARG	3.0
1	A	192	ASP	3.0
1	C	205	GLU	3.0
1	A	117	ALA	2.9
1	A	168	ASP	2.8
1	A	203	SER	2.8
1	B	155	LYS	2.7
1	A	217	GLN	2.7
1	A	205	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	206	GLU	2.7
1	A	70	ASP	2.7
1	C	155	LYS	2.7
1	A	147	GLU	2.6
1	A	154	TYR	2.5
1	A	155	LYS	2.5
1	A	165	ASN	2.5
1	A	69	ALA	2.5
1	C	201	GLY	2.4
1	C	14	ALA	2.4
1	C	218	ILE	2.4
1	A	158	GLN	2.4
1	C	203	SER	2.3
1	A	215	VAL	2.2
1	C	35	GLY	2.1
1	A	200	THR	2.1
1	C	34	THR	2.1
1	A	118	GLU	2.1
1	A	16	LYS	2.1
1	C	8	LEU	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
4	PG4	B	1001	12/13	0.90	0.15	1.00	14,58,79,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	SO4	C	1402	5/5	0.89	0.24	0.81	54,69,91,111	0
3	C5P	A	1300	21/21	0.98	0.20	0.58	22,26,38,41	0
3	C5P	C	1302	21/21	0.98	0.21	0.57	15,22,31,33	0
3	C5P	B	1301	21/21	0.99	0.17	0.15	4,19,23,32	0
2	SO4	A	1400	5/5	0.97	0.18	-0.03	54,73,84,106	0
2	SO4	B	1401	5/5	0.99	0.15	-0.57	39,43,45,71	0

6.5 Other polymers (i)

There are no such residues in this entry.