



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1K39  
Title : The structure of yeast delta3-delta2-enoyl-CoA isomerase complexed with octanoyl-CoA  
Authors : Mursula, A.M.; Geerlof, A.; Hiltunen, J.K.; Wierenga, R.K.  
Deposited on : 2001-10-02  
Resolution : 3.29 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](mailto: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.

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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

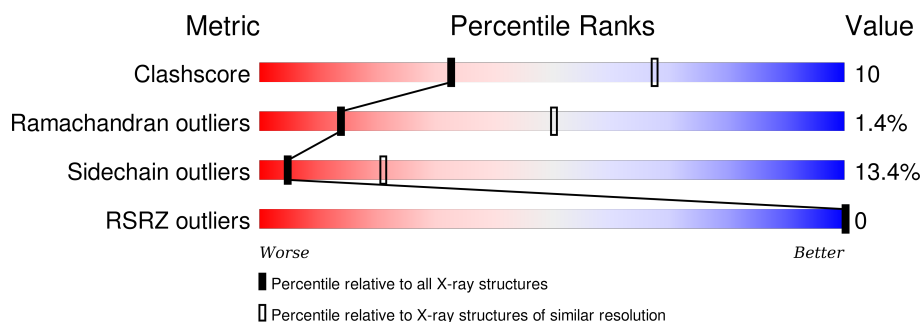
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 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	280	
1	B	280	
1	C	280	

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
3	CO8	A	300	-	-	-	X
3	CO8	B	301	-	-	-	X
3	CO8	C	302	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6587 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.

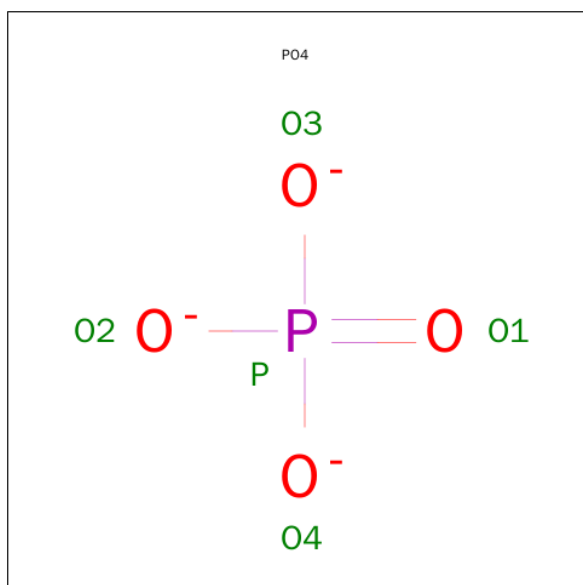
- Molecule 1 is a protein called d3,d2-enoyl CoA isomerase ECI1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	48	0	0
			2135	1375	351	399	10			
1	B	271	Total	C	N	O	S	73	0	0
			2150	1384	354	402	10			
1	C	266	Total	C	N	O	S	35	0	0
			2114	1362	348	394	10			

There are 3 discrepancies between the modelled and reference sequences:

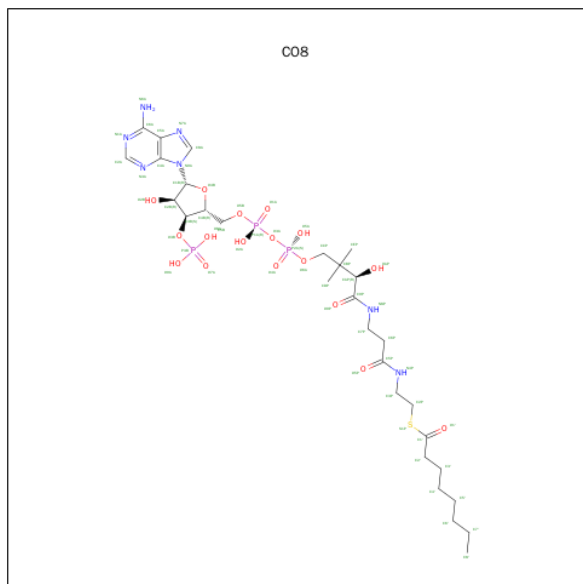
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ILE	MET	ENGINEERED	UNP Q05871
B	25	ILE	MET	ENGINEERED	UNP Q05871
C	25	ILE	MET	ENGINEERED	UNP Q05871

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula:  $C_{29}H_{50}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

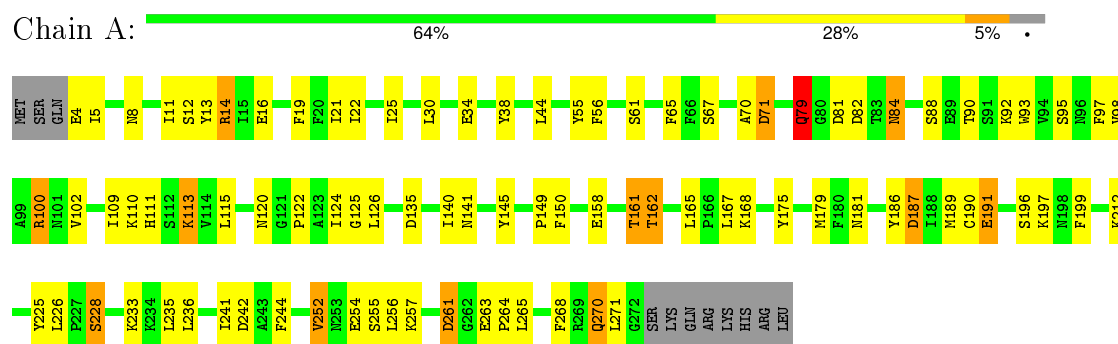
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	O	0	0
			2	2		

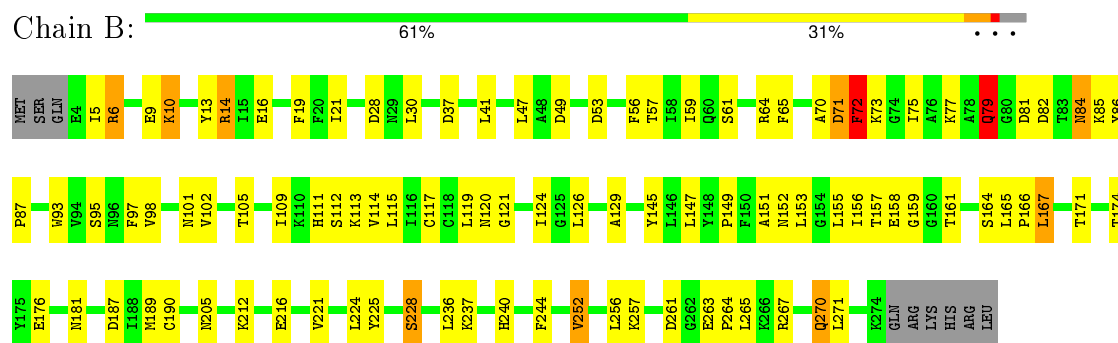
### 3 Residue-property plots

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.

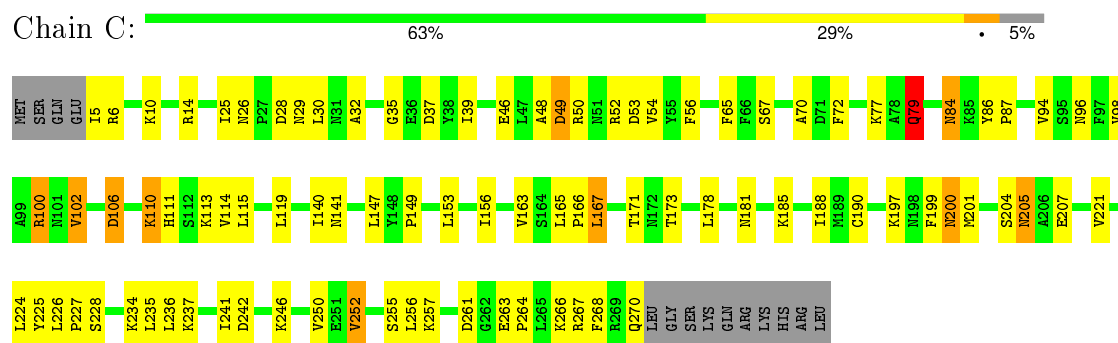
- Molecule 1: d3,d2-enoyl CoA isomerase ECI1



- Molecule 1: d3,d2-enoyl CoA isomerase ECI1



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.65Å 116.65Å 216.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.29 19.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-3.29) 97.4 (19.92-3.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.62 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.205 , 0.262 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22527 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO8, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.30	2/2181 (0.1%)	1.33	10/2947 (0.3%)
1	B	1.27	3/2196 (0.1%)	1.61	16/2966 (0.5%)
1	C	1.04	1/2160 (0.0%)	0.98	11/2919 (0.4%)
All	All	1.21	6/6537 (0.1%)	1.33	37/8832 (0.4%)

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	3
1	B	0	5
1	C	0	2
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLN	C-O	46.03	2.10	1.23
1	B	72	PHE	C-N	-45.04	0.30	1.34
1	C	84	ASN	C-N	-43.22	0.34	1.34
1	A	84	ASN	C-N	-32.29	0.59	1.34
1	B	79	GLN	C-N	-25.61	0.86	1.33
1	B	84	ASN	C-N	-18.40	0.91	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	ASP	O-C-N	-66.27	16.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	GLN	CA-C-N	-39.69	29.89	117.20
1	A	270	GLN	C-N-CA	-29.65	47.57	121.70
1	B	72	PHE	O-C-N	-28.65	76.86	122.70
1	A	270	GLN	O-C-N	-25.87	81.30	122.70
1	A	270	GLN	CA-C-O	-22.55	72.74	120.10
1	B	79	GLN	O-C-N	-21.32	86.95	123.20
1	C	84	ASN	O-C-N	-18.68	92.82	122.70
1	C	84	ASN	C-N-CA	17.53	165.51	121.70
1	C	79	GLN	O-C-N	16.45	151.17	123.20
1	C	79	GLN	CA-C-N	-14.97	86.26	116.20
1	C	84	ASN	CA-C-N	12.98	145.75	117.20
1	B	72	PHE	CA-C-N	11.71	142.96	117.20
1	B	84	ASN	C-N-CA	10.99	149.18	121.70
1	B	79	GLN	C-N-CA	9.55	142.36	122.30
1	C	79	GLN	C-N-CA	-9.34	102.69	122.30
1	A	79	GLN	O-C-N	-8.79	108.26	123.20
1	B	72	PHE	C-N-CA	7.43	140.28	121.70
1	B	28	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	79	GLN	CA-C-N	6.51	129.23	116.20
1	A	82	ASP	CB-CG-OD2	6.03	123.73	118.30
1	C	53	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	82	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	261	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	187	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	261	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	53	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	187	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	81	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	28	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	37	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	71	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	71	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	81	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	261	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	270	GLN	C-N-CA	-5.06	109.06	121.70
1	C	49	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	79	GLN	Mainchain
1	A	84	ASN	Mainchain
1	B	71	ASP	Mainchain
1	B	72	PHE	Mainchain,Peptide
1	B	79	GLN	Mainchain
1	B	84	ASN	Mainchain
1	C	84	ASN	Mainchain,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	2135	0	2125	43	0
1	B	2150	0	2142	47	0
1	C	2114	0	2106	40	0
2	A	10	0	0	0	0
2	C	5	0	0	0	0
3	A	57	0	46	5	0
3	B	57	0	46	8	0
3	C	57	0	46	5	0
4	B	2	0	0	0	0
All	All	6587	0	6511	133	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 10.

All (133) 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)
3:C:302:CO8:C9P	3:C:302:CO8:O9P	1.80	1.29
3:B:301:CO8:OAP	3:B:301:CO8:CAP	1.80	1.29
3:A:300:CO8:C9P	3:A:300:CO8:O9P	1.81	1.28
3:C:302:CO8:OAP	3:C:302:CO8:CAP	1.80	1.27
3:A:300:CO8:OAP	3:A:300:CO8:CAP	1.80	1.27
3:B:301:CO8:O9P	3:B:301:CO8:C9P	1.81	1.26
1:B:98:VAL:HG13	1:B:252:VAL:CG1	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:NH1	1:B:16:GLU:OE2	2.16	0.77
1:B:225:TYR:O	1:B:228:SER:HB2	1.87	0.75
1:A:70:ALA:H	3:A:300:CO8:H22	1.52	0.73
1:A:140:ILE:HG23	1:A:141:ASN:H	1.54	0.71
1:C:98:VAL:O	1:C:102:VAL:HG22	1.91	0.70
1:C:102:VAL:HG13	1:C:252:VAL:HG21	1.76	0.66
1:A:225:TYR:O	1:A:228:SER:HB2	1.94	0.66
1:B:98:VAL:HG13	1:B:252:VAL:HG11	1.80	0.63
1:A:19:PHE:HD2	1:A:56:PHE:HB2	1.64	0.63
1:C:70:ALA:H	3:C:302:CO8:H22	1.63	0.62
1:B:105:THR:OG1	1:B:159:GLY:HA2	2.02	0.60
1:A:149:PRO:HA	1:A:181:ASN:OD1	2.02	0.59
1:B:149:PRO:HA	1:B:181:ASN:OD1	2.02	0.59
1:B:61:SER:HB3	1:B:120:ASN:OD1	2.03	0.59
1:C:30:LEU:HD12	3:C:302:CO8:H8A	1.84	0.59
1:C:94:VAL:HA	1:C:98:VAL:HB	1.85	0.58
1:A:167:LEU:HD13	1:A:168:LYS:HG2	1.85	0.58
1:B:70:ALA:H	3:B:301:CO8:H22	1.67	0.58
1:C:39:ILE:HD11	1:C:100:ARG:HH11	1.70	0.57
1:C:54:VAL:O	1:C:113:LYS:HD2	2.05	0.56
1:C:165:LEU:HB2	1:C:166:PRO:HD3	1.86	0.55
1:B:158:GLU:OE2	3:B:301:CO8:H2'2	2.07	0.54
1:B:109:ILE:HD13	1:B:244:PHE:HB3	1.89	0.54
1:B:98:VAL:HG13	1:B:252:VAL:HG13	1.88	0.54
1:A:140:ILE:HG23	1:A:141:ASN:N	2.20	0.54
1:B:97:PHE:HE1	3:B:301:CO8:H4'1	1.74	0.53
1:A:161:THR:O	1:A:162:THR:C	2.47	0.53
1:A:55:TYR:CD2	1:A:226:LEU:HB3	2.43	0.53
1:B:145:TYR:HA	1:B:189:MET:CE	2.39	0.53
1:C:140:ILE:HG23	1:C:141:ASN:N	2.24	0.53
1:B:161:THR:HA	1:B:164:SER:OG	2.09	0.52
1:B:57:THR:OG1	1:B:111:HIS:HE1	1.91	0.52
1:C:96:ASN:O	1:C:100:ARG:HG3	2.10	0.51
1:B:30:LEU:HD22	1:B:65:PHE:HB2	1.94	0.50
1:A:71:ASP:OD1	3:A:300:CO8:H2A	2.12	0.50
1:A:61:SER:HB3	1:A:120:ASN:OD1	2.12	0.50
1:C:225:TYR:O	1:C:228:SER:HB2	2.11	0.50
1:C:56:PHE:CD2	1:C:114:VAL:HB	2.47	0.50
1:B:119:LEU:HD22	1:B:121:GLY:O	2.12	0.49
1:C:30:LEU:HD22	1:C:65:PHE:HB2	1.94	0.49
1:C:94:VAL:HG22	1:C:256:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:HA	1:C:224:LEU:HD12	1.93	0.49
1:A:228:SER:HB3	1:B:151:ALA:HA	1.93	0.49
1:A:235:LEU:HD11	1:B:156:ILE:HD12	1.94	0.48
1:B:13:TYR:HA	1:B:21:ILE:O	2.12	0.48
1:B:165:LEU:HB2	1:B:166:PRO:HD3	1.95	0.48
1:B:153:LEU:O	1:B:264:PRO:HA	2.14	0.47
1:B:30:LEU:HD12	3:B:301:CO8:H8A	1.95	0.47
1:A:98:VAL:HG13	1:A:252:VAL:HG13	1.97	0.47
1:A:97:PHE:HE1	3:A:300:CO8:H4'1	1.80	0.47
1:C:29:ASN:ND2	1:C:32:ALA:HB3	2.30	0.47
1:B:109:ILE:CD1	1:B:244:PHE:HB3	2.44	0.47
1:A:97:PHE:HE2	1:A:255:SER:HB3	1.79	0.46
1:B:166:PRO:HG3	1:B:174:THR:HG21	1.96	0.46
1:A:187:ASP:O	1:A:191:GLU:HB2	2.15	0.46
1:A:109:ILE:HD13	1:A:244:PHE:HB3	1.97	0.46
1:A:38:TYR:CZ	1:A:126:LEU:HD23	2.51	0.46
1:C:111:HIS:CD2	1:C:113:LYS:H	2.34	0.45
1:B:145:TYR:HA	1:B:189:MET:HE1	1.97	0.45
1:C:49:ASP:HA	1:C:113:LYS:HE3	1.97	0.45
1:C:98:VAL:HG22	1:C:252:VAL:HG13	1.98	0.45
1:C:140:ILE:HG23	1:C:141:ASN:H	1.81	0.45
1:B:221:VAL:HA	1:B:224:LEU:HD12	1.98	0.45
1:B:97:PHE:CE1	3:B:301:CO8:H4'1	2.52	0.45
1:B:111:HIS:O	1:B:237:LYS:NZ	2.40	0.45
1:C:199:PHE:O	1:C:200:ASN:C	2.54	0.45
1:A:263:GLU:HB3	1:A:264:PRO:HD3	1.97	0.45
1:A:93:TRP:CZ2	1:A:265:LEU:HD21	2.52	0.45
1:C:197:LYS:HD3	1:C:199:PHE:CE1	2.51	0.45
1:A:241:ILE:HG23	1:A:242:ASP:N	2.32	0.45
1:C:241:ILE:HG23	1:C:242:ASP:N	2.32	0.45
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.79	0.45
1:C:86:TYR:HA	1:C:87:PRO:HD3	1.86	0.45
1:C:263:GLU:HG3	1:C:267:ARG:HG3	1.98	0.45
1:B:5:ILE:HG12	1:B:6:ARG:H	1.83	0.44
1:B:19:PHE:HD2	1:B:56:PHE:HB2	1.83	0.44
1:A:197:LYS:HG2	1:A:199:PHE:CE1	2.52	0.44
1:B:49:ASP:HA	1:B:113:LYS:HE3	2.00	0.44
1:B:263:GLU:N	1:B:264:PRO:HD2	2.33	0.44
1:C:29:ASN:HD21	1:C:32:ALA:HB3	1.82	0.44
1:B:124:ILE:HA	1:B:147:LEU:O	2.18	0.44
1:C:72:PHE:C	1:C:72:PHE:CD1	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:CD2	1:A:56:PHE:HB2	2.48	0.43
1:C:226:LEU:N	1:C:227:PRO:CD	2.81	0.43
1:A:93:TRP:HZ2	1:A:265:LEU:HD21	1.83	0.43
1:B:101:ASN:OD1	3:B:301:CO8:H6'1	2.19	0.43
1:C:149:PRO:HA	1:C:181:ASN:OD1	2.18	0.42
1:A:22:ILE:HG12	1:A:44:LEU:HD13	2.01	0.42
1:C:48:ALA:HB3	1:C:111:HIS:HE1	1.84	0.42
1:B:155:LEU:HD21	1:B:264:PRO:HB3	2.01	0.42
1:C:26:ASN:ND2	1:C:29:ASN:HB3	2.35	0.42
1:B:93:TRP:CZ2	1:B:265:LEU:HD21	2.55	0.42
1:C:35:GLY:O	1:C:39:ILE:HG12	2.20	0.42
1:C:100:ARG:HB2	3:C:302:CO8:C8'	2.50	0.42
1:A:124:ILE:CG2	1:A:125:GLY:N	2.83	0.42
1:A:186:TYR:HA	1:A:189:MET:HG3	2.01	0.42
1:A:145:TYR:HA	1:A:189:MET:CE	2.50	0.42
1:B:5:ILE:HG12	1:B:6:ARG:N	2.34	0.41
1:B:56:PHE:CD2	1:B:114:VAL:HB	2.55	0.41
1:B:126:LEU:O	1:B:129:ALA:HB3	2.20	0.41
1:A:150:PHE:CE2	1:A:158:GLU:HG2	2.54	0.41
1:A:14:ARG:NH1	1:A:16:GLU:OE2	2.53	0.41
1:C:163:VAL:O	1:C:167:LEU:HB2	2.21	0.41
1:A:8:ASN:HB3	1:A:11:ILE:H	1.86	0.41
1:C:178:LEU:HA	1:C:178:LEU:HD23	1.91	0.41
1:C:5:ILE:HG23	1:C:6:ARG:O	2.20	0.41
1:A:140:ILE:CG2	1:A:141:ASN:H	2.30	0.41
1:C:205:ASN:HD21	1:C:207:GLU:HB3	1.85	0.41
1:A:13:TYR:HA	1:A:21:ILE:O	2.21	0.41
1:A:167:LEU:CD1	1:A:168:LYS:HG2	2.50	0.41
1:B:9:GLU:H	1:B:9:GLU:CD	2.24	0.41
1:C:115:LEU:HA	1:C:115:LEU:HD12	1.93	0.41
1:B:86:TYR:HA	1:B:87:PRO:HD3	1.90	0.41
1:A:175:TYR:O	1:A:179:MET:HG2	2.21	0.41
1:B:10:LYS:HD3	1:B:37:ASP:OD2	2.21	0.41
1:C:153:LEU:O	1:C:264:PRO:HA	2.20	0.41
1:B:152:ASN:O	1:B:267:ARG:HD3	2.20	0.41
1:A:196:SER:HB3	1:B:176:GLU:HG2	2.02	0.41
1:A:100:ARG:H	1:A:100:ARG:HG2	1.48	0.41
1:B:57:THR:OG1	1:B:111:HIS:CE1	2.73	0.40
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.90	0.40
1:A:14:ARG:HD2	1:A:16:GLU:OE2	2.21	0.40
1:C:106:ASP:O	1:C:110:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:LEU:HD21	1:B:240:HIS:CE1	2.57	0.40
1:A:65:PHE:HA	1:A:122:PRO:HD2	2.03	0.40
1:A:111:HIS:CE1	1:A:113:LYS:HG3	2.57	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	267/280 (95%)	240 (90%)	23 (9%)	4 (2%)	13	49
1	B	269/280 (96%)	248 (92%)	17 (6%)	4 (2%)	13	49
1	C	264/280 (94%)	245 (93%)	16 (6%)	3 (1%)	17	57
All	All	800/840 (95%)	733 (92%)	56 (7%)	11 (1%)	14	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	LEU
1	B	73	LYS
1	B	85	LYS
1	B	72	PHE
1	A	67	SER
1	A	79	GLN
1	C	200	ASN
1	B	271	LEU
1	A	162	THR
1	C	67	SER
1	C	79	GLN

### 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	234/245 (96%)	204 (87%)	30 (13%)	5	23
1	B	236/245 (96%)	208 (88%)	28 (12%)	6	27
1	C	232/245 (95%)	196 (84%)	36 (16%)	3	16
All	All	702/735 (96%)	608 (87%)	94 (13%)	5	21

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	5	ILE
1	A	12	SER
1	A	14	ARG
1	A	25	ILE
1	A	30	LEU
1	A	34	GLU
1	A	79	GLN
1	A	88	SER
1	A	90	THR
1	A	92	LYS
1	A	95	SER
1	A	100	ARG
1	A	102	VAL
1	A	110	LYS
1	A	113	LYS
1	A	135	ASP
1	A	161	THR
1	A	190	CYS
1	A	191	GLU
1	A	212	LYS
1	A	228	SER
1	A	233	LYS
1	A	236	LEU
1	A	252	VAL
1	A	254	GLU

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Mol	Chain	Res	Type
1	A	256	LEU
1	A	257	LYS
1	A	261	ASP
1	A	268	PHE
1	B	6	ARG
1	B	10	LYS
1	B	14	ARG
1	B	41	LEU
1	B	47	LEU
1	B	59	ILE
1	B	64	ARG
1	B	75	ILE
1	B	77	LYS
1	B	79	GLN
1	B	95	SER
1	B	102	VAL
1	B	112	SER
1	B	115	LEU
1	B	117	CYS
1	B	157	THR
1	B	167	LEU
1	B	171	THR
1	B	190	CYS
1	B	205	ASN
1	B	212	LYS
1	B	216	GLU
1	B	228	SER
1	B	236	LEU
1	B	252	VAL
1	B	256	LEU
1	B	257	LYS
1	B	270	GLN
1	C	10	LYS
1	C	14	ARG
1	C	25	ILE
1	C	46	GLU
1	C	50	ARG
1	C	52	ARG
1	C	77	LYS
1	C	79	GLN
1	C	100	ARG
1	C	102	VAL

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Mol	Chain	Res	Type
1	C	106	ASP
1	C	110	LYS
1	C	119	LEU
1	C	147	LEU
1	C	156	ILE
1	C	167	LEU
1	C	171	THR
1	C	173	THR
1	C	185	LYS
1	C	188	ILE
1	C	190	CYS
1	C	201	MET
1	C	204	SER
1	C	205	ASN
1	C	234	LYS
1	C	235	LEU
1	C	236	LEU
1	C	237	LYS
1	C	246	LYS
1	C	250	VAL
1	C	252	VAL
1	C	255	SER
1	C	257	LYS
1	C	266	LYS
1	C	268	PHE
1	C	270	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	198	ASN
1	B	79	GLN
1	B	111	HIS
1	B	198	ASN
1	B	205	ASN
1	B	240	HIS
1	C	26	ASN
1	C	29	ASN
1	C	198	ASN
1	C	205	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 ⓘ

6 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	PO4	A	281	-	4,4,4	0.56	0	6,6,6	0.27	0
2	PO4	A	282	-	4,4,4	0.47	0	6,6,6	0.26	0
3	CO8	A	300	-	49,59,59	5.10	6 (12%)	61,85,85	2.15	9 (14%)
3	CO8	B	301	-	49,59,59	5.11	6 (12%)	61,85,85	2.17	8 (13%)
2	PO4	C	281	-	4,4,4	0.41	0	6,6,6	0.27	0
3	CO8	C	302	-	49,59,59	5.10	6 (12%)	61,85,85	2.09	7 (11%)

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	PO4	A	281	-	-	0/0/0/0	0/0/0/0
2	PO4	A	282	-	-	0/0/0/0	0/0/0/0
3	CO8	A	300	-	-	0/54/74/74	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CO8	B	301	-	-	0/54/74/74	0/3/3/3
2	PO4	C	281	-	-	0/0/0/0	0/0/0/0
3	CO8	C	302	-	-	0/54/74/74	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	CO8	P1A-O1A	2.31	1.59	1.51
3	A	300	CO8	P1A-O1A	2.35	1.59	1.51
3	C	302	CO8	P1A-O1A	2.36	1.59	1.51
3	B	301	CO8	C2A-N1A	2.43	1.38	1.33
3	A	300	CO8	P2A-O4A	2.45	1.60	1.51
3	A	300	CO8	C2A-N1A	2.46	1.38	1.33
3	C	302	CO8	P2A-O4A	2.48	1.60	1.51
3	B	301	CO8	P2A-O4A	2.51	1.60	1.51
3	C	302	CO8	C2A-N1A	2.62	1.38	1.33
3	B	301	CO8	C2A-N3A	3.55	1.38	1.32
3	A	300	CO8	C2A-N3A	3.65	1.38	1.32
3	C	302	CO8	C2A-N3A	3.75	1.38	1.32
3	A	300	CO8	OAP-CAP	19.05	1.80	1.42
3	C	302	CO8	OAP-CAP	19.10	1.80	1.42
3	B	301	CO8	OAP-CAP	19.15	1.80	1.42
3	C	302	CO8	O9P-C9P	29.27	1.80	1.23
3	B	301	CO8	O9P-C9P	29.37	1.81	1.23
3	A	300	CO8	O9P-C9P	29.37	1.81	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	CO8	N3A-C2A-N1A	-11.15	120.36	128.89
3	B	301	CO8	N3A-C2A-N1A	-10.98	120.49	128.89
3	A	300	CO8	N3A-C2A-N1A	-10.74	120.67	128.89
3	B	301	CO8	O1'-C1'-S1P	-6.21	117.91	122.83
3	A	300	CO8	O1'-C1'-S1P	-5.93	118.13	122.83
3	C	302	CO8	O1'-C1'-S1P	-5.28	118.64	122.83
3	C	302	CO8	P2A-O3A-P1A	-4.20	120.95	132.73
3	A	300	CO8	P2A-O3A-P1A	-3.90	121.78	132.73
3	B	301	CO8	P2A-O3A-P1A	-3.82	122.00	132.73
3	A	300	CO8	O1'-C1'-C2'	-2.98	121.89	123.94
3	A	300	CO8	C2B-C1B-N9A	-2.92	109.83	114.29
3	B	301	CO8	O1'-C1'-C2'	-2.86	121.97	123.94
3	C	302	CO8	O1'-C1'-C2'	-2.68	122.09	123.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	CO8	C2B-C1B-N9A	-2.64	110.25	114.29
3	C	302	CO8	C2B-C1B-N9A	-2.59	110.33	114.29
3	B	301	CO8	C7P-C6P-C5P	-2.12	108.82	112.31
3	A	300	CO8	C7P-C6P-C5P	-2.01	108.99	112.31
3	A	300	CO8	C4A-C5A-N7A	-2.01	107.63	109.48
3	A	300	CO8	O4B-C1B-N9A	2.30	112.91	108.10
3	C	302	CO8	O4B-C1B-N9A	2.48	113.30	108.10
3	B	301	CO8	O4B-C1B-N9A	2.57	113.47	108.10
3	C	302	CO8	C2'-C1'-S1P	6.56	119.26	113.36
3	A	300	CO8	C2'-C1'-S1P	7.36	119.98	113.36
3	B	301	CO8	C2'-C1'-S1P	7.52	120.12	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	CO8	5	0
3	B	301	CO8	8	0
3	C	302	CO8	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/280 (93%)	-0.72	0 100 100	5, 16, 36, 60	1 (0%)
1	B	261/280 (93%)	-0.77	0 100 100	5, 16, 37, 58	0
1	C	261/280 (93%)	-0.68	0 100 100	9, 19, 38, 55	0
All	All	784/840 (93%)	-0.72	0 100 100	5, 16, 38, 60	1 (0%)

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CO8	C	302	57/57	0.70	0.42	3.29	55,56,57,58	57
3	CO8	B	301	57/57	0.76	0.37	3.07	55,56,57,58	57
3	CO8	A	300	57/57	0.78	0.37	2.63	55,56,57,58	57

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	281	5/5	0.92	0.29	0.82	78,79,79,79	5
2	PO4	A	282	5/5	0.90	0.33	-	52,53,53,53	5
2	PO4	C	281	5/5	0.91	0.29	-	54,54,55,55	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.