



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2020 – 02:13 PM JST

PDB ID : 6L8A  
Title : Tetrathionate hydrolase from Acidithiobacillus ferrooxidans  
Authors : Tamada, T.; Hirano, Y.  
Deposited on : 2019-11-05  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

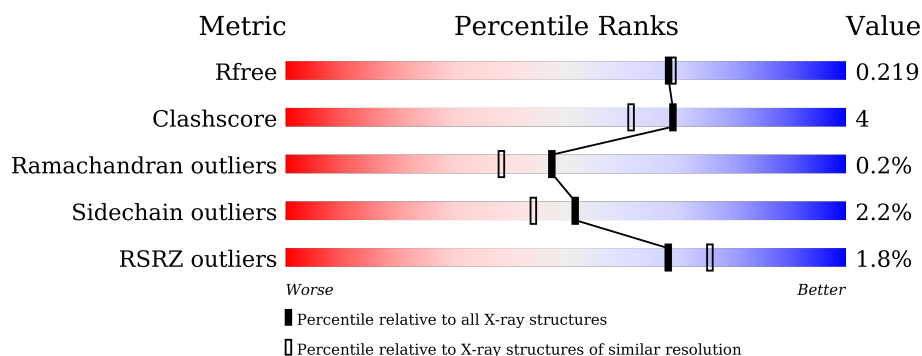
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	470	<div> <div>3%</div> <div>89% 8%</div> </div>
1	B	470	<div> <div>2%</div> <div>90% 6%</div> </div>
1	C	470	<div> <div>3%</div> <div>83% 8% 9%</div> </div>
1	D	470	<div> <div>%</div> <div>85% 11%</div> </div>
1	E	470	<div> <div>%</div> <div>88% 8%</div> </div>
1	F	470	<div> <div>%</div> <div>85% 12%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21302 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 Tetrathionate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3421	2196	581	632	12			
1	B	456	Total	C	N	O	S	0	0	0
			3441	2210	586	633	12			
1	C	429	Total	C	N	O	S	0	0	0
			3242	2084	548	599	11			
1	D	459	Total	C	N	O	S	0	0	0
			3459	2221	590	637	11			
1	E	452	Total	C	N	O	S	0	0	0
			3413	2193	581	627	12			
1	F	457	Total	C	N	O	S	0	0	0
			3451	2217	589	633	12			

There are 18 discrepancies between the modelled and reference sequences:

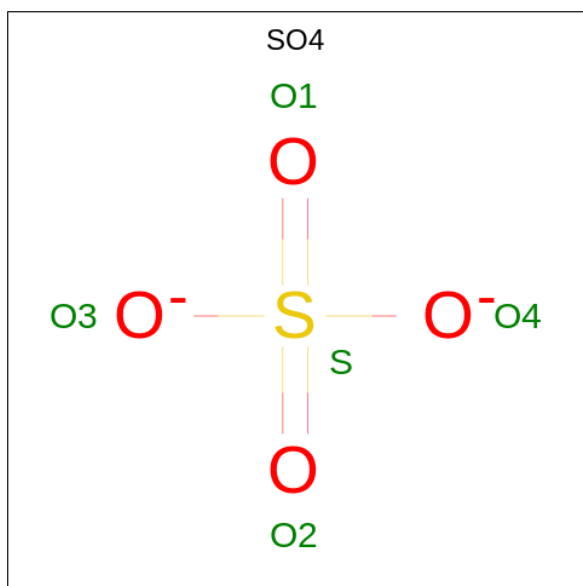
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP B7J3C9
A	31	ALA	-	expression tag	UNP B7J3C9
A	32	SER	-	expression tag	UNP B7J3C9
B	30	MET	-	expression tag	UNP B7J3C9
B	31	ALA	-	expression tag	UNP B7J3C9
B	32	SER	-	expression tag	UNP B7J3C9
C	30	MET	-	expression tag	UNP B7J3C9
C	31	ALA	-	expression tag	UNP B7J3C9
C	32	SER	-	expression tag	UNP B7J3C9
D	30	MET	-	expression tag	UNP B7J3C9
D	31	ALA	-	expression tag	UNP B7J3C9
D	32	SER	-	expression tag	UNP B7J3C9
E	30	MET	-	expression tag	UNP B7J3C9
E	31	ALA	-	expression tag	UNP B7J3C9
E	32	SER	-	expression tag	UNP B7J3C9
F	30	MET	-	expression tag	UNP B7J3C9
F	31	ALA	-	expression tag	UNP B7J3C9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	32	SER	-	expression tag	UNP B7J3C9

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



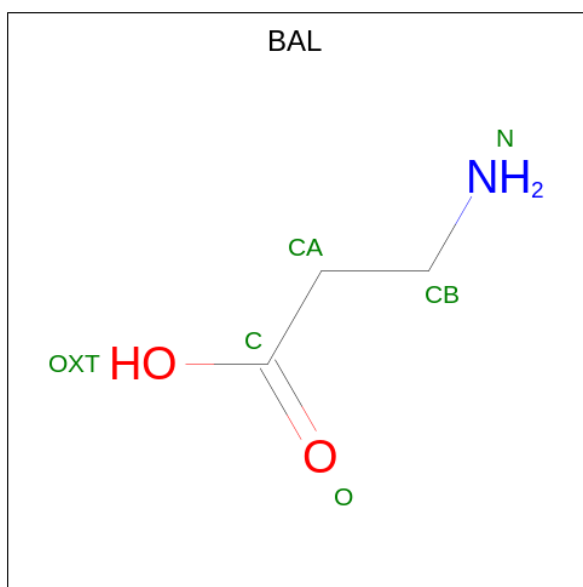
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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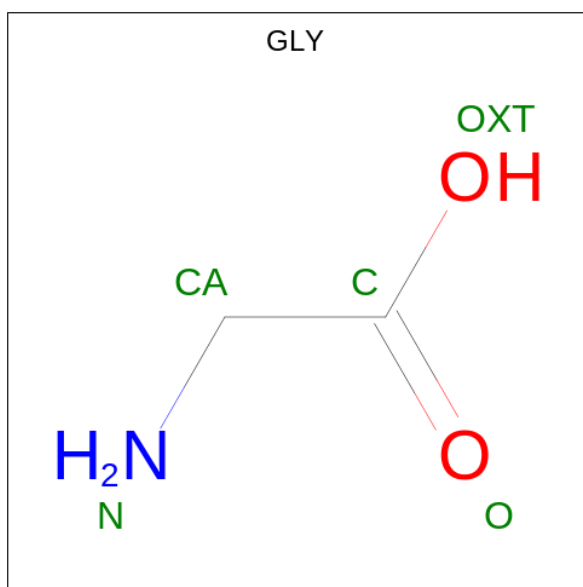
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total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

- Molecule 3 is BETA-ALANINE (three-letter code: BAL) (formula:  $C_3H_7NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			6	3	1	2		
3	D	1	Total	C	N	O	0	0
			6	3	1	2		
3	E	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			5	2	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			5	2	1	2		

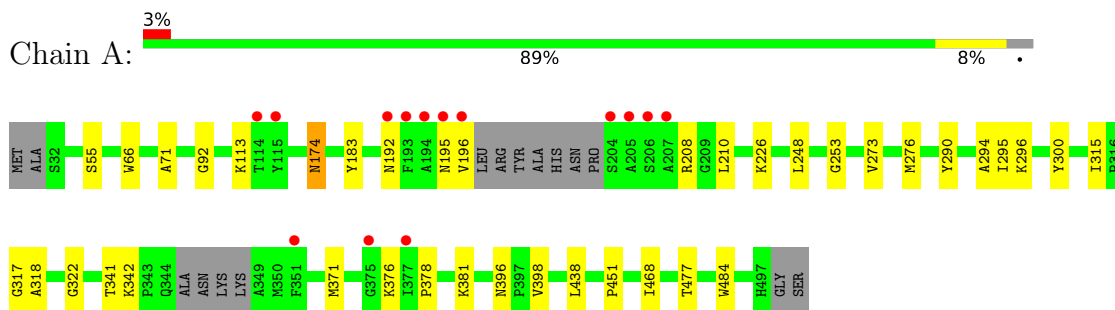
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	126	Total	O	0	0
			126	126		
5	B	127	Total	O	0	0
			127	127		
5	C	80	Total	O	0	0
			80	80		
5	D	82	Total	O	0	0
			82	82		
5	E	140	Total	O	0	0
			140	140		
5	F	142	Total	O	0	0
			142	142		

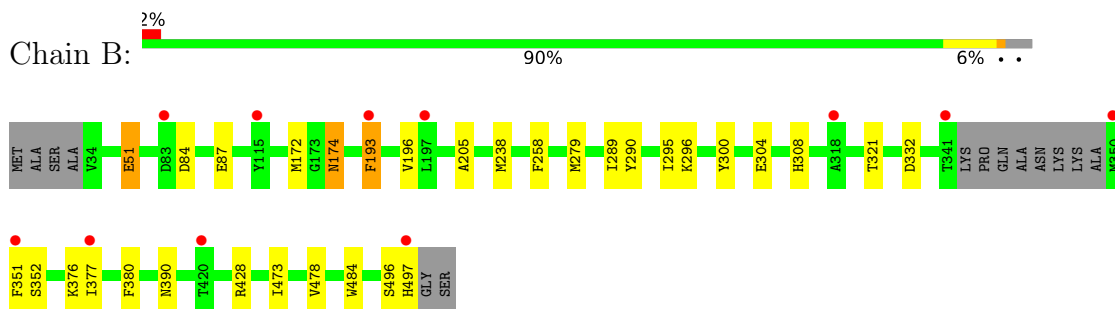
### 3 Residue-property plots [i](#)

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

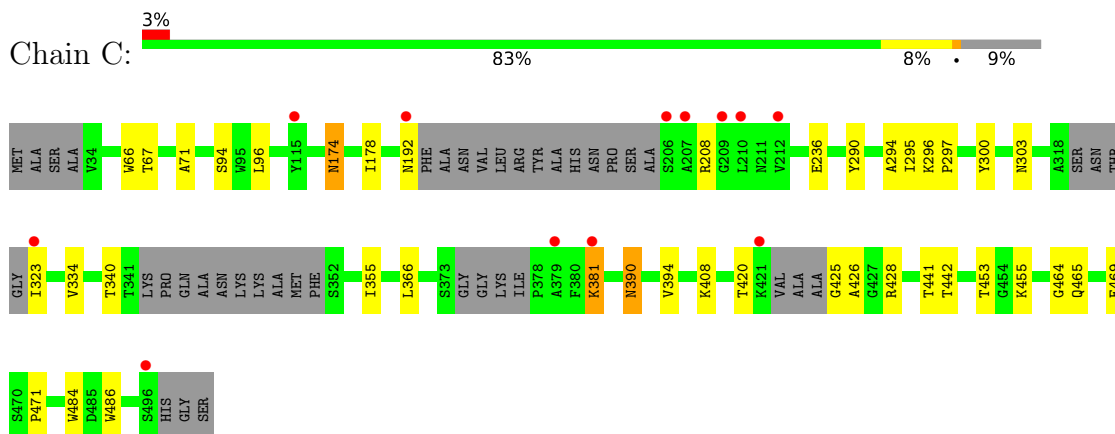
- Molecule 1: Tetrathionate hydrolase



- Molecule 1: Tetrathionate hydrolase

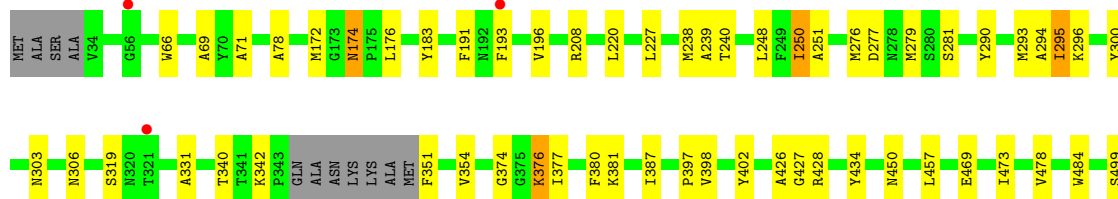
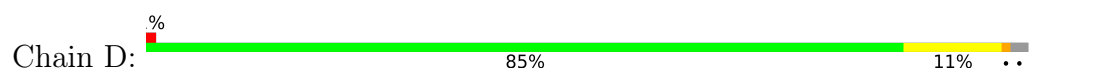


- Molecule 1: Tetrathionate hydrolase

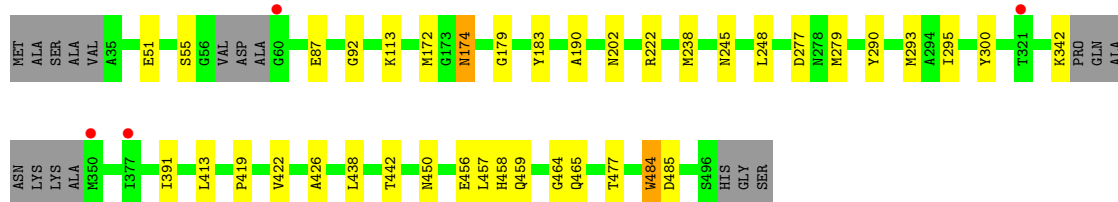
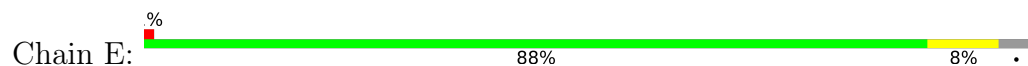


- Molecule 1: Tetrathionate hydrolase

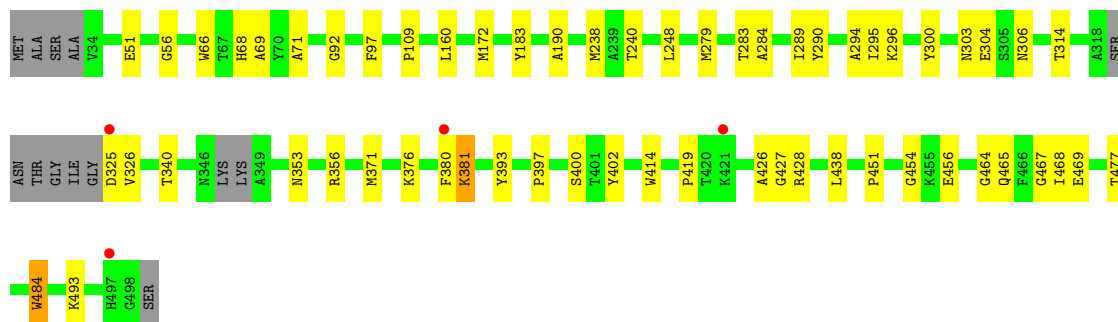
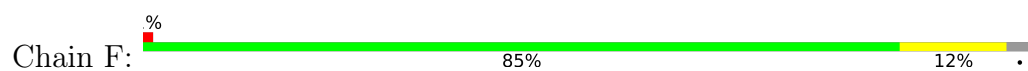




- Molecule 1: Tetrathionate hydrolase



- Molecule 1: Tetrathionate hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.03Å 91.03Å 231.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.36 – 1.95 44.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.36-1.95) 99.7 (44.66-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.177 , 0.219 0.178 , 0.219	Depositor DCC
$R_{free}$ test set	8100 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.041 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/3525	0.61	0/4826
1	B	0.40	0/3548	0.61	0/4860
1	C	0.37	0/3339	0.58	0/4569
1	D	0.37	0/3567	0.60	0/4886
1	E	0.42	0/3518	0.63	1/4815 (0.0%)
1	F	0.43	0/3558	0.63	0/4872
All	All	0.40	0/21055	0.61	1/28828 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	438	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	258	PHE	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	3421	0	3308	21	0
1	B	3441	0	3324	19	0
1	C	3242	0	3129	19	0
1	D	3459	0	3343	38	0
1	E	3413	0	3302	23	0
1	F	3451	0	3335	39	0
2	A	35	0	0	0	0
2	B	45	0	0	0	0
2	C	15	0	0	0	0
2	D	30	0	0	1	0
2	E	10	0	0	0	0
2	F	15	0	0	1	0
3	C	6	0	6	3	0
3	D	6	0	6	0	0
3	E	6	0	6	0	0
4	E	5	0	2	1	0
4	F	5	0	2	0	0
5	A	126	0	0	0	0
5	B	127	0	0	3	0
5	C	80	0	0	0	0
5	D	82	0	0	3	0
5	E	140	0	0	4	0
5	F	142	0	0	3	0
All	All	21302	0	19763	148	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 4.

All (148) 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:E:172:MET:SD	5:E:505:HOH:O	2.10	1.05
1:D:172:MET:SD	5:D:508:HOH:O	2.17	1.03
1:F:172:MET:SD	5:F:505:HOH:O	2.23	0.95
1:B:172:MET:SD	5:B:510:HOH:O	2.27	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:MET:SD	5:F:505:HOH:O	2.37	0.81
1:D:340:THR:HG21	1:D:381:LYS:HB2	1.63	0.80
1:D:354:VAL:HG21	1:F:51:GLU:HB2	1.65	0.78
1:F:467:GLY:N	1:F:469:GLU:OE2	2.16	0.78
1:B:238:MET:SD	5:B:510:HOH:O	2.43	0.76
1:D:238:MET:SD	5:D:508:HOH:O	2.47	0.73
1:C:340:THR:HB	1:C:381:LYS:HB3	1.68	0.73
1:E:238:MET:SD	5:E:505:HOH:O	2.46	0.73
1:B:279:MET:SD	5:B:510:HOH:O	2.46	0.73
1:E:450:ASN:HB2	1:E:457:LEU:HD11	1.75	0.69
1:D:279:MET:SD	5:D:508:HOH:O	2.51	0.69
1:F:68:HIS:CE1	1:F:284:ALA:H	2.11	0.69
1:C:174:ASN:HD22	1:C:174:ASN:C	1.93	0.68
1:E:87:GLU:OE1	5:E:601:HOH:O	2.12	0.67
1:F:279:MET:SD	5:F:505:HOH:O	2.53	0.66
1:D:354:VAL:CG2	1:F:51:GLU:HB2	2.28	0.64
1:B:380:PHE:HB3	1:B:428:ARG:HD2	1.80	0.62
3:C:504:BAL:HB2	1:E:458:HIS:CE1	2.34	0.62
1:A:192:ASN:HB3	1:A:195:ASN:HD22	1.66	0.61
1:D:319:SER:HA	1:D:342:LYS:HE2	1.82	0.60
1:B:496:SER:HB2	1:B:497:HIS:CD2	2.37	0.60
1:D:380:PHE:O	1:D:428:ARG:NE	2.36	0.58
1:F:68:HIS:HE1	1:F:283:THR:HA	1.69	0.57
1:C:297:PRO:HB2	1:C:323:ILE:HD12	1.86	0.56
1:E:279:MET:SD	5:E:505:HOH:O	2.58	0.56
1:C:67:THR:HG22	1:C:178:ILE:HD11	1.88	0.56
1:E:245:ASN:H	4:E:504:GLY:N	2.03	0.56
1:B:193:PHE:HZ	1:D:295:ILE:HD11	1.71	0.55
1:D:402:TYR:CZ	1:D:427:GLY:HA2	2.41	0.55
2:D:506:SO4:O3	1:F:56:GLY:N	2.35	0.55
1:A:315:ILE:HB	1:A:318:ALA:HB2	1.87	0.55
1:C:426:ALA:HA	1:C:442:THR:OG1	2.06	0.55
1:D:191:PHE:CE1	1:D:208:ARG:HG3	2.41	0.55
1:B:174:ASN:HD22	1:B:174:ASN:C	2.08	0.55
1:F:314:THR:HG23	1:F:356:ARG:HH12	1.73	0.54
1:F:289:ILE:HG12	1:F:304:GLU:HG2	1.88	0.54
1:B:193:PHE:CE2	1:D:276:MET:HE1	2.44	0.53
1:C:290:TYR:HA	1:C:300:TYR:O	2.09	0.53
1:F:314:THR:HG23	1:F:356:ARG:NH1	2.24	0.53
1:A:183:TYR:CE1	1:A:248:LEU:HD11	2.45	0.52
1:B:321:THR:HB	1:D:193:PHE:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ALA:C	1:C:296:LYS:H	2.13	0.52
1:F:303:ASN:HD21	1:F:306:ASN:HD22	1.56	0.52
1:F:66:TRP:CZ2	1:F:71:ALA:HB2	2.45	0.52
1:E:391:ILE:HD12	1:E:413:LEU:HD11	1.91	0.52
1:D:174:ASN:ND2	1:D:174:ASN:O	2.42	0.52
1:A:174:ASN:HD22	1:A:174:ASN:C	2.14	0.51
1:C:66:TRP:CZ2	1:C:71:ALA:HB2	2.45	0.51
1:B:332:ASP:OD2	1:B:390:ASN:ND2	2.44	0.51
1:F:397:PRO:HA	1:F:426:ALA:O	2.11	0.51
1:F:353:ASN:HB3	1:F:371:MET:HE3	1.90	0.51
1:B:193:PHE:HD2	1:D:208:ARG:NH2	2.08	0.50
1:A:376:LYS:HE2	1:A:378:PRO:HA	1.93	0.50
1:A:294:ALA:C	1:A:296:LYS:H	2.16	0.50
1:D:397:PRO:HA	1:D:426:ALA:O	2.11	0.50
1:A:195:ASN:HD21	1:A:210:LEU:HD23	1.76	0.49
1:C:208:ARG:O	1:C:236:GLU:HG3	2.13	0.49
1:F:380:PHE:O	1:F:428:ARG:NE	2.45	0.49
1:D:66:TRP:CZ2	1:D:71:ALA:HB2	2.47	0.49
1:F:68:HIS:CE1	1:F:283:THR:HA	2.48	0.49
1:D:354:VAL:HG21	1:F:51:GLU:CB	2.39	0.49
1:F:438:LEU:HG	1:F:451:PRO:HB3	1.95	0.49
1:F:493:LYS:HE2	2:F:502:SO4:O3	2.12	0.49
1:A:253:GLY:O	1:A:276:MET:HG2	2.12	0.49
1:E:426:ALA:HA	1:E:442:THR:OG1	2.13	0.49
1:D:377:ILE:HG13	1:D:381:LYS:HG2	1.95	0.48
1:C:192:ASN:N	1:C:192:ASN:OD1	2.46	0.48
1:E:419:PRO:HB2	1:E:422:VAL:HG22	1.94	0.48
1:A:371:MET:O	1:A:396:ASN:ND2	2.46	0.48
1:A:317:GLY:O	1:A:342:LYS:HG2	2.14	0.48
1:E:174:ASN:HD22	1:E:174:ASN:C	2.17	0.48
1:C:390:ASN:HD21	1:C:408:LYS:HZ2	1.62	0.47
1:C:425:GLY:HA2	1:C:428:ARG:HD2	1.96	0.47
1:F:92:GLY:HA2	1:F:477:THR:OG1	2.14	0.47
1:D:473:ILE:HG12	1:D:478:VAL:HG22	1.96	0.47
1:D:450:ASN:HB2	1:D:457:LEU:HD11	1.97	0.47
1:A:318:ALA:HA	1:A:341:THR:HG22	1.97	0.47
1:D:290:TYR:HA	1:D:300:TYR:O	2.15	0.47
1:F:340:THR:OG1	1:F:381:LYS:HG3	2.15	0.47
1:D:183:TYR:CE1	1:D:248:LEU:HD11	2.51	0.46
1:D:78:ALA:HB1	1:D:434:TYR:HD1	1.80	0.46
1:F:402:TYR:CE1	1:F:427:GLY:HA2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASN:ND2	1:C:174:ASN:C	2.65	0.46
1:B:51:GLU:H	1:B:51:GLU:HG3	1.36	0.46
1:D:294:ALA:C	1:D:296:LYS:H	2.18	0.46
1:B:351:PHE:CE1	1:B:377:ILE:HG12	2.51	0.46
1:D:303:ASN:ND2	1:D:306:ASN:OD1	2.49	0.46
1:D:69:ALA:HB2	1:D:240:THR:HB	1.98	0.45
3:C:504:BAL:HA1	1:E:459:GLN:HG2	1.97	0.45
1:A:192:ASN:HB2	1:A:210:LEU:O	2.16	0.45
1:A:290:TYR:HA	1:A:300:TYR:O	2.15	0.45
1:B:296:LYS:NZ	1:E:55:SER:HB3	2.32	0.45
1:F:402:TYR:CZ	1:F:427:GLY:HA2	2.51	0.45
1:D:220:LEU:HD23	1:D:227:LEU:HA	1.98	0.45
1:D:174:ASN:HD22	1:D:174:ASN:C	2.17	0.45
1:E:183:TYR:CE1	1:E:248:LEU:HD11	2.52	0.45
1:A:322:GLY:HA3	1:A:381:LYS:HG3	1.99	0.44
1:C:355:ILE:HD12	1:C:394:VAL:HG11	1.99	0.44
1:B:196:VAL:HG22	1:D:196:VAL:HG22	2.00	0.44
1:C:441:THR:HG23	1:C:471:PRO:HG3	1.99	0.44
1:A:208:ARG:HE	1:A:276:MET:HE3	1.83	0.43
1:E:464:GLY:HA2	1:E:484:TRP:CD1	2.54	0.43
1:E:92:GLY:HA2	1:E:477:THR:OG1	2.18	0.43
1:E:179:GLY:O	1:E:222:ARG:NH1	2.50	0.43
1:F:69:ALA:HB2	1:F:240:THR:HB	2.00	0.43
1:F:400:SER:HA	1:F:426:ALA:O	2.18	0.43
1:D:351:PHE:CE2	1:D:376:LYS:HD2	2.54	0.43
1:A:92:GLY:HA2	1:A:477:THR:OG1	2.18	0.43
1:D:239:ALA:HB1	1:D:281:SER:HA	2.00	0.43
1:D:331:ALA:HB3	1:D:387:ILE:HG21	2.01	0.43
1:E:277:ASP:HB2	1:E:293:MET:SD	2.59	0.43
1:F:464:GLY:HA2	1:F:484:TRP:CD1	2.53	0.43
1:A:192:ASN:O	1:A:196:VAL:HG23	2.18	0.43
1:A:66:TRP:CZ2	1:A:71:ALA:HB2	2.54	0.43
3:C:504:BAL:HB2	1:E:458:HIS:HE1	1.81	0.43
1:D:319:SER:HA	1:D:342:LYS:HG2	2.01	0.43
1:A:438:LEU:HG	1:A:451:PRO:HB3	2.01	0.42
1:D:374:GLY:HA3	1:D:398:VAL:O	2.19	0.42
1:F:381:LYS:HG2	1:F:381:LYS:H	1.67	0.42
1:F:393:TYR:CD2	1:F:438:LEU:HD11	2.55	0.42
1:E:190:ALA:HB1	1:F:190:ALA:HB1	2.01	0.42
1:B:205:ALA:HA	1:E:51:GLU:HG3	2.01	0.42
1:B:289:ILE:HG23	1:B:304:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ILE:HG12	1:B:478:VAL:HG22	2.01	0.42
1:F:294:ALA:C	1:F:296:LYS:H	2.22	0.42
1:F:414:TRP:CD2	1:F:454:GLY:HA3	2.55	0.41
1:C:96:LEU:HG	1:C:486:TRP:CE3	2.55	0.41
1:D:250:ILE:HD12	1:D:251:ALA:H	1.85	0.41
1:F:97:PHE:CZ	1:F:160:LEU:HD13	2.56	0.41
1:B:290:TYR:HA	1:B:300:TYR:O	2.21	0.41
1:E:290:TYR:HA	1:E:300:TYR:O	2.20	0.41
1:D:176:LEU:HB2	1:D:183:TYR:HB2	2.03	0.41
1:A:226:LYS:HA	1:A:226:LYS:HD3	1.87	0.41
1:F:183:TYR:CD1	1:F:248:LEU:HD11	2.56	0.41
1:F:183:TYR:CE1	1:F:248:LEU:HD11	2.56	0.41
1:A:322:GLY:HA3	1:A:381:LYS:CB	2.51	0.41
1:C:334:VAL:HG13	1:C:366:LEU:HD12	2.03	0.41
1:C:464:GLY:O	1:C:465:GLN:HG2	2.21	0.41
1:C:453:THR:HB	1:C:455:LYS:HG3	2.03	0.40
1:E:456:GLU:OE2	1:E:459:GLN:HB3	2.22	0.40
1:D:277:ASP:HB2	1:D:293:MET:SD	2.61	0.40
1:F:290:TYR:HA	1:F:300:TYR:O	2.21	0.40
1:F:353:ASN:HB3	1:F:371:MET:CE	2.51	0.40
1:F:419:PRO:HG3	1:F:456:GLU:OE1	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	449/470 (96%)	439 (98%)	9 (2%)	1 (0%)	47	38
1	B	452/470 (96%)	442 (98%)	9 (2%)	1 (0%)	47	38
1	C	417/470 (89%)	407 (98%)	9 (2%)	1 (0%)	47	38
1	D	455/470 (97%)	447 (98%)	7 (2%)	1 (0%)	47	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	446/470 (95%)	436 (98%)	9 (2%)	1 (0%)	47	38
1	F	451/470 (96%)	440 (98%)	10 (2%)	1 (0%)	47	38
All	All	2670/2820 (95%)	2611 (98%)	53 (2%)	6 (0%)	47	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	ILE
1	C	295	ILE
1	D	295	ILE
1	F	295	ILE
1	B	295	ILE
1	E	295	ILE

### 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	350/361 (97%)	343 (98%)	7 (2%)	55	48
1	B	352/361 (98%)	343 (97%)	9 (3%)	46	36
1	C	333/361 (92%)	325 (98%)	8 (2%)	49	40
1	D	354/361 (98%)	348 (98%)	6 (2%)	60	55
1	E	349/361 (97%)	342 (98%)	7 (2%)	55	48
1	F	352/361 (98%)	344 (98%)	8 (2%)	50	42
All	All	2090/2166 (96%)	2045 (98%)	45 (2%)	52	44

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

Mol	Chain	Res	Type
1	A	55	SER
1	A	113	LYS
1	A	174	ASN
1	A	273	VAL

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Mol	Chain	Res	Type
1	A	398	VAL
1	A	468	ILE
1	A	484	TRP
1	B	51	GLU
1	B	84	ASP
1	B	87	GLU
1	B	174	ASN
1	B	193	PHE
1	B	308	HIS
1	B	352	SER
1	B	376	LYS
1	B	484	TRP
1	C	94	SER
1	C	174	ASN
1	C	303	ASN
1	C	381	LYS
1	C	390	ASN
1	C	420	THR
1	C	469	GLU
1	C	484	TRP
1	D	174	ASN
1	D	250	ILE
1	D	376	LYS
1	D	469	GLU
1	D	484	TRP
1	D	499	SER
1	E	113	LYS
1	E	174	ASN
1	E	202	ASN
1	E	342	LYS
1	E	465	GLN
1	E	484	TRP
1	E	485	ASP
1	F	109	PRO
1	F	325	ASP
1	F	326	VAL
1	F	376	LYS
1	F	381	LYS
1	F	465	GLN
1	F	468	ILE
1	F	484	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	497	HIS
1	B	497	HIS
1	C	390	ASN
1	E	202	ASN
1	E	459	GLN
1	E	465	GLN
1	F	68	HIS
1	F	306	ASN
1	F	460	HIS
1	F	465	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	C	502	-	4,4,4	0.19	0	6,6,6	0.32	0
2	SO4	B	507	-	4,4,4	0.17	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	C	501	-	4,4,4	0.11	0	6,6,6	0.18	0
2	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	D	501	-	4,4,4	0.16	0	6,6,6	0.31	0
3	BAL	D	507	-	1,5,5	0.27	0	0,5,5	0.00	-
2	SO4	B	505	-	4,4,4	0.12	0	6,6,6	0.17	0
2	SO4	A	505	-	4,4,4	0.30	0	6,6,6	0.16	0
2	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	D	502	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	A	501	-	4,4,4	0.10	0	6,6,6	0.16	0
2	SO4	A	506	-	4,4,4	0.18	0	6,6,6	0.34	0
4	GLY	F	504	-	1,4,4	0.13	0	0,4,4	0.00	-
2	SO4	D	504	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	F	503	-	4,4,4	0.13	0	6,6,6	0.23	0
2	SO4	D	503	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	B	506	-	4,4,4	0.20	0	6,6,6	0.09	0
3	BAL	C	504	-	1,5,5	0.25	0	0,5,5	0.00	-
2	SO4	F	501	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	E	501	-	4,4,4	0.10	0	6,6,6	0.14	0
2	SO4	E	502	-	4,4,4	0.24	0	6,6,6	0.35	0
2	SO4	B	503	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	D	506	-	4,4,4	0.11	0	6,6,6	0.17	0
3	BAL	E	503	-	1,5,5	0.22	0	0,5,5	0.00	-
2	SO4	F	502	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	B	502	-	4,4,4	0.13	0	6,6,6	0.32	0
2	SO4	B	508	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	B	501	-	4,4,4	0.11	0	6,6,6	0.23	0
2	SO4	A	502	-	4,4,4	0.20	0	6,6,6	0.21	0
4	GLY	E	504	-	1,4,4	0.10	0	0,4,4	0.00	-
2	SO4	A	507	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	B	509	-	4,4,4	0.18	0	6,6,6	0.20	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	BAL	E	503	-	-	0/1/3/3	-
4	GLY	F	504	-	-	0/0/2/2	-
3	BAL	C	504	-	-	0/1/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLY	E	504	-	-	0/0/2/2	-
3	BAL	D	507	-	-	0/1/3/3	-

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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	BAL	3	0
2	D	506	SO4	1	0
2	F	502	SO4	1	0
4	E	504	GLY	1	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

### 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	455/470 (96%)	-0.11	14 (3%)	49	58	14, 22, 45, 57	0
1	B	456/470 (97%)	-0.16	11 (2%)	59	68	14, 22, 41, 59	0
1	C	429/470 (91%)	-0.10	12 (2%)	53	62	18, 28, 47, 68	0
1	D	459/470 (97%)	-0.19	3 (0%)	87	92	19, 27, 41, 53	0
1	E	452/470 (96%)	-0.32	4 (0%)	84	89	12, 21, 38, 56	0
1	F	457/470 (97%)	-0.31	4 (0%)	84	89	14, 22, 40, 54	0
All	All	2708/2820 (96%)	-0.20	48 (1%)	68	76	12, 24, 42, 68	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ALA	5.1
1	B	377	ILE	4.9
1	A	115	TYR	4.8
1	A	375	GLY	4.6
1	A	192	ASN	4.4
1	C	207	ALA	3.9
1	C	210	LEU	3.9
1	A	193	PHE	3.7
1	A	206	SER	3.5
1	A	377	ILE	3.4
1	A	204	SER	3.3
1	C	209	GLY	3.3
1	A	207	ALA	3.2
1	F	380	PHE	3.2
1	B	341	THR	3.1
1	C	323	ILE	3.1
1	C	115	TYR	3.0
1	B	318	ALA	3.0
1	C	379	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	193	PHE	2.8
1	C	496	SER	2.7
1	C	206	SER	2.7
1	E	377	ILE	2.7
1	B	351	PHE	2.7
1	B	497	HIS	2.7
1	D	321	THR	2.6
1	B	197	LEU	2.6
1	B	83	ASP	2.5
1	F	421	LYS	2.5
1	A	205	ALA	2.4
1	D	56	GLY	2.4
1	C	192	ASN	2.4
1	A	196	VAL	2.4
1	F	325	ASP	2.3
1	A	195	ASN	2.3
1	E	321	THR	2.3
1	D	193	PHE	2.2
1	B	420	THR	2.2
1	C	212	VAL	2.2
1	E	60	GLY	2.2
1	C	381	LYS	2.2
1	C	421	LYS	2.2
1	A	351	PHE	2.1
1	A	114	THR	2.1
1	B	115	TYR	2.1
1	E	350	MET	2.1
1	B	350	MET	2.1
1	F	497	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	D	505	5/5	0.81	0.20	46,52,57,68	0
4	GLY	E	504	5/5	0.84	0.12	28,32,38,42	0
3	BAL	D	507	6/6	0.86	0.12	32,37,40,44	0
3	BAL	C	504	6/6	0.86	0.25	27,34,37,38	0
2	SO4	A	505	5/5	0.86	0.15	30,33,44,55	0
2	SO4	A	502	5/5	0.87	0.25	38,44,51,65	0
2	SO4	A	503	5/5	0.88	0.16	51,55,69,73	0
3	BAL	E	503	6/6	0.88	0.21	26,31,35,37	0
2	SO4	B	508	5/5	0.89	0.18	35,40,44,57	0
2	SO4	A	504	5/5	0.90	0.11	53,54,66,67	0
2	SO4	D	502	5/5	0.91	0.18	41,47,53,54	0
2	SO4	B	504	5/5	0.91	0.22	43,44,55,58	0
4	GLY	F	504	5/5	0.92	0.09	29,30,37,41	0
2	SO4	C	503	5/5	0.92	0.09	49,56,62,63	0
2	SO4	A	506	5/5	0.94	0.12	25,35,37,39	0
2	SO4	B	509	5/5	0.94	0.12	35,48,52,57	0
2	SO4	A	501	5/5	0.95	0.21	42,48,52,58	0
2	SO4	A	507	5/5	0.95	0.10	32,32,45,55	0
2	SO4	D	503	5/5	0.95	0.16	46,50,55,58	0
2	SO4	F	503	5/5	0.96	0.08	31,32,39,40	0
2	SO4	B	506	5/5	0.96	0.20	38,39,44,50	0
2	SO4	B	505	5/5	0.97	0.10	35,38,41,44	0
2	SO4	D	506	5/5	0.98	0.12	34,40,45,47	0
2	SO4	B	507	5/5	0.98	0.06	32,40,41,43	0
2	SO4	F	502	5/5	0.98	0.11	37,41,45,48	0
2	SO4	D	504	5/5	0.98	0.06	26,31,34,34	0
2	SO4	B	501	5/5	0.98	0.09	36,39,40,44	0
2	SO4	D	501	5/5	0.98	0.06	26,31,36,40	0
2	SO4	E	501	5/5	0.98	0.06	29,29,31,31	0
2	SO4	E	502	5/5	0.98	0.08	31,32,35,35	0
2	SO4	C	501	5/5	0.98	0.09	34,36,41,41	0
2	SO4	C	502	5/5	0.99	0.08	23,25,27,29	0
2	SO4	B	502	5/5	0.99	0.08	19,24,25,28	0
2	SO4	F	501	5/5	0.99	0.04	24,25,31,31	0
2	SO4	B	503	5/5	0.99	0.06	24,26,29,30	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.