



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 01:31 AM EST

PDB ID : 1OTG
Title : 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE
Authors : Subramanya, H.S.; Roper, D.I.; Dauter, Z.; Dodson, E.J.; Davies, G.J.; Wilson, K.S.; Wigley, D.B.
Deposited on : 1995-11-09
Resolution : 2.10 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

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>.

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

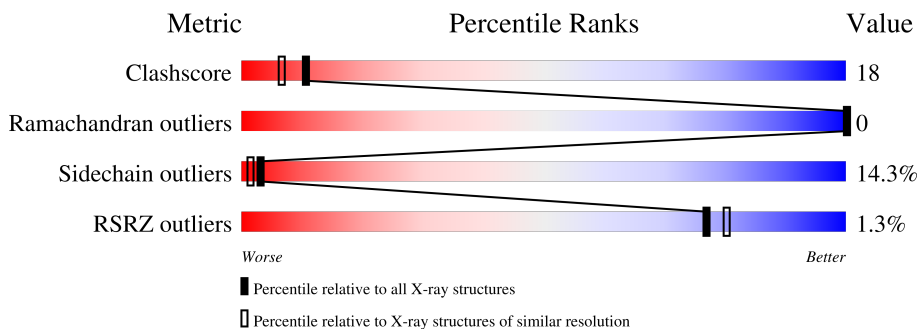
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	125	 2% 55% 31% 12%
1	B	125	 2% 48% 36% 13%
1	C	125	 % 59% 27% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3227 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.

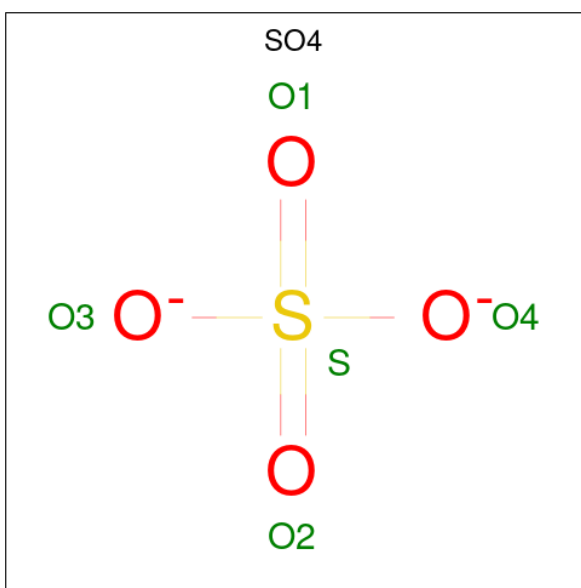
- Molecule 1 is a protein called 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	125	997	640	174	178	5	0	0	0
1	B	125	997	640	174	178	5	0	0	0
1	C	125	997	640	174	178	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	PHE	SER	conflict	UNP Q05354
B	61	PHE	SER	conflict	UNP Q05354
C	61	PHE	SER	conflict	UNP Q05354

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

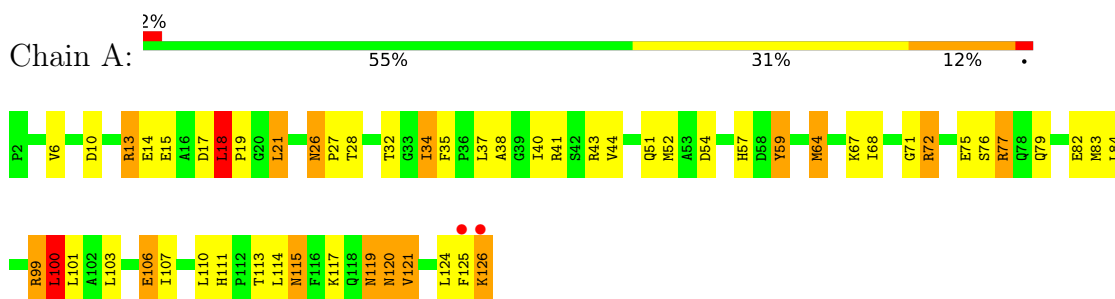
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	64	Total	O	0	0
			64	64		
3	C	80	Total	O	0	0
			80	80		

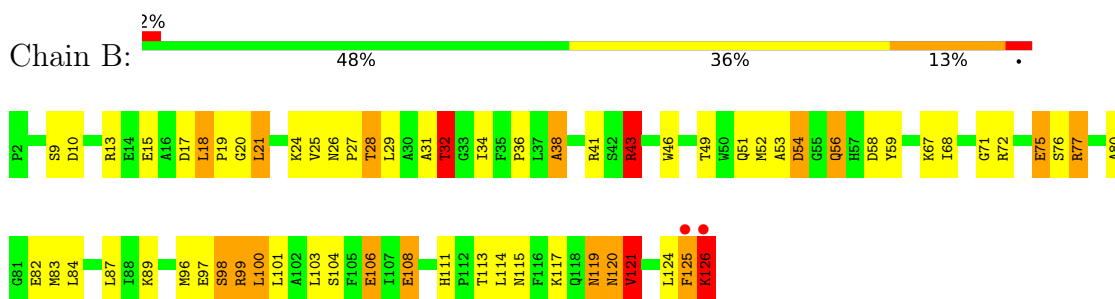
3 Residue-property plots [i](#)

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.

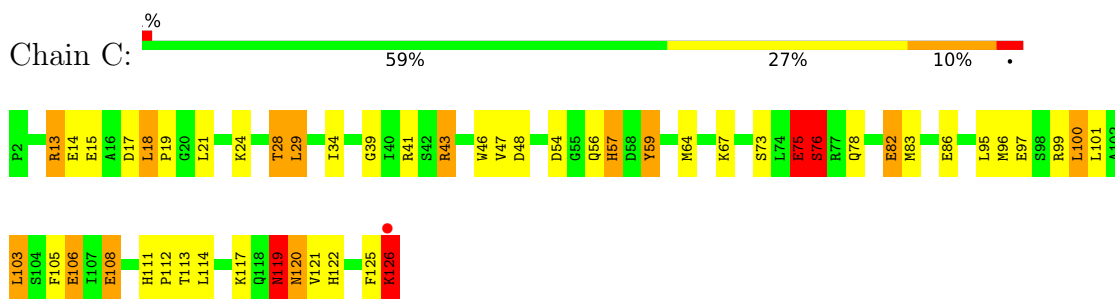
- Molecule 1: 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE



- Molecule 1: 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE



- Molecule 1: 5-CARBOXYMETHYL-2-HYDROXYMUCONATE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.30Å 90.30Å 129.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.10) 89.6 (19.95-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.09Å)	Xtrriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 92.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3227	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4

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	0.92	0/1022	2.18	38/1382 (2.7%)
1	B	1.00	0/1022	2.28	56/1382 (4.1%)
1	C	0.98	0/1022	1.98	30/1382 (2.2%)
All	All	0.97	0/3066	2.15	124/4146 (3.0%)

There are no bond length outliers.

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	NE-CZ-NH2	-20.49	110.06	120.30
1	A	99	ARG	NE-CZ-NH1	19.02	129.81	120.30
1	B	99	ARG	NE-CZ-NH2	-18.26	111.17	120.30
1	B	77	ARG	NE-CZ-NH1	15.26	127.93	120.30
1	B	10	ASP	CB-CG-OD2	-12.26	107.27	118.30
1	B	41	ARG	NE-CZ-NH2	-12.07	114.27	120.30
1	A	41	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	B	99	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	C	99	ARG	NE-CZ-NH1	-11.04	114.78	120.30
1	B	10	ASP	CB-CG-OD1	10.88	128.09	118.30
1	C	75	GLU	CB-CG-CD	10.82	143.41	114.20
1	B	41	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	C	106	GLU	CG-CD-OE2	-10.44	97.43	118.30
1	C	48	ASP	CB-CG-OD1	10.39	127.66	118.30
1	B	54	ASP	CB-CG-OD1	10.15	127.44	118.30
1	C	106	GLU	CG-CD-OE1	10.02	138.34	118.30
1	A	77	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	A	54	ASP	CB-CG-OD1	8.94	126.35	118.30
1	B	43	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	13	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	79	GLN	CA-CB-CG	8.37	131.80	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ARG	CD-NE-CZ	-8.05	112.33	123.60
1	A	15	GLU	CG-CD-OE2	8.00	134.30	118.30
1	A	10	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	17	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	C	14	GLU	CG-CD-OE1	7.55	133.41	118.30
1	B	72	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	76	SER	CB-CA-C	-7.48	95.88	110.10
1	A	106	GLU	OE1-CD-OE2	7.47	132.26	123.30
1	C	97	GLU	CG-CD-OE1	7.46	133.22	118.30
1	C	99	ARG	NH1-CZ-NH2	7.12	127.23	119.40
1	C	18	LEU	CA-CB-CG	-7.03	99.14	115.30
1	C	75	GLU	OE1-CD-OE2	-6.87	115.05	123.30
1	B	20	GLY	CA-C-O	-6.75	108.46	120.60
1	C	59	TYR	CB-CG-CD2	6.63	124.97	121.00
1	C	17	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	76	SER	CB-CA-C	-6.53	97.69	110.10
1	B	18	LEU	CB-CA-C	6.45	122.46	110.20
1	A	51	GLN	N-CA-CB	6.44	122.19	110.60
1	A	71	GLY	CA-C-O	-6.42	109.04	120.60
1	C	41	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	64	MET	CA-CB-CG	-6.38	102.44	113.30
1	A	14	GLU	CG-CD-OE1	6.38	131.06	118.30
1	A	72	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	18	LEU	CA-CB-CG	-6.35	100.70	115.30
1	B	75	GLU	CG-CD-OE1	6.26	130.81	118.30
1	B	99	ARG	CD-NE-CZ	6.26	132.36	123.60
1	A	115	ASN	CA-CB-CG	-6.25	99.65	113.40
1	B	52	MET	CG-SD-CE	-6.24	90.21	100.20
1	A	106	GLU	CG-CD-OE2	-6.12	106.06	118.30
1	C	41	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	48	ASP	OD1-CG-OD2	-6.09	111.72	123.30
1	B	97	GLU	CA-CB-CG	6.07	126.74	113.40
1	A	72	ARG	CA-CB-CG	-6.03	100.14	113.40
1	B	121	VAL	CA-CB-CG1	6.01	119.92	110.90
1	B	59	TYR	CA-CB-CG	5.98	124.76	113.40
1	C	43	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	C	59	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	B	77	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	14	GLU	CG-CD-OE2	-5.94	106.42	118.30
1	C	126	LYS	CA-CB-CG	5.94	126.46	113.40
1	A	72	ARG	CB-CA-C	5.93	122.25	110.40
1	B	126	LYS	CA-C-O	-5.90	107.71	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ARG	CD-NE-CZ	5.87	131.81	123.60
1	A	115	ASN	OD1-CG-ND2	5.86	135.38	121.90
1	B	52	MET	CA-CB-CG	-5.86	103.34	113.30
1	A	17	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	75	GLU	CG-CD-OE2	-5.84	106.62	118.30
1	B	108	GLU	CA-CB-CG	5.83	126.23	113.40
1	A	13	ARG	NH1-CZ-NH2	5.81	125.80	119.40
1	B	117	LYS	CA-CB-CG	-5.81	100.61	113.40
1	B	125	PHE	CB-CA-C	5.80	122.00	110.40
1	C	82	GLU	CB-CA-C	-5.79	98.82	110.40
1	A	15	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	A	21	LEU	CA-CB-CG	5.74	128.49	115.30
1	B	32	THR	N-CA-CB	-5.72	99.43	110.30
1	B	31	ALA	C-N-CA	5.69	135.93	121.70
1	B	82	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	B	17	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	32	THR	O-C-N	-5.63	113.62	123.20
1	A	13	ARG	CB-CG-CD	-5.62	96.99	111.60
1	A	100	LEU	N-CA-CB	-5.59	99.22	110.40
1	B	89	LYS	CA-CB-CG	5.58	125.68	113.40
1	A	99	ARG	O-C-N	5.57	131.61	122.70
1	B	31	ALA	O-C-N	-5.57	113.79	122.70
1	A	82	GLU	CG-CD-OE1	-5.56	107.18	118.30
1	B	98	SER	CA-C-O	-5.56	108.43	120.10
1	C	15	GLU	CG-CD-OE2	-5.54	107.22	118.30
1	B	51	GLN	N-CA-CB	5.54	120.57	110.60
1	A	40	ILE	CA-CB-CG1	5.49	121.43	111.00
1	C	108	GLU	CB-CA-C	-5.48	99.44	110.40
1	A	115	ASN	N-CA-CB	-5.48	100.74	110.60
1	B	56	GLN	CB-CG-CD	-5.44	97.44	111.60
1	B	67	LYS	N-CA-CB	5.42	120.35	110.60
1	C	119	ASN	O-C-N	-5.36	114.12	122.70
1	B	115	ASN	N-CA-CB	-5.35	100.96	110.60
1	B	20	GLY	O-C-N	5.34	131.25	122.70
1	B	106	GLU	CB-CG-CD	5.34	128.61	114.20
1	B	15	GLU	N-CA-CB	5.32	120.17	110.60
1	C	97	GLU	CB-CA-C	-5.31	99.78	110.40
1	B	9	SER	N-CA-CB	5.29	118.44	110.50
1	B	82	GLU	CB-CA-C	-5.29	99.83	110.40
1	B	72	ARG	CA-CB-CG	-5.25	101.86	113.40
1	C	86	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	B	71	GLY	CA-C-O	-5.24	111.17	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	GLY	CA-C-O	-5.22	111.21	120.60
1	B	117	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	B	36	PRO	N-CD-CG	-5.20	95.39	103.20
1	B	84	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	A	76	SER	N-CA-CB	-5.19	102.71	110.50
1	B	56	GLN	CA-CB-CG	-5.14	102.09	113.40
1	B	32	THR	CA-C-O	5.14	130.89	120.10
1	A	59	TYR	CB-CG-CD2	5.10	124.06	121.00
1	B	18	LEU	CB-CG-CD1	5.10	119.66	111.00
1	C	57	HIS	O-C-N	5.10	130.85	122.70
1	A	10	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	14	GLU	CG-CD-OE2	-5.06	108.18	118.30
1	C	29	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	56	GLN	N-CA-CB	-5.03	101.54	110.60
1	B	38	ALA	CB-CA-C	5.03	117.64	110.10
1	C	13	ARG	CA-CB-CG	-5.02	102.36	113.40
1	A	84	LEU	CB-CA-C	5.01	119.73	110.20
1	A	52	MET	O-C-N	-5.01	114.69	122.70
1	B	76	SER	N-CA-CB	5.01	118.01	110.50

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	997	0	982	41	0
1	B	997	0	982	42	0
1	C	997	0	982	41	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	57	0	0	0	0
3	B	64	0	0	1	0
3	C	80	0	0	2	0
All	All	3227	0	2946	110	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 18.

All (110) 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:B:54:ASP:OD1	1:B:56:GLN:HB2	1.51	1.09
1:A:111:HIS:CD2	1:A:114:LEU:H	1.89	0.91
1:C:126:LYS:HE2	1:C:126:LYS:C	1.93	0.88
1:A:120:ASN:HD21	1:B:100:LEU:HA	1.40	0.85
1:C:24:LYS:O	1:C:28:THR:HG23	1.79	0.82
1:B:106:GLU:OE1	3:B:139:HOH:O	1.97	0.81
1:B:125:PHE:O	1:B:126:LYS:HE3	1.81	0.80
1:A:111:HIS:HD2	1:A:114:LEU:H	1.27	0.80
1:A:6:VAL:HG22	1:A:64:MET:HG2	1.66	0.78
1:A:28:THR:HG22	1:A:83:MET:HE1	1.66	0.78
1:C:119:ASN:HD21	1:C:121:VAL:HG13	1.49	0.77
1:B:54:ASP:CG	1:B:56:GLN:HB2	2.05	0.77
1:C:111:HIS:CD2	1:C:114:LEU:H	2.03	0.77
1:B:120:ASN:HD21	1:C:100:LEU:HA	1.51	0.76
1:A:111:HIS:CD2	1:A:113:THR:H	2.04	0.76
1:A:126:LYS:HE2	1:A:126:LYS:C	2.06	0.76
1:B:24:LYS:O	1:B:28:THR:HG23	1.86	0.74
1:B:32:THR:HG22	1:B:34:ILE:H	1.55	0.72
1:C:126:LYS:C	1:C:126:LYS:CE	2.58	0.71
1:A:106:GLU:HG2	1:A:107:ILE:N	2.04	0.71
1:A:111:HIS:HD2	1:A:113:THR:H	1.38	0.71
1:A:28:THR:HG22	1:A:83:MET:CE	2.20	0.70
1:A:68:ILE:HD11	1:A:77:ARG:HD3	1.72	0.70
1:C:111:HIS:HD2	1:C:113:THR:H	1.39	0.70
1:C:119:ASN:ND2	1:C:121:VAL:HG13	2.07	0.69
1:C:96:MET:CE	1:C:103:LEU:HD22	2.24	0.68
1:B:32:THR:CG2	1:B:34:ILE:HB	2.24	0.68
1:C:111:HIS:CD2	1:C:113:THR:H	2.13	0.67
1:C:78:GLN:O	1:C:82:GLU:HG3	1.94	0.66
1:A:26:ASN:HB2	1:A:27:PRO:HD3	1.77	0.66
1:B:38:ALA:HB2	1:B:125:PHE:CD2	2.32	0.65
1:C:57:HIS:HD2	1:C:59:TYR:OH	1.78	0.65
1:C:111:HIS:HD2	1:C:114:LEU:H	1.44	0.64
1:A:38:ALA:HB2	1:A:125:PHE:CD1	2.35	0.61
1:A:100:LEU:HA	1:C:120:ASN:HD21	1.64	0.61
1:B:18:LEU:N	1:B:19:PRO:CD	2.64	0.60
1:A:37:LEU:HD21	1:B:54:ASP:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:CG2	1:B:34:ILE:H	2.16	0.58
1:A:125:PHE:O	1:A:126:LYS:HD3	2.03	0.58
1:B:111:HIS:HD2	1:B:113:THR:H	1.51	0.58
1:B:24:LYS:O	1:B:28:THR:CG2	2.52	0.57
1:A:32:THR:OG1	1:A:34:ILE:HG13	2.05	0.56
1:B:111:HIS:HD2	1:B:114:LEU:H	1.53	0.56
1:B:120:ASN:C	1:B:120:ASN:HD22	2.09	0.56
1:C:13:ARG:HG3	1:C:46:TRP:CH2	2.40	0.56
1:B:111:HIS:CD2	1:B:114:LEU:H	2.24	0.55
1:A:26:ASN:HD22	1:A:26:ASN:N	2.05	0.55
1:A:67:LYS:NZ	1:B:108:GLU:OE2	2.38	0.55
1:B:21:LEU:HD22	1:B:25:VAL:HG23	1.87	0.54
1:C:13:ARG:O	1:C:13:ARG:HG2	2.05	0.54
1:A:121:VAL:HG23	1:A:125:PHE:HE1	1.71	0.54
1:A:101:LEU:H	1:C:120:ASN:HD21	1.56	0.54
1:C:24:LYS:O	1:C:28:THR:CG2	2.52	0.53
1:B:111:HIS:CD2	1:B:113:THR:H	2.27	0.53
1:C:18:LEU:N	1:C:19:PRO:CD	2.71	0.53
1:C:96:MET:HE3	1:C:103:LEU:HD22	1.90	0.52
1:C:122:HIS:O	1:C:126:LYS:HB3	2.09	0.52
1:A:68:ILE:C	1:A:110:LEU:HD12	2.30	0.51
1:A:26:ASN:CB	1:A:27:PRO:HD3	2.40	0.50
1:A:34:ILE:HD12	1:A:35:PHE:CZ	2.47	0.50
1:A:120:ASN:HD21	1:B:101:LEU:H	1.58	0.49
1:B:29:LEU:O	1:B:32:THR:HB	2.11	0.49
1:C:54:ASP:OD1	1:C:56:GLN:HB2	2.12	0.49
1:A:120:ASN:ND2	1:B:101:LEU:H	2.10	0.49
1:C:75:GLU:HB2	3:C:198:HOH:O	2.12	0.48
1:C:120:ASN:C	1:C:120:ASN:HD22	2.17	0.48
1:B:96:MET:HG2	1:B:101:LEU:HD23	1.95	0.48
1:B:119:ASN:HD22	1:B:121:VAL:H	1.62	0.48
1:C:119:ASN:ND2	1:C:121:VAL:H	2.12	0.48
1:B:18:LEU:HD12	1:B:46:TRP:CH2	2.48	0.48
1:A:13:ARG:HH11	1:A:13:ARG:HD2	1.44	0.47
1:A:101:LEU:H	1:C:120:ASN:ND2	2.13	0.47
1:A:18:LEU:N	1:A:19:PRO:CD	2.76	0.47
1:B:119:ASN:ND2	1:B:121:VAL:H	2.12	0.47
1:C:34:ILE:HD11	3:C:144:HOH:O	2.15	0.47
1:C:73:SER:O	1:C:76:SER:HB2	2.14	0.47
1:B:34:ILE:HG21	1:B:34:ILE:HD13	1.50	0.46
1:C:67:LYS:HA	1:C:108:GLU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ALA:HB2	1:B:125:PHE:HD2	1.81	0.46
1:C:96:MET:HE1	1:C:101:LEU:HD23	1.98	0.46
1:C:126:LYS:C	1:C:126:LYS:NZ	2.71	0.44
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.85	0.44
1:C:13:ARG:HH11	1:C:13:ARG:HD3	1.65	0.44
1:A:28:THR:HG22	1:A:83:MET:HE3	1.98	0.44
1:A:111:HIS:HD2	1:A:113:THR:N	2.09	0.43
1:A:57:HIS:HD2	1:A:59:TYR:OH	2.01	0.43
1:A:34:ILE:O	1:A:72:ARG:NH1	2.52	0.43
1:A:121:VAL:HG23	1:A:125:PHE:CE1	2.52	0.43
1:B:80:ALA:HA	1:B:83:MET:HE3	2.01	0.43
1:C:125:PHE:O	1:C:126:LYS:C	2.57	0.42
1:B:119:ASN:ND2	1:B:121:VAL:HG13	2.34	0.42
1:B:120:ASN:ND2	1:C:101:LEU:H	2.17	0.42
1:B:58:ASP:O	1:B:99:ARG:NH2	2.52	0.42
1:A:119:ASN:C	1:A:119:ASN:HD22	2.22	0.42
1:A:120:ASN:HD22	1:A:120:ASN:C	2.23	0.42
1:A:34:ILE:HD12	1:A:35:PHE:CE2	2.55	0.42
1:B:126:LYS:HE3	1:B:126:LYS:C	2.40	0.42
1:B:43:ARG:HB2	1:C:47:VAL:HG11	2.02	0.41
1:C:13:ARG:HG3	1:C:46:TRP:CZ3	2.55	0.41
1:B:68:ILE:HD11	1:B:77:ARG:HD3	2.02	0.41
1:B:26:ASN:N	1:B:27:PRO:CD	2.84	0.41
1:C:95:LEU:HD23	1:C:95:LEU:HA	1.85	0.41
1:B:43:ARG:HB2	1:C:47:VAL:CG1	2.50	0.41
1:C:111:HIS:HA	1:C:112:PRO:HD3	1.89	0.41
1:A:44:VAL:CG1	1:B:49:THR:HB	2.51	0.41
1:A:37:LEU:O	1:B:53:ALA:HA	2.21	0.41
1:A:106:GLU:CG	1:A:107:ILE:N	2.79	0.40
1:C:64:MET:O	1:C:105:PHE:HA	2.22	0.40
1:C:111:HIS:HD2	1:C:113:THR:N	2.14	0.40
1:A:121:VAL:O	1:A:124:LEU:HB2	2.22	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	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	B	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	C	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
All	All	369/375 (98%)	360 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	105/105 (100%)	90 (86%)	15 (14%)	3	1
1	B	105/105 (100%)	89 (85%)	16 (15%)	3	1
1	C	105/105 (100%)	91 (87%)	14 (13%)	4	2
All	All	315/315 (100%)	270 (86%)	45 (14%)	3	1

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	21	LEU
1	A	26	ASN
1	A	34	ILE
1	A	43	ARG
1	A	75	GLU
1	A	99	ARG
1	A	100	LEU
1	A	103	LEU
1	A	115	ASN
1	A	117	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	119	ASN
1	A	120	ASN
1	A	121	VAL
1	A	126	LYS
1	B	13	ARG
1	B	21	LEU
1	B	28	THR
1	B	32	THR
1	B	43	ARG
1	B	75	GLU
1	B	87	LEU
1	B	98	SER
1	B	100	LEU
1	B	103	LEU
1	B	104	SER
1	B	119	ASN
1	B	120	ASN
1	B	121	VAL
1	B	124	LEU
1	B	126	LYS
1	C	21	LEU
1	C	28	THR
1	C	29	LEU
1	C	43	ARG
1	C	75	GLU
1	C	76	SER
1	C	83	MET
1	C	100	LEU
1	C	103	LEU
1	C	106	GLU
1	C	117	LYS
1	C	119	ASN
1	C	120	ASN
1	C	126	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	57	HIS
1	A	111	HIS
1	A	119	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	ASN
1	B	57	HIS
1	B	111	HIS
1	B	115	ASN
1	B	118	GLN
1	B	119	ASN
1	B	120	ASN
1	C	57	HIS
1	C	111	HIS
1	C	118	GLN
1	C	119	ASN
1	C	120	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 monosaccharides 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	$\# Z > 2$
2	SO4	C	128	-	4,4,4	0.60	0	6,6,6	0.75	0
2	SO4	B	128	-	4,4,4	0.46	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	127	-	4,4,4	0.88	0	6,6,6	0.28	0
2	SO4	B	127	-	4,4,4	0.68	0	6,6,6	0.39	0
2	SO4	A	128	-	4,4,4	0.76	0	6,6,6	0.91	0
2	SO4	A	1	-	4,4,4	0.86	0	6,6,6	0.74	0
2	SO4	C	127	-	4,4,4	0.86	0	6,6,6	0.72	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	125/125 (100%)	-0.58	2 (1%) 72 75	18, 30, 55, 74	0
1	B	125/125 (100%)	-0.59	2 (1%) 72 75	19, 28, 51, 68	0
1	C	125/125 (100%)	-0.78	1 (0%) 86 88	15, 26, 45, 64	0
All	All	375/375 (100%)	-0.65	5 (1%) 77 80	15, 28, 52, 74	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	LYS	3.7
1	B	126	LYS	3.3
1	B	125	PHE	3.2
1	C	126	LYS	3.1
1	A	125	PHE	2.3

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, 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	B-factors(\AA^2)	Q<0.9
2	SO4	A	127	5/5	0.92	0.16	99,99,99,99	0
2	SO4	A	1	5/5	0.97	0.09	72,72,72,72	0
2	SO4	A	128	5/5	0.97	0.09	62,62,63,63	0
2	SO4	B	127	5/5	0.98	0.09	45,46,47,47	0
2	SO4	B	128	5/5	0.98	0.12	50,50,50,51	0
2	SO4	C	127	5/5	0.98	0.07	48,49,49,50	0
2	SO4	C	128	5/5	0.99	0.10	41,42,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.