



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2023 – 10:29 PM EDT

PDB ID : 1XG3  
Title : Crystal structure of the C123S 2-methylisocitrate lyase mutant from Escherichia coli in complex with the reaction product, Mg(II)-pyruvate and succinate  
Authors : Liu, S.; Lu, Z.; Han, Y.; Melamud, E.; Dunaway-Mariano, D.; Herzberg, O.  
Deposited on : 2004-09-16  
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

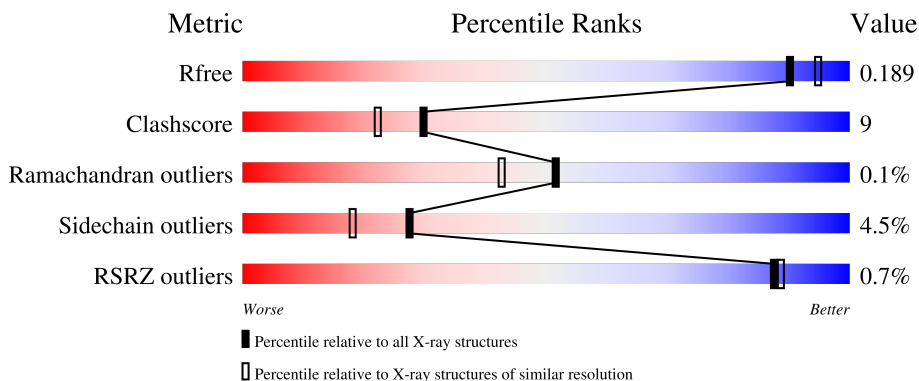
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	295	 2% 81% 14% ..
1	B	295	 80% 15% ..
1	C	295	 77% 18% ..
1	D	295	 2% 79% 13% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9815 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 Probable methylisocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2190	1375	383	423	9	0	0	0
1	B	286	2176	1366	381	420	9	0	0	0
1	C	287	2184	1372	382	421	9	0	0	0
1	D	283	2152	1352	377	414	9	0	0	0

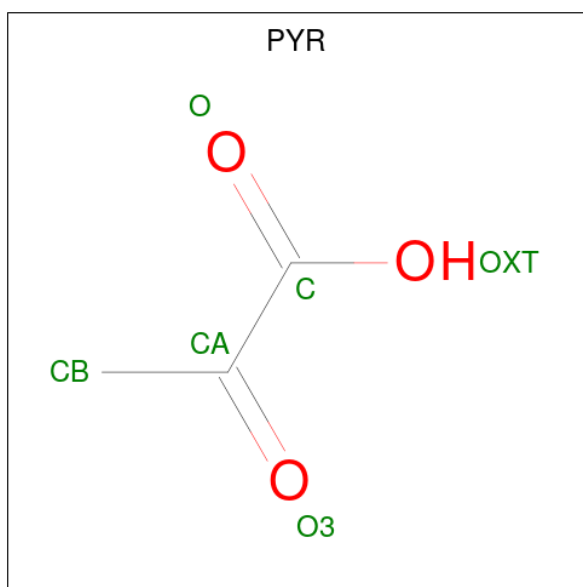
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	SER	CYS	engineered mutation	UNP P77541
B	123	SER	CYS	engineered mutation	UNP P77541
C	123	SER	CYS	engineered mutation	UNP P77541
D	123	SER	CYS	engineered mutation	UNP P77541

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

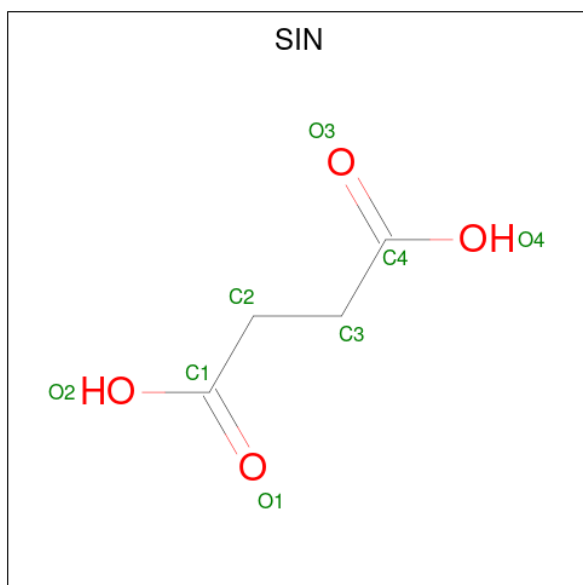
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula:  $C_4H_6O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 4 4	0	0
4	B	1	Total C O 8 4 4	0	0
4	D	1	Total C O 8 4 4	0	0

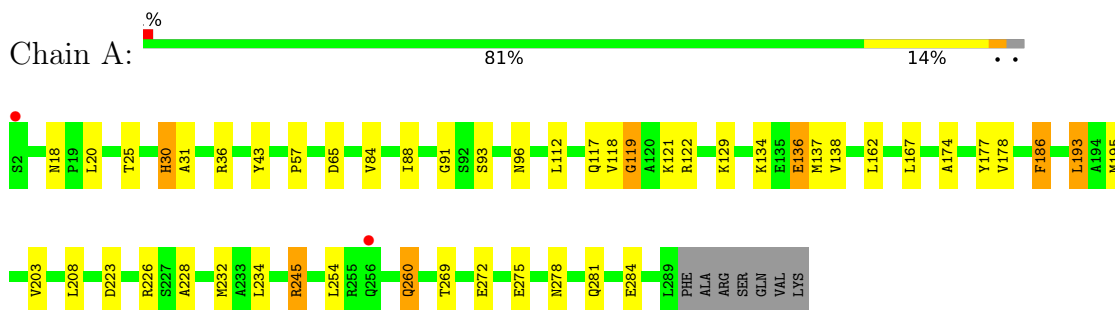
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	250	Total O 250 250	0	0
5	B	277	Total O 277 277	0	0
5	C	267	Total O 267 267	0	0
5	D	267	Total O 267 267	0	0

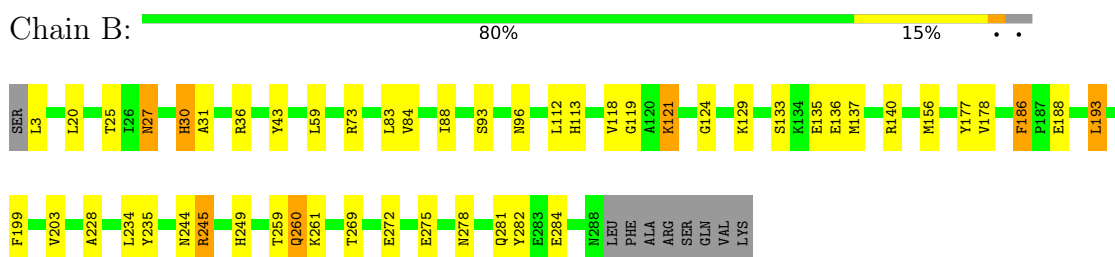
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

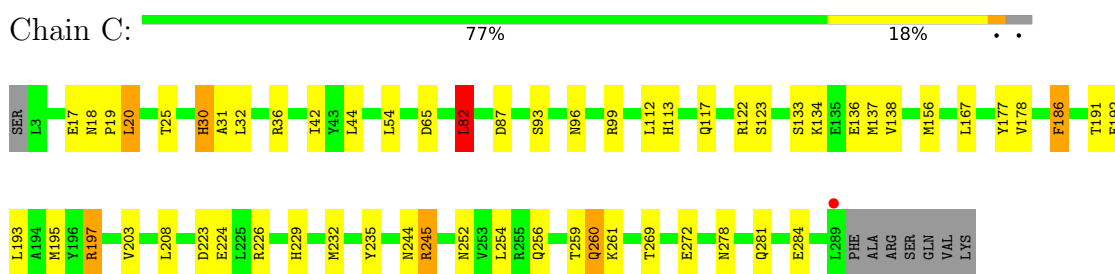
- Molecule 1: Probable methylisocitrate lyase



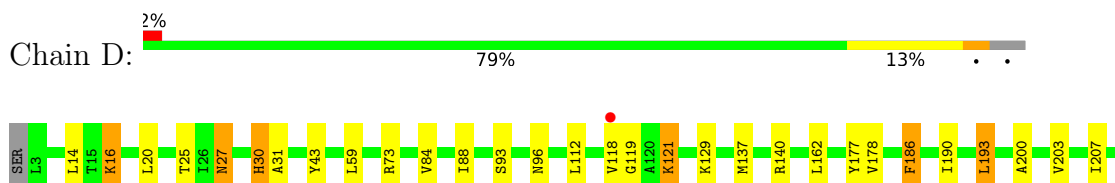
- Molecule 1: Probable methylisocitrate lyase

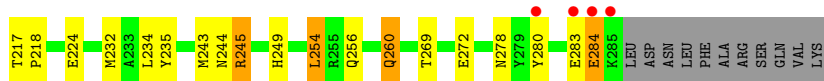


- Molecule 1: Probable methylisocitrate lyase



- Molecule 1: Probable methylisocitrate lyase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.36Å 85.99Å 99.60Å 90.00° 108.28° 90.00°	Depositor
Resolution (Å)	25.85 – 1.90 25.85 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.3 (25.85-1.90) 88.6 (25.85-1.90)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.98 (at 1.91Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.161 , 0.195 0.156 , 0.189	Depositor DCC
$R_{free}$ test set	3591 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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, 0.333 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, SIN, PYR

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	0.41	1/2224 (0.0%)	0.64	0/3016
1	B	0.42	1/2210 (0.0%)	0.65	0/2997
1	C	0.42	1/2218 (0.0%)	0.66	1/3008 (0.0%)
1	D	0.43	1/2186 (0.0%)	0.66	0/2964
All	All	0.42	4/8838 (0.0%)	0.65	1/11985 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	GLU	CD-OE2	7.34	1.33	1.25
1	D	284	GLU	CD-OE2	7.25	1.33	1.25
1	A	284	GLU	CD-OE2	7.21	1.33	1.25
1	C	284	GLU	CD-OE2	6.01	1.32	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	LEU	CA-CB-CG	5.31	127.52	115.30

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	2190	0	2189	42	0
1	B	2176	0	2173	43	0
1	C	2184	0	2184	45	0
1	D	2152	0	2152	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	8	0	4	0	0
4	B	8	0	4	0	0
4	D	8	0	4	0	0
5	A	250	0	0	7	0
5	B	277	0	0	8	0
5	C	267	0	0	6	0
5	D	267	0	0	8	0
All	All	9815	0	8710	164	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 9.

All (164) 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:A:260:GLN:HE21	1:A:260:GLN:H	1.08	0.97
1:B:260:GLN:H	1:B:260:GLN:HE21	1.01	0.96
1:C:260:GLN:HE21	1:C:260:GLN:H	1.03	0.96
1:D:260:GLN:HE21	1:D:260:GLN:H	0.98	0.91
1:A:117:GLN:HE22	1:A:122:ARG:H	1.27	0.80
1:B:88:ILE:HD13	1:B:119:GLY:HA2	1.64	0.79
1:C:93:SER:H	1:C:96:ASN:HD22	1.30	0.77
1:D:260:GLN:HE21	1:D:260:GLN:N	1.81	0.77
1:A:167:LEU:HD23	1:A:195:MET:HE3	1.66	0.76
1:B:93:SER:H	1:B:96:ASN:HD22	1.34	0.76
1:D:93:SER:H	1:D:96:ASN:HD22	1.32	0.76
1:B:260:GLN:HE21	1:B:260:GLN:N	1.82	0.74
1:C:260:GLN:HE21	1:C:260:GLN:N	1.85	0.72
5:C:2333:HOH:O	1:D:73:ARG:HD2	1.90	0.71
1:D:260:GLN:H	1:D:260:GLN:NE2	1.82	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ARG:HD3	5:B:2426:HOH:O	1.93	0.69
1:C:245:ARG:HD3	5:D:2473:HOH:O	1.91	0.69
1:A:93:SER:H	1:A:96:ASN:HD22	1.40	0.69
1:B:88:ILE:CD1	1:B:119:GLY:HA2	2.23	0.68
1:D:280:TYR:HA	1:D:283:GLU:HG2	1.76	0.68
5:A:2171:HOH:O	1:B:245:ARG:HD3	1.93	0.67
1:C:197:ARG:HG3	5:C:2459:HOH:O	1.98	0.64
1:B:118:VAL:HG12	1:B:119:GLY:N	2.11	0.64
1:A:167:LEU:HD23	1:A:195:MET:CE	2.27	0.64
1:C:42:ILE:HG13	1:C:82:LEU:HD23	1.80	0.63
1:D:200:ALA:HB2	1:D:207:ILE:HD13	1.81	0.63
1:A:245:ARG:HD3	5:A:2147:HOH:O	1.99	0.63
5:C:2449:HOH:O	1:D:245:ARG:HD3	1.99	0.62
1:B:129:LYS:HG2	5:B:2252:HOH:O	1.99	0.62
1:D:88:ILE:HD13	1:D:119:GLY:HA2	1.82	0.61
1:B:27:ASN:HD22	1:B:27:ASN:C	2.04	0.61
1:B:140:ARG:HD3	5:B:2268:HOH:O	2.01	0.61
1:C:254:LEU:HD21	1:D:235:TYR:CG	2.36	0.60
1:C:197:ARG:HG3	1:C:197:ARG:HH11	1.66	0.60
1:D:16:LYS:HE2	5:D:2566:HOH:O	2.02	0.60
1:B:259:THR:OG1	1:B:261:LYS:HG3	2.02	0.59
1:D:140:ARG:HD3	5:D:2633:HOH:O	2.01	0.59
1:D:193:LEU:HD11	1:D:224:GLU:HB3	1.84	0.59
1:D:112:LEU:HD12	1:D:112:LEU:C	2.23	0.59
1:A:117:GLN:NE2	1:A:122:ARG:H	1.99	0.59
1:B:278:ASN:HD21	1:B:281:GLN:NE2	2.00	0.59
1:D:88:ILE:CD1	1:D:119:GLY:HA2	2.34	0.58
1:A:260:GLN:HE21	1:A:260:GLN:N	1.89	0.58
1:B:27:ASN:ND2	1:B:30:HIS:H	2.02	0.56
1:C:65:ASP:HB2	5:C:2450:HOH:O	2.05	0.56
1:C:117:GLN:HE22	1:C:123:SER:H	1.53	0.56
1:D:118:VAL:HG12	1:D:119:GLY:N	2.19	0.56
1:B:260:GLN:H	1:B:260:GLN:NE2	1.86	0.56
1:A:118:VAL:HG12	1:A:119:GLY:N	2.20	0.56
1:C:223:ASP:OD1	1:C:226:ARG:NH2	2.40	0.55
1:C:252:ASN:O	1:C:256:GLN:HG3	2.07	0.54
1:C:87:ASP:HB2	5:C:2522:HOH:O	2.08	0.54
1:D:27:ASN:ND2	1:D:30:HIS:H	2.06	0.54
1:D:269:THR:OG1	1:D:272:GLU:HG3	2.08	0.54
1:C:112:LEU:HD12	1:C:112:LEU:C	2.28	0.54
1:A:129:LYS:HG2	5:A:2244:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG12	1:B:119:GLY:H	1.74	0.53
1:C:32:LEU:O	1:C:36:ARG:HG3	2.09	0.52
1:B:30:HIS:HD2	5:B:2235:HOH:O	1.92	0.52
1:C:254:LEU:HD21	1:D:235:TYR:CD2	2.45	0.52
1:D:118:VAL:HG12	1:D:119:GLY:H	1.73	0.52
1:D:278:ASN:ND2	5:D:2567:HOH:O	2.40	0.52
1:D:283:GLU:HG3	1:D:284:GLU:N	2.25	0.52
1:A:223:ASP:OD1	1:A:226:ARG:NH2	2.42	0.51
5:A:2339:HOH:O	1:C:99:ARG:HD3	2.10	0.51
1:B:112:LEU:C	1:B:112:LEU:HD12	2.31	0.51
1:C:25:THR:HG21	1:C:31:ALA:HA	1.93	0.51
1:A:30:HIS:HE1	1:B:244:ASN:OD1	1.94	0.51
1:B:124:GLY:HA3	1:B:188:GLU:HG2	1.93	0.51
1:D:27:ASN:C	1:D:27:ASN:HD22	2.14	0.50
1:D:162:LEU:HD22	1:D:190:ILE:HD13	1.93	0.50
1:C:244:ASN:OD1	1:D:30:HIS:HE1	1.94	0.50
1:D:25:THR:HG21	1:D:31:ALA:HA	1.93	0.50
1:B:199:PHE:O	1:B:203:VAL:HG22	2.11	0.50
1:A:36:ARG:NH2	1:A:275:GLU:HG2	2.27	0.49
1:A:137:MET:HG2	1:A:177:TYR:CZ	2.48	0.49
1:C:113:HIS:HA	1:C:156:MET:O	2.11	0.49
1:A:25:THR:HG21	1:A:31:ALA:HA	1.95	0.49
1:A:178:VAL:HG21	1:A:203:VAL:HB	1.95	0.49
1:D:186:PHE:CD1	1:D:186:PHE:C	2.87	0.49
1:C:259:THR:OG1	1:C:261:LYS:HG3	2.13	0.48
1:A:167:LEU:C	1:A:167:LEU:HD13	2.34	0.48
1:B:118:VAL:CG1	1:B:119:GLY:N	2.76	0.48
1:B:137:MET:HG2	1:B:177:TYR:CZ	2.48	0.48
1:B:178:VAL:HG21	1:B:203:VAL:HB	1.96	0.48
1:A:254:LEU:HD21	1:B:235:TYR:CG	2.49	0.47
1:D:59:LEU:HA	1:D:121:LYS:O	2.14	0.47
1:A:18:ASN:O	1:A:226:ARG:HD3	2.15	0.47
1:A:88:ILE:CD1	1:A:119:GLY:HA2	2.45	0.47
1:A:134:LYS:O	1:A:138:VAL:HG23	2.14	0.47
1:B:25:THR:HG21	1:B:31:ALA:HA	1.96	0.47
1:B:275:GLU:HG2	5:B:2446:HOH:O	2.15	0.46
1:C:93:SER:H	1:C:96:ASN:ND2	2.07	0.46
1:C:191:THR:H	1:C:195:MET:CE	2.28	0.46
1:C:269:THR:OG1	1:C:272:GLU:HG3	2.15	0.46
1:A:118:VAL:HG12	1:A:119:GLY:H	1.80	0.46
1:C:117:GLN:HE21	1:C:122:ARG:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:OG1	1:A:272:GLU:HG3	2.15	0.46
1:D:84:VAL:O	1:D:112:LEU:HA	2.16	0.46
1:D:137:MET:HG2	1:D:177:TYR:CZ	2.50	0.46
1:C:278:ASN:HD21	1:C:281:GLN:CD	2.19	0.46
1:D:129:LYS:HG2	5:D:2493:HOH:O	2.16	0.46
1:A:91:GLY:HA3	1:A:96:ASN:CB	2.46	0.46
1:C:178:VAL:HG21	1:C:203:VAL:HB	1.97	0.46
5:A:2150:HOH:O	1:B:73:ARG:HD2	2.15	0.46
1:B:113:HIS:HA	1:B:156:MET:O	2.17	0.45
1:A:43:TYR:CG	1:A:234:LEU:HD11	2.52	0.45
1:A:84:VAL:O	1:A:112:LEU:HA	2.16	0.45
1:A:57:PRO:HG2	1:B:282:TYR:CD1	2.52	0.45
1:B:135:GLU:H	1:B:135:GLU:CD	2.20	0.45
1:B:249:HIS:HE1	5:B:2414:HOH:O	1.99	0.45
1:C:30:HIS:HE1	1:D:244:ASN:OD1	1.99	0.45
1:D:30:HIS:HD2	5:D:2411:HOH:O	1.99	0.45
1:A:186:PHE:CD1	1:A:186:PHE:C	2.89	0.45
1:A:65:ASP:OD1	1:C:65:ASP:HB3	2.17	0.45
1:C:193:LEU:HD11	1:C:224:GLU:HB3	1.99	0.45
1:C:192:GLU:H	1:C:195:MET:HE3	1.83	0.44
1:D:178:VAL:HG21	1:D:203:VAL:HB	2.00	0.44
1:A:88:ILE:HD13	1:A:119:GLY:HA2	1.98	0.44
1:B:84:VAL:O	1:B:112:LEU:HA	2.17	0.44
1:C:208:LEU:C	1:C:208:LEU:HD23	2.37	0.44
1:D:249:HIS:HD2	5:D:2572:HOH:O	2.00	0.44
1:C:54:LEU:HD23	1:D:73:ARG:HG2	1.99	0.44
1:A:162:LEU:CD1	1:A:195:MET:HE1	2.48	0.44
1:B:118:VAL:CG1	1:B:119:GLY:H	2.30	0.44
1:D:186:PHE:C	1:D:186:PHE:HD1	2.21	0.44
1:A:260:GLN:H	1:A:260:GLN:NE2	1.93	0.44
1:D:14:LEU:HD21	1:D:232:MET:CG	2.47	0.44
1:C:260:GLN:H	1:C:260:GLN:NE2	1.88	0.44
1:C:134:LYS:O	1:C:138:VAL:HG23	2.18	0.43
1:B:269:THR:OG1	1:B:272:GLU:HG3	2.17	0.43
1:C:18:ASN:HA	1:C:19:PRO:HA	1.90	0.43
1:A:208:LEU:C	1:A:208:LEU:HD23	2.38	0.43
1:C:30:HIS:HD2	5:C:2314:HOH:O	2.00	0.43
1:C:32:LEU:O	1:C:36:ARG:CG	2.66	0.43
1:C:192:GLU:H	1:C:195:MET:CE	2.32	0.43
1:B:249:HIS:HD2	5:B:2347:HOH:O	2.01	0.43
1:C:235:TYR:CG	1:D:254:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:PHE:C	1:B:186:PHE:CD1	2.91	0.42
1:D:280:TYR:HD2	1:D:283:GLU:OE2	2.02	0.42
1:C:137:MET:HG2	1:C:177:TYR:CZ	2.55	0.42
1:D:256:GLN:HG2	5:D:2644:HOH:O	2.19	0.42
1:C:17:GLU:HG2	1:C:20:LEU:HA	2.01	0.42
1:A:30:HIS:HD2	5:A:2112:HOH:O	2.02	0.42
1:A:136:GLU:HG3	5:A:2310:HOH:O	2.19	0.42
1:B:3:LEU:N	5:B:2377:HOH:O	2.53	0.42
1:B:43:TYR:CG	1:B:234:LEU:HD11	2.55	0.42
1:D:217:THR:HA	1:D:218:PRO:HD3	1.97	0.42
1:A:193:LEU:HD22	1:A:228:ALA:HB2	2.02	0.41
1:C:186:PHE:C	1:C:186:PHE:CD1	2.92	0.41
1:D:200:ALA:HB2	1:D:207:ILE:CD1	2.47	0.41
1:B:193:LEU:HD22	1:B:228:ALA:HB2	2.02	0.41
1:C:133:SER:OG	1:C:136:GLU:HG3	2.20	0.41
1:B:59:LEU:HA	1:B:121:LYS:O	2.20	0.41
1:A:112:LEU:C	1:A:112:LEU:HD12	2.41	0.41
1:B:133:SER:OG	1:B:136:GLU:HG3	2.20	0.41
1:A:174:ALA:O	1:A:178:VAL:HG23	2.21	0.41
1:C:254:LEU:HD11	1:D:235:TYR:CE1	2.56	0.41
1:A:118:VAL:CG1	1:A:119:GLY:N	2.84	0.41
1:A:186:PHE:C	1:A:186:PHE:HD1	2.24	0.41
1:A:278:ASN:HD21	1:A:281:GLN:NE2	2.20	0.40
1:D:43:TYR:CG	1:D:234:LEU:HD11	2.56	0.40
1:B:186:PHE:C	1:B:186:PHE:HD1	2.25	0.40
1:A:167:LEU:CD2	1:A:195:MET:HE3	2.42	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	286/295 (97%)	279 (98%)	6 (2%)	1 (0%)	41	31
1	B	284/295 (96%)	277 (98%)	7 (2%)	0	100	100
1	C	285/295 (97%)	279 (98%)	6 (2%)	0	100	100
1	D	281/295 (95%)	271 (96%)	10 (4%)	0	100	100
All	All	1136/1180 (96%)	1106 (97%)	29 (3%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLY

### 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	226/232 (97%)	217 (96%)	9 (4%)	31	22
1	B	224/232 (97%)	215 (96%)	9 (4%)	31	22
1	C	225/232 (97%)	214 (95%)	11 (5%)	25	15
1	D	221/232 (95%)	210 (95%)	11 (5%)	24	15
All	All	896/928 (97%)	856 (96%)	40 (4%)	27	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	30	HIS
1	A	121	LYS
1	A	136	GLU
1	A	186	PHE
1	A	193	LEU
1	A	232	MET
1	A	245	ARG
1	A	260	GLN
1	B	20	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	27	ASN
1	B	30	HIS
1	B	83	LEU
1	B	121	LYS
1	B	186	PHE
1	B	193	LEU
1	B	245	ARG
1	B	260	GLN
1	C	20	LEU
1	C	30	HIS
1	C	44	LEU
1	C	82	LEU
1	C	167	LEU
1	C	186	PHE
1	C	197	ARG
1	C	229	HIS
1	C	232	MET
1	C	245	ARG
1	C	260	GLN
1	D	16	LYS
1	D	20	LEU
1	D	27	ASN
1	D	30	HIS
1	D	121	LYS
1	D	186	PHE
1	D	193	LEU
1	D	243	MET
1	D	245	ARG
1	D	254	LEU
1	D	260	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	4	HIS
1	A	30	HIS
1	A	96	ASN
1	A	117	GLN
1	A	204	GLN
1	A	229	HIS
1	A	260	GLN
1	A	278	ASN

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Mol	Chain	Res	Type
1	B	27	ASN
1	B	30	HIS
1	B	96	ASN
1	B	249	HIS
1	B	260	GLN
1	B	278	ASN
1	B	281	GLN
1	C	4	HIS
1	C	30	HIS
1	C	96	ASN
1	C	117	GLN
1	C	260	GLN
1	C	271	ASN
1	C	278	ASN
1	C	281	GLN
1	D	4	HIS
1	D	27	ASN
1	D	30	HIS
1	D	96	ASN
1	D	204	GLN
1	D	249	HIS
1	D	260	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PYR	A	2105	2	5,5,5	1.30	0	3,6,6	1.91	1 (33%)
3	PYR	C	2305	2	5,5,5	1.51	1 (20%)	3,6,6	1.75	1 (33%)
3	PYR	B	2205	2	5,5,5	1.47	1 (20%)	3,6,6	1.90	1 (33%)
3	PYR	D	2405	2	5,5,5	1.40	0	3,6,6	1.85	1 (33%)
4	SIN	A	2106	-	7,7,7	1.11	0	8,8,8	1.14	0
4	SIN	D	2406	-	7,7,7	1.24	0	8,8,8	1.22	0
4	SIN	B	2206	-	7,7,7	1.14	0	8,8,8	1.21	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	PYR	A	2105	2	-	0/4/4/4	-
3	PYR	C	2305	2	-	0/4/4/4	-
3	PYR	B	2205	2	-	0/4/4/4	-
3	PYR	D	2405	2	-	0/4/4/4	-
4	SIN	A	2106	-	-	2/5/5/5	-
4	SIN	D	2406	-	-	1/5/5/5	-
4	SIN	B	2206	-	-	3/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2205	PYR	OXT-C	-2.16	1.24	1.30
3	C	2305	PYR	O-C	2.01	1.28	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2105	PYR	OXT-C-CA	3.01	122.21	113.97
3	B	2205	PYR	OXT-C-CA	3.01	122.19	113.97
3	D	2405	PYR	OXT-C-CA	2.91	121.93	113.97
3	C	2305	PYR	OXT-C-CA	2.69	121.34	113.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2106	SIN	C1-C2-C3-C4
4	D	2406	SIN	C1-C2-C3-C4
4	B	2206	SIN	C1-C2-C3-C4
4	B	2206	SIN	O2-C1-C2-C3
4	A	2106	SIN	O1-C1-C2-C3
4	B	2206	SIN	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

## 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	288/295 (97%)	-0.36	2 (0%) 87   88	10, 19, 31, 41	0
1	B	286/295 (96%)	-0.50	0 100   100	11, 18, 27, 35	0
1	C	287/295 (97%)	-0.45	1 (0%) 94   94	10, 17, 29, 39	0
1	D	283/295 (95%)	-0.44	5 (1%) 68   71	9, 16, 29, 64	0
All	All	1144/1180 (96%)	-0.44	8 (0%) 87   88	9, 18, 29, 64	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	4.6
1	D	284	GLU	3.9
1	D	283	GLU	3.5
1	A	256	GLN	2.8
1	D	280	TYR	2.8
1	D	285	LYS	2.2
1	C	289	LEU	2.1
1	D	118	VAL	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	SIN	A	2106	8/8	0.90	0.16	30,37,38,40	0
4	SIN	B	2206	8/8	0.90	0.13	22,26,28,30	0
4	SIN	D	2406	8/8	0.92	0.13	18,22,26,29	0
3	PYR	A	2105	6/6	0.96	0.13	14,16,17,17	0
3	PYR	D	2405	6/6	0.97	0.07	12,13,14,15	0
3	PYR	C	2305	6/6	0.97	0.07	16,18,18,19	0
3	PYR	B	2205	6/6	0.98	0.10	13,16,16,16	0
2	MG	B	2201	1/1	0.98	0.05	15,15,15,15	0
2	MG	D	2401	1/1	0.99	0.06	14,14,14,14	0
2	MG	A	2101	1/1	0.99	0.04	15,15,15,15	0
2	MG	C	2301	1/1	1.00	0.02	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.