



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:05 AM GMT

PDB ID : 2FEL  
Title : 3-carboxy-cis,cis-muconate lactonizing enzyme from Agrobacterium radiobacter S2  
Authors : Lehtio, L.; Goldman, A.  
Deposited on : 2005-12-16  
Resolution : 2.20 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

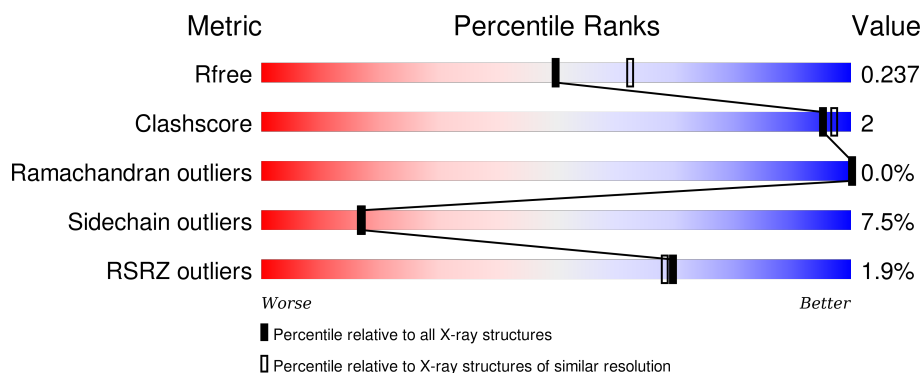
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	359	 2% 86% 7% • 6%
1	B	359	 1% 89% 5% • 6%
1	C	359	 3% 85% 8% • 6%
1	D	359	 2% 84% 8% • 6%
1	E	359	 87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	359	
1	G	359	
1	H	359	
1	I	359	
1	J	359	
1	K	359	
1	L	359	

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
2	CL	L	1511	-	-	-	X
3	SO4	A	1602	-	-	-	X
3	SO4	B	1610	-	-	-	X
3	SO4	C	1608	-	-	-	X
3	SO4	D	1609	-	-	-	X
3	SO4	E	1607	-	-	-	X
3	SO4	F	1611	-	-	-	X
3	SO4	G	1605	-	-	-	X
3	SO4	H	1606	-	-	-	X
3	SO4	I	1603	-	-	-	X
3	SO4	J	1612	-	-	-	X
3	SO4	K	1601	-	-	-	X
3	SO4	L	1604	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31917 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 3-carboxy-cis,cis-muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	2	0
			2544	1598	450	487	9			
1	B	339	Total	C	N	O	S	0	1	0
			2545	1598	452	486	9			
1	D	337	Total	C	N	O	S	0	3	0
			2552	1602	452	489	9			
1	C	337	Total	C	N	O	S	0	3	0
			2551	1602	451	489	9			
1	E	338	Total	C	N	O	S	0	4	0
			2572	1616	455	492	9			
1	F	339	Total	C	N	O	S	0	2	0
			2551	1601	453	488	9			
1	G	338	Total	C	N	O	S	0	2	0
			2557	1608	453	487	9			
1	H	338	Total	C	N	O	S	0	2	0
			2548	1600	451	488	9			
1	I	337	Total	C	N	O	S	0	1	0
			2537	1594	450	484	9			
1	J	338	Total	C	N	O	S	0	2	0
			2547	1599	452	487	9			
1	L	338	Total	C	N	O	S	0	2	0
			2547	1599	452	487	9			
1	K	337	Total	C	N	O	S	0	2	0
			2543	1597	451	486	9			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Cl	0	0
			2	2		
2	D	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		
2	I	2	Total	Cl	0	0
			2	2		
2	A	1	Total	Cl	0	0
			1	1		
2	L	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	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	B	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

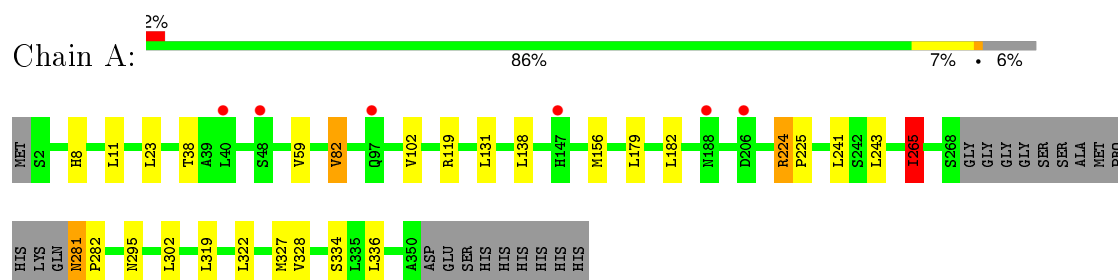
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	132	Total	O	0	0
			132	132		
4	C	70	Total	O	0	0
			70	70		
4	D	100	Total	O	0	0
			100	100		
4	E	142	Total	O	0	0
			142	142		
4	F	107	Total	O	0	0
			107	107		
4	G	119	Total	O	0	0
			119	119		
4	H	114	Total	O	0	0
			114	114		
4	I	92	Total	O	0	0
			92	92		
4	J	100	Total	O	0	0
			100	100		
4	K	87	Total	O	0	0
			87	87		
4	L	79	Total	O	0	0
			79	79		

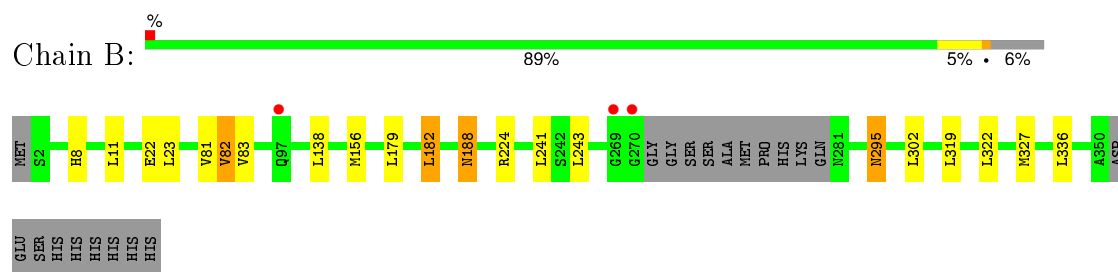
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

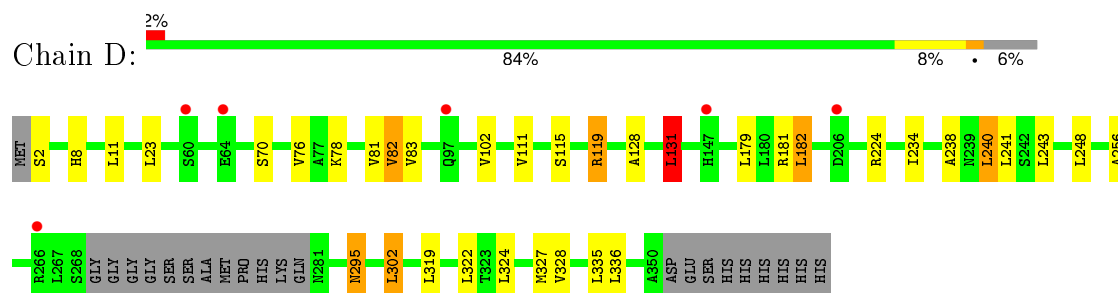
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



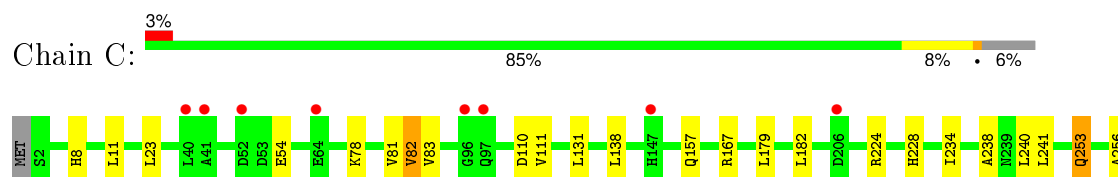
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

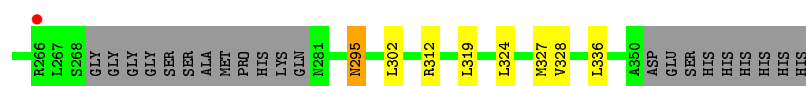


- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



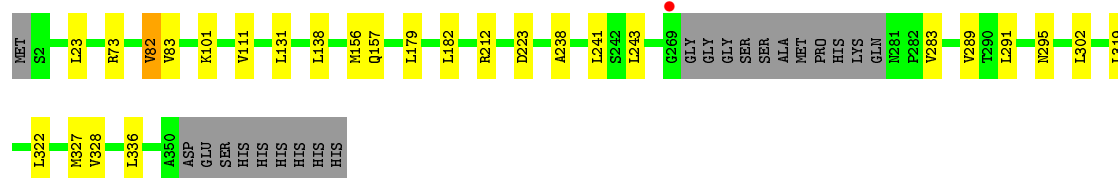
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme





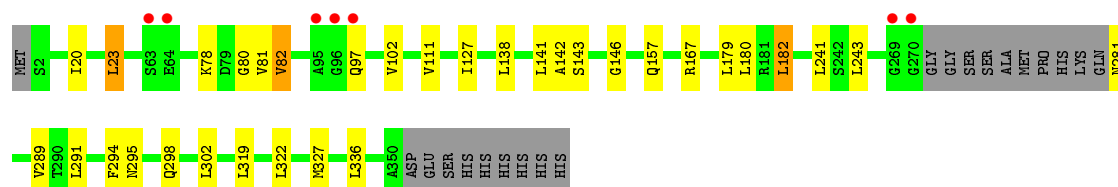
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

Chain E: 87% 7% 6%



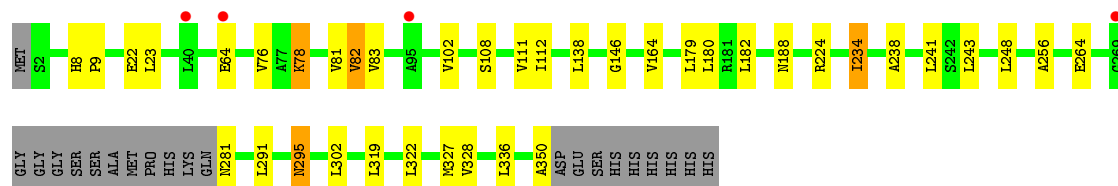
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

Chain F: 85% 8% 6%



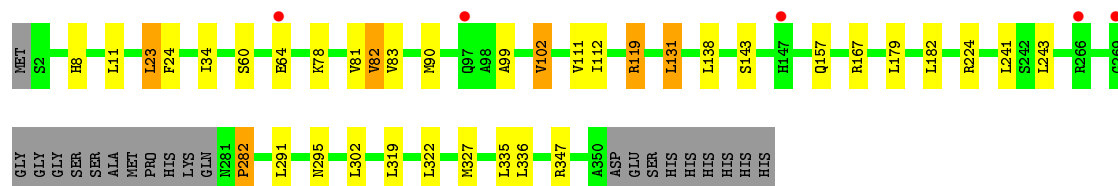
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

Chain G: 83% 10% 6%



- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

Chain H: 84% 9% 6%

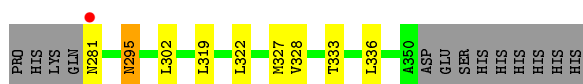


- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

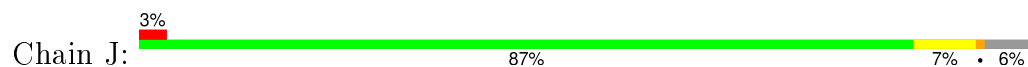
Chain I: 86% 7% 6%



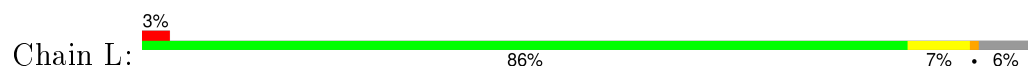




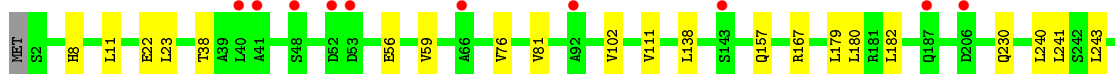
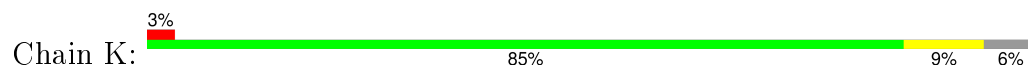
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.86Å 208.51Å 123.93Å 90.00° 108.35° 90.00°	Depositor
Resolution (Å)	19.96 – 2.20 19.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-2.20) 99.7 (19.92-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.188 , 0.236 0.191 , 0.237	Depositor DCC
$R_{free}$ test set	10998 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 219958 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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	0.47	0/2581	0.73	4/3493 (0.1%)
1	B	0.49	0/2582	0.74	2/3494 (0.1%)
1	C	0.60	2/2589 (0.1%)	0.73	1/3504 (0.0%)
1	D	0.44	0/2589	0.71	4/3504 (0.1%)
1	E	0.50	0/2609	0.72	1/3531 (0.0%)
1	F	0.49	0/2588	0.72	2/3502 (0.1%)
1	G	0.47	0/2594	0.72	1/3511 (0.0%)
1	H	0.50	0/2585	0.75	4/3498 (0.1%)
1	I	0.47	0/2574	0.68	2/3484 (0.1%)
1	J	0.46	0/2584	0.68	2/3497 (0.1%)
1	K	0.43	0/2580	0.65	0/3492
1	L	0.46	1/2584 (0.0%)	0.68	2/3497 (0.1%)
All	All	0.48	3/31039 (0.0%)	0.71	25/42007 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	GLU	CD-OE1	13.47	1.40	1.25
1	C	54	GLU	CD-OE2	12.93	1.39	1.25
1	L	148	LYS	CD-CE	5.07	1.64	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	82	VAL	CB-CA-C	-8.64	94.98	111.40
1	F	82	VAL	CB-CA-C	-8.63	95.01	111.40
1	H	82	VAL	CB-CA-C	-8.04	96.12	111.40
1	L	82	VAL	CB-CA-C	-7.73	96.72	111.40
1	A	82	VAL	CB-CA-C	-7.64	96.89	111.40
1	E	82	VAL	CB-CA-C	-7.62	96.91	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	302	LEU	CA-CB-CG	-7.57	97.89	115.30
1	D	119	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	L	302	LEU	CA-CB-CG	-7.27	98.58	115.30
1	C	82	VAL	CB-CA-C	-7.18	97.75	111.40
1	B	82	VAL	CB-CA-C	-7.03	98.05	111.40
1	F	302	LEU	CA-CB-CG	-6.92	99.38	115.30
1	D	82	VAL	CB-CA-C	-6.88	98.32	111.40
1	A	302	LEU	CA-CB-CG	-6.83	99.60	115.30
1	H	302	LEU	CA-CB-CG	-6.39	100.61	115.30
1	A	119	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	H	119	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	J	302	LEU	CA-CB-CG	-6.12	101.22	115.30
1	J	119	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	I	265	ILE	CB-CA-C	-6.00	99.60	111.60
1	D	119	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	302	LEU	CA-CB-CG	-5.41	102.86	115.30
1	H	23	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	265	ILE	CB-CA-C	-5.29	101.03	111.60
1	D	131	LEU	CA-CB-CG	5.07	126.95	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	2544	0	2545	7	0
1	B	2545	0	2547	5	0
1	C	2551	0	2550	13	0
1	D	2552	0	2550	12	0
1	E	2572	0	2574	9	0
1	F	2551	0	2551	8	0
1	G	2557	0	2565	14	0
1	H	2548	0	2548	10	0
1	I	2537	0	2541	6	0
1	J	2547	0	2548	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2543	0	2545	8	0
1	L	2547	0	2548	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	L	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	110	0	0	0	0
4	B	132	0	0	0	0
4	C	70	0	0	0	0
4	D	100	0	0	0	0
4	E	142	0	0	0	0
4	F	107	0	0	0	0
4	G	119	0	0	0	0
4	H	114	0	0	0	0
4	I	92	0	0	0	0
4	J	100	0	0	1	0
4	K	87	0	0	0	0
4	L	79	0	0	0	0
All	All	31917	0	30612	96	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 2.

All (96) 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:F:281:ASN:HB3	1:H:157:GLN:HG3	1.61	0.80
1:E:157:GLN:HG3	1:G:281:ASN:HB3	1.68	0.74
1:A:281:ASN:HB3	1:C:157:GLN:HG3	1.74	0.70
1:E:302[A]:LEU:HD23	1:E:327:MET:CE	2.23	0.67
1:L:181:ARG:HB3	1:L:240:LEU:HD21	1.79	0.63
1:D:302:LEU:HD11	1:D:324:LEU:HD13	1.81	0.62
1:C:238:ALA:HB2	1:C:302:LEU:HD12	1.87	0.57
1:I:6:PHE:HE2	1:I:333:THR:HG21	1.72	0.55
1:K:38:THR:HG23	1:K:59:VAL:HG22	1.88	0.55
1:C:295:ASN:ND2	1:C:327:MET:HG2	2.22	0.55
1:K:295:ASN:HD21	1:K:327:MET:HA	1.72	0.54
1:H:24:PHE:HA	1:H:119:ARG:HH21	1.73	0.54
1:D:238:ALA:HB2	1:D:302:LEU:HD12	1.90	0.54
1:I:295:ASN:HD21	1:I:327:MET:HA	1.71	0.53
1:I:6:PHE:CE2	1:I:333:THR:HG21	2.44	0.53
1:C:8:HIS:HB3	1:C:11:LEU:HB2	1.91	0.53
1:G:238:ALA:HB2	1:G:302[B]:LEU:HD12	1.91	0.52
1:J:117:MET:HG3	1:J:191:ALA:O	2.11	0.51
1:A:224:ARG:HG3	1:A:225:PRO:HD2	1.91	0.51
1:L:170:GLY:HA2	1:K:230:GLN:HE21	1.75	0.51
1:I:157:GLN:HG3	1:K:281:ASN:HB3	1.93	0.51
1:C:295:ASN:HD21	1:C:327:MET:HA	1.76	0.49
1:H:81:VAL:HG23	1:H:112:ILE:HD11	1.95	0.49
1:F:294:PHE:O	1:F:298:GLN:HG2	2.12	0.49
1:J:295:ASN:HD21	1:J:327:MET:HA	1.78	0.49
1:F:295:ASN:HD21	1:F:327:MET:HA	1.79	0.48
1:E:238:ALA:HB2	1:E:302[C]:LEU:HD12	1.96	0.48
1:C:253:GLN:HE21	1:C:253:GLN:HA	1.78	0.48
1:L:83:VAL:HA	1:L:86:LEU:HB3	1.96	0.48
1:K:8:HIS:HB3	1:K:11:LEU:HB2	1.96	0.47
1:G:180:LEU:HA	1:G:180:LEU:HD12	1.68	0.47
1:B:8:HIS:HB3	1:B:11:LEU:HB2	1.97	0.47
1:G:81:VAL:HG21	1:G:108:SER:HB3	1.96	0.47
1:E:295:ASN:HD21	1:E:327:MET:HA	1.78	0.47
1:D:295:ASN:HD21	1:D:327:MET:HA	1.78	0.47
1:K:302:LEU:HD23	1:K:302:LEU:HA	1.46	0.46
1:B:295:ASN:HD21	1:B:327:MET:HA	1.80	0.46
1:H:8:HIS:HB3	1:H:11:LEU:HB2	1.97	0.46
1:L:126:ILE:O	1:L:130:ARG:HG3	2.15	0.46
1:F:157:GLN:HG2	1:H:282:PRO:HD3	1.97	0.46
1:C:238:ALA:CB	1:C:302:LEU:HD12	2.45	0.45
1:L:295:ASN:HD21	1:L:327:MET:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.70	0.45
1:J:157:GLN:HG2	1:L:282:PRO:HD3	1.99	0.45
1:H:295:ASN:HD21	1:H:327:MET:HA	1.82	0.45
1:J:281:ASN:HB3	1:L:157:GLN:HG3	1.99	0.45
1:G:264:GLU:HG2	1:G:350:ALA:HB2	1.99	0.45
1:J:156:MET:HG3	1:L:256:ALA:HB1	1.99	0.45
1:B:156:MET:HG3	1:D:256:ALA:HB1	1.99	0.44
1:D:181:ARG:HB3	1:D:240:LEU:HD21	1.98	0.44
1:E:212:ARG:HD2	1:E:223:ASP:OD1	2.17	0.44
1:C:110:ASP:OD1	1:C:228:HIS:HE1	1.99	0.44
1:J:24:PHE:HA	1:J:119:ARG:HH21	1.83	0.44
1:G:295:ASN:HD21	1:G:327:MET:HA	1.82	0.44
1:D:295:ASN:ND2	1:D:327:MET:HG2	2.33	0.44
1:E:283:VAL:HG11	1:F:80:GLY:HA3	2.00	0.43
1:E:302[B]:LEU:HA	1:E:302[B]:LEU:HD12	1.49	0.43
1:F:127:ILE:HG22	1:F:182:LEU:HD11	2.01	0.43
1:C:234:ILE:HG22	1:C:302:LEU:HD13	2.00	0.43
1:G:78:LYS:HE3	1:G:78:LYS:HB3	1.56	0.43
1:H:99:ALA:O	1:H:102:VAL:HG13	2.18	0.43
1:F:142:ALA:O	1:F:146:GLY:HA3	2.18	0.43
1:D:8:HIS:HB3	1:D:11:LEU:HB2	2.00	0.43
1:H:34:ILE:HG12	1:H:90:MET:HE2	2.01	0.43
1:L:20:ILE:O	1:L:23:LEU:HB2	2.18	0.43
1:G:81:VAL:HG23	1:G:112:ILE:HD11	2.00	0.43
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.91	0.42
1:A:8:HIS:HB3	1:A:11:LEU:HB2	1.99	0.42
1:D:128:ALA:HB2	1:D:182:LEU:HD13	2.01	0.42
1:E:302[A]:LEU:HA	1:E:302[A]:LEU:HD13	1.82	0.42
1:F:20:ILE:O	1:F:23:LEU:HB2	2.20	0.42
1:J:228:HIS:HD2	4:J:1627:HOH:O	2.02	0.42
1:H:78:LYS:HB2	1:H:78:LYS:HE3	1.78	0.42
1:D:248:LEU:HA	1:D:248:LEU:HD23	1.86	0.42
1:D:234:ILE:HG22	1:D:302:LEU:HD13	2.02	0.42
1:D:131:LEU:HD13	1:D:335:LEU:HD21	2.01	0.42
1:I:81:VAL:HG11	1:I:108:SER:HB3	2.01	0.41
1:B:188[A]:ASN:HB3	1:B:224:ARG:HH12	1.84	0.41
1:A:38:THR:HG23	1:A:59:VAL:HG22	2.02	0.41
1:A:265:ILE:HD13	1:A:265:ILE:HG21	1.72	0.41
1:A:156:MET:HG3	1:C:256:ALA:HB1	2.01	0.41
1:E:156:MET:HG3	1:G:256:ALA:HB1	2.01	0.41
1:K:308:GLN:HG2	1:K:316:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HD11	1:C:324:LEU:HD13	2.01	0.41
1:H:131:LEU:HD13	1:H:335:LEU:HD21	2.03	0.41
1:G:146:GLY:HA2	1:G:164:VAL:HB	2.03	0.41
1:G:248:LEU:HD23	1:G:248:LEU:HA	1.86	0.41
1:G:188[B]:ASN:HA	1:G:188[B]:ASN:HD22	1.59	0.41
1:C:228:HIS:CD2	1:C:312:ARG:HH21	2.39	0.40
1:G:234:ILE:HG23	1:G:234:ILE:HD13	1.77	0.40
1:A:295:ASN:HD21	1:A:327:MET:HA	1.86	0.40
1:J:138:LEU:HA	1:J:138:LEU:HD12	1.93	0.40
1:L:118:LEU:HA	1:L:118:LEU:HD23	1.92	0.40
1:D:115:SER:O	1:D:119:ARG:HD3	2.21	0.40
1:G:8:HIS:HA	1:G:9:PRO:HD3	1.96	0.40
1:I:281:ASN:HB2	1:K:157:GLN:HG3	2.03	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	335/359 (93%)	327 (98%)	7 (2%)	1 (0%)	46	50
1	B	336/359 (94%)	328 (98%)	8 (2%)	0	100	100
1	C	336/359 (94%)	327 (97%)	9 (3%)	0	100	100
1	D	336/359 (94%)	331 (98%)	5 (2%)	0	100	100
1	E	339/359 (94%)	328 (97%)	11 (3%)	0	100	100
1	F	337/359 (94%)	325 (96%)	12 (4%)	0	100	100
1	G	337/359 (94%)	328 (97%)	9 (3%)	0	100	100
1	H	336/359 (94%)	328 (98%)	7 (2%)	1 (0%)	46	50
1	I	334/359 (93%)	321 (96%)	13 (4%)	0	100	100
1	J	336/359 (94%)	329 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	335/359 (93%)	328 (98%)	7 (2%)	0	100	100
1	L	336/359 (94%)	325 (97%)	11 (3%)	0	100	100
All	All	4033/4308 (94%)	3925 (97%)	106 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	282	PRO
1	A	282	PRO

### 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	256/271 (94%)	239 (93%)	17 (7%)	21	22
1	B	255/271 (94%)	239 (94%)	16 (6%)	22	24
1	C	257/271 (95%)	238 (93%)	19 (7%)	17	17
1	D	257/271 (95%)	234 (91%)	23 (9%)	12	11
1	E	259/271 (96%)	241 (93%)	18 (7%)	19	20
1	F	256/271 (94%)	235 (92%)	21 (8%)	14	13
1	G	257/271 (95%)	235 (91%)	22 (9%)	13	12
1	H	256/271 (94%)	235 (92%)	21 (8%)	14	13
1	I	255/271 (94%)	234 (92%)	21 (8%)	14	13
1	J	256/271 (94%)	239 (93%)	17 (7%)	21	22
1	K	256/271 (94%)	235 (92%)	21 (8%)	14	13
1	L	256/271 (94%)	242 (94%)	14 (6%)	27	30
All	All	3076/3252 (95%)	2846 (92%)	230 (8%)	17	17

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	82	VAL
1	A	102	VAL
1	A	131	LEU
1	A	138	LEU
1	A	179	LEU
1	A	182	LEU
1	A	224	ARG
1	A	241	LEU
1	A	243	LEU
1	A	265	ILE
1	A	281	ASN
1	A	319	LEU
1	A	322	LEU
1	A	328	VAL
1	A	334	SER
1	A	336	LEU
1	B	22	GLU
1	B	23	LEU
1	B	81	VAL
1	B	82	VAL
1	B	83	VAL
1	B	138	LEU
1	B	179	LEU
1	B	182	LEU
1	B	188[A]	ASN
1	B	188[B]	ASN
1	B	241	LEU
1	B	243	LEU
1	B	295	ASN
1	B	319	LEU
1	B	322	LEU
1	B	336	LEU
1	D	2	SER
1	D	23	LEU
1	D	70	SER
1	D	76	VAL
1	D	78	LYS
1	D	81	VAL
1	D	82	VAL
1	D	83	VAL
1	D	102	VAL
1	D	111	VAL

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Mol	Chain	Res	Type
1	D	131	LEU
1	D	179	LEU
1	D	182	LEU
1	D	224	ARG
1	D	240	LEU
1	D	241	LEU
1	D	243	LEU
1	D	295	ASN
1	D	302	LEU
1	D	319	LEU
1	D	322	LEU
1	D	328	VAL
1	D	336	LEU
1	C	23	LEU
1	C	78	LYS
1	C	81	VAL
1	C	82	VAL
1	C	83	VAL
1	C	111	VAL
1	C	131	LEU
1	C	138	LEU
1	C	167	ARG
1	C	179	LEU
1	C	182	LEU
1	C	224	ARG
1	C	240	LEU
1	C	241	LEU
1	C	253	GLN
1	C	295	ASN
1	C	319	LEU
1	C	328	VAL
1	C	336	LEU
1	E	23	LEU
1	E	73	ARG
1	E	82	VAL
1	E	83	VAL
1	E	101	LYS
1	E	111	VAL
1	E	131	LEU
1	E	138	LEU
1	E	179	LEU
1	E	182	LEU

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Mol	Chain	Res	Type
1	E	241	LEU
1	E	243	LEU
1	E	289	VAL
1	E	291	LEU
1	E	319	LEU
1	E	322	LEU
1	E	328	VAL
1	E	336	LEU
1	F	23	LEU
1	F	78	LYS
1	F	81	VAL
1	F	82	VAL
1	F	97	GLN
1	F	102	VAL
1	F	111	VAL
1	F	138	LEU
1	F	141	LEU
1	F	143	SER
1	F	167	ARG
1	F	179	LEU
1	F	180	LEU
1	F	182	LEU
1	F	241	LEU
1	F	243	LEU
1	F	289	VAL
1	F	291	LEU
1	F	319	LEU
1	F	322	LEU
1	F	336	LEU
1	G	22	GLU
1	G	23	LEU
1	G	64	GLU
1	G	76	VAL
1	G	78	LYS
1	G	82	VAL
1	G	83	VAL
1	G	102	VAL
1	G	111	VAL
1	G	138	LEU
1	G	179	LEU
1	G	182	LEU
1	G	224	ARG

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Mol	Chain	Res	Type
1	G	234	ILE
1	G	241	LEU
1	G	243	LEU
1	G	291	LEU
1	G	295	ASN
1	G	319	LEU
1	G	322	LEU
1	G	328	VAL
1	G	336	LEU
1	H	23	LEU
1	H	60	SER
1	H	64	GLU
1	H	82	VAL
1	H	83	VAL
1	H	102	VAL
1	H	111	VAL
1	H	131	LEU
1	H	138	LEU
1	H	143	SER
1	H	167	ARG
1	H	179	LEU
1	H	182	LEU
1	H	224	ARG
1	H	241	LEU
1	H	243	LEU
1	H	291	LEU
1	H	319	LEU
1	H	322	LEU
1	H	336	LEU
1	H	347	ARG
1	I	4	SER
1	I	23	LEU
1	I	38	THR
1	I	53	ASP
1	I	60	SER
1	I	76	VAL
1	I	81	VAL
1	I	83	VAL
1	I	102	VAL
1	I	111	VAL
1	I	138	LEU
1	I	143	SER

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Mol	Chain	Res	Type
1	I	179	LEU
1	I	182	LEU
1	I	241	LEU
1	I	265	ILE
1	I	295	ASN
1	I	319	LEU
1	I	322	LEU
1	I	328	VAL
1	I	336	LEU
1	J	23	LEU
1	J	54	GLU
1	J	56	GLU
1	J	81	VAL
1	J	83	VAL
1	J	88	ARG
1	J	138	LEU
1	J	179	LEU
1	J	182	LEU
1	J	187	GLN
1	J	241	LEU
1	J	243	LEU
1	J	295	ASN
1	J	319	LEU
1	J	322	LEU
1	J	328	VAL
1	J	336	LEU
1	L	23	LEU
1	L	82	VAL
1	L	83	VAL
1	L	102	VAL
1	L	179	LEU
1	L	182	LEU
1	L	206	ASP
1	L	224	ARG
1	L	241	LEU
1	L	243	LEU
1	L	266	ARG
1	L	319	LEU
1	L	328	VAL
1	L	336	LEU
1	K	22	GLU
1	K	23	LEU

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Mol	Chain	Res	Type
1	K	56	GLU
1	K	76	VAL
1	K	81	VAL
1	K	102	VAL
1	K	111	VAL
1	K	138	LEU
1	K	167	ARG
1	K	179	LEU
1	K	180	LEU
1	K	182	LEU
1	K	240	LEU
1	K	241	LEU
1	K	243	LEU
1	K	295	ASN
1	K	311	GLU
1	K	319	LEU
1	K	322	LEU
1	K	328	VAL
1	K	336	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	281	ASN
1	A	295	ASN
1	A	298	GLN
1	A	326	GLN
1	B	187	GLN
1	B	295	ASN
1	D	207	ASN
1	D	295	ASN
1	D	298	GLN
1	D	326	GLN
1	C	187	GLN
1	C	207	ASN
1	C	228	HIS
1	C	253	GLN
1	C	295	ASN
1	E	187	GLN
1	E	295	ASN
1	E	298	GLN

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Mol	Chain	Res	Type
1	F	97	GLN
1	F	187	GLN
1	F	295	ASN
1	F	298	GLN
1	G	295	ASN
1	G	326	GLN
1	H	187	GLN
1	H	295	ASN
1	H	326	GLN
1	I	187	GLN
1	I	228	HIS
1	I	295	ASN
1	J	228	HIS
1	J	295	ASN
1	J	298	GLN
1	J	326	GLN
1	L	187	GLN
1	L	295	ASN
1	K	207	ASN
1	K	253	GLN
1	K	295	ASN
1	K	298	GLN
1	K	326	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 ⓘ

Of 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 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	SO4	A	1602	-	4,4,4	0.23	0	6,6,6	0.22	0
3	SO4	B	1610	-	4,4,4	0.29	0	6,6,6	0.34	0
3	SO4	C	1608	-	4,4,4	0.30	0	6,6,6	0.37	0
3	SO4	D	1609	-	4,4,4	0.20	0	6,6,6	0.23	0
3	SO4	E	1607	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	F	1611	-	4,4,4	0.19	0	6,6,6	0.26	0
3	SO4	G	1605	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	H	1606	-	4,4,4	0.26	0	6,6,6	0.26	0
3	SO4	I	1603	-	4,4,4	0.20	0	6,6,6	0.33	0
3	SO4	J	1612	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	K	1601	-	4,4,4	0.16	0	6,6,6	0.26	0
3	SO4	L	1604	-	4,4,4	0.23	0	6,6,6	0.21	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	SO4	A	1602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1610	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1608	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1609	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1607	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1611	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1605	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1606	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1603	-	-	0/0/0/0	0/0/0/0
3	SO4	J	1612	-	-	0/0/0/0	0/0/0/0
3	SO4	K	1601	-	-	0/0/0/0	0/0/0/0
3	SO4	L	1604	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	337/359 (93%)	-0.21	6 (1%) 71 70	23, 30, 37, 42	1 (0%)
1	B	339/359 (94%)	-0.32	3 (0%) 85 85	23, 30, 36, 43	0
1	C	337/359 (93%)	-0.12	9 (2%) 58 57	18, 30, 37, 43	0
1	D	337/359 (93%)	-0.15	6 (1%) 71 70	25, 31, 37, 42	0
1	E	338/359 (94%)	-0.34	1 (0%) 94 94	23, 30, 37, 46	0
1	F	339/359 (94%)	-0.15	7 (2%) 67 65	22, 30, 37, 50	0
1	G	338/359 (94%)	-0.22	4 (1%) 81 80	25, 30, 38, 47	0
1	H	338/359 (94%)	-0.30	5 (1%) 76 75	24, 30, 38, 46	0
1	I	337/359 (93%)	-0.09	7 (2%) 67 65	19, 30, 38, 43	0
1	J	338/359 (94%)	-0.11	9 (2%) 58 57	24, 30, 37, 45	0
1	K	337/359 (93%)	0.04	11 (3%) 50 49	25, 31, 35, 43	0
1	L	338/359 (94%)	0.04	9 (2%) 58 57	25, 31, 37, 42	1 (0%)
All	All	4053/4308 (94%)	-0.16	77 (1%) 70 68	18, 30, 37, 50	2 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	269	GLY	7.9
1	B	270	GLY	7.9
1	L	269	GLY	7.4
1	G	269	GLY	6.4
1	F	270	GLY	5.4
1	B	269	GLY	5.1
1	H	269	GLY	5.0
1	E	269	GLY	4.8
1	J	350	ALA	4.5
1	F	64	GLU	4.4
1	G	64	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	206	ASP	3.6
1	J	269	GLY	3.5
1	A	40	LEU	3.5
1	F	97	GLN	3.4
1	C	96	GLY	3.4
1	I	95	ALA	3.4
1	G	95	ALA	3.4
1	C	97	GLN	3.3
1	I	64	GLU	3.1
1	J	147	HIS	3.1
1	J	64	GLU	3.1
1	K	206	ASP	3.1
1	B	97	GLN	3.1
1	C	64	GLU	3.1
1	J	143	SER	3.1
1	H	266	ARG	3.0
1	K	40	LEU	3.0
1	A	147	HIS	2.9
1	I	41	ALA	2.9
1	D	64	GLU	2.9
1	L	97	GLN	2.8
1	H	97	GLN	2.8
1	A	97	GLN	2.7
1	K	66	ALA	2.7
1	L	206	ASP	2.7
1	C	40	LEU	2.7
1	D	97	GLN	2.6
1	H	147	HIS	2.6
1	F	95	ALA	2.6
1	H	64	GLU	2.6
1	L	22	GLU	2.6
1	F	96	GLY	2.5
1	C	147	HIS	2.5
1	K	187	GLN	2.5
1	D	147	HIS	2.5
1	D	266	ARG	2.5
1	C	41	ALA	2.4
1	G	40	LEU	2.4
1	A	206	ASP	2.4
1	L	187	GLN	2.4
1	K	48	SER	2.4
1	I	63	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	97	GLN	2.3
1	C	52	ASP	2.3
1	A	188	ASN	2.3
1	C	266	ARG	2.3
1	J	63[A]	SER	2.3
1	L	268	SER	2.3
1	K	41	ALA	2.2
1	K	92	ALA	2.2
1	I	40	LEU	2.2
1	D	60	SER	2.2
1	C	206	ASP	2.2
1	J	56	GLU	2.1
1	K	143	SER	2.1
1	I	281	ASN	2.1
1	A	48	SER	2.1
1	L	147	HIS	2.1
1	I	56	GLU	2.1
1	K	281	ASN	2.0
1	K	52	ASP	2.0
1	F	63[A]	SER	2.0
1	L	350	ALA	2.0
1	J	53	ASP	2.0
1	K	53	ASP	2.0
1	L	95	ALA	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 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( $\text{\AA}^2$ )	Q<0.9
3	SO4	F	1611	5/5	0.92	0.30	22.13	70,71,72,72	0
3	SO4	B	1610	5/5	0.98	0.28	16.61	54,54,55,56	0
3	SO4	E	1607	5/5	0.94	0.28	14.49	70,71,71,71	0
3	SO4	C	1608	5/5	0.95	0.34	13.51	57,57,58,60	0
3	SO4	K	1601	5/5	0.86	0.39	11.47	80,80,81,81	0
3	SO4	D	1609	5/5	0.92	0.28	9.25	74,75,76,76	0
3	SO4	H	1606	5/5	0.95	0.28	7.93	61,62,62,63	0
3	SO4	A	1602	5/5	0.95	0.30	4.56	68,68,68,69	0
3	SO4	J	1612	5/5	0.94	0.35	3.98	70,71,72,73	0
3	SO4	L	1604	5/5	0.93	0.23	3.19	70,71,71,71	0
3	SO4	I	1603	5/5	0.95	0.26	3.13	68,68,69,69	0
3	SO4	G	1605	5/5	0.98	0.20	2.57	56,56,57,57	0
2	CL	L	1511	1/1	0.98	0.14	2.35	44,44,44,44	0
2	CL	G	1506	1/1	0.99	0.14	1.82	39,39,39,39	0
2	CL	I	1510	1/1	0.98	0.10	-0.80	52,52,52,52	0
2	CL	D	1503	1/1	0.99	0.08	-1.59	41,41,41,41	0
2	CL	D	1508	1/1	0.98	0.17	-	43,43,43,43	0
2	CL	H	1505	1/1	0.98	0.12	-	38,38,38,38	0
2	CL	G	1502	1/1	0.96	0.13	-	38,38,38,38	0
2	CL	B	1504	1/1	0.99	0.16	-	37,37,37,37	0
2	CL	I	1509	1/1	0.98	0.12	-	34,34,34,34	0
2	CL	H	1501	1/1	0.99	0.13	-	33,33,33,33	0
2	CL	A	1507	1/1	0.98	0.13	-	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.