



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:52 PM GMT

PDB ID : 1VH3
Title : Crystal structure of CMP-KDO synthetase
Authors : Structural GenomiX
Deposited on : 2003-12-01
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

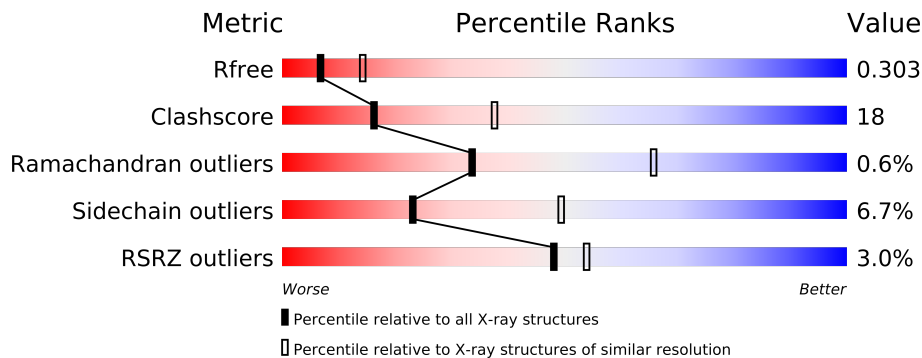
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	262	
1	B	262	
1	C	262	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CMK	B	263[A]	-	X
2	CMK	B	263[B]	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5485 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-deoxy-manno-octulosonatecytidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	Se	0	0	0
			1653	1056	281	311	1	4			
1	B	246	Total	C	N	O	S	Se	0	0	0
			1864	1187	320	352	1	4			
1	C	238	Total	C	N	O	S	Se	0	1	0
			1766	1129	300	333	1	3			

There are 39 discrepancies between the modelled and reference sequences:

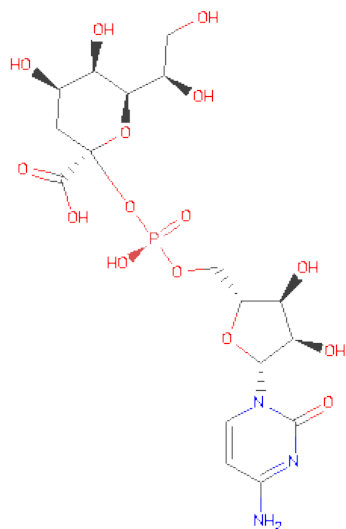
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP P44490
A	29	MSE	MET	modified residue	UNP P44490
A	67	MSE	MET	modified residue	UNP P44490
A	123	MSE	MET	modified residue	UNP P44490
A	168	MSE	MET	modified residue	UNP P44490
A	255	GLY	-	cloning artifact	UNP P44490
A	256	SER	-	cloning artifact	UNP P44490
A	257	HIS	-	cloning artifact	UNP P44490
A	258	HIS	-	cloning artifact	UNP P44490
A	259	HIS	-	cloning artifact	UNP P44490
A	260	HIS	-	cloning artifact	UNP P44490
A	261	HIS	-	cloning artifact	UNP P44490
A	262	HIS	-	cloning artifact	UNP P44490
B	1	MSE	-	cloning artifact	UNP P44490
B	29	MSE	MET	modified residue	UNP P44490
B	67	MSE	MET	modified residue	UNP P44490
B	123	MSE	MET	modified residue	UNP P44490
B	168	MSE	MET	modified residue	UNP P44490
B	255	GLY	-	cloning artifact	UNP P44490
B	256	SER	-	cloning artifact	UNP P44490
B	257	HIS	-	cloning artifact	UNP P44490
B	258	HIS	-	cloning artifact	UNP P44490
B	259	HIS	-	cloning artifact	UNP P44490

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Chain	Residue	Modelled	Actual	Comment	Reference
B	260	HIS	-	cloning artifact	UNP P44490
B	261	HIS	-	cloning artifact	UNP P44490
B	262	HIS	-	cloning artifact	UNP P44490
C	1	MSE	-	cloning artifact	UNP P44490
C	29	MSE	MET	modified residue	UNP P44490
C	67	MSE	MET	modified residue	UNP P44490
C	123	MSE	MET	modified residue	UNP P44490
C	168	MSE	MET	modified residue	UNP P44490
C	255	GLY	-	cloning artifact	UNP P44490
C	256	SER	-	cloning artifact	UNP P44490
C	257	HIS	-	cloning artifact	UNP P44490
C	258	HIS	-	cloning artifact	UNP P44490
C	259	HIS	-	cloning artifact	UNP P44490
C	260	HIS	-	cloning artifact	UNP P44490
C	261	HIS	-	cloning artifact	UNP P44490
C	262	HIS	-	cloning artifact	UNP P44490

- Molecule 2 is CYTIDINE 5'-MONOPHOSPHATE 3-DEOXY-BETA-D-GULO-OCT-2-UL O-PYRANOSONICACID (three-letter code: CMK) (formula: C₁₇H₂₆N₃O₁₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	17	3	15	1		
2	B	1	Total	C	N	O	P	0	1
			72	34	6	30	2		

- Molecule 3 is water.

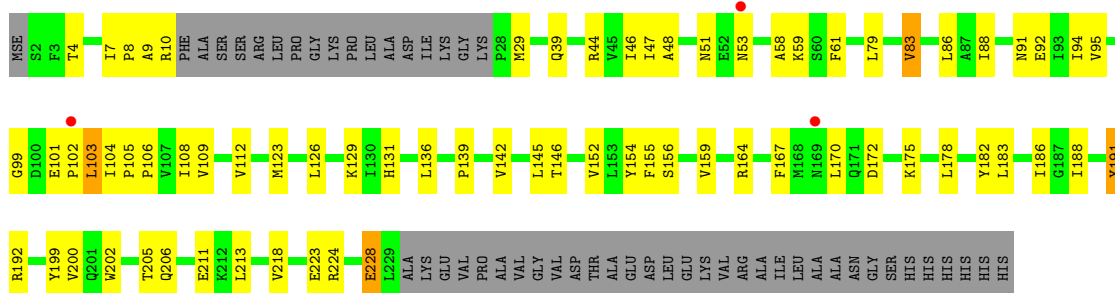
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	29	Total 29	O 29	0	0
3	C	20	Total 20	O 20	0	0

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.

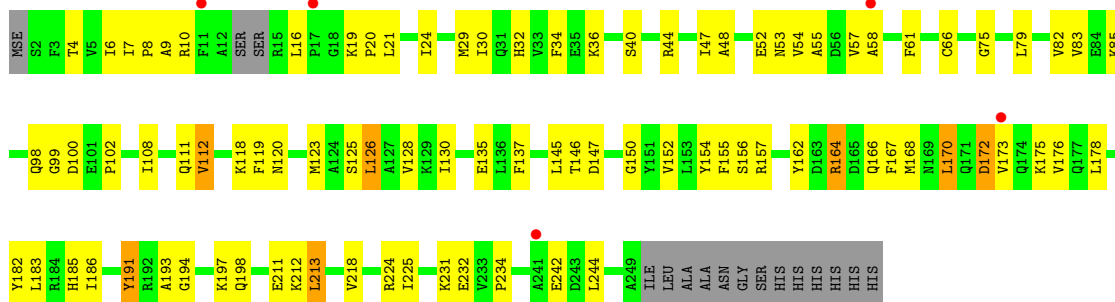
- Molecule 1: 3-deoxy-manno-octulosonatecytidyltransferase

Chain A: 



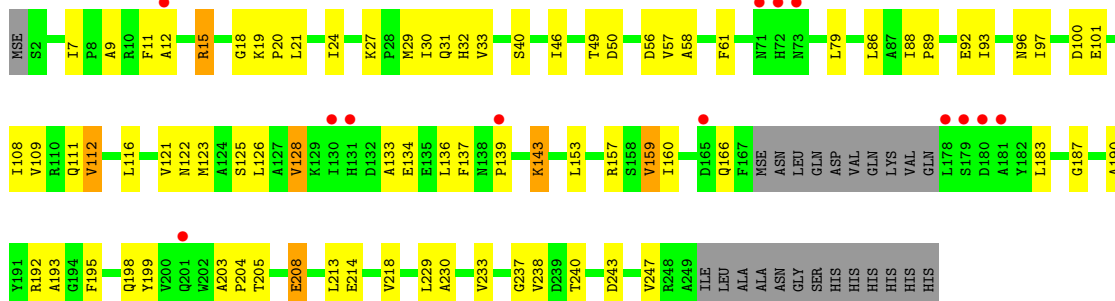
- Molecule 1: 3-deoxy-manno-octulosonatecytidyltransferase

Chain B: 



- Molecule 1: 3-deoxy-manno-octulosonatecytidyltransferase

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.48Å 48.28Å 96.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.70 19.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.95-2.70) 96.6 (19.95-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.27 (at 2.71Å)	Xtriage
Refinement program	REFMAC 4	Depositor
R, R_{free}	0.256 , 0.307 0.259 , 0.303	Depositor DCC
R_{free} test set	1162 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22724 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5485	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CMK

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	0.52	0/1679	0.93	1/2277 (0.0%)
1	B	0.48	0/1894	0.82	0/2567
1	C	0.45	0/1801	0.82	2/2453 (0.1%)
All	All	0.48	0/5374	0.86	3/7297 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LEU	CA-CB-CG	6.69	130.68	115.30
1	C	12	ALA	CA-C-N	-5.44	105.24	117.20
1	C	56	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1653	0	1637	54	0
1	B	1864	0	1817	76	0
1	C	1766	0	1709	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	24	2	0
2	B	72	0	48	18	0
3	A	45	0	0	3	0
3	B	29	0	0	1	0
3	C	20	0	0	0	0
All	All	5485	0	5235	193	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (193) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:123:MSE:HE1	1:C:218:VAL:HG21	1.31	1.09
1:A:172:ASP:HB3	1:A:175:LYS:HG3	1.51	0.92
1:B:157:ARG:HH22	2:B:263[B]:CMK:H7	1.42	0.83
1:A:139:PRO:HB2	1:B:168:MSE:HE2	1.59	0.83
1:C:123:MSE:HE2	1:C:195:PHE:HE2	1.44	0.82
1:A:105:PRO:HD2	1:A:108:ILE:HD13	1.63	0.80
1:B:8:PRO:HB2	2:B:263[B]:CMK:H1'	1.64	0.80
1:A:8:PRO:HB2	2:A:263:CMK:H1'	1.66	0.77
1:C:128:VAL:HG21	1:C:233:VAL:HG22	1.67	0.77
1:B:8:PRO:HB2	2:B:263[A]:CMK:H1'	1.69	0.75
1:A:4:THR:HG23	1:A:44:ARG:HB3	1.69	0.75
1:A:104:ILE:HG23	1:A:108:ILE:HD11	1.67	0.75
1:C:93:ILE:HG23	1:C:116:LEU:HD22	1.69	0.73
1:C:123:MSE:HE2	1:C:195:PHE:CE2	2.26	0.69
2:B:263[B]:CMK:O1Y	2:B:263[B]:CMK:H6	1.94	0.67
1:C:205:THR:HG22	1:C:208:GLU:H	1.60	0.67
1:C:143:LYS:H	1:C:143:LYS:HD2	1.59	0.66
1:C:79:LEU:HD21	1:C:96:ASN:ND2	2.10	0.66
1:B:164:ARG:HG2	1:B:168:MSE:HE3	1.78	0.66
1:C:19:LYS:HE3	1:C:238:VAL:O	1.96	0.65
1:B:167:PHE:HA	1:B:170:LEU:HD22	1.78	0.64
1:C:123:MSE:HE1	1:C:218:VAL:CG2	2.19	0.64
1:A:105:PRO:O	1:A:108:ILE:HG12	1.98	0.64
1:A:112:VAL:CG1	1:A:126:LEU:HD13	2.28	0.64
1:B:19:LYS:HG2	1:B:20:PRO:HD3	1.79	0.63
3:A:265:HOH:O	1:B:168:MSE:HE1	1.97	0.63
1:C:139:PRO:O	1:C:157:ARG:HD2	1.98	0.63
1:B:166:GLN:O	1:B:170:LEU:HB3	1.99	0.62
1:C:208:GLU:HG3	1:C:214:GLU:HA	1.81	0.62
1:B:83:VAL:HG11	1:B:193:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:11:PHE:HD2	1:C:20:PRO:HG2	1.65	0.62
1:B:58:ALA:HA	1:B:61:PHE:CE1	2.35	0.61
1:A:104:ILE:HD11	1:A:188:ILE:HD11	1.81	0.61
1:B:172:ASP:HB3	1:B:175:LYS:HB2	1.81	0.61
1:C:143:LYS:N	1:C:143:LYS:HD2	2.16	0.60
1:A:136:LEU:HD11	1:A:182:TYR:CG	2.36	0.60
1:A:211:GLU:HG2	1:B:162:TYR:O	2.01	0.60
1:B:9:ALA:HB2	1:B:30:ILE:HD13	1.85	0.58
1:B:232:GLU:O	1:B:234:PRO:HD3	2.04	0.57
1:B:112:VAL:HG13	1:B:126:LEU:HD22	1.86	0.57
1:C:11:PHE:HA	1:C:20:PRO:CG	2.35	0.57
1:B:178:LEU:HD22	1:B:182:TYR:CE1	2.40	0.56
1:A:108:ILE:HB	1:A:126:LEU:HD21	1.88	0.56
1:A:145:LEU:HD12	1:A:146:THR:N	2.21	0.56
1:C:58:ALA:HA	1:C:61:PHE:CE1	2.41	0.55
1:B:146:THR:CG2	1:B:150:GLY:HA2	2.36	0.55
1:B:154:TYR:CE2	1:B:156:SER:HB2	2.41	0.55
1:A:46:ILE:HD13	1:A:86:LEU:HD12	1.88	0.55
1:B:186:ILE:HD13	1:B:234:PRO:HG2	1.89	0.55
1:B:194:GLY:HA2	1:B:197:LYS:HE2	1.89	0.54
1:C:9:ALA:HB3	1:C:49:THR:HB	1.90	0.54
1:C:123:MSE:CE	1:C:218:VAL:HG11	2.38	0.54
1:C:123:MSE:HE3	1:C:218:VAL:HG11	1.90	0.54
1:A:186:ILE:HG22	1:A:188:ILE:HD12	1.90	0.54
1:B:111:GLN:HG3	1:B:231:LYS:HE3	1.91	0.53
1:C:203:ALA:HB1	1:C:204:PRO:HD2	1.89	0.53
1:A:167:PHE:HA	1:A:170:LEU:HB2	1.91	0.53
1:B:19:LYS:N	1:B:20:PRO:CD	2.71	0.53
1:A:164:ARG:HH22	2:B:263[B]:CMK:H6	1.73	0.53
1:C:108:ILE:O	1:C:112:VAL:HG23	2.09	0.53
1:A:95:VAL:HG11	1:A:109:VAL:HG13	1.91	0.53
1:C:93:ILE:HG12	1:C:116:LEU:HD23	1.91	0.52
1:B:185:HIS:ND1	2:B:263[A]:CMK:C7	2.73	0.52
1:C:21:LEU:HD22	1:C:57:VAL:HG21	1.92	0.52
1:A:101:GLU:OE2	1:A:102:PRO:HD2	2.10	0.52
1:B:137:PHE:HE2	1:B:173:VAL:HG13	1.73	0.51
1:A:123:MSE:HE2	1:A:191:TYR:CE1	2.45	0.51
1:C:27:LYS:HD3	1:C:31:GLN:NE2	2.25	0.51
1:C:19:LYS:HE2	1:C:100:ASP:HB3	1.93	0.51
1:B:173:VAL:HA	1:B:176:VAL:HG23	1.91	0.51
1:A:104:ILE:CD1	1:A:188:ILE:HD11	2.39	0.51
1:B:100:ASP:O	1:B:102:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:263[B]:CMK:O1Y	2:B:263[B]:CMK:C6	2.57	0.51
1:B:98:GLN:CG	2:B:263[B]:CMK:H4'	2.41	0.50
1:C:238:VAL:HG21	1:C:247:VAL:HG21	1.94	0.50
1:B:146:THR:HG21	1:B:150:GLY:HA2	1.94	0.50
1:C:11:PHE:HA	1:C:20:PRO:CD	2.42	0.50
1:B:170:LEU:CD1	1:B:176:VAL:HG22	2.41	0.50
1:B:16:LEU:O	1:B:19:LYS:HB3	2.12	0.50
1:B:130:ILE:HG12	1:B:135:GLU:OE2	2.11	0.50
1:B:211:GLU:HB3	1:B:213:LEU:HD22	1.94	0.50
1:A:7:ILE:HD12	1:A:47:ILE:CD1	2.42	0.50
1:B:83:VAL:CG1	1:B:193:ALA:HB1	2.41	0.50
1:C:88:ILE:HG23	1:C:89:PRO:HD2	1.93	0.50
1:B:29:MSE:HE3	1:B:99:GLY:O	2.11	0.50
1:C:11:PHE:HA	1:C:20:PRO:HG2	1.94	0.50
1:C:243:ASP:O	1:C:247:VAL:HG23	2.11	0.50
1:C:238:VAL:CG2	1:C:247:VAL:HG21	2.41	0.50
1:B:4:THR:HG23	1:B:44:ARG:HB3	1.94	0.50
1:C:108:ILE:HA	1:C:111:GLN:HB3	1.94	0.49
1:B:213:LEU:HD12	2:B:263[A]:CMK:H4	1.94	0.49
1:C:229:LEU:HD13	1:C:230:ALA:O	2.12	0.49
1:C:40:SER:HB2	1:C:109:VAL:HB	1.94	0.49
1:A:139:PRO:CB	1:B:168:MSE:HE2	2.37	0.48
1:C:125:SER:OG	1:C:126:LEU:N	2.46	0.48
1:A:152:VAL:HG11	1:A:155:PHE:CE1	2.47	0.48
1:C:24:ILE:CD1	1:C:29:MSE:HG3	2.43	0.48
1:B:185:HIS:ND1	2:B:263[A]:CMK:O7	2.36	0.48
1:C:137:PHE:O	1:C:139:PRO:HD3	2.12	0.48
1:A:136:LEU:HG	1:A:159:VAL:HG23	1.95	0.48
1:A:112:VAL:HG12	1:A:126:LEU:HD13	1.95	0.48
1:B:29:MSE:O	1:B:32:HIS:HB2	2.14	0.48
1:C:24:ILE:HB	1:C:32:HIS:NE2	2.28	0.48
1:A:92:GLU:O	1:A:192:ARG:HA	2.14	0.48
1:B:6:ILE:HB	1:B:79:LEU:HD13	1.95	0.47
1:B:112:VAL:HG22	1:B:126:LEU:CD2	2.43	0.47
1:C:122:ASN:OD1	1:C:192:ARG:HG3	2.15	0.47
1:B:172:ASP:CB	1:B:175:LYS:HB2	2.44	0.47
1:C:11:PHE:CE2	1:C:18:GLY:HA2	2.49	0.47
1:A:136:LEU:HD11	1:A:182:TYR:CD2	2.49	0.47
1:B:98:GLN:HG2	2:B:263[B]:CMK:H4'	1.96	0.47
1:A:192:ARG:HG3	3:A:272:HOH:O	2.14	0.47
1:B:120:ASN:HB3	1:B:224:ARG:HH21	1.80	0.47
1:A:154:TYR:CE2	1:A:156:SER:HB2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:LEU:O	1:A:83:VAL:HG13	2.15	0.46
1:C:15:ARG:HB3	1:C:240:THR:HG22	1.97	0.46
1:A:126:LEU:HD12	1:A:228:GLU:HB3	1.97	0.46
1:C:24:ILE:HB	1:C:32:HIS:CD2	2.51	0.46
1:C:58:ALA:HA	1:C:61:PHE:CZ	2.50	0.46
1:C:46:ILE:HD13	1:C:86:LEU:HD23	1.98	0.46
1:A:46:ILE:HD13	1:A:86:LEU:CD1	2.46	0.46
1:C:160:ILE:O	1:C:160:ILE:HG13	2.15	0.46
1:B:183:LEU:HG	3:B:275:HOH:O	2.16	0.46
1:B:52:GLU:O	1:B:53:ASN:C	2.54	0.46
1:C:97:ILE:HD11	1:C:109:VAL:HG11	1.96	0.46
1:C:203:ALA:HB1	1:C:204:PRO:CD	2.46	0.46
1:A:123:MSE:HE2	1:A:191:TYR:HE1	1.81	0.46
1:A:101:GLU:HA	1:A:102:PRO:HD2	1.62	0.45
1:A:105:PRO:HD2	1:A:108:ILE:CD1	2.42	0.45
1:A:58:ALA:HA	1:A:61:PHE:CE1	2.52	0.45
1:C:89:PRO:O	1:C:193:ALA:HB3	2.17	0.45
1:B:211:GLU:O	1:B:212:LYS:HB2	2.17	0.45
1:A:9:ALA:N	1:A:48:ALA:O	2.45	0.45
1:C:19:LYS:N	1:C:20:PRO:HD2	2.32	0.45
1:B:75:GLY:O	1:B:79:LEU:HG	2.16	0.45
1:B:7:ILE:HA	1:B:8:PRO:HD3	1.81	0.44
1:B:118:LYS:HE2	1:B:119:PHE:CE1	2.52	0.44
1:B:66:CYS:SG	1:B:85:LYS:HD3	2.57	0.44
1:B:112:VAL:CG1	1:B:126:LEU:HD22	2.47	0.44
1:C:24:ILE:HD11	1:C:29:MSE:HG3	1.99	0.44
2:B:263[B]:CMK:H6C	2:B:263[B]:CMK:H5'2	1.99	0.44
2:B:263[A]:CMK:H4	2:B:263[A]:CMK:O1Y	2.17	0.44
1:C:89:PRO:HG2	1:C:92:GLU:HB2	1.99	0.44
1:A:51:ASN:OD1	1:A:53:ASN:HB2	2.18	0.44
1:A:39:GLN:HB3	1:A:106:PRO:HG2	1.98	0.44
1:B:19:LYS:N	1:B:20:PRO:HD2	2.33	0.44
1:B:19:LYS:CG	1:B:20:PRO:HD3	2.47	0.43
1:B:152:VAL:HG11	1:B:155:PHE:CE1	2.54	0.43
1:C:46:ILE:HD13	1:C:86:LEU:CD2	2.49	0.43
1:A:205:THR:HG22	1:A:206:GLN:N	2.33	0.43
1:B:54:VAL:O	1:B:55:ALA:C	2.57	0.43
1:B:185:HIS:ND1	2:B:263[A]:CMK:H7	2.34	0.43
1:C:19:LYS:N	1:C:20:PRO:CD	2.82	0.43
1:B:48:ALA:HB2	1:B:82:VAL:HG21	2.00	0.43
1:C:7:ILE:HD13	1:C:33:VAL:HG12	2.01	0.43
2:B:263[B]:CMK:H6C	2:B:263[B]:CMK:C5'	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:LEU:CD1	1:A:228:GLU:HB3	2.49	0.42
1:A:88:ILE:HG21	1:A:94:ILE:HD11	2.01	0.42
1:A:218:VAL:CG1	1:A:223:GLU:HB3	2.49	0.42
1:A:199:TYR:HA	1:A:202:TRP:CE3	2.54	0.42
1:B:128:VAL:CG1	1:B:234:PRO:HD2	2.49	0.42
2:A:263:CMK:H6C	2:A:263:CMK:H5'1	2.00	0.42
1:B:125:SER:O	1:B:126:LEU:HD13	2.20	0.42
1:A:142:VAL:HG21	1:A:213:LEU:HD11	2.02	0.42
1:B:108:ILE:HD13	1:B:234:PRO:HG3	2.01	0.42
1:B:146:THR:HG23	1:B:150:GLY:HA2	2.00	0.42
1:A:7:ILE:HB	1:A:47:ILE:HD12	2.02	0.42
1:A:29:MSE:HB3	3:A:282:HOH:O	2.20	0.42
1:A:91:ASN:HD21	1:A:192:ARG:NH1	2.17	0.42
1:C:123:MSE:HA	1:C:190:ALA:O	2.20	0.42
1:B:157:ARG:NH2	2:B:263[B]:CMK:H5	2.35	0.42
1:B:146:THR:HG22	1:B:147:ASP:O	2.20	0.42
1:B:123:MSE:SE	1:B:218:VAL:HG21	2.70	0.42
1:B:21:LEU:HD22	1:B:57:VAL:HG11	2.02	0.42
1:B:36:LYS:HD2	1:B:102:PRO:O	2.20	0.42
1:C:101:GLU:HG2	1:C:237:GLY:HA2	2.01	0.42
1:C:143:LYS:NZ	1:C:157:ARG:O	2.48	0.41
1:A:145:LEU:HD12	1:A:146:THR:H	1.84	0.41
1:B:128:VAL:HG11	1:B:234:PRO:HD2	2.01	0.41
1:B:123:MSE:HE3	1:B:191:TYR:HE1	1.84	0.41
1:B:218:VAL:HB	1:B:225:ILE:HD11	2.02	0.41
1:B:185:HIS:CE1	2:B:263[A]:CMK:H7	2.55	0.41
1:C:136:LEU:O	1:C:143:LYS:NZ	2.43	0.41
1:A:136:LEU:HD11	1:A:182:TYR:CB	2.51	0.41
1:B:146:THR:HG23	1:B:150:GLY:CA	2.51	0.41
1:C:136:LEU:O	1:C:159:VAL:HG13	2.21	0.41
1:B:34:PHE:HD1	1:B:47:ILE:HD11	1.86	0.40
1:C:133:ALA:O	1:C:134:GLU:C	2.58	0.40
1:B:98:GLN:CG	2:B:263[A]:CMK:H4'	2.50	0.40
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.93	0.40
1:B:172:ASP:HB3	1:B:175:LYS:H	1.87	0.40
1:A:136:LEU:HA	1:A:136:LEU:HD12	1.93	0.40
1:A:129:LYS:HB3	1:A:131:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/262 (79%)	193 (93%)	13 (6%)	1 (0%)	38	70
1	B	242/262 (92%)	218 (90%)	23 (10%)	1 (0%)	43	76
1	C	235/262 (90%)	219 (93%)	14 (6%)	2 (1%)	25	55
All	All	684/786 (87%)	630 (92%)	50 (7%)	4 (1%)	33	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	GLN
1	C	187	GLY
1	A	99	GLY
1	B	24	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/218 (82%)	168 (94%)	10 (6%)	30	59
1	B	193/218 (88%)	180 (93%)	13 (7%)	23	49
1	C	179/218 (82%)	165 (92%)	14 (8%)	18	40
All	All	550/654 (84%)	513 (93%)	37 (7%)	23	49

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

Mol	Chain	Res	Type
1	A	10	ARG
1	A	59	LYS

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Mol	Chain	Res	Type
1	A	83	VAL
1	A	103	LEU
1	A	178	LEU
1	A	183	LEU
1	A	191	TYR
1	A	200	VAL
1	A	224	ARG
1	A	228	GLU
1	B	10	ARG
1	B	40	SER
1	B	112	VAL
1	B	126	LEU
1	B	145	LEU
1	B	164	ARG
1	B	170	LEU
1	B	172	ASP
1	B	191	TYR
1	B	198	GLN
1	B	213	LEU
1	B	242	GLU
1	B	244	LEU
1	C	15	ARG
1	C	30	ILE
1	C	50	ASP
1	C	112	VAL
1	C	121	VAL
1	C	128	VAL
1	C	143	LYS
1	C	153	LEU
1	C	159	VAL
1	C	183	LEU
1	C	198	GLN
1	C	199	TYR
1	C	208	GLU
1	C	213	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	122	ASN
1	A	131	HIS

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	177	GLN
1	A	198	GLN
1	B	98	GLN
1	B	140	ASN
1	C	53	ASN
1	C	96	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 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
2	CMK	A	263	-	38,38,38	2.37	8 (21%)	55,58,58	2.90	13 (23%)
2	CMK	B	263[A]	-	38,38,38	2.10	5 (13%)	55,58,58	2.79	14 (25%)
2	CMK	B	263[B]	-	38,38,38	2.19	7 (18%)	55,58,58	3.46	14 (25%)

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	CMK	A	263	-	-	0/24/62/62	0/3/3/3
2	CMK	B	263[A]	-	-	0/24/62/62	0/3/3/3
2	CMK	B	263[B]	-	-	0/24/62/62	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	263[B]	CMK	O2-C2	-10.67	1.18	1.43
2	B	263[A]	CMK	O2-C2	-10.38	1.18	1.43
2	A	263	CMK	O2-C2	-10.24	1.19	1.43
2	A	263	CMK	C4-C5	-5.80	1.44	1.52
2	A	263	CMK	C2'-C1'	-5.39	1.45	1.53
2	B	263[B]	CMK	PA-O5'	-3.92	1.41	1.59
2	B	263[A]	CMK	PA-O5'	-3.34	1.44	1.59
2	B	263[B]	CMK	PA-O2	-2.81	1.49	1.59
2	B	263[B]	CMK	C5-C6	2.77	1.60	1.52
2	A	263	CMK	PA-O5'	-2.76	1.46	1.59
2	B	263[A]	CMK	PA-O2	-2.75	1.49	1.59
2	A	263	CMK	PA-O2	-2.60	1.50	1.59
2	B	263[A]	CMK	C3-C2	2.46	1.55	1.52
2	B	263[B]	CMK	C3-C2	2.24	1.55	1.52
2	A	263	CMK	C3-C4	-2.14	1.49	1.53
2	B	263[B]	CMK	O1Y-C1	2.13	1.29	1.22
2	B	263[A]	CMK	O1Y-C1	2.08	1.29	1.22
2	B	263[B]	CMK	C2C-N1C	-2.08	1.35	1.38
2	A	263	CMK	O6-C6	2.04	1.47	1.44
2	A	263	CMK	C5-C6	2.02	1.58	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	263[B]	CMK	PA-O2-C2	17.82	159.62	125.56
2	A	263	CMK	PA-O2-C2	15.31	154.81	125.56
2	B	263[A]	CMK	PA-O2-C2	13.50	151.35	125.56
2	B	263[B]	CMK	C3-C4-C5	-9.34	101.86	110.79
2	B	263[B]	CMK	O4'-C1'-N1C	-8.96	89.17	108.06
2	B	263[A]	CMK	O4'-C1'-N1C	-8.60	89.94	108.06
2	A	263	CMK	O4'-C1'-N1C	-7.63	91.98	108.06
2	B	263[B]	CMK	O5-C5-C4	-6.15	98.91	110.03
2	B	263[A]	CMK	C2'-C1'-N1C	-5.58	98.89	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	263	CMK	C3-C4-C5	5.55	116.09	110.79
2	B	263[B]	CMK	C2'-C1'-N1C	-5.49	99.11	113.26
2	B	263[A]	CMK	C3-C4-C5	-4.95	106.05	110.79
2	A	263	CMK	C2-C3-C4	4.93	121.16	110.76
2	A	263	CMK	C2'-C1'-N1C	-4.64	101.31	113.26
2	B	263[A]	CMK	C7-C6-C5	3.68	119.95	114.09
2	B	263[A]	CMK	O5-C5-C4	-3.66	103.42	110.03
2	A	263	CMK	C6C-N1C-C1'	3.40	127.77	119.33
2	B	263[B]	CMK	O6-C6-C5	-3.10	104.19	108.69
2	B	263[B]	CMK	C4-C5-C6	-3.02	104.32	110.56
2	B	263[B]	CMK	O1Y-C1-C2	-2.96	113.97	124.03
2	A	263	CMK	C2C-N3C-C4C	2.83	119.67	115.57
2	B	263[B]	CMK	O3'-C3'-C4'	-2.82	102.76	111.08
2	B	263[A]	CMK	O2-C2-C1	2.80	116.97	109.91
2	A	263	CMK	C5'-C4'-C3'	-2.78	104.09	115.21
2	B	263[A]	CMK	O3'-C3'-C4'	-2.76	102.93	111.08
2	B	263[B]	CMK	C5'-C4'-C3'	-2.63	104.69	115.21
2	B	263[A]	CMK	C5'-C4'-C3'	-2.62	104.72	115.21
2	B	263[B]	CMK	C2C-N3C-C4C	2.58	119.31	115.57
2	A	263	CMK	C3'-C2'-C1'	2.50	104.81	100.91
2	B	263[A]	CMK	O4'-C1'-C2'	-2.39	103.11	106.77
2	B	263[A]	CMK	C6C-N1C-C1'	2.29	125.00	119.33
2	B	263[A]	CMK	C2C-N3C-C4C	2.29	118.89	115.57
2	B	263[B]	CMK	C6C-N1C-C1'	2.29	125.00	119.33
2	A	263	CMK	C2C-N1C-C1'	-2.26	115.94	119.03
2	A	263	CMK	O1A-PA-O2	2.16	114.18	105.38
2	B	263[B]	CMK	O4-C4-C5	-2.16	106.03	110.23
2	A	263	CMK	C8-C7-C6	2.13	116.70	112.14
2	A	263	CMK	C2-O6-C6	-2.11	110.29	113.99
2	B	263[A]	CMK	O7-C7-C6	2.11	114.21	109.06
2	B	263[B]	CMK	C3-C2-C1	-2.10	106.69	111.63
2	B	263[A]	CMK	O1Y-C1-C2	-2.09	116.91	124.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	211/262 (80%)	-0.30	3 (1%) 72 77	24, 40, 68, 76	0
1	B	246/262 (93%)	-0.07	5 (2%) 62 68	25, 47, 91, 105	0
1	C	238/262 (90%)	0.26	13 (5%) 24 26	35, 60, 85, 97	0
All	All	695/786 (88%)	-0.03	21 (3%) 48 54	24, 50, 85, 105	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	PRO	6.6
1	C	73	ASN	5.3
1	C	12	ALA	3.9
1	C	178	LEU	3.6
1	C	131	HIS	3.4
1	C	165	ASP	3.3
1	B	241	ALA	3.3
1	C	71	ASN	3.0
1	C	72	HIS	2.9
1	C	180	ASP	2.7
1	C	139	PRO	2.5
1	C	181	ALA	2.5
1	A	169	ASN	2.4
1	B	58	ALA	2.4
1	C	179	SER	2.4
1	A	53	ASN	2.3
1	B	11	PHE	2.3
1	C	201	GLN	2.2
1	C	130	ILE	2.2
1	B	17	PRO	2.1
1	B	173	VAL	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CMK	B	263[A]	36/36	0.48	7.16	37,41,44,45	36
2	CMK	B	263[B]	36/36	0.48	6.90	33,37,39,39	36
2	CMK	A	263	36/36	0.21	1.00	38,42,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.