



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:05 AM GMT

PDB ID : 2FEN  
Title : 3-carboxy-cis,cis-muconate lactonizing enzyme from Agrobacterium radiobacter S2  
Authors : Lehtio, L.; Goldman, A.  
Deposited on : 2005-12-16  
Resolution : 2.60 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

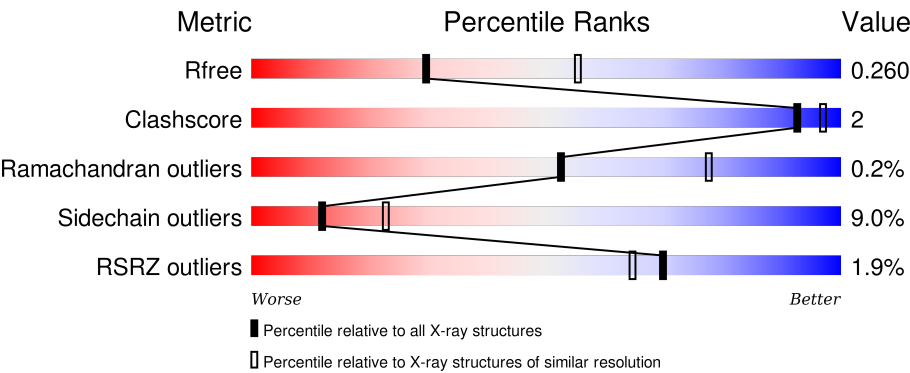
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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 <sub>free</sub>	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	<div><div>2%</div><div><div></div><div>87%</div><div>8%</div><div>5%</div></div></div>
1	B	359	<div><div>%</div><div><div></div><div>82%</div><div>11%</div><div>6%</div></div></div>
1	C	359	<div><div></div><div><div></div><div>83%</div><div>11%</div><div>6%</div></div></div>
1	D	359	<div><div>2%</div><div><div></div><div>84%</div><div>10%</div><div></div></div></div>
1	E	359	<div><div>3%</div><div><div></div><div>85%</div><div>9%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	359	 84% 9% • 6%
1	G	359	 82% 12% • 6%
1	H	359	 84% 8% • 6%
1	I	359	 83% 10% • 6%
1	J	359	 80% 13% • 6%
1	K	359	 84% 9% • 6%
1	L	359	 85% 8% • 6%

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	SO4	B	1001	-	-	-	X
2	SO4	C	1003	-	-	-	X
2	SO4	H	1002	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31433 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	342	Total	C	N	O	S	0	2	0
			2574	1615	457	493	9			
1	B	339	Total	C	N	O	S	0	1	0
			2545	1598	452	486	9			
1	D	343	Total	C	N	O	S	0	0	0
			2564	1610	456	489	9			
1	C	338	Total	C	N	O	S	0	1	0
			2543	1597	450	487	9			
1	E	337	Total	C	N	O	S	0	2	0
			2544	1598	450	487	9			
1	F	339	Total	C	N	O	S	0	0	0
			2537	1594	450	484	9			
1	H	337	Total	C	N	O	S	0	3	0
			2552	1602	452	489	9			
1	G	337	Total	C	N	O	S	0	3	0
			2551	1602	451	489	9			
1	I	337	Total	C	N	O	S	0	2	0
			2544	1598	450	487	9			
1	J	339	Total	C	N	O	S	0	1	0
			2545	1598	452	486	9			
1	L	337	Total	C	N	O	S	0	3	0
			2552	1602	452	489	9			
1	K	336	Total	C	N	O	S	0	1	0
			2532	1592	448	483	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	C	2	Total Cl 2 2	0	0
3	I	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	79	Total O 79 79	0	0

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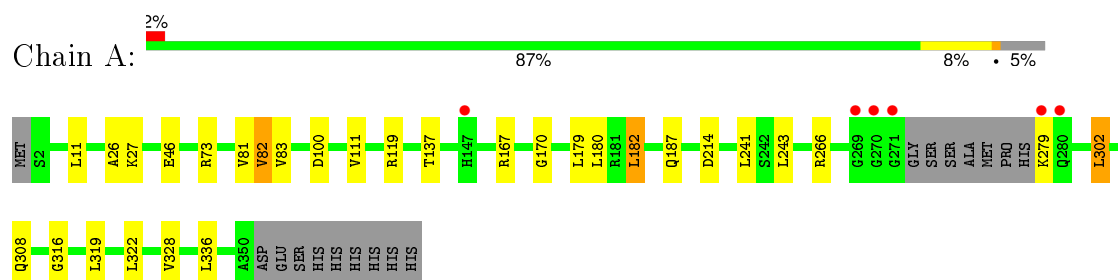
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	79	Total 79	O 79	0	0
4	C	103	Total 103	O 103	0	0
4	D	98	Total 98	O 98	0	0
4	E	45	Total 45	O 45	0	0
4	F	72	Total 72	O 72	0	0
4	G	72	Total 72	O 72	0	0
4	H	74	Total 74	O 74	0	0
4	I	50	Total 50	O 50	0	0
4	J	53	Total 53	O 53	0	0
4	K	70	Total 70	O 70	0	0
4	L	30	Total 30	O 30	0	0

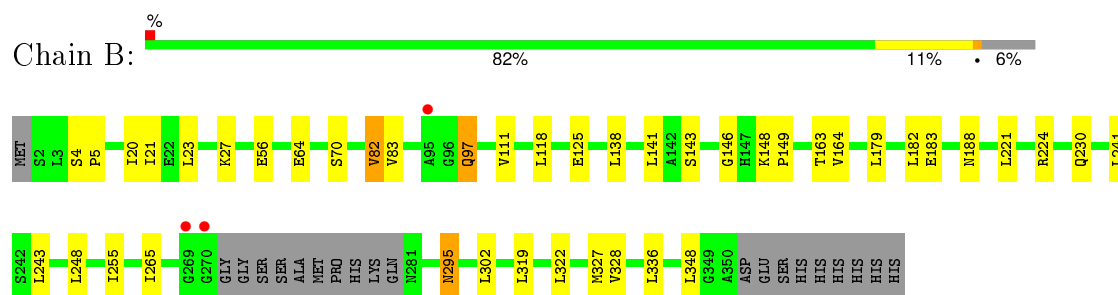
### 3 Residue-property plots [i](#)

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

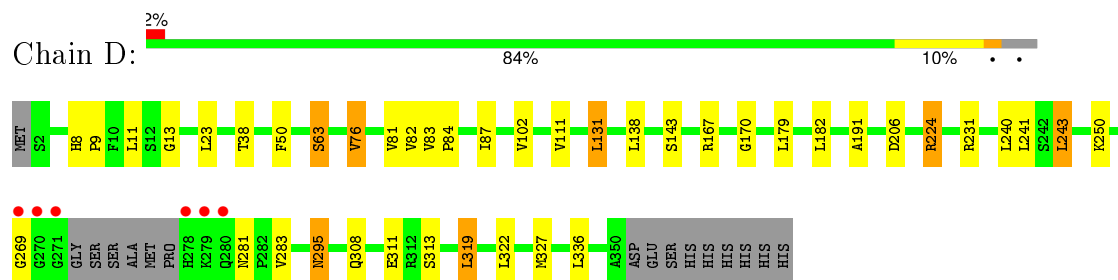
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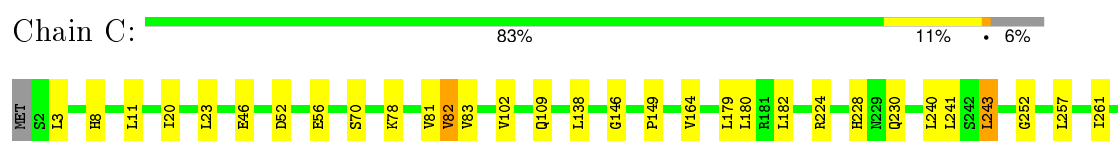
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



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

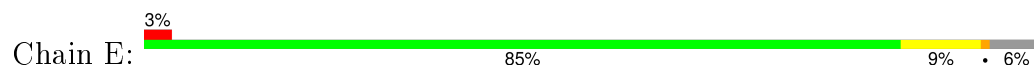


- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

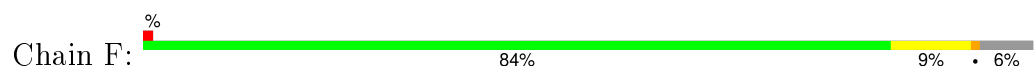




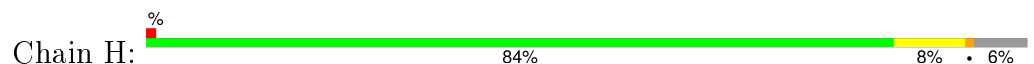
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



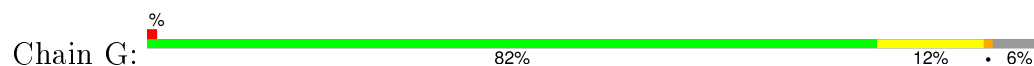
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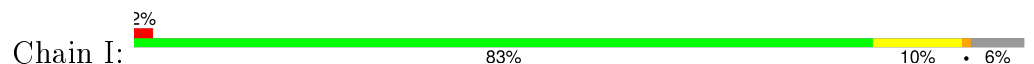
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

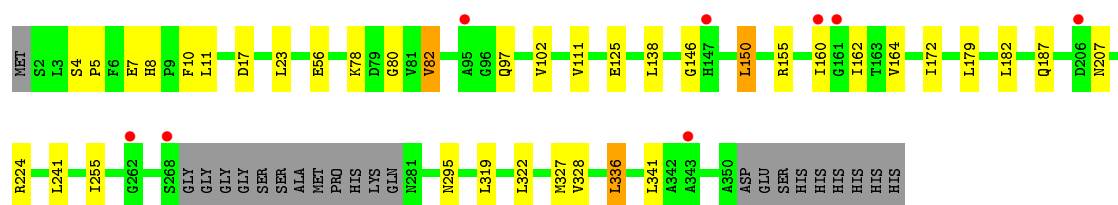


- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

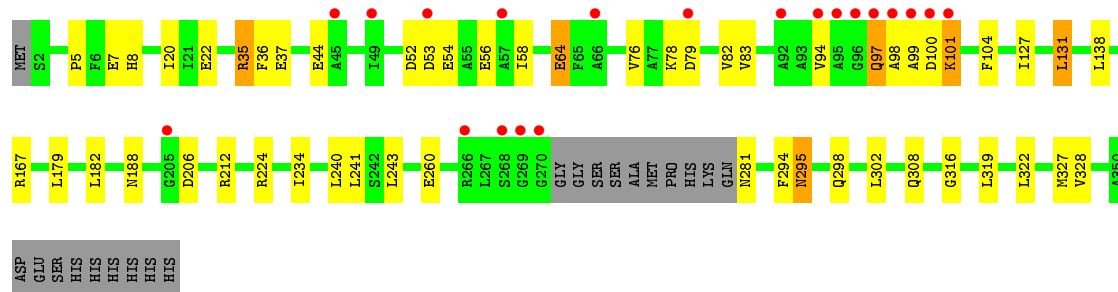
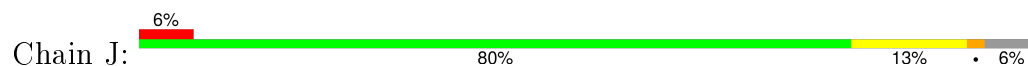


- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme

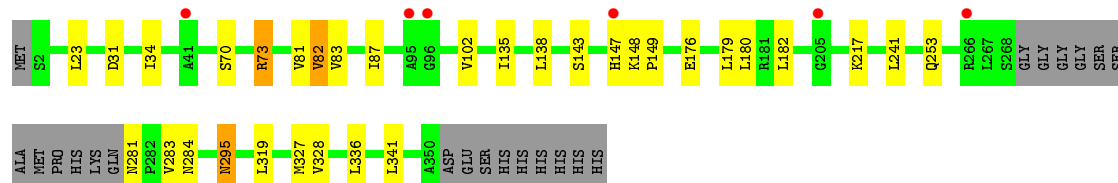
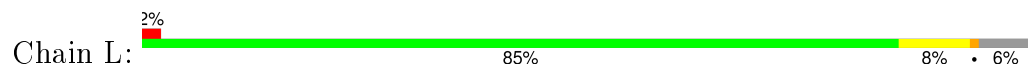




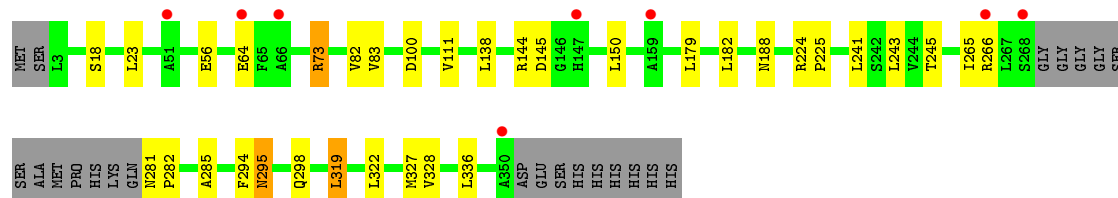
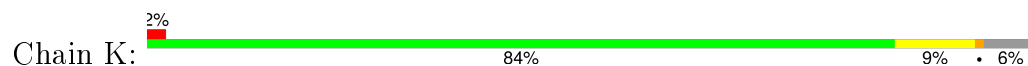
- Molecule 1: 3-carboxy-cis,cis-muconate lactonizing enzyme



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.03Å 205.32Å 235.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.60) 94.9 (19.99-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.262 0.200 , 0.260	Depositor DCC
$R_{free}$ test set	6657 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 133155 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	31433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.42% 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	0.52	0/2611	0.72	1/3531 (0.0%)
1	B	0.52	0/2582	0.72	2/3494 (0.1%)
1	C	0.57	0/2580	0.76	2/3492 (0.1%)
1	D	0.53	0/2601	0.75	1/3518 (0.0%)
1	E	0.42	0/2581	0.63	0/3493
1	F	0.46	0/2574	0.71	3/3483 (0.1%)
1	G	0.48	0/2589	0.70	1/3504 (0.0%)
1	H	0.49	2/2589 (0.1%)	0.68	2/3504 (0.1%)
1	I	0.51	0/2581	0.71	1/3493 (0.0%)
1	J	0.88	18/2582 (0.7%)	0.73	3/3494 (0.1%)
1	K	0.45	0/2569	0.67	0/3477
1	L	0.49	0/2589	0.67	1/3504 (0.0%)
All	All	0.54	20/31028 (0.1%)	0.71	17/41987 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	64	GLU	CD-OE2	12.99	1.40	1.25
1	J	56	GLU	CD-OE2	12.34	1.39	1.25
1	J	52	ASP	CG-OD1	11.13	1.50	1.25
1	J	56	GLU	CD-OE1	8.90	1.35	1.25
1	J	56	GLU	CG-CD	8.17	1.64	1.51
1	J	104	PHE	CG-CD2	8.03	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	52	ASP	CG-OD2	7.71	1.43	1.25
1	J	37	GLU	CD-OE1	7.12	1.33	1.25
1	H	44	GLU	CD-OE1	6.66	1.32	1.25
1	J	104	PHE	CE1-CZ	6.56	1.49	1.37
1	J	54	GLU	CD-OE1	6.25	1.32	1.25
1	J	53	ASP	CG-OD1	6.14	1.39	1.25
1	J	36	PHE	CG-CD2	5.93	1.47	1.38
1	J	36	PHE	CG-CD1	5.81	1.47	1.38
1	J	64	GLU	CD-OE1	5.80	1.32	1.25
1	H	44	GLU	CD-OE2	5.76	1.31	1.25
1	J	104	PHE	CG-CD1	5.60	1.47	1.38
1	J	36	PHE	CE2-CZ	5.32	1.47	1.37
1	J	44	GLU	CD-OE1	5.29	1.31	1.25
1	J	97	GLN	CD-NE2	5.09	1.45	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	302	LEU	CA-CB-CG	-6.82	99.62	115.30
1	B	302	LEU	CA-CB-CG	-6.72	99.85	115.30
1	I	82	VAL	CB-CA-C	-6.14	99.74	111.40
1	L	82	VAL	CB-CA-C	-6.05	99.91	111.40
1	G	302	LEU	CA-CB-CG	-5.98	101.54	115.30
1	A	82	VAL	CB-CA-C	-5.87	100.25	111.40
1	J	212	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	J	53	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	F	240	LEU	CA-CB-CG	5.45	127.83	115.30
1	D	131	LEU	CA-CB-CG	5.40	127.72	115.30
1	F	82	VAL	CB-CA-C	-5.32	101.29	111.40
1	H	82	VAL	CB-CA-C	-5.29	101.34	111.40
1	B	82	VAL	CB-CA-C	-5.12	101.67	111.40
1	J	35	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	82	VAL	CB-CA-C	-5.06	101.78	111.40
1	C	302	LEU	CA-CB-CG	-5.04	103.70	115.30
1	F	131	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	281	ASN	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2574	0	2575	10	0
1	B	2545	0	2547	14	0
1	C	2543	0	2544	16	0
1	D	2564	0	2568	15	0
1	E	2544	0	2545	8	0
1	F	2537	0	2542	13	0
1	G	2551	0	2550	11	0
1	H	2552	0	2550	12	0
1	I	2544	0	2545	14	0
1	J	2545	0	2547	9	0
1	K	2532	0	2536	8	0
1	L	2552	0	2550	9	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	79	0	0	0	0
4	B	79	0	0	0	0
4	C	103	0	0	0	0
4	D	98	0	0	0	0
4	E	45	0	0	0	0
4	F	72	0	0	1	0
4	G	72	0	0	0	0
4	H	74	0	0	0	0
4	I	50	0	0	0	0
4	J	53	0	0	0	0
4	K	70	0	0	1	0
4	L	30	0	0	0	0
All	All	31433	0	30599	123	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 (123) 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:295:ASN:HD21	1:C:327:MET:HA	1.40	0.87
1:D:170:GLY:HA2	1:C:230:GLN:HE21	1.50	0.76
1:A:170:GLY:HA2	1:B:230:GLN:HE21	1.58	0.67
1:F:283:VAL:HG11	1:G:80:GLY:HA3	1.77	0.65
1:J:58:ILE:HD11	1:J:101:LYS:HB2	1.79	0.65
1:A:73:ARG:HH11	1:D:13:GLY:HA2	1.66	0.61
1:D:281:ASN:HB3	1:D:283:VAL:HG23	1.82	0.60
1:L:295:ASN:HD21	1:L:327:MET:HA	1.67	0.60
1:K:295:ASN:HD21	1:K:327:MET:HA	1.66	0.59
1:H:295:ASN:HD21	1:H:327:MET:HA	1.67	0.57
1:J:295:ASN:HD21	1:J:327:MET:HA	1.70	0.57
1:E:322:LEU:HD12	1:H:5:PRO:HG2	1.88	0.56
1:D:295:ASN:HD21	1:D:327:MET:HA	1.71	0.56
1:I:295:ASN:HD21	1:I:327:MET:HA	1.71	0.56
1:F:224:ARG:HG3	1:F:225:PRO:HD2	1.88	0.55
1:B:295:ASN:HD21	1:B:327:MET:HA	1.72	0.55
1:B:21:ILE:HG12	1:C:3:LEU:HD21	1.90	0.52
1:B:146:GLY:HA2	1:B:164:VAL:HB	1.91	0.52
1:K:224:ARG:HG3	1:K:225:PRO:HD2	1.92	0.52
1:C:146:GLY:HA2	1:C:164:VAL:HB	1.91	0.52
1:F:73:ARG:HD3	1:G:9:PRO:O	2.09	0.52
1:F:80:GLY:HA3	1:G:283:VAL:HG11	1.92	0.51
1:I:10:PHE:HA	1:L:73:ARG:HB3	1.92	0.51
1:I:255:ILE:HG21	1:I:341:LEU:HD11	1.92	0.50
1:E:5:PRO:HG2	1:H:322:LEU:HD12	1.94	0.49
1:I:150:LEU:HB3	1:I:162:ILE:HG13	1.94	0.49
1:F:266:ARG:HB2	4:F:398:HOH:O	2.12	0.49
1:E:295:ASN:HD21	1:E:327:MET:HA	1.78	0.48
1:C:295:ASN:ND2	1:C:327:MET:HA	2.20	0.47
1:C:295:ASN:HA	1:C:295:ASN:HD22	1.52	0.47
1:K:282:PRO:HB2	1:K:285:ALA:HB3	1.96	0.47
1:J:5:PRO:HA	1:J:8:HIS:HB2	1.95	0.47
1:B:188[A]:ASN:HB3	1:B:224:ARG:HH12	1.80	0.47
1:E:257:LEU:HD23	1:E:257:LEU:HA	1.76	0.47
1:I:80:GLY:HA3	1:L:283:VAL:HG11	1.96	0.46
1:A:26:ALA:HB2	1:D:9:PRO:HG2	1.98	0.46
1:C:149:PRO:HG2	1:C:350:ALA:HB3	1.98	0.46
1:L:87:ILE:HD13	1:L:87:ILE:HA	1.76	0.46
1:B:265:ILE:HG13	1:B:348:LEU:HD23	1.98	0.45
1:G:294:PHE:O	1:G:298:GLN:HG2	2.17	0.45
1:C:252:GLY:HA3	1:C:288:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ILE:HD13	1:F:176:GLU:HG3	1.97	0.45
1:B:5:PRO:HG2	1:C:322:LEU:HD12	1.99	0.45
1:E:78:LYS:HB2	1:E:78:LYS:HE3	1.69	0.45
1:G:160:ILE:HG12	1:G:160:ILE:H	1.54	0.45
1:B:148:LYS:HA	1:B:149:PRO:HD3	1.86	0.45
1:L:284:ASN:HB2	1:L:341:LEU:HD13	1.98	0.45
1:I:138:LEU:HB3	1:I:172:ILE:HG12	1.98	0.45
1:L:135:ILE:HD13	1:L:176:GLU:HG3	1.99	0.45
1:K:144:ARG:HB3	1:K:144:ARG:HE	1.60	0.44
1:F:8:HIS:HB3	1:F:11:LEU:HB2	1.99	0.44
1:K:281:ASN:HA	4:K:383:HOH:O	2.17	0.44
1:K:319:LEU:HA	1:K:319:LEU:HD23	1.76	0.44
1:D:319:LEU:HD23	1:D:319:LEU:HA	1.88	0.44
1:C:257:LEU:O	1:C:261:ILE:HG13	2.18	0.44
1:C:8:HIS:HB3	1:C:11:LEU:HB2	2.00	0.44
1:D:231:ARG:HG3	1:D:308:GLN:NE2	2.32	0.44
1:F:295:ASN:HD21	1:F:327:MET:HA	1.83	0.44
1:I:155:ARG:HE	1:I:155:ARG:HB3	1.66	0.43
1:D:8:HIS:HB3	1:D:11:LEU:HB2	2.00	0.43
1:A:302:LEU:HA	1:A:302:LEU:HD13	1.48	0.43
1:K:73:ARG:HB3	1:K:73:ARG:HE	1.36	0.43
1:B:20:ILE:HD13	1:B:20:ILE:HA	1.89	0.43
1:G:173:ALA:HA	1:G:176:GLU:HG3	2.00	0.43
1:I:8:HIS:HB3	1:I:11:LEU:HB2	1.99	0.43
1:A:46:GLU:HG2	1:A:214:ASP:OD1	2.18	0.43
1:B:295:ASN:HD22	1:B:295:ASN:HA	1.53	0.43
1:H:243:LEU:HA	1:H:243:LEU:HD12	1.80	0.43
1:B:118:LEU:HG	1:B:221:LEU:HD11	2.01	0.43
1:L:217:LYS:HB3	1:L:217:LYS:HE2	1.65	0.42
1:C:109:GLN:HG2	1:C:228:HIS:CD2	2.54	0.42
1:B:255:ILE:HA	1:B:255:ILE:HD13	1.90	0.42
1:D:308:GLN:HB3	1:D:313:SER:HB3	2.00	0.42
1:H:4:SER:HA	1:H:5:PRO:HD3	1.91	0.42
1:C:243:LEU:HA	1:C:243:LEU:HD12	1.80	0.42
1:D:240:LEU:HA	1:D:243:LEU:HB2	2.00	0.42
1:A:11:LEU:HA	1:D:76:VAL:HG21	2.00	0.42
1:J:234:ILE:HG22	1:J:302:LEU:HD23	2.02	0.42
1:I:150:LEU:HD23	1:I:150:LEU:HA	1.87	0.42
1:H:180:LEU:HD13	1:H:180:LEU:HA	1.79	0.42
1:G:8:HIS:HB3	1:G:11:LEU:HB2	2.00	0.42
1:G:293:ARG:O	1:G:297:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:LEU:HD23	1:H:141:LEU:HA	1.88	0.42
1:E:248:LEU:HB3	1:E:288:LEU:HD22	2.00	0.42
1:I:4:SER:HA	1:I:5:PRO:HD3	1.88	0.42
1:G:150:LEU:HD23	1:G:349:GLY:HA2	2.02	0.41
1:H:8:HIS:HB3	1:H:11:LEU:HB2	2.02	0.41
1:E:243:LEU:HD12	1:F:306:LEU:HD11	2.02	0.41
1:H:155:ARG:HB3	1:H:155:ARG:HE	1.60	0.41
1:C:299:ILE:HA	1:C:299:ILE:HD12	1.85	0.41
1:E:348:LEU:HA	1:E:348:LEU:HD23	1.95	0.41
1:I:187:GLN:HE21	1:I:187:GLN:HB2	1.68	0.41
1:H:105:GLY:HA2	1:H:203:LYS:HB2	2.02	0.41
1:A:308:GLN:HG2	1:A:316:GLY:HA3	2.03	0.41
1:G:248:LEU:HD23	1:G:248:LEU:HA	1.89	0.41
1:I:336:LEU:HA	1:I:336:LEU:HD12	1.88	0.41
1:D:81:VAL:HG12	1:D:84:PRO:HD2	2.03	0.41
1:D:191:ALA:HB2	1:D:224:ARG:HH21	1.86	0.41
1:A:187:GLN:HE21	1:A:187:GLN:HB2	1.65	0.41
1:F:150:LEU:HD23	1:F:349:GLY:HA2	2.03	0.41
1:J:308:GLN:HG2	1:J:316:GLY:HA3	2.02	0.41
1:J:98:ALA:HB3	1:J:101:LYS:HD2	2.03	0.41
1:F:295:ASN:HD22	1:F:295:ASN:HA	1.58	0.41
1:G:212:ARG:HG2	1:G:223:ASP:OD1	2.21	0.41
1:L:148:LYS:HA	1:L:149:PRO:HD3	1.93	0.41
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.77	0.41
1:D:170:GLY:HA2	1:C:230:GLN:NE2	2.28	0.41
1:I:146:GLY:HA2	1:I:164:VAL:HB	2.01	0.41
1:F:255:ILE:HA	1:F:255:ILE:HD13	1.88	0.41
1:A:119:ARG:HH11	1:A:119:ARG:HD3	1.72	0.40
1:L:31:ASP:HA	1:L:34:ILE:HD12	2.03	0.40
1:J:127:ILE:O	1:J:131:LEU:HB2	2.21	0.40
1:C:257:LEU:HA	1:C:257:LEU:HD23	1.95	0.40
1:A:182:LEU:HA	1:A:182:LEU:HD23	1.65	0.40
1:F:120:LEU:HD11	1:F:324:LEU:HD21	2.02	0.40
1:H:101:LYS:HA	1:H:101:LYS:HD2	1.94	0.40
1:B:97:GLN:H	1:B:97:GLN:HG3	1.78	0.40
1:I:295:ASN:HA	1:I:295:ASN:HD22	1.56	0.40
1:J:243:LEU:HA	1:J:243:LEU:HD12	1.91	0.40
1:K:294:PHE:O	1:K:298:GLN:HG2	2.20	0.40
1:D:87:ILE:HD13	1:D:87:ILE:HA	1.88	0.40
1:J:294:PHE:O	1:J:298:GLN:HG2	2.21	0.40
1:H:131:LEU:HD13	1:H:335:LEU:HD21	2.02	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	340/359 (95%)	328 (96%)	12 (4%)	0	100	100
1	B	336/359 (94%)	326 (97%)	10 (3%)	0	100	100
1	C	335/359 (93%)	318 (95%)	17 (5%)	0	100	100
1	D	339/359 (94%)	326 (96%)	11 (3%)	2 (1%)	30	56
1	E	335/359 (93%)	321 (96%)	12 (4%)	2 (1%)	30	56
1	F	335/359 (93%)	326 (97%)	9 (3%)	0	100	100
1	G	336/359 (94%)	322 (96%)	14 (4%)	0	100	100
1	H	336/359 (94%)	321 (96%)	15 (4%)	0	100	100
1	I	335/359 (93%)	322 (96%)	12 (4%)	1 (0%)	46	72
1	J	336/359 (94%)	315 (94%)	20 (6%)	1 (0%)	46	72
1	K	333/359 (93%)	321 (96%)	11 (3%)	1 (0%)	46	72
1	L	336/359 (94%)	323 (96%)	13 (4%)	0	100	100
All	All	4032/4308 (94%)	3869 (96%)	156 (4%)	7 (0%)	52	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	63	SER
1	E	189	GLY
1	J	99	ALA
1	I	17	ASP
1	K	64	GLU
1	D	269	GLY
1	E	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	258/271 (95%)	238 (92%)	20 (8%)	16	30
1	B	255/271 (94%)	230 (90%)	25 (10%)	10	19
1	C	256/271 (94%)	233 (91%)	23 (9%)	12	23
1	D	256/271 (94%)	231 (90%)	25 (10%)	10	19
1	E	256/271 (94%)	233 (91%)	23 (9%)	12	23
1	F	254/271 (94%)	235 (92%)	19 (8%)	17	33
1	G	257/271 (95%)	230 (90%)	27 (10%)	8	16
1	H	257/271 (95%)	238 (93%)	19 (7%)	17	34
1	I	256/271 (94%)	236 (92%)	20 (8%)	16	30
1	J	255/271 (94%)	224 (88%)	31 (12%)	6	11
1	K	254/271 (94%)	230 (91%)	24 (9%)	11	20
1	L	257/271 (95%)	237 (92%)	20 (8%)	16	30
All	All	3071/3252 (94%)	2795 (91%)	276 (9%)	12	23

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	81	VAL
1	A	82	VAL
1	A	83	VAL
1	A	100	ASP
1	A	111	VAL
1	A	137	THR
1	A	167	ARG
1	A	179	LEU
1	A	180	LEU
1	A	182	LEU
1	A	241	LEU
1	A	243	LEU
1	A	266	ARG

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Mol	Chain	Res	Type
1	A	279	LYS
1	A	302	LEU
1	A	319	LEU
1	A	322	LEU
1	A	328	VAL
1	A	336	LEU
1	B	4	SER
1	B	23	LEU
1	B	27	LYS
1	B	56	GLU
1	B	64	GLU
1	B	70	SER
1	B	82	VAL
1	B	83	VAL
1	B	97	GLN
1	B	111	VAL
1	B	125	GLU
1	B	138	LEU
1	B	141	LEU
1	B	143	SER
1	B	163	THR
1	B	179	LEU
1	B	182	LEU
1	B	183	GLU
1	B	241	LEU
1	B	243	LEU
1	B	295	ASN
1	B	319	LEU
1	B	322	LEU
1	B	328	VAL
1	B	336	LEU
1	D	23	LEU
1	D	38	THR
1	D	50	PHE
1	D	63	SER
1	D	76	VAL
1	D	82	VAL
1	D	83	VAL
1	D	102	VAL
1	D	111	VAL
1	D	131	LEU
1	D	138	LEU

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Mol	Chain	Res	Type
1	D	143	SER
1	D	167	ARG
1	D	179	LEU
1	D	182	LEU
1	D	206	ASP
1	D	224	ARG
1	D	241	LEU
1	D	243	LEU
1	D	250	LYS
1	D	295	ASN
1	D	311	GLU
1	D	319	LEU
1	D	322	LEU
1	D	336	LEU
1	C	20	ILE
1	C	23	LEU
1	C	46	GLU
1	C	52	ASP
1	C	56	GLU
1	C	70	SER
1	C	78	LYS
1	C	81	VAL
1	C	82	VAL
1	C	83	VAL
1	C	102	VAL
1	C	138	LEU
1	C	179	LEU
1	C	180	LEU
1	C	182	LEU
1	C	224	ARG
1	C	240	LEU
1	C	241	LEU
1	C	243	LEU
1	C	295	ASN
1	C	319	LEU
1	C	328	VAL
1	C	336	LEU
1	E	23	LEU
1	E	48	SER
1	E	81	VAL
1	E	82	VAL
1	E	83	VAL

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Mol	Chain	Res	Type
1	E	102	VAL
1	E	111	VAL
1	E	121	LYS
1	E	147	HIS
1	E	151	THR
1	E	179	LEU
1	E	182	LEU
1	E	188	ASN
1	E	224	ARG
1	E	240	LEU
1	E	241	LEU
1	E	243	LEU
1	E	266	ARG
1	E	295	ASN
1	E	302	LEU
1	E	319	LEU
1	E	334	SER
1	E	336	LEU
1	F	54	GLU
1	F	68	ASP
1	F	79	ASP
1	F	81	VAL
1	F	82	VAL
1	F	83	VAL
1	F	111	VAL
1	F	138	LEU
1	F	179	LEU
1	F	182	LEU
1	F	240	LEU
1	F	241	LEU
1	F	243	LEU
1	F	295	ASN
1	F	319	LEU
1	F	322	LEU
1	F	328	VAL
1	F	334	SER
1	F	336	LEU
1	H	27	LYS
1	H	56	GLU
1	H	64	GLU
1	H	70	SER
1	H	76	VAL

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Mol	Chain	Res	Type
1	H	82	VAL
1	H	83	VAL
1	H	121	LYS
1	H	131	LEU
1	H	138	LEU
1	H	167	ARG
1	H	179	LEU
1	H	180	LEU
1	H	182	LEU
1	H	224	ARG
1	H	241	LEU
1	H	243	LEU
1	H	319	LEU
1	H	336	LEU
1	G	2	SER
1	G	4	SER
1	G	7	GLU
1	G	23	LEU
1	G	27	LYS
1	G	76	VAL
1	G	81	VAL
1	G	82	VAL
1	G	83	VAL
1	G	111	VAL
1	G	125	GLU
1	G	138	LEU
1	G	155	ARG
1	G	160	ILE
1	G	167	ARG
1	G	179	LEU
1	G	180	LEU
1	G	182	LEU
1	G	241	LEU
1	G	243	LEU
1	G	281	ASN
1	G	295	ASN
1	G	319	LEU
1	G	322	LEU
1	G	328	VAL
1	G	336	LEU
1	G	347	ARG
1	I	7	GLU

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Mol	Chain	Res	Type
1	I	23	LEU
1	I	56	GLU
1	I	78	LYS
1	I	82	VAL
1	I	97	GLN
1	I	102	VAL
1	I	111	VAL
1	I	125	GLU
1	I	150	LEU
1	I	160	ILE
1	I	179	LEU
1	I	182	LEU
1	I	207	ASN
1	I	224	ARG
1	I	241	LEU
1	I	319	LEU
1	I	322	LEU
1	I	328	VAL
1	I	336	LEU
1	J	7	GLU
1	J	20	ILE
1	J	22	GLU
1	J	35	ARG
1	J	64	GLU
1	J	76	VAL
1	J	78	LYS
1	J	79	ASP
1	J	82	VAL
1	J	83	VAL
1	J	94	VAL
1	J	97	GLN
1	J	100	ASP
1	J	101	LYS
1	J	131	LEU
1	J	138	LEU
1	J	167	ARG
1	J	179	LEU
1	J	182	LEU
1	J	188[A]	ASN
1	J	188[B]	ASN
1	J	206	ASP
1	J	224	ARG

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Mol	Chain	Res	Type
1	J	240	LEU
1	J	241	LEU
1	J	260	GLU
1	J	281	ASN
1	J	295	ASN
1	J	319	LEU
1	J	322	LEU
1	J	328	VAL
1	L	23	LEU
1	L	70	SER
1	L	73	ARG
1	L	81	VAL
1	L	82	VAL
1	L	83	VAL
1	L	102	VAL
1	L	138	LEU
1	L	143	SER
1	L	147	HIS
1	L	179	LEU
1	L	180	LEU
1	L	182	LEU
1	L	241	LEU
1	L	253	GLN
1	L	281	ASN
1	L	295	ASN
1	L	319	LEU
1	L	328	VAL
1	L	336	LEU
1	K	18	SER
1	K	23	LEU
1	K	56	GLU
1	K	73	ARG
1	K	82	VAL
1	K	83	VAL
1	K	100	ASP
1	K	111	VAL
1	K	138	LEU
1	K	145	ASP
1	K	150	LEU
1	K	179	LEU
1	K	182	LEU
1	K	188	ASN

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Mol	Chain	Res	Type
1	K	241	LEU
1	K	243	LEU
1	K	245	THR
1	K	265	ILE
1	K	266	ARG
1	K	295	ASN
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 (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	253	GLN
1	A	280	GLN
1	A	295	ASN
1	A	298	GLN
1	A	326	GLN
1	B	187	GLN
1	B	295	ASN
1	B	326	GLN
1	D	147	HIS
1	D	295	ASN
1	D	298	GLN
1	D	326	GLN
1	C	147	HIS
1	C	295	ASN
1	C	326	GLN
1	E	187	GLN
1	E	207	ASN
1	E	295	ASN
1	F	187	GLN
1	F	207	ASN
1	F	281	ASN
1	F	295	ASN
1	F	298	GLN
1	H	187	GLN
1	H	295	ASN
1	G	187	GLN
1	G	281	ASN

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Mol	Chain	Res	Type
1	G	295	ASN
1	G	298	GLN
1	I	187	GLN
1	I	295	ASN
1	J	295	ASN
1	J	298	GLN
1	L	253	GLN
1	L	281	ASN
1	L	295	ASN
1	K	295	ASN
1	K	298	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	$\# Z  > 2$
2	SO4	B	1001	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	C	1003	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	G	1004	-	4,4,4	0.16	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	H	1002	-	4,4,4	0.25	0	6,6,6	0.09	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
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1002	-	-	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 [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

### 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	342/359 (95%)	-0.33	6 (1%) 71 66	20, 28, 36, 52	1 (0%)
1	B	339/359 (94%)	-0.43	3 (0%) 85 83	20, 28, 36, 52	0
1	C	338/359 (94%)	-0.51	1 (0%) 94 93	17, 27, 34, 39	0
1	D	343/359 (95%)	-0.37	6 (1%) 73 68	20, 28, 37, 50	1 (0%)
1	E	337/359 (93%)	-0.10	9 (2%) 58 51	22, 28, 34, 37	1 (0%)
1	F	339/359 (94%)	-0.34	5 (1%) 76 71	21, 28, 36, 45	0
1	G	337/359 (93%)	-0.41	2 (0%) 90 88	19, 28, 35, 41	0
1	H	337/359 (93%)	-0.21	5 (1%) 76 71	22, 28, 35, 39	0
1	I	337/359 (93%)	-0.36	8 (2%) 62 56	20, 28, 34, 38	1 (0%)
1	J	339/359 (94%)	0.06	20 (5%) 26 19	22, 29, 36, 41	0
1	K	336/359 (93%)	-0.10	8 (2%) 62 56	19, 29, 36, 40	0
1	L	337/359 (93%)	-0.25	6 (1%) 71 66	21, 28, 36, 40	0
All	All	4061/4308 (94%)	-0.28	79 (1%) 70 64	17, 28, 36, 52	4 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	99	ALA	7.5
1	J	97	GLN	7.0
1	A	271	GLY	6.1
1	B	270	GLY	5.9
1	J	269	GLY	5.2
1	D	270	GLY	5.0
1	J	270	GLY	4.9
1	L	147	HIS	4.3
1	K	350	ALA	4.3
1	J	101	LYS	4.1
1	F	270	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLY	4.0
1	E	147	HIS	3.9
1	E	97	GLN	3.9
1	D	278	HIS	3.8
1	J	95	ALA	3.8
1	J	53	ASP	3.7
1	D	279	LYS	3.4
1	J	100	ASP	3.3
1	A	279	LYS	3.3
1	E	60	SER	3.2
1	I	147	HIS	3.2
1	A	269	GLY	3.2
1	E	64	GLU	3.2
1	H	64	GLU	3.1
1	L	96	GLY	3.1
1	J	92	ALA	3.1
1	J	57	ALA	3.0
1	L	266	ARG	2.9
1	J	268	SER	2.9
1	D	269	GLY	2.9
1	D	280	GLN	2.9
1	J	96	GLY	2.9
1	J	94	VAL	2.8
1	F	95	ALA	2.8
1	G	350	ALA	2.8
1	I	206	ASP	2.7
1	K	64	GLU	2.7
1	K	147	HIS	2.7
1	J	98	ALA	2.7
1	K	51	ALA	2.6
1	E	281	ASN	2.6
1	A	280	GLN	2.6
1	F	64	GLU	2.6
1	E	66	ALA	2.5
1	K	266	ARG	2.5
1	I	95	ALA	2.5
1	I	268	SER	2.5
1	J	49	ILE	2.4
1	J	66	ALA	2.4
1	E	40	LEU	2.4
1	H	97	GLN	2.4
1	J	266	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	77	ALA	2.3
1	K	66	ALA	2.3
1	J	79	ASP	2.3
1	B	95	ALA	2.3
1	I	343	ALA	2.3
1	D	271	GLY	2.3
1	A	147	HIS	2.2
1	L	95	ALA	2.2
1	L	41	ALA	2.2
1	C	351	ASP	2.2
1	I	160	ILE	2.2
1	J	45	ALA	2.2
1	F	206	ASP	2.2
1	L	205	GLY	2.1
1	E	96	GLY	2.1
1	F	40	LEU	2.1
1	K	268	SER	2.1
1	K	159	ALA	2.1
1	H	266	ARG	2.1
1	E	63[A]	SER	2.1
1	H	70	SER	2.1
1	B	269	GLY	2.0
1	I	262	GLY	2.0
1	J	205	GLY	2.0
1	G	53	ASP	2.0
1	I	161	GLY	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
2	SO4	B	1001	5/5	0.97	0.22	9.84	54,55,56,56	0
2	SO4	C	1003	5/5	0.97	0.25	5.92	64,65,65,65	0
2	SO4	H	1002	5/5	0.93	0.29	2.70	87,87,87,87	0
3	CL	C	2004	1/1	0.89	0.17	1.15	40,40,40,40	0
3	CL	J	2001	1/1	0.94	0.17	-	35,35,35,35	0
3	CL	I	2005	1/1	0.99	0.07	-	24,24,24,24	0
3	CL	C	2003	1/1	0.99	0.08	-	25,25,25,25	0
2	SO4	G	1004	5/5	0.94	0.32	-	65,65,66,67	0
3	CL	A	2002	1/1	0.97	0.12	-	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.