



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 18, 2021 – 10:11 AM JST

PDB ID : 7CQY
Title : Tetrathionate hydrolase from Acidithiobacillus ferrooxidans mutant - D325N
Authors : Tamada, T.; Hirano, Y.
Deposited on : 2020-08-12
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

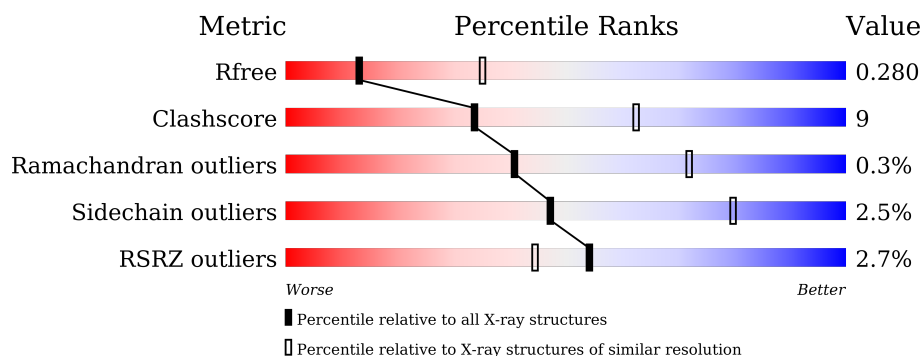
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 75%, yellow 75%, yellow 86%, grey 86%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 15% • 10% </div> </div>
1	B	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 74%, yellow 74%, yellow 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 74% 18% • 7% </div> </div>
1	C	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 7%, green 7%, green 65%, yellow 65%, yellow 86%, grey 86%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 7% 65% 21% • 13% </div> </div>
1	D	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 75%, yellow 75%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 75% 22% •• </div> </div>
1	E	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 77%, yellow 77%, yellow 95%, grey 95%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 77% 18% •• </div> </div>
1	F	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 76%, yellow 76%, yellow 93%, grey 93%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 76% 17% • 5% </div> </div>

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	E	501	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19937 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	425	Total	C	N	O	S	0	0	0
			3202	2058	541	591	12			
1	B	436	Total	C	N	O	S	0	0	0
			3302	2120	562	609	11			
1	C	409	Total	C	N	O	S	0	0	0
			3105	1997	524	574	10			
1	D	464	Total	C	N	O	S	0	0	0
			3502	2248	600	642	12			
1	E	451	Total	C	N	O	S	0	0	0
			3406	2185	582	627	12			
1	F	445	Total	C	N	O	S	0	0	0
			3365	2161	575	618	11			

There are 24 discrepancies between the modelled and reference sequences:

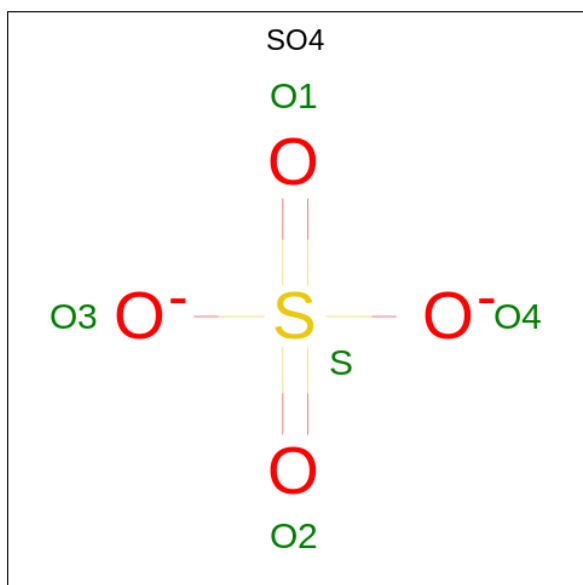
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP B7J3C9
A	31	SER	-	expression tag	UNP B7J3C9
A	32	ALA	-	expression tag	UNP B7J3C9
A	325	ASN	ASP	engineered mutation	UNP B7J3C9
B	30	MET	-	expression tag	UNP B7J3C9
B	31	SER	-	expression tag	UNP B7J3C9
B	32	ALA	-	expression tag	UNP B7J3C9
B	325	ASN	ASP	engineered mutation	UNP B7J3C9
C	30	MET	-	expression tag	UNP B7J3C9
C	31	SER	-	expression tag	UNP B7J3C9
C	32	ALA	-	expression tag	UNP B7J3C9
C	325	ASN	ASP	engineered mutation	UNP B7J3C9
D	30	MET	-	expression tag	UNP B7J3C9
D	31	SER	-	expression tag	UNP B7J3C9
D	32	ALA	-	expression tag	UNP B7J3C9
D	325	ASN	ASP	engineered mutation	UNP B7J3C9
E	30	MET	-	expression tag	UNP B7J3C9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	31	SER	-	expression tag	UNP B7J3C9
E	32	ALA	-	expression tag	UNP B7J3C9
E	325	ASN	ASP	engineered mutation	UNP B7J3C9
F	30	MET	-	expression tag	UNP B7J3C9
F	31	SER	-	expression tag	UNP B7J3C9
F	32	ALA	-	expression tag	UNP B7J3C9
F	325	ASN	ASP	engineered mutation	UNP B7J3C9

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



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

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

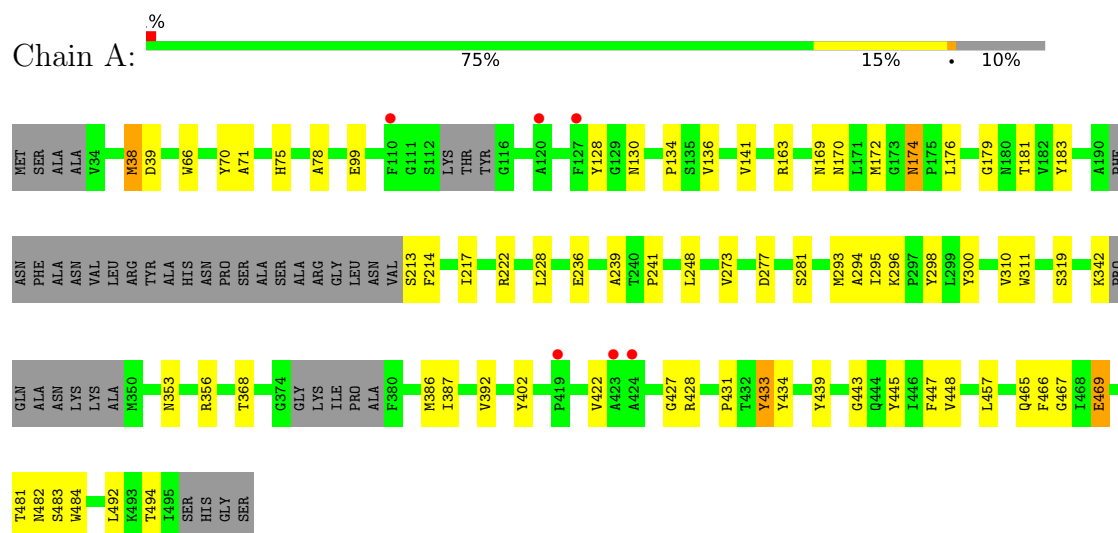
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		
3	D	4	Total	O	0	0
			4	4		
3	E	1	Total	O	0	0
			1	1		
3	F	1	Total	O	0	0
			1	1		

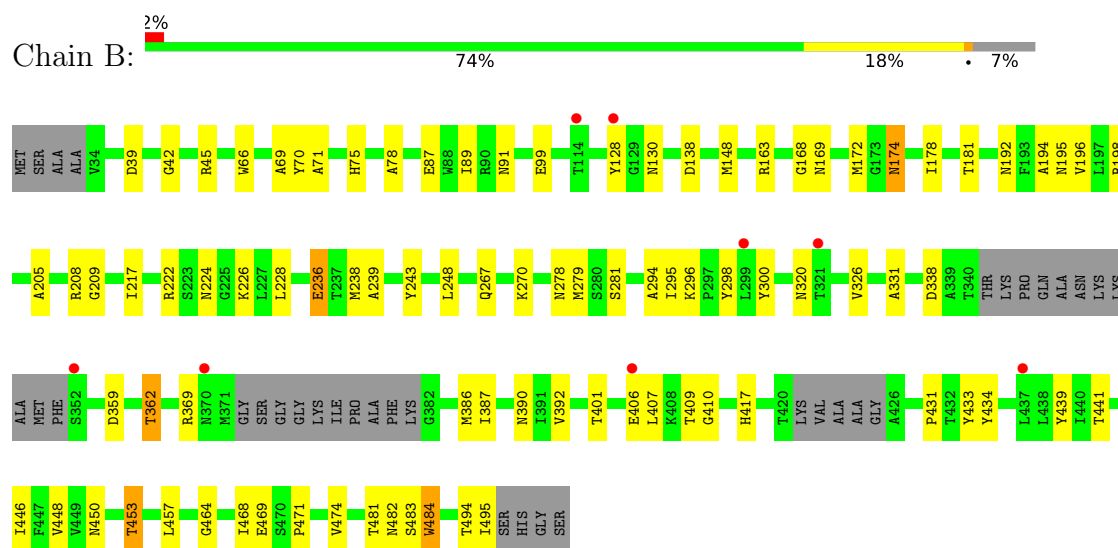
3 Residue-property plots [i](#)

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

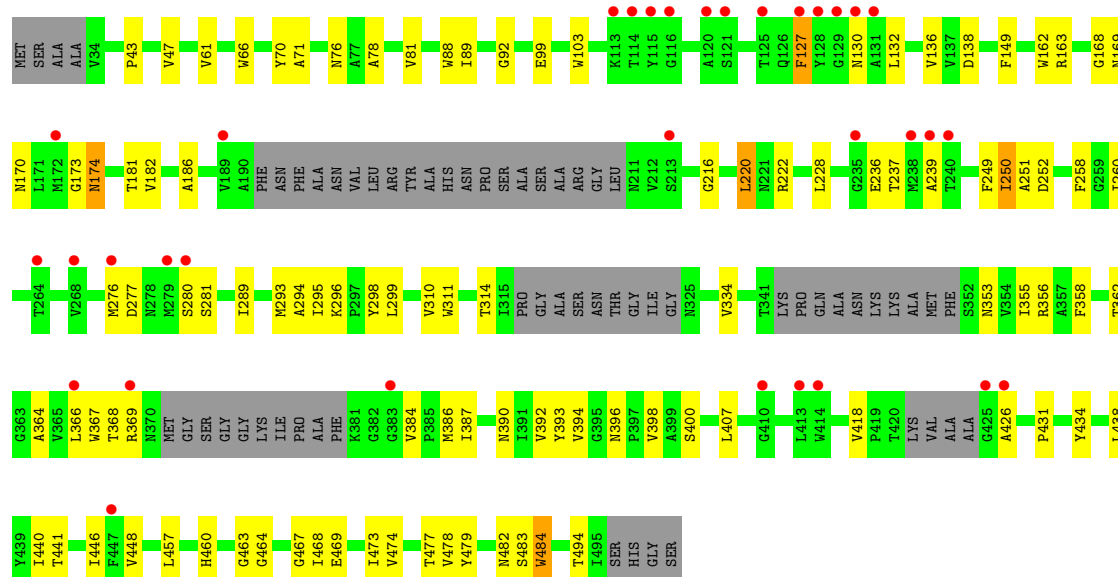


• Molecule 1: Tetrathionate hydrolase

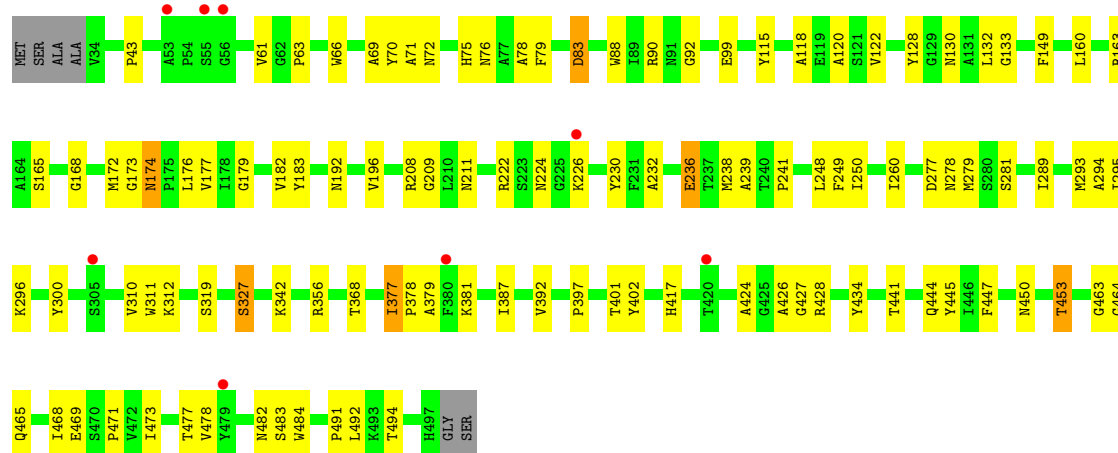
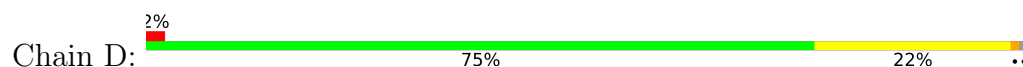


• Molecule 1: Tetrathionate hydrolase

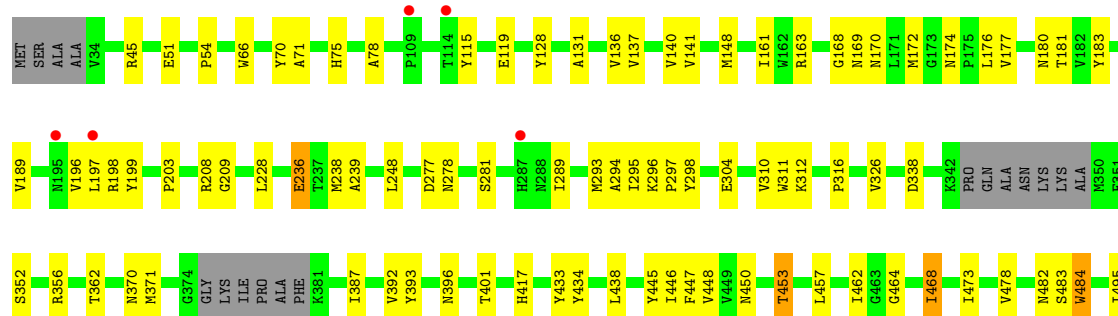
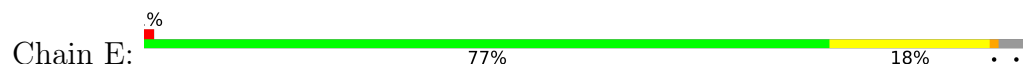




- Molecule 1: Tetrathionate hydrolase

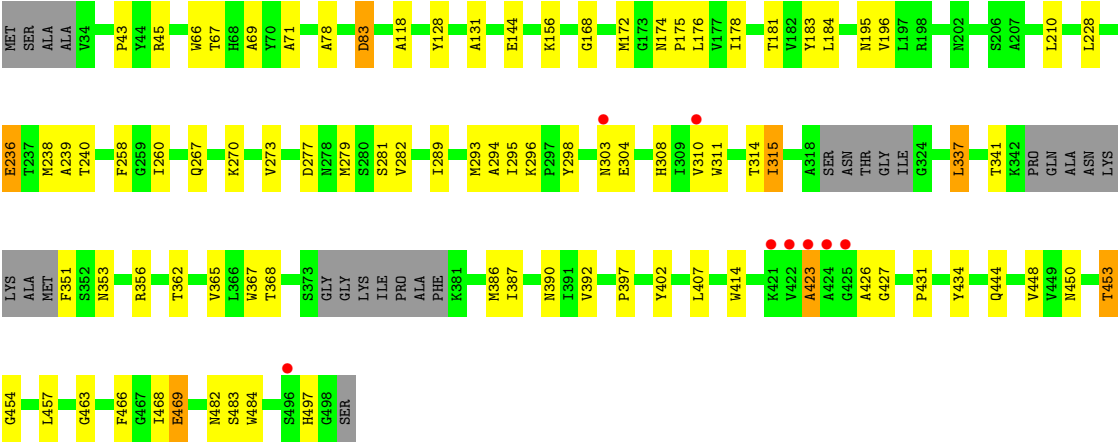
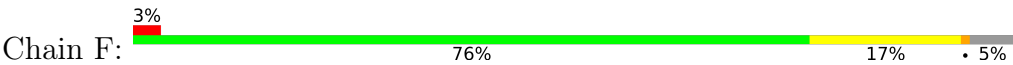


- Molecule 1: Tetrathionate hydrolase





● Molecule 1: Tetrathionate hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	94.31Å 94.31Å 235.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.24 – 2.80 46.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.24-2.80) 99.6 (46.24-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.225 , 0.280 0.226 , 0.280	Depositor DCC
R_{free} test set	2770 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.034 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19937	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/3298	0.53	0/4514
1	B	0.27	0/3403	0.52	0/4664
1	C	0.27	0/3198	0.52	0/4381
1	D	0.27	0/3611	0.50	0/4945
1	E	0.27	0/3510	0.52	0/4806
1	F	0.28	0/3468	0.52	1/4748 (0.0%)
All	All	0.27	0/20488	0.52	1/28058 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	337	LEU	CA-CB-CG	5.66	128.31	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3202	0	3092	44	0
1	B	3302	0	3180	57	0
1	C	3105	0	2993	64	0
1	D	3502	0	3397	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3406	0	3290	55	0
1	F	3365	0	3248	57	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	D	5	0	0	0	0
2	E	15	0	0	2	0
2	F	10	0	0	1	0
3	A	2	0	0	1	0
3	B	2	0	0	2	0
3	D	4	0	0	4	0
3	E	1	0	0	0	0
3	F	1	0	0	2	0
All	All	19937	0	19200	334	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 9.

All (334) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ASN:ND2	1:B:453:THR:OG1	2.16	0.78
1:D:172:MET:SD	3:D:604:HOH:O	2.42	0.76
1:D:132:LEU:HD22	1:D:173:GLY:HA2	1.70	0.73
1:F:78:ALA:HB1	1:F:434:TYR:HD1	1.54	0.72
1:B:172:MET:SD	3:B:602:HOH:O	2.47	0.71
1:F:448:VAL:HG12	1:F:457:LEU:HB2	1.73	0.71
1:D:441:THR:HG23	1:D:471:PRO:HG3	1.73	0.70
1:B:448:VAL:HG12	1:B:457:LEU:HB2	1.74	0.69
1:A:172:MET:SD	3:A:602:HOH:O	2.50	0.69
1:C:186:ALA:O	1:C:237:THR:OG1	2.10	0.69
1:D:450:ASN:ND2	1:D:453:THR:OG1	2.25	0.68
1:D:78:ALA:HB1	1:D:434:TYR:HD1	1.59	0.67
1:F:239:ALA:HB1	1:F:281:SER:HA	1.75	0.67
1:A:78:ALA:HB1	1:A:434:TYR:HD1	1.60	0.67
1:F:83:ASP:N	1:F:83:ASP:OD1	2.24	0.67
1:C:387:ILE:HG12	1:C:392:VAL:HG22	1.77	0.66
1:B:441:THR:HG23	1:B:471:PRO:HG3	1.78	0.66
1:F:156:LYS:NZ	2:F:501:SO4:O1	2.26	0.66
1:D:279:MET:SD	3:D:604:HOH:O	2.54	0.65
1:E:239:ALA:HB1	1:E:281:SER:HA	1.78	0.65
1:C:89:ILE:HD11	1:C:474:VAL:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ASN:HD22	1:D:211:ASN:HB2	1.61	0.65
1:D:281:SER:H	1:D:327:SER:HB3	1.60	0.64
1:D:239:ALA:HB1	1:D:281:SER:HA	1.81	0.63
1:D:69:ALA:HA	1:D:174:ASN:HD21	1.63	0.63
1:B:267:GLN:NE2	1:B:270:LYS:HB2	2.14	0.63
1:C:136:VAL:HG21	1:C:479:TYR:HD2	1.62	0.63
1:F:356:ARG:HH21	1:F:365:VAL:HG11	1.64	0.62
1:B:209:GLY:HA3	1:B:236:GLU:HB3	1.81	0.62
1:F:176:LEU:HB2	1:F:183:TYR:HB2	1.80	0.62
1:E:78:ALA:HB1	1:E:434:TYR:HD1	1.64	0.62
1:F:172:MET:SD	3:F:601:HOH:O	2.56	0.62
1:A:448:VAL:HG12	1:A:457:LEU:HB2	1.82	0.62
1:B:390:ASN:HD22	1:B:407:LEU:HD23	1.65	0.60
1:B:469:GLU:OE1	1:B:481:THR:OG1	2.14	0.60
1:B:196:VAL:HG22	1:D:196:VAL:HG22	1.83	0.60
1:F:267:GLN:NE2	1:F:270:LYS:HB2	2.16	0.60
1:C:239:ALA:HB1	1:C:281:SER:HA	1.83	0.60
1:C:277:ASP:OD1	1:C:280:SER:OG	2.20	0.60
1:D:277:ASP:HB2	1:D:293:MET:SD	2.42	0.59
1:E:448:VAL:HG12	1:E:457:LEU:HB2	1.84	0.59
1:F:118:ALA:HA	1:F:423:ALA:HB1	1.85	0.59
1:E:131:ALA:O	1:E:468:ILE:HG22	2.03	0.59
1:B:205:ALA:HB2	1:E:51:GLU:HG3	1.85	0.59
1:A:387:ILE:HG12	1:A:392:VAL:HG22	1.85	0.58
1:F:289:ILE:HG12	1:F:304:GLU:HG2	1.86	0.58
1:A:66:TRP:CZ2	1:A:71:ALA:HB2	2.38	0.58
1:F:144:GLU:HG3	1:F:175:PRO:HG3	1.86	0.58
1:E:128:TYR:HE1	1:F:168:GLY:HA3	1.69	0.58
1:D:176:LEU:HB2	1:D:183:TYR:HB2	1.85	0.58
1:F:66:TRP:CZ2	1:F:71:ALA:HB2	2.39	0.57
1:C:464:GLY:HA2	1:C:484:TRP:CD1	2.39	0.57
1:A:128:TYR:HE1	1:C:168:GLY:HA3	1.70	0.57
1:E:45:ARG:NH1	2:E:501:SO4:O1	2.38	0.57
1:B:294:ALA:C	1:B:296:LYS:H	2.07	0.57
1:D:238:MET:SD	3:D:604:HOH:O	2.58	0.57
1:C:362:THR:HG23	1:C:364:ALA:H	1.70	0.57
1:F:294:ALA:C	1:F:296:LYS:H	2.08	0.57
1:A:277:ASP:HB2	1:A:293:MET:SD	2.45	0.57
1:D:294:ALA:C	1:D:296:LYS:H	2.08	0.56
1:E:208:ARG:HD2	1:E:236:GLU:OE2	2.04	0.56
1:F:67:THR:HG22	1:F:178:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ILE:HG12	1:C:478:VAL:HG22	1.86	0.56
1:E:66:TRP:CZ2	1:E:71:ALA:HB2	2.40	0.56
1:C:138:ASP:HB2	1:C:222:ARG:HH22	1.71	0.55
1:D:473:ILE:HG23	1:D:492:LEU:HD11	1.89	0.55
1:E:294:ALA:C	1:E:296:LYS:H	2.10	0.55
1:F:387:ILE:HG12	1:F:392:VAL:HG22	1.88	0.55
1:A:179:GLY:O	1:A:222:ARG:NH1	2.38	0.54
1:A:294:ALA:C	1:A:296:LYS:H	2.09	0.54
1:A:356:ARG:NE	1:A:368:THR:OG1	2.37	0.54
1:B:78:ALA:HB1	1:B:434:TYR:HD1	1.71	0.54
1:C:78:ALA:HB1	1:C:434:TYR:HD1	1.72	0.54
1:B:239:ALA:HB1	1:B:281:SER:HA	1.89	0.54
1:D:83:ASP:O	1:D:90:ARG:NH1	2.41	0.54
1:F:66:TRP:NE1	1:F:174:ASN:OD1	2.40	0.54
1:B:99:GLU:OE1	1:B:130:ASN:ND2	2.32	0.53
1:B:87:GLU:HG2	1:B:91:ASN:HD22	1.73	0.53
1:F:181:THR:HG23	1:F:228:LEU:HD12	1.91	0.52
1:B:208:ARG:HD2	1:B:236:GLU:OE2	2.09	0.52
1:D:133:GLY:HA2	1:D:469:GLU:HG2	1.90	0.52
1:C:482:ASN:OD1	1:C:483:SER:N	2.42	0.52
1:D:118:ALA:HB1	1:D:378:PRO:HG3	1.92	0.52
1:D:478:VAL:HG23	1:D:492:LEU:HD12	1.91	0.52
1:E:473:ILE:HG12	1:E:478:VAL:HG22	1.90	0.52
1:F:303:ASN:HD22	1:F:308:HIS:HB3	1.73	0.52
1:A:239:ALA:HB1	1:A:281:SER:HA	1.90	0.52
1:F:314:THR:O	1:F:356:ARG:NH1	2.42	0.52
1:A:298:TYR:HB2	1:A:300:TYR:CE2	2.44	0.52
1:D:402:TYR:CZ	1:D:427:GLY:HA2	2.46	0.51
1:F:450:ASN:ND2	1:F:453:THR:OG1	2.43	0.51
1:A:70:TYR:HB2	1:A:75:HIS:HA	1.91	0.51
1:C:236:GLU:O	1:C:252:ASP:HA	2.09	0.51
1:C:446:ILE:HG23	1:C:460:HIS:HB3	1.91	0.51
1:B:387:ILE:HG12	1:B:392:VAL:HG22	1.92	0.51
1:F:386:MET:HE1	1:F:431:PRO:HB2	1.92	0.51
1:C:66:TRP:CZ2	1:C:71:ALA:HB2	2.45	0.51
1:B:128:TYR:HE1	1:D:168:GLY:HA3	1.75	0.51
1:F:367:TRP:NE1	1:F:407:LEU:O	2.38	0.51
1:B:279:MET:SD	3:B:602:HOH:O	2.60	0.51
1:D:482:ASN:OD1	1:D:483:SER:N	2.44	0.51
1:A:181:THR:HG23	1:A:228:LEU:HD12	1.92	0.50
1:C:250:ILE:HG12	1:C:251:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:GLY:N	1:C:469:GLU:OE1	2.45	0.50
1:B:406:GLU:OE1	1:B:409:THR:OG1	2.27	0.50
1:D:66:TRP:CZ2	1:D:71:ALA:HB2	2.46	0.50
1:D:397:PRO:HA	1:D:426:ALA:O	2.12	0.50
1:C:174:ASN:C	1:C:174:ASN:HD22	2.14	0.50
1:B:66:TRP:CE2	1:B:71:ALA:HB2	2.47	0.50
1:D:192:ASN:ND2	1:D:211:ASN:HB2	2.25	0.50
1:E:131:ALA:HB3	1:E:172:MET:O	2.12	0.50
1:C:356:ARG:HG2	1:C:358:PHE:HE1	1.76	0.50
1:C:367:TRP:NE1	1:C:407:LEU:O	2.39	0.50
1:A:217:ILE:HG21	1:A:248:LEU:HD13	1.93	0.49
1:F:315:ILE:HG22	1:F:356:ARG:HD3	1.93	0.49
1:B:446:ILE:HD13	1:B:495:ILE:HD13	1.94	0.49
1:A:443:GLY:HA2	1:A:465:GLN:NE2	2.27	0.49
1:D:444:GLN:HB3	1:D:463:GLY:HA2	1.94	0.49
1:E:401:THR:HG22	1:E:417:HIS:HA	1.93	0.49
1:D:69:ALA:HA	1:D:174:ASN:ND2	2.27	0.49
1:F:397:PRO:HA	1:F:426:ALA:O	2.13	0.49
1:D:377:ILE:HG12	1:D:381:LYS:HG2	1.95	0.49
1:E:196:VAL:HG22	1:F:196:VAL:HG22	1.95	0.49
1:E:238:MET:HB2	1:E:278:ASN:O	2.13	0.49
1:F:414:TRP:CD2	1:F:454:GLY:HA3	2.47	0.49
1:F:341:THR:O	1:F:351:PHE:HB3	2.12	0.49
1:C:441:THR:OG1	1:C:469:GLU:O	2.30	0.49
1:D:133:GLY:CA	1:D:469:GLU:HG2	2.43	0.49
1:D:249:PHE:CG	1:D:289:ILE:HG21	2.47	0.49
1:A:386:MET:HE2	1:A:431:PRO:HB2	1.95	0.49
1:C:386:MET:HE3	1:C:393:TYR:CD1	2.48	0.49
1:D:122:VAL:HG11	1:D:379:ALA:HB3	1.95	0.49
1:A:273:VAL:HG13	1:A:300:TYR:CZ	2.47	0.49
1:B:70:TYR:HB2	1:B:75:HIS:HA	1.94	0.49
1:F:279:MET:SD	3:F:601:HOH:O	2.60	0.49
1:B:386:MET:HE2	1:B:431:PRO:HB2	1.94	0.48
1:B:482:ASN:OD1	1:B:483:SER:N	2.46	0.48
1:D:387:ILE:HG12	1:D:392:VAL:HG22	1.95	0.48
1:E:277:ASP:HB2	1:E:293:MET:SD	2.53	0.48
1:D:444:GLN:NE2	3:D:601:HOH:O	2.45	0.48
1:B:39:ASP:HB2	1:D:99:GLU:O	2.13	0.48
1:B:66:TRP:CZ2	1:B:71:ALA:HB2	2.48	0.48
1:D:78:ALA:HB1	1:D:434:TYR:CD1	2.46	0.48
1:A:176:LEU:HB2	1:A:183:TYR:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLY:HA3	1:D:128:TYR:HE1	1.77	0.48
1:D:465:GLN:HB2	1:D:483:SER:HB2	1.96	0.48
1:E:352:SER:OG	1:E:370:ASN:OD1	2.32	0.48
1:F:466:PHE:HA	1:F:469:GLU:OE2	2.13	0.48
1:B:320:ASN:OD1	1:B:320:ASN:N	2.46	0.48
1:C:70:TYR:CE2	1:C:384:VAL:HG11	2.48	0.48
1:A:78:ALA:HB1	1:A:434:TYR:CD1	2.44	0.48
1:B:401:THR:HG22	1:B:417:HIS:HA	1.96	0.48
1:C:418:VAL:HG11	1:C:426:ALA:HB3	1.95	0.48
1:B:464:GLY:HA2	1:B:484:TRP:CD1	2.49	0.47
1:D:401:THR:HG22	1:D:417:HIS:HD2	1.79	0.47
1:F:310:VAL:HG12	1:F:311:TRP:HD1	1.78	0.47
1:A:183:TYR:CD1	1:A:248:LEU:HD11	2.49	0.47
1:B:267:GLN:HE22	1:B:270:LYS:HB2	1.77	0.47
1:D:209:GLY:HA3	1:D:236:GLU:HB3	1.96	0.47
1:B:138:ASP:HB2	1:B:222:ARG:NH2	2.29	0.47
1:C:149:PHE:HD2	1:C:163:ARG:HG2	1.80	0.47
1:A:38:MET:HG3	1:A:39:ASP:N	2.30	0.47
1:C:438:LEU:O	1:C:448:VAL:HA	2.14	0.47
1:D:281:SER:N	1:D:327:SER:HB3	2.29	0.47
1:F:236:GLU:CG	1:F:238:MET:HG3	2.44	0.47
1:C:386:MET:HE2	1:C:431:PRO:HB2	1.96	0.47
1:B:178:ILE:HG21	1:B:243:TYR:CZ	2.50	0.47
1:F:144:GLU:OE2	1:F:184:LEU:HA	2.15	0.47
1:A:428:ARG:HG3	1:A:467:GLY:O	2.14	0.47
1:A:174:ASN:HD22	1:A:174:ASN:C	2.18	0.47
1:A:465:GLN:HB3	1:A:483:SER:OG	2.15	0.47
1:A:163:ARG:NH1	1:C:43:PRO:HD3	2.30	0.46
1:C:99:GLU:OE1	1:C:130:ASN:ND2	2.44	0.46
1:D:160:LEU:HD11	1:D:163:ARG:HB3	1.98	0.46
1:E:387:ILE:HG12	1:E:392:VAL:HG22	1.97	0.46
1:F:390:ASN:HD22	1:F:407:LEU:HD23	1.79	0.46
1:C:81:VAL:HG11	1:C:89:ILE:HD13	1.97	0.46
1:E:326:VAL:HG11	1:E:338:ASP:OD1	2.16	0.46
1:B:194:ALA:O	1:B:198:ARG:HG3	2.15	0.46
1:A:213:SER:HB2	1:C:127:PHE:CD2	2.51	0.46
1:C:448:VAL:HG13	1:C:457:LEU:HB2	1.97	0.46
1:D:70:TYR:HB2	1:D:75:HIS:HA	1.98	0.46
1:A:217:ILE:HD12	1:A:241:PRO:HG3	1.98	0.46
1:C:355:ILE:HD12	1:C:394:VAL:HG11	1.98	0.46
1:D:491:PRO:O	1:D:494:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:TRP:CE2	1:D:71:ALA:HB2	2.50	0.46
1:E:482:ASN:OD1	1:E:483:SER:N	2.49	0.46
1:F:402:TYR:CZ	1:F:427:GLY:HA2	2.51	0.46
1:C:216:GLY:HA2	1:C:237:THR:HG21	1.98	0.46
1:C:181:THR:HG23	1:C:228:LEU:HD12	1.97	0.46
1:C:294:ALA:C	1:C:296:LYS:H	2.20	0.46
1:F:482:ASN:OD1	1:F:483:SER:N	2.49	0.46
1:A:134:PRO:HD3	1:A:481:THR:HG23	1.97	0.45
1:D:182:VAL:HG23	1:D:222:ARG:HG2	1.98	0.45
1:D:424:ALA:O	1:D:428:ARG:NH2	2.48	0.45
1:D:72:ASN:ND2	1:D:76:ASN:O	2.29	0.45
1:D:177:VAL:HG13	1:D:222:ARG:HD2	1.99	0.45
1:D:356:ARG:NE	1:D:368:THR:OG1	2.43	0.45
1:A:136:VAL:HG22	1:A:141:VAL:HG22	1.99	0.45
1:B:174:ASN:HD22	1:B:174:ASN:C	2.19	0.45
1:E:180:ASN:N	1:E:180:ASN:OD1	2.34	0.45
1:E:297:PRO:O	1:E:298:TYR:HD1	2.00	0.45
1:A:99:GLU:OE1	1:A:130:ASN:ND2	2.43	0.45
1:B:298:TYR:HB2	1:B:300:TYR:CE1	2.52	0.45
1:B:89:ILE:HD11	1:B:474:VAL:HG12	1.99	0.45
1:E:464:GLY:HA2	1:E:484:TRP:CD1	2.52	0.45
1:A:466:PHE:HD1	1:A:469:GLU:HG3	1.82	0.45
1:E:169:ASN:OD1	1:E:170:ASN:N	2.49	0.45
1:E:310:VAL:HG12	1:E:311:TRP:HD1	1.81	0.45
1:B:69:ALA:HA	1:B:174:ASN:HD21	1.82	0.44
1:C:310:VAL:HG12	1:C:311:TRP:HD1	1.81	0.44
1:C:311:TRP:CH2	1:C:358:PHE:HD2	2.35	0.44
1:C:353:ASN:ND2	1:C:398:VAL:HG23	2.32	0.44
1:B:45:ARG:NH2	2:B:502:SO4:O4	2.41	0.44
1:B:39:ASP:HB3	1:B:42:GLY:HA3	2.00	0.44
1:B:181:THR:HG23	1:B:228:LEU:HD12	1.98	0.44
1:F:195:ASN:HD21	1:F:210:LEU:HD23	1.81	0.44
1:F:273:VAL:HG21	1:F:293:MET:HE3	1.99	0.44
1:C:76:ASN:HB2	1:C:386:MET:HG3	1.98	0.44
1:D:248:LEU:HB2	1:D:260:ILE:HB	2.00	0.44
1:D:445:TYR:HB2	1:D:447:PHE:CE1	2.53	0.44
1:D:92:GLY:HA2	1:D:477:THR:OG1	2.18	0.44
1:C:258:PHE:HB2	1:C:260:ILE:HD11	2.00	0.44
1:E:183:TYR:CD1	1:E:248:LEU:HD11	2.53	0.44
1:A:66:TRP:CE2	1:A:71:ALA:HB2	2.52	0.44
1:C:66:TRP:CE2	1:C:71:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:GLY:HA2	1:C:477:THR:OG1	2.18	0.44
1:F:131:ALA:O	1:F:468:ILE:HG13	2.18	0.44
1:C:356:ARG:HG2	1:C:358:PHE:CE1	2.53	0.44
1:A:482:ASN:OD1	1:A:483:SER:N	2.51	0.43
1:D:241:PRO:HB3	1:D:250:ILE:HB	1.99	0.43
1:E:446:ILE:HG22	1:E:462:ILE:HD11	1.99	0.43
1:C:299:LEU:HD23	1:C:358:PHE:CE2	2.53	0.43
1:F:497:HIS:ND1	1:F:497:HIS:O	2.51	0.43
1:A:319:SER:HA	1:A:342:LYS:HB3	2.00	0.43
1:B:217:ILE:HG21	1:B:248:LEU:HD13	2.00	0.43
1:D:319:SER:HB3	1:D:342:LYS:HG2	1.99	0.43
1:E:208:ARG:HB3	1:E:236:GLU:HG2	2.01	0.43
1:C:396:ASN:O	1:C:400:SER:N	2.51	0.43
1:C:390:ASN:HD22	1:C:407:LEU:HD23	1.84	0.43
1:C:132:LEU:HD22	1:C:173:GLY:HA2	2.00	0.43
1:E:445:TYR:HB2	1:E:447:PHE:CE1	2.54	0.43
1:A:310:VAL:HG12	1:A:311:TRP:HD1	1.83	0.43
1:A:402:TYR:CZ	1:A:427:GLY:HA2	2.54	0.43
1:B:369:ARG:HD3	1:B:410:GLY:O	2.19	0.43
1:C:103:TRP:HD1	1:C:484:TRP:CD1	2.36	0.43
1:E:199:TYR:CE1	1:E:203:PRO:HB3	2.54	0.43
1:E:371:MET:HE2	1:E:396:ASN:HB2	2.01	0.43
1:A:445:TYR:HB2	1:A:447:PHE:CE1	2.54	0.43
1:B:464:GLY:HA2	1:B:484:TRP:CE2	2.53	0.43
1:E:393:TYR:CD2	1:E:438:LEU:HD11	2.54	0.43
1:C:127:PHE:N	1:C:127:PHE:CD1	2.87	0.42
1:D:238:MET:HB2	1:D:278:ASN:O	2.19	0.42
1:E:78:ALA:HB1	1:E:434:TYR:CD1	2.50	0.42
1:B:224:ASN:CG	1:B:226:LYS:HG2	2.39	0.42
1:D:149:PHE:CD1	1:D:165:SER:HB2	2.54	0.42
1:E:450:ASN:ND2	1:E:453:THR:OG1	2.51	0.42
1:F:69:ALA:HB2	1:F:240:THR:HB	2.02	0.42
1:A:433:TYR:C	1:A:433:TYR:CD1	2.93	0.42
2:E:501:SO4:O2	1:F:45:ARG:NH2	2.49	0.42
1:F:258:PHE:HB2	1:F:260:ILE:HD11	2.01	0.42
1:F:444:GLN:HB3	1:F:463:GLY:HA2	2.00	0.42
1:B:464:GLY:HA2	1:B:484:TRP:NE1	2.35	0.42
1:C:169:ASN:OD1	1:C:170:ASN:N	2.49	0.42
1:D:61:VAL:HG21	1:D:88:TRP:CZ2	2.55	0.42
1:D:300:TYR:HE1	1:D:312:LYS:HE2	1.85	0.42
1:E:209:GLY:HA3	1:E:236:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:THR:HG23	1:E:228:LEU:HD12	2.01	0.42
1:E:289:ILE:HG23	1:E:304:GLU:HG2	2.00	0.42
1:C:61:VAL:HG21	1:C:88:TRP:CZ2	2.55	0.42
1:E:371:MET:HB3	1:E:371:MET:HE2	1.90	0.42
1:E:446:ILE:HD13	1:E:495:ILE:HD13	2.02	0.42
1:B:326:VAL:HG11	1:B:338:ASP:OD1	2.19	0.42
1:D:224:ASN:CG	1:D:226:LYS:HG2	2.40	0.42
1:E:316:PRO:HD3	1:E:356:ARG:CZ	2.50	0.42
1:E:66:TRP:CH2	1:E:71:ALA:HB2	2.55	0.42
1:F:402:TYR:CE2	1:F:427:GLY:HA2	2.55	0.42
1:B:359:ASP:OD2	1:B:362:THR:HG23	2.20	0.42
1:C:296:LYS:HA	1:C:296:LYS:HD2	1.87	0.42
1:D:179:GLY:O	1:D:222:ARG:HD3	2.19	0.42
1:B:163:ARG:CZ	1:D:43:PRO:HG3	2.50	0.42
1:E:54:PRO:HD3	1:E:161:ILE:HD11	2.02	0.42
1:E:128:TYR:CE1	1:F:168:GLY:HA3	2.52	0.42
1:B:224:ASN:OD1	1:B:226:LYS:HG2	2.20	0.42
1:D:174:ASN:HD22	1:D:174:ASN:C	2.21	0.42
1:E:70:TYR:HB2	1:E:75:HIS:HA	2.02	0.42
1:F:356:ARG:HG2	1:F:368:THR:HG23	2.01	0.42
1:A:213:SER:OG	1:A:214:PHE:N	2.47	0.41
1:A:402:TYR:CE1	1:A:427:GLY:HA2	2.55	0.41
1:E:168:GLY:HA3	1:F:128:TYR:HE1	1.85	0.41
1:F:277:ASP:HB2	1:F:293:MET:SD	2.60	0.41
1:A:169:ASN:OD1	1:A:170:ASN:N	2.52	0.41
1:C:463:GLY:O	1:C:482:ASN:ND2	2.53	0.41
1:E:115:TYR:O	1:E:119:GLU:HB2	2.20	0.41
1:F:282:VAL:HG13	1:F:289:ILE:HG23	2.00	0.41
1:F:296:LYS:HG2	1:F:298:TYR:CD2	2.55	0.41
1:B:192:ASN:OD1	1:B:195:ASN:ND2	2.38	0.41
1:A:439:TYR:CE1	1:A:492:LEU:HD11	2.55	0.41
1:B:238:MET:HB2	1:B:278:ASN:O	2.21	0.41
1:C:251:ALA:HB1	1:C:293:MET:CE	2.51	0.41
1:F:386:MET:HG2	1:F:387:ILE:N	2.36	0.41
1:C:334:VAL:HG13	1:C:366:LEU:HD12	2.02	0.41
1:E:298:TYR:HD2	1:E:312:LYS:HD2	1.85	0.41
1:B:148:MET:HG2	1:B:169:ASN:O	2.20	0.41
1:D:63:PRO:HG3	1:D:79:PHE:CZ	2.56	0.41
1:F:267:GLN:HE21	1:F:270:LYS:HB2	1.85	0.41
1:C:356:ARG:NE	1:C:368:THR:OG1	2.53	0.41
1:C:369:ARG:HA	1:C:369:ARG:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:VAL:HG12	1:D:311:TRP:HD1	1.86	0.41
1:F:78:ALA:HB1	1:F:434:TYR:CD1	2.44	0.41
1:D:208:ARG:HD2	1:D:236:GLU:OE2	2.21	0.41
1:E:136:VAL:HG22	1:E:141:VAL:HG22	2.02	0.41
1:F:315:ILE:H	1:F:315:ILE:HD13	1.86	0.41
1:B:439:TYR:CE1	1:B:448:VAL:HG22	2.56	0.41
1:C:298:TYR:CD1	1:C:314:THR:HG22	2.56	0.41
1:C:47:VAL:O	1:C:162:TRP:HA	2.20	0.41
1:D:99:GLU:OE1	1:D:130:ASN:ND2	2.50	0.41
1:E:140:VAL:HG13	1:E:161:ILE:HD12	2.03	0.41
1:E:189:VAL:HG12	1:E:238:MET:SD	2.61	0.41
1:E:163:ARG:NH1	1:F:43:PRO:HD3	2.35	0.41
1:C:249:PHE:CG	1:C:289:ILE:HG21	2.56	0.41
1:D:444:GLN:HG2	1:D:464:GLY:O	2.21	0.41
1:B:483:SER:C	1:B:484:TRP:HE3	2.24	0.40
1:C:182:VAL:HB	1:C:220:LEU:HD12	2.03	0.40
1:E:176:LEU:HB2	1:E:183:TYR:HB2	2.03	0.40
1:B:331:ALA:HB3	1:B:387:ILE:HG21	2.02	0.40
1:D:115:TYR:HB2	1:D:120:ALA:HB2	2.04	0.40
1:A:469:GLU:H	1:A:469:GLU:HG2	1.48	0.40
1:E:148:MET:HG2	1:E:169:ASN:O	2.21	0.40
1:D:230:TYR:HE1	1:D:232:ALA:HB2	1.86	0.40
1:E:137:VAL:HG21	1:E:177:VAL:HB	2.02	0.40
1:C:440:ILE:O	1:C:446:ILE:HD12	2.22	0.40
1:D:473:ILE:HG12	1:D:478:VAL:HG22	2.04	0.40
1:E:297:PRO:C	1:E:298:TYR:HD1	2.25	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	415/470 (88%)	402 (97%)	12 (3%)	1 (0%)	47	78
1	B	428/470 (91%)	413 (96%)	14 (3%)	1 (0%)	47	78
1	C	397/470 (84%)	380 (96%)	16 (4%)	1 (0%)	41	72
1	D	462/470 (98%)	445 (96%)	16 (4%)	1 (0%)	47	78
1	E	445/470 (95%)	429 (96%)	15 (3%)	1 (0%)	47	78
1	F	437/470 (93%)	417 (95%)	18 (4%)	2 (0%)	29	61
All	All	2584/2820 (92%)	2486 (96%)	91 (4%)	7 (0%)	41	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	ILE
1	B	295	ILE
1	C	295	ILE
1	D	295	ILE
1	E	295	ILE
1	F	295	ILE
1	F	423	ALA

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	328/361 (91%)	319 (97%)	9 (3%)	44	78
1	B	339/361 (94%)	331 (98%)	8 (2%)	49	81
1	C	320/361 (89%)	312 (98%)	8 (2%)	47	80
1	D	358/361 (99%)	350 (98%)	8 (2%)	52	83
1	E	349/361 (97%)	340 (97%)	9 (3%)	46	79
1	F	344/361 (95%)	335 (97%)	9 (3%)	46	79
All	All	2038/2166 (94%)	1987 (98%)	51 (2%)	47	80

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	MET
1	A	174	ASN
1	A	236	GLU
1	A	353	ASN
1	A	422	VAL
1	A	433	TYR
1	A	469	GLU
1	A	484	TRP
1	A	494	THR
1	B	174	ASN
1	B	236	GLU
1	B	362	THR
1	B	433	TYR
1	B	453	THR
1	B	468	ILE
1	B	484	TRP
1	B	494	THR
1	C	127	PHE
1	C	174	ASN
1	C	220	LEU
1	C	250	ILE
1	C	276	MET
1	C	468	ILE
1	C	484	TRP
1	C	494	THR
1	D	83	ASP
1	D	174	ASN
1	D	236	GLU
1	D	327	SER
1	D	377	ILE
1	D	453	THR
1	D	468	ILE
1	D	484	TRP
1	E	174	ASN
1	E	197	LEU
1	E	198	ARG
1	E	236	GLU
1	E	362	THR
1	E	433	TYR
1	E	453	THR
1	E	468	ILE
1	E	484	TRP
1	F	83	ASP

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Mol	Chain	Res	Type
1	F	236	GLU
1	F	315	ILE
1	F	337	LEU
1	F	353	ASN
1	F	362	THR
1	F	453	THR
1	F	469	GLU
1	F	484	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	ASN
1	A	465	GLN
1	B	267	GLN
1	B	388	HIS
1	B	390	ASN
1	C	353	ASN
1	C	388	HIS
1	C	390	ASN
1	C	458	HIS
1	D	49	HIS
1	D	91	ASN
1	D	388	HIS
1	D	417	HIS
1	D	450	ASN
1	F	211	ASN
1	F	267	GLN
1	F	303	ASN
1	F	353	ASN
1	F	388	HIS
1	F	390	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	E	501	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	F	502	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	E	503	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	E	502	-	4,4,4	0.15	0	6,6,6	0.18	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	SO4	2	0
2	F	501	SO4	1	0
2	B	502	SO4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/470 (90%)	0.14	6 (1%) 75 70	43, 60, 80, 100	0
1	B	436/470 (92%)	0.16	8 (1%) 68 61	43, 63, 82, 92	0
1	C	409/470 (87%)	0.52	33 (8%) 12 6	57, 75, 93, 100	0
1	D	464/470 (98%)	0.09	8 (1%) 70 63	47, 61, 74, 86	0
1	E	451/470 (95%)	-0.04	5 (1%) 80 75	38, 53, 77, 89	0
1	F	445/470 (94%)	0.11	12 (2%) 54 44	41, 59, 79, 89	0
All	All	2630/2820 (93%)	0.16	72 (2%) 54 44	38, 62, 85, 100	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	PRO	4.8
1	D	55	SER	4.7
1	C	114	THR	4.4
1	D	380	PHE	4.3
1	C	238	MET	3.9
1	A	120	ALA	3.8
1	A	423	ALA	3.5
1	C	239	ALA	3.5
1	A	424	ALA	3.4
1	F	202	ASN	3.2
1	C	129	GLY	3.2
1	C	213	SER	3.0
1	F	303	ASN	3.0
1	C	121	SER	3.0
1	F	207	ALA	3.0
1	C	131	ALA	2.9
1	C	113	LYS	2.9
1	C	128	TYR	2.9
1	E	195	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	437	LEU	2.9
1	C	366	LEU	2.8
1	C	240	THR	2.8
1	C	127	PHE	2.8
1	C	116	GLY	2.7
1	C	447	PHE	2.7
1	F	206	SER	2.7
1	C	426	ALA	2.7
1	C	413	LEU	2.6
1	C	172	MET	2.6
1	C	280	SER	2.6
1	A	127	PHE	2.6
1	A	110	PHE	2.6
1	C	279	MET	2.5
1	F	422	VAL	2.5
1	C	235	GLY	2.5
1	F	310	VAL	2.5
1	C	410	GLY	2.5
1	C	268	VAL	2.4
1	C	125	THR	2.4
1	F	423	ALA	2.4
1	E	109	PRO	2.3
1	C	120	ALA	2.3
1	D	226	LYS	2.3
1	E	114	THR	2.3
1	C	425	GLY	2.3
1	C	130	ASN	2.2
1	C	414	TRP	2.2
1	F	424	ALA	2.2
1	D	53	ALA	2.2
1	E	197	LEU	2.2
1	F	496	SER	2.2
1	B	128	TYR	2.2
1	C	276	MET	2.2
1	F	421	LYS	2.2
1	C	115	TYR	2.2
1	C	383	GLY	2.2
1	F	198	ARG	2.2
1	C	189	VAL	2.2
1	C	369	ARG	2.1
1	D	305	SER	2.1
1	E	287	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	299	LEU	2.1
1	D	420	THR	2.1
1	D	56	GLY	2.1
1	B	321	THR	2.1
1	C	264	THR	2.1
1	F	425	GLY	2.1
1	B	406	GLU	2.1
1	B	114	THR	2.0
1	B	352	SER	2.0
1	D	479	TYR	2.0
1	B	370	ASN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	502	5/5	0.91	0.14	81,83,86,102	0
2	SO4	E	503	5/5	0.92	0.20	71,75,83,89	0
2	SO4	E	501	5/5	0.93	0.16	57,65,73,90	0
2	SO4	E	502	5/5	0.93	0.19	50,55,63,70	0
2	SO4	A	501	5/5	0.94	0.16	70,74,87,92	0
2	SO4	D	501	5/5	0.95	0.14	67,69,78,86	0
2	SO4	F	501	5/5	0.95	0.10	54,56,65,70	0
2	SO4	B	501	5/5	0.96	0.11	54,60,64,72	0
2	SO4	F	502	5/5	0.97	0.18	62,65,72,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.