



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:00 am BST

PDB ID : 3MB2
Title : Kinetic and Structural Characterization of a Heterohexamer 4-Oxalocrotonate Tautomerase from *Chloroflexus aurantiacus* J-10-fl: Implications for Functional and Structural Diversity in the Tautomerase Superfamily
Authors : Burks, E.A.; Fleming, C.D.; Mesecar, A.D.; Whitman, C.P.; Pegan, S.D.
Deposited on : 2010-03-24
Resolution : 2.41 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 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 : 2.11
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) : 2.11

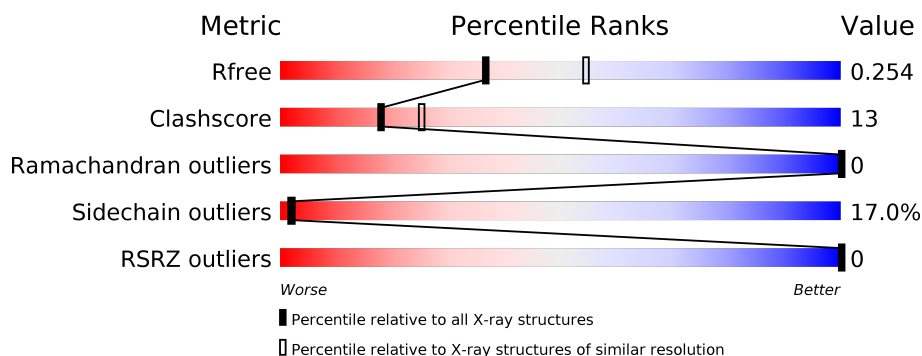
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 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	72	<div> <div>53%</div> <div>25%</div> <div>6%</div> <div>•</div> <div>15%</div> </div>
1	C	72	<div> <div>61%</div> <div>18%</div> <div>7%</div> <div></div> <div>14%</div> </div>
1	E	72	<div> <div>54%</div> <div>19%</div> <div>7%</div> <div>•</div> <div>15%</div> </div>
1	G	72	<div> <div>53%</div> <div>18%</div> <div>11%</div> <div>•</div> <div>15%</div> </div>
1	I	72	<div> <div>54%</div> <div>24%</div> <div>•</div> <div>•</div> <div>17%</div> </div>
1	K	72	<div> <div>57%</div> <div>19%</div> <div>10%</div> <div></div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	72	
2	D	72	
2	F	72	
2	H	72	
2	J	72	
2	L	72	

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	SO4	C	73	-	-	X	-
3	SO4	C	74	-	-	X	-
3	SO4	C	75	-	-	X	-
3	SO4	I	74	-	-	X	-
3	SO4	K	74	-	-	X	-
3	SO4	L	73	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5781 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 4-oxalocrotonate tautomerase family enzyme - alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	S	0	0	0
			458	292	79	84	3			
1	C	62	Total	C	N	O	S	0	0	0
			469	298	83	85	3			
1	E	61	Total	C	N	O	S	0	0	0
			458	292	79	84	3			
1	G	61	Total	C	N	O	S	0	0	0
			458	292	79	84	3			
1	I	60	Total	C	N	O	S	0	0	0
			450	286	78	83	3			
1	K	62	Total	C	N	O	S	0	0	0
			469	298	83	85	3			

- Molecule 2 is a protein called 4-oxalocrotonate tautomerase family enzyme - beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	59	Total	C	N	O	S	0	0	0
			459	293	80	85	1			
2	D	58	Total	C	N	O	S	0	1	0
			460	294	80	85	1			
2	F	54	Total	C	N	O	S	0	1	0
			427	272	76	78	1			
2	H	58	Total	C	N	O	S	0	0	0
			451	289	79	82	1			
2	J	59	Total	C	N	O	S	0	1	0
			468	298	81	88	1			
2	L	54	Total	C	N	O	S	0	0	0
			420	268	75	76	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

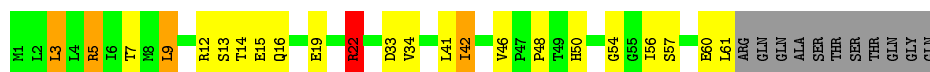
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	21	Total	O	0	0
			21	21		
4	C	27	Total	O	0	0
			27	27		
4	D	23	Total	O	0	0
			23	23		
4	E	8	Total	O	0	0
			8	8		
4	F	26	Total	O	0	0
			26	26		
4	G	14	Total	O	0	0
			14	14		
4	H	21	Total	O	0	0
			21	21		
4	I	28	Total	O	0	0
			28	28		
4	J	22	Total	O	0	0
			22	22		
4	K	17	Total	O	0	0
			17	17		
4	L	26	Total	O	0	0
			26	26		

3 Residue-property plots [i](#)

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

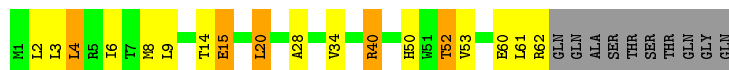
- Molecule 1: 4-oxalocrotonate tautomerase family enzyme - alpha subunit

Chain A: 



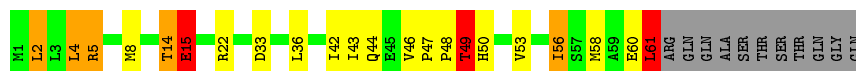
- Molecule 1: 4-oxalocrotonate tautomerase family enzyme - alpha subunit

Chain C: 



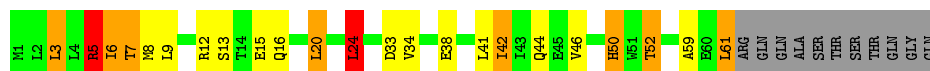
- Molecule 1: 4-oxalocrotonate tautomerase family enzyme - alpha subunit

Chain E: 



- Molecule 1: 4-oxalocrotonate tautomerase family enzyme - alpha subunit

Chain G: 



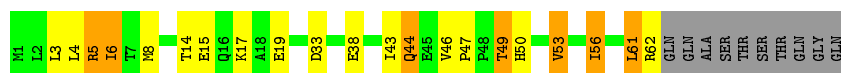
- Molecule 1: 4-oxalocrotonate tautomerase family enzyme - alpha subunit

Chain I: 



- Molecule 1: 4-oxalocrotonate tautomerase family enzyme - alpha subunit

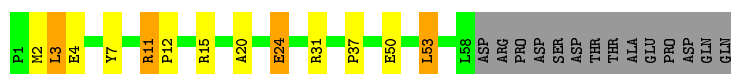
Chain K: 



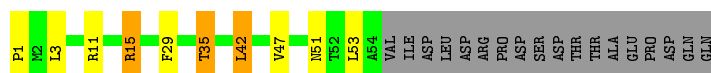
- Molecule 2: 4-oxalocrotonate tautomerase family enzyme - beta subunit



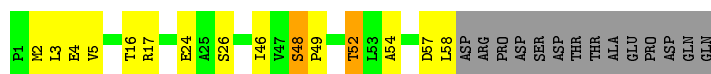
- Molecule 2: 4-oxalocrotonate tautomerase family enzyme - beta subunit



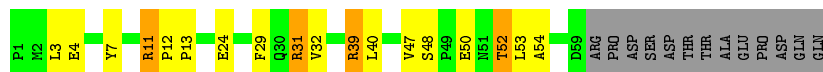
- Molecule 2: 4-oxalocrotonate tautomerase family enzyme - beta subunit



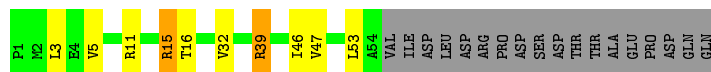
- Molecule 2: 4-oxalocrotonate tautomerase family enzyme - beta subunit



- Molecule 2: 4-oxalocrotonate tautomerase family enzyme - beta subunit



- Molecule 2: 4-oxalocrotonate tautomerase family enzyme - beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	106.06Å 106.06Å 109.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.85 – 2.41 47.77 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.6 (91.85-2.41) 98.6 (47.77-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.203 , 0.250 0.209 , 0.254	Depositor DCC
R_{free} test set	2670 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 20.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.477 for h,-h-k,-l 0.006 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5781	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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

5.1 Standard geometry

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	1.13	2/464 (0.4%)	1.32	8/630 (1.3%)
1	C	1.13	2/475 (0.4%)	1.19	4/644 (0.6%)
1	E	1.13	1/464 (0.2%)	1.27	6/630 (1.0%)
1	G	1.12	2/464 (0.4%)	1.18	6/630 (1.0%)
1	I	1.20	2/456 (0.4%)	1.09	2/619 (0.3%)
1	K	1.09	1/475 (0.2%)	1.26	4/644 (0.6%)
2	B	1.12	0/468	1.02	1/636 (0.2%)
2	D	1.24	2/469 (0.4%)	1.21	4/637 (0.6%)
2	F	1.11	0/436	1.03	1/593 (0.2%)
2	H	1.10	0/460	0.98	1/625 (0.2%)
2	J	1.21	2/477 (0.4%)	1.03	2/648 (0.3%)
2	L	1.16	0/429	1.07	1/582 (0.2%)
All	All	1.15	14/5537 (0.3%)	1.14	40/7518 (0.5%)

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
2	D	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	GLU	CG-CD	7.12	1.62	1.51
1	E	15	GLU	CB-CG	6.94	1.65	1.52
1	A	15	GLU	CB-CG	6.87	1.65	1.52
1	G	38	GLU	CG-CD	6.68	1.61	1.51
1	A	15	GLU	CG-CD	6.64	1.61	1.51
2	D	24	GLU	CG-CD	6.07	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	24	GLU	CD-OE2	5.83	1.32	1.25
2	J	24	GLU	CG-CD	5.79	1.60	1.51
1	I	15	GLU	CG-CD	5.62	1.60	1.51
1	C	15	GLU	CB-CG	5.62	1.62	1.52
1	K	15	GLU	CG-CD	5.59	1.60	1.51
1	I	18	ALA	CA-CB	5.46	1.64	1.52
2	J	24	GLU	CD-OE2	5.34	1.31	1.25
1	G	15	GLU	CG-CD	5.10	1.59	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	31	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	E	5	ARG	NE-CZ-NH2	-12.71	113.95	120.30
1	K	5	ARG	NE-CZ-NH2	-12.07	114.27	120.30
2	D	31	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	K	5	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	E	5	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	5	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	A	5	ARG	NE-CZ-NH2	-9.01	115.80	120.30
2	J	31	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	C	40	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	A	22	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	K	61	LEU	CA-CB-CG	7.57	132.72	115.30
2	J	31	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	12	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	22	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	I	41	LEU	CA-CB-CG	6.84	131.02	115.30
1	A	3	LEU	CA-CB-CG	6.71	130.73	115.30
2	F	42	LEU	CB-CG-CD2	6.44	121.94	111.00
1	G	12	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	D	3	LEU	CB-CG-CD2	6.07	121.31	111.00
1	G	5	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	G	12	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	D	53	LEU	CA-CB-CG	6.01	129.12	115.30
1	E	61	LEU	CA-CB-CG	5.85	128.76	115.30
1	G	24	LEU	CA-CB-CG	5.62	128.22	115.30
1	C	61	LEU	CA-CB-CG	5.59	128.17	115.30
1	E	2	LEU	CB-CG-CD2	5.58	120.48	111.00
1	E	49	THR	N-CA-CB	-5.54	99.77	110.30
1	C	20	LEU	CB-CG-CD1	5.53	120.40	111.00
1	C	40	ARG	NE-CZ-NH2	5.52	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	H	57	ASP	CB-CG-OD2	-5.36	113.47	118.30
2	L	39	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	G	3	LEU	CA-CB-CG	5.27	127.42	115.30
1	G	24	LEU	CB-CG-CD1	5.25	119.92	111.00
1	E	22	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	B	31	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	3	LEU	CB-CG-CD1	5.08	119.64	111.00
1	I	20	LEU	CA-CB-CG	5.05	126.92	115.30
1	K	49	THR	N-CA-CB	-5.04	100.72	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	37	PRO	Peptide

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	458	0	483	16	0
1	C	469	0	496	13	0
1	E	458	0	483	15	0
1	G	458	0	483	17	0
1	I	450	0	472	27	0
1	K	469	0	496	22	0
2	B	459	0	471	14	0
2	D	460	0	472	11	0
2	F	427	0	439	9	0
2	H	451	0	467	15	0
2	J	468	0	476	15	0
2	L	420	0	432	6	0
3	A	10	0	0	1	0
3	C	15	0	0	6	0
3	D	5	0	0	1	0
3	E	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	10	0	0	3	0
3	K	10	0	0	5	0
3	L	10	0	0	4	0
4	A	16	0	0	0	0
4	B	21	0	0	0	0
4	C	27	0	0	2	0
4	D	23	0	0	1	0
4	E	8	0	0	0	0
4	F	26	0	0	1	0
4	G	14	0	0	1	0
4	H	21	0	0	1	0
4	I	28	0	0	4	0
4	J	22	0	0	3	0
4	K	17	0	0	2	0
4	L	26	0	0	1	0
All	All	5781	0	5670	151	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 13.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:THR:CG2	3:C:74:SO4:O2	1.83	1.27
1:I:14:THR:HG22	3:I:74:SO4:O4	1.12	1.26
1:C:40:ARG:NH1	3:C:73:SO4:O2	1.75	1.19
1:A:14:THR:HG23	1:I:14:THR:HG23	1.33	1.11
1:A:14:THR:HG22	3:A:74:SO4:O1	1.53	1.07
1:C:14:THR:HG22	3:C:74:SO4:O2	0.89	1.06
1:G:6:ILE:HD11	1:G:8:MET:HB3	1.39	1.05
1:I:14:THR:CG2	3:I:74:SO4:O4	2.08	0.99
1:C:40:ARG:NH1	3:C:73:SO4:S	2.36	0.98
1:I:6:ILE:HG21	1:I:8:MET:HE2	1.44	0.96
2:J:52:THR:HG22	2:J:54:ALA:H	1.31	0.94
2:H:52:THR:HG22	2:H:54:ALA:H	1.33	0.93
2:F:29:PHE:HB3	2:F:35[A]:THR:CG2	2.00	0.92
1:G:5:ARG:HD2	2:J:4:GLU:OE1	1.72	0.88
2:L:39:ARG:NH1	3:L:73:SO4:O2	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HD12	1:A:57:SER:H	1.42	0.85
1:G:13:SER:H	1:G:16:GLN:HE21	1.25	0.84
1:A:13:SER:H	1:A:16:GLN:HE21	1.25	0.83
2:H:2:MET:CE	1:I:42:ILE:HD12	2.08	0.83
2:B:15:ARG:HG2	2:B:15:ARG:HH11	1.44	0.82
1:G:52:THR:HG22	4:K:164:HOH:O	1.79	0.82
2:H:2:MET:CE	1:I:42:ILE:CD1	2.58	0.82
2:H:2:MET:HE1	1:I:42:ILE:HD12	1.60	0.81
2:F:29:PHE:HB3	2:F:35[A]:THR:HG21	1.63	0.79
1:G:52:THR:CG2	4:K:164:HOH:O	2.30	0.78
3:C:75:SO4:O3	2:F:1:PRO:HD3	1.83	0.77
1:K:8:MET:HE1	1:K:17:LYS:HG3	1.66	0.77
1:I:59:ALA:O	1:I:60:GLU:HB2	1.85	0.75
2:B:15:ARG:CG	2:B:15:ARG:HH11	1.99	0.74
3:I:74:SO4:O1	1:K:50:HIS:HE1	1.70	0.73
1:I:6:ILE:CG2	1:I:8:MET:HE2	2.16	0.73
1:C:60:GLU:N	1:C:60:GLU:OE2	2.22	0.73
1:E:49:THR:HG23	1:E:50:HIS:CD2	2.24	0.73
2:L:39:ARG:NH1	3:L:73:SO4:S	2.63	0.70
3:D:73:SO4:O2	4:D:172:HOH:O	2.09	0.70
2:H:5:VAL:HG13	1:K:4:LEU:HD22	1.72	0.69
2:L:39:ARG:NH1	3:L:73:SO4:O3	2.25	0.68
1:A:5:ARG:HD2	2:D:4:GLU:OE1	1.95	0.66
2:J:50[A]:GLU:OE1	4:J:233:HOH:O	2.14	0.65
1:E:49:THR:HG23	1:E:50:HIS:HD2	1.62	0.64
2:F:35[A]:THR:HB	4:F:243:HOH:O	1.98	0.63
1:G:46:VAL:HG13	1:G:50:HIS:HB2	1.79	0.63
3:L:74:SO4:O4	4:L:208:HOH:O	2.13	0.63
1:K:8:MET:HE2	1:K:43:ILE:CG2	2.29	0.62
1:A:56:ILE:HD12	1:A:57:SER:N	2.13	0.62
1:K:47:PRO:HB2	1:K:49:THR:HG22	1.81	0.62
1:A:13:SER:H	1:A:16:GLN:NE2	1.97	0.60
2:H:52:THR:CG2	2:H:54:ALA:H	2.10	0.60
2:L:11:ARG:HG3	2:L:11:ARG:O	2.01	0.60
1:K:46:VAL:HG13	1:K:50:HIS:HB2	1.83	0.60
1:E:53:VAL:O	1:E:56:ILE:HD13	2.02	0.59
3:C:75:SO4:S	2:F:1:PRO:HD3	2.42	0.59
1:K:17:LYS:CE	3:K:74:SO4:O2	2.51	0.59
1:G:13:SER:H	1:G:16:GLN:NE2	1.99	0.59
2:B:18:LYS:HZ2	2:F:51:ASN:HD21	1.52	0.57
2:B:5:VAL:HG13	1:E:4:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLU:HG3	2:D:15:ARG:HH21	1.69	0.57
1:I:6:ILE:HG21	1:I:8:MET:CE	2.26	0.57
2:D:50[B]:GLU:H	2:D:50[B]:GLU:CD	2.08	0.56
2:J:52:THR:CG2	2:J:54:ALA:H	2.13	0.56
1:A:19:GLU:OE1	1:A:22:ARG:NH1	2.38	0.56
1:I:59:ALA:O	1:I:60:GLU:CB	2.55	0.55
1:K:6:ILE:C	1:K:6:ILE:HD13	2.27	0.54
1:K:8:MET:HE2	1:K:43:ILE:HG21	1.89	0.54
2:B:50:GLU:HG3	2:D:15:ARG:HE	1.72	0.54
1:K:17:LYS:HE2	3:K:74:SO4:O2	2.08	0.54
1:K:8:MET:CE	1:K:43:ILE:HG21	2.38	0.53
2:H:26:SER:HB2	4:H:131:HOH:O	2.08	0.53
1:I:12:ARG:HD3	4:I:224:HOH:O	2.09	0.53
1:K:14:THR:OG1	3:K:74:SO4:O1	2.18	0.53
2:H:52:THR:HG22	2:H:54:ALA:N	2.13	0.53
1:I:12:ARG:HB2	4:I:77:HOH:O	2.09	0.53
1:K:6:ILE:HD11	1:K:8:MET:SD	2.50	0.52
1:I:9:LEU:HD11	1:I:58:MET:HG3	1.91	0.52
1:C:52:THR:CG2	4:C:88:HOH:O	2.58	0.52
1:A:46:VAL:HG13	1:A:50:HIS:HB2	1.93	0.52
1:A:9:LEU:HD11	1:A:48:PRO:HA	1.92	0.51
1:K:8:MET:HE2	1:K:43:ILE:HG23	1.93	0.51
1:G:7:THR:HG23	4:J:79:HOH:O	2.10	0.51
2:J:52:THR:CG2	2:J:53:LEU:N	2.74	0.51
2:B:15:ARG:NH1	2:B:15:ARG:CG	2.62	0.51
2:B:18:LYS:NZ	2:F:51:ASN:HD21	2.08	0.50
1:E:15:GLU:OE1	1:K:14:THR:HB	2.10	0.50
2:J:52:THR:HG22	2:J:54:ALA:N	2.12	0.50
2:B:10:ASP:N	2:B:10:ASP:OD1	2.35	0.50
1:A:54:GLY:HA2	1:E:36:LEU:O	2.12	0.49
2:H:2:MET:CE	1:I:42:ILE:HD11	2.42	0.49
1:G:46:VAL:HG13	1:G:50:HIS:CB	2.42	0.49
1:C:4:LEU:HD23	1:C:4:LEU:N	2.28	0.49
2:H:4:GLU:OE1	1:K:5:ARG:HD2	2.13	0.48
2:D:2:MET:HE2	1:E:42:ILE:CD1	2.41	0.48
2:H:2:MET:HE2	1:I:42:ILE:HD11	1.96	0.48
1:E:46:VAL:HG13	1:E:50:HIS:HB2	1.95	0.48
2:B:4:GLU:OE1	1:E:5:ARG:HD2	2.13	0.48
1:I:60:GLU:C	4:I:182:HOH:O	2.51	0.47
1:A:14:THR:HG23	1:I:14:THR:CG2	2.23	0.47
1:I:4:LEU:HD22	2:L:5:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HG21	1:C:8:MET:CE	2.44	0.47
1:E:14:THR:OG1	3:E:74:SO4:O4	2.22	0.47
1:G:41:LEU:HB3	1:I:52:THR:CG2	2.46	0.46
1:K:53:VAL:O	1:K:56:ILE:HD13	2.15	0.46
1:I:4:LEU:O	1:I:41:LEU:HA	2.16	0.46
2:H:2:MET:HE3	1:I:42:ILE:CD1	2.45	0.46
1:I:57:SER:HB3	4:I:116:HOH:O	2.15	0.46
1:K:6:ILE:HD11	1:K:8:MET:CG	2.46	0.46
1:G:20:LEU:O	1:G:24:LEU:HB2	2.16	0.46
1:K:49:THR:HG23	1:K:50:HIS:ND1	2.31	0.46
1:A:7:THR:HB	2:D:2:MET:HE3	1.97	0.45
1:I:6:ILE:CG2	1:I:8:MET:CE	2.90	0.45
2:D:2:MET:CE	1:E:42:ILE:CD1	2.95	0.45
1:K:8:MET:HE1	1:K:17:LYS:CG	2.40	0.45
1:A:42:ILE:HD13	1:A:42:ILE:N	2.33	0.44
1:E:60:GLU:HA	1:E:61:LEU:HA	1.52	0.44
2:H:46:ILE:N	2:H:46:ILE:HD12	2.33	0.44
1:C:3:LEU:C	1:C:4:LEU:HD23	2.38	0.44
1:C:52:THR:HG22	4:C:88:HOH:O	2.17	0.43
2:D:11:ARG:HA	2:D:12:PRO:HD2	1.74	0.43
1:E:49:THR:CG2	1:E:50:HIS:CD2	2.98	0.43
2:J:11:ARG:HA	2:J:12:PRO:HD2	1.90	0.43
1:C:2:LEU:HD21	1:C:28:ALA:HB1	2.00	0.43
2:D:20:ALA:O	2:D:24:GLU:HG3	2.19	0.43
1:G:24:LEU:HD21	2:J:29:PHE:CE2	2.54	0.43
2:J:52:THR:HG23	2:J:53:LEU:N	2.34	0.43
1:G:7:THR:CG2	4:J:79:HOH:O	2.67	0.43
2:J:50[B]:GLU:CD	2:J:50[B]:GLU:H	2.22	0.43
1:K:3:LEU:HD13	1:K:4:LEU:N	2.34	0.42
1:G:42:ILE:N	1:G:42:ILE:CD1	2.82	0.42
2:H:2:MET:HE2	1:I:42:ILE:CD1	2.45	0.42
2:J:50[B]:GLU:HG2	2:L:15:ARG:HH11	1.85	0.42
1:C:6:ILE:HG21	1:C:8:MET:HE1	2.01	0.42
1:A:42:ILE:CD1	1:A:42:ILE:N	2.81	0.42
2:B:56:ILE:HA	2:B:56:ILE:HD13	1.74	0.42
1:G:59:ALA:O	1:G:61:LEU:N	2.51	0.42
2:B:48:SER:HA	2:B:49:PRO:HD3	2.00	0.42
4:G:160:HOH:O	1:I:52:THR:CG2	2.68	0.41
2:B:46:ILE:HD13	2:B:46:ILE:N	2.35	0.41
2:F:29:PHE:HB3	2:F:35[A]:THR:HG23	1.93	0.41
1:E:48:PRO:O	1:E:58:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:LEU:HD13	2:J:32:VAL:HG11	2.02	0.41
1:K:44:GLN:HE21	1:K:44:GLN:HA	1.86	0.41
1:A:41:LEU:HB3	1:C:52:THR:CG2	2.51	0.41
2:J:12:PRO:HA	2:J:13:PRO:HD3	1.97	0.41
2:D:50[B]:GLU:HG2	2:F:15:ARG:NH1	2.36	0.41
2:J:7:TYR:CD2	2:J:7:TYR:C	2.94	0.41
2:B:17:ARG:HH11	2:B:17:ARG:HG2	1.86	0.41
1:E:8:MET:HE3	1:E:43:ILE:HG21	2.03	0.40
1:I:8:MET:HE3	1:I:43:ILE:HG23	2.03	0.40
2:D:7:TYR:C	2:D:7:TYR:CD2	2.94	0.40
1:G:50:HIS:HE1	3:K:74:SO4:O2	2.04	0.40
2:H:48:SER:HA	2:H:49:PRO:HD3	1.94	0.40
2:J:39:ARG:HG2	3:K:73:SO4:O4	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	59/72 (82%)	59 (100%)	0	0	100	100
1	C	60/72 (83%)	58 (97%)	2 (3%)	0	100	100
1	E	59/72 (82%)	57 (97%)	2 (3%)	0	100	100
1	G	59/72 (82%)	57 (97%)	2 (3%)	0	100	100
1	I	58/72 (81%)	57 (98%)	1 (2%)	0	100	100
1	K	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
2	B	57/72 (79%)	56 (98%)	1 (2%)	0	100	100
2	D	57/72 (79%)	55 (96%)	2 (4%)	0	100	100
2	F	53/72 (74%)	53 (100%)	0	0	100	100
2	H	56/72 (78%)	56 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	58/72 (81%)	58 (100%)	0	0	100	100
2	L	52/72 (72%)	52 (100%)	0	0	100	100
All	All	688/864 (80%)	675 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	47/56 (84%)	39 (83%)	8 (17%)	2	2
1	C	48/56 (86%)	39 (81%)	9 (19%)	1	1
1	E	47/56 (84%)	37 (79%)	10 (21%)	1	1
1	G	47/56 (84%)	33 (70%)	14 (30%)	0	0
1	I	46/56 (82%)	38 (83%)	8 (17%)	2	2
1	K	48/56 (86%)	39 (81%)	9 (19%)	1	1
2	B	50/62 (81%)	43 (86%)	7 (14%)	3	4
2	D	50/62 (81%)	47 (94%)	3 (6%)	19	30
2	F	46/62 (74%)	38 (83%)	8 (17%)	2	2
2	H	49/62 (79%)	42 (86%)	7 (14%)	3	3
2	J	51/62 (82%)	43 (84%)	8 (16%)	2	3
2	L	45/62 (73%)	38 (84%)	7 (16%)	2	3
All	All	574/708 (81%)	476 (83%)	98 (17%)	2	2

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	LEU
1	A	22	ARG
1	A	33	ASP

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Mol	Chain	Res	Type
1	A	34	VAL
1	A	42	ILE
1	A	60	GLU
1	A	61	LEU
2	B	3	LEU
2	B	10	ASP
2	B	17	ARG
2	B	30	GLN
2	B	40	LEU
2	B	58	LEU
2	B	59	ASP
1	C	4	LEU
1	C	9	LEU
1	C	15	GLU
1	C	20	LEU
1	C	34	VAL
1	C	50	HIS
1	C	52	THR
1	C	53	VAL
1	C	62	ARG
2	D	3	LEU
2	D	11	ARG
2	D	53	LEU
1	E	2	LEU
1	E	4	LEU
1	E	14	THR
1	E	15	GLU
1	E	33	ASP
1	E	44	GLN
1	E	47	PRO
1	E	49	THR
1	E	56	ILE
1	E	61	LEU
2	F	3	LEU
2	F	11	ARG
2	F	15	ARG
2	F	35[A]	THR
2	F	35[B]	THR
2	F	42	LEU
2	F	47	VAL
2	F	53	LEU
1	G	3	LEU

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Mol	Chain	Res	Type
1	G	5	ARG
1	G	6	ILE
1	G	7	THR
1	G	9	LEU
1	G	20	LEU
1	G	24	LEU
1	G	33	ASP
1	G	34	VAL
1	G	42	ILE
1	G	44	GLN
1	G	50	HIS
1	G	52	THR
1	G	61	LEU
2	H	3	LEU
2	H	16	THR
2	H	17	ARG
2	H	24	GLU
2	H	48	SER
2	H	52	THR
2	H	58	LEU
1	I	1	MET
1	I	4	LEU
1	I	12	ARG
1	I	34	VAL
1	I	41	LEU
1	I	50	HIS
1	I	52	THR
1	I	53	VAL
2	J	3	LEU
2	J	11	ARG
2	J	31	ARG
2	J	39	ARG
2	J	40	LEU
2	J	47	VAL
2	J	48	SER
2	J	52	THR
1	K	6	ILE
1	K	19	GLU
1	K	33	ASP
1	K	38	GLU
1	K	44	GLN
1	K	53	VAL

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Mol	Chain	Res	Type
1	K	56	ILE
1	K	61	LEU
1	K	62	ARG
2	L	3	LEU
2	L	15	ARG
2	L	16	THR
2	L	32	VAL
2	L	46	ILE
2	L	47	VAL
2	L	53	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	16	GLN
1	E	44	GLN
2	F	41	GLN
2	F	51	ASN
1	G	16	GLN
1	G	50	HIS
1	I	44	GLN
2	J	51	ASN
1	K	44	GLN
2	L	41	GLN

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

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	73	-	4,4,4	1.40	1 (25%)	6,6,6	1.02	1 (16%)
3	SO4	C	73	-	4,4,4	0.35	0	6,6,6	0.76	0
3	SO4	F	73	-	4,4,4	0.35	0	6,6,6	0.31	0
3	SO4	E	73	-	4,4,4	0.54	0	6,6,6	1.01	0
3	SO4	L	74	-	4,4,4	0.92	0	6,6,6	1.16	1 (16%)
3	SO4	A	73	-	4,4,4	0.95	0	6,6,6	1.08	0
3	SO4	L	73	-	4,4,4	0.41	0	6,6,6	0.66	0
3	SO4	K	73	-	4,4,4	0.56	0	6,6,6	0.93	0
3	SO4	A	74	-	4,4,4	0.94	0	6,6,6	1.34	2 (33%)
3	SO4	H	73	-	4,4,4	1.35	1 (25%)	6,6,6	0.60	0
3	SO4	G	73	-	4,4,4	0.98	0	6,6,6	0.66	0
3	SO4	E	74	-	4,4,4	0.93	0	6,6,6	0.46	0
3	SO4	C	74	-	4,4,4	1.06	0	6,6,6	0.84	0
3	SO4	K	74	-	4,4,4	0.95	0	6,6,6	0.50	0
3	SO4	I	74	-	4,4,4	1.06	0	6,6,6	1.37	1 (16%)
3	SO4	C	75	-	4,4,4	1.28	1 (25%)	6,6,6	2.15	1 (16%)
3	SO4	I	73	-	4,4,4	0.26	0	6,6,6	0.72	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	75	SO4	O2-S	2.28	1.58	1.46
3	D	73	SO4	O2-S	2.21	1.58	1.46
3	H	73	SO4	O1-S	2.01	1.56	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	75	SO4	O4-S-O3	-4.68	89.09	109.06
3	I	74	SO4	O4-S-O2	-2.55	96.01	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	74	SO4	O4-S-O3	2.38	119.23	109.06
3	A	74	SO4	O3-S-O1	-2.18	97.94	109.31
3	L	74	SO4	O4-S-O3	2.17	118.33	109.06
3	D	73	SO4	O4-S-O3	-2.06	100.28	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	73	SO4	1	0
3	C	73	SO4	2	0
3	L	74	SO4	1	0
3	L	73	SO4	3	0
3	K	73	SO4	1	0
3	A	74	SO4	1	0
3	E	74	SO4	1	0
3	C	74	SO4	2	0
3	K	74	SO4	4	0
3	I	74	SO4	3	0
3	C	75	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	61/72 (84%)	-0.20	0 100 100	28, 31, 38, 46	0
1	C	62/72 (86%)	-0.09	0 100 100	19, 30, 38, 46	0
1	E	61/72 (84%)	-0.22	0 100 100	27, 32, 42, 44	0
1	G	61/72 (84%)	-0.19	0 100 100	23, 30, 37, 42	0
1	I	60/72 (83%)	-0.15	0 100 100	27, 31, 38, 46	0
1	K	62/72 (86%)	-0.15	0 100 100	24, 32, 41, 50	0
2	B	59/72 (81%)	-0.20	0 100 100	12, 32, 41, 47	0
2	D	58/72 (80%)	-0.21	0 100 100	23, 29, 38, 41	0
2	F	54/72 (75%)	-0.13	0 100 100	21, 30, 38, 40	0
2	H	58/72 (80%)	-0.23	0 100 100	24, 32, 40, 46	0
2	J	59/72 (81%)	-0.18	0 100 100	16, 30, 39, 42	0
2	L	54/72 (75%)	-0.15	0 100 100	24, 31, 38, 43	0
All	All	709/864 (82%)	-0.17	0 100 100	12, 31, 40, 50	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 ⓘ

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(Å ²)	Q<0.9
3	SO4	I	74	5/5	0.87	0.23	55,55,59,62	0
3	SO4	L	74	5/5	0.88	0.15	45,51,57,57	0
3	SO4	C	75	5/5	0.93	0.20	60,65,70,70	0
3	SO4	E	74	5/5	0.94	0.22	56,57,61,61	0
3	SO4	D	73	5/5	0.94	0.12	46,52,57,59	0
3	SO4	A	74	5/5	0.94	0.28	61,64,65,68	0
3	SO4	K	74	5/5	0.95	0.19	59,61,62,63	0
3	SO4	H	73	5/5	0.96	0.09	63,66,71,72	0
3	SO4	C	74	5/5	0.97	0.21	54,58,60,60	0
3	SO4	G	73	5/5	0.97	0.27	58,59,63,65	0
3	SO4	A	73	5/5	0.97	0.11	53,59,63,64	0
3	SO4	F	73	5/5	0.98	0.12	51,54,56,57	0
3	SO4	E	73	5/5	0.98	0.10	55,58,60,60	0
3	SO4	C	73	5/5	0.98	0.11	49,53,55,57	0
3	SO4	L	73	5/5	0.99	0.08	52,53,57,59	0
3	SO4	K	73	5/5	0.99	0.08	54,54,58,59	0
3	SO4	I	73	5/5	0.99	0.14	54,54,56,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.