



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:16 am GMT

PDB ID : 1UQR  
Title : TYPE II 3-DEHYDROQUINATE DEHYDRATASE (DHQASE) FROM  
ACTINOBACILLUS PLEUROPNEUMONIAE  
Authors : Maes, D.; Gonzalez-Ramirez, L.A.; Lopez-Jaramillo, J.; Yu, B.; De Bondt, H.;  
Zegers, I.; Afonina, E.; Garcia-Ruiz, J.M.; Gulnik, S.  
Deposited on : 2003-10-16  
Resolution : 1.70 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

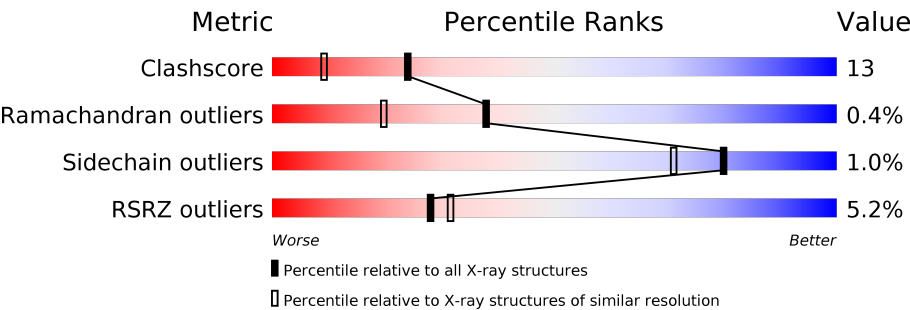
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	154	<div><div>7%</div><div><div></div><div>77%</div><div>17%</div><div>• 5%</div></div></div>
1	B	154	<div><div>3%</div><div><div></div><div>77%</div><div>12%</div><div>• 10%</div></div></div>
1	C	154	<div><div>3%</div><div><div></div><div>77%</div><div>18%</div><div>• •</div></div></div>
1	D	154	<div><div>6%</div><div><div></div><div>75%</div><div>22%</div><div>• • •</div></div></div>
1	E	154	<div><div>5%</div><div><div></div><div>75%</div><div>18%</div><div>7%</div></div></div>
1	F	154	<div><div>5%</div><div><div></div><div>81%</div><div>14%</div><div>5%</div></div></div>
1	G	154	<div><div>4%</div><div><div></div><div>71%</div><div>19%</div><div>• 9%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	H	154	
1	I	154	
1	J	154	
1	K	154	
1	L	154	

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	C	1156	-	-	-	X
2	SO4	F	1155	-	-	-	X
2	SO4	H	1157	-	-	-	X
3	TRS	B	1149	-	-	-	X
3	TRS	E	1150	-	-	-	X
3	TRS	K	1155	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16147 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-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	1	0
			1156	736	201	214	5			
1	B	138	Total	C	N	O	S	0	1	0
			1089	694	188	202	5			
1	C	148	Total	C	N	O	S	0	1	1
			1161	735	203	216	7			
1	D	152	Total	C	N	O	S	0	1	1
			1195	759	208	222	6			
1	E	143	Total	C	N	O	S	0	1	0
			1130	720	196	209	5			
1	F	146	Total	C	N	O	S	0	1	1
			1145	726	200	213	6			
1	G	140	Total	C	N	O	S	0	1	0
			1106	703	193	205	5			
1	H	148	Total	C	N	O	S	0	1	1
			1161	735	203	216	7			
1	I	141	Total	C	N	O	S	0	1	0
			1115	708	194	208	5			
1	J	146	Total	C	N	O	S	0	1	0
			1156	736	201	214	5			
1	K	152	Total	C	N	O	S	0	1	1
			1195	759	208	222	6			
1	L	138	Total	C	N	O	S	0	1	0
			1089	694	188	202	5			

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



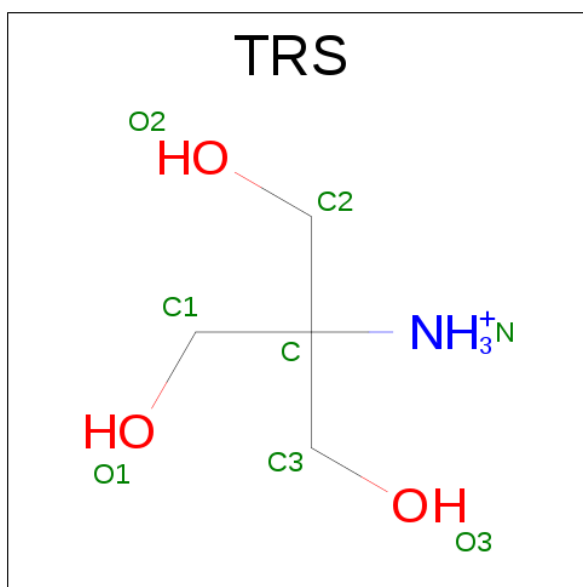
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	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		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	E	1	Total	C	N	O	0	0
			8	4	1	3		
3	H	1	Total	C	N	O	0	0
			8	4	1	3		
3	K	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	204	Total	O	0	0
			204	204		
4	C	216	Total	O	0	0
			216	216		
4	D	203	Total	O	0	0
			203	203		
4	E	162	Total	O	0	0
			162	162		
4	F	216	Total	O	0	0
			216	216		
4	G	156	Total	O	0	0
			156	156		
4	H	199	Total	O	0	0
			199	199		

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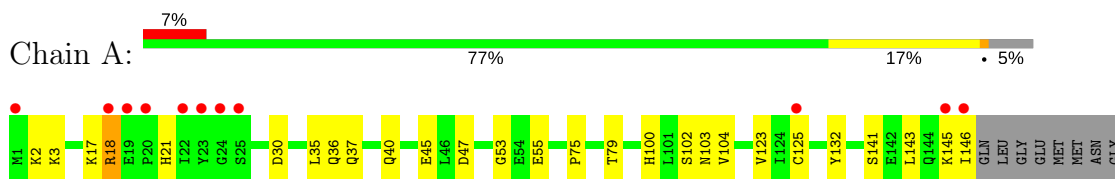
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	179	Total 179	O 179	0	0
4	J	152	Total 152	O 152	0	0
4	K	199	Total 199	O 199	0	0
4	L	181	Total 181	O 181	0	0



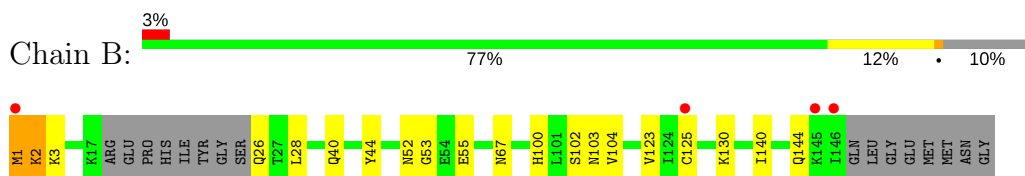
### 3 Residue-property plots [i](#)

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

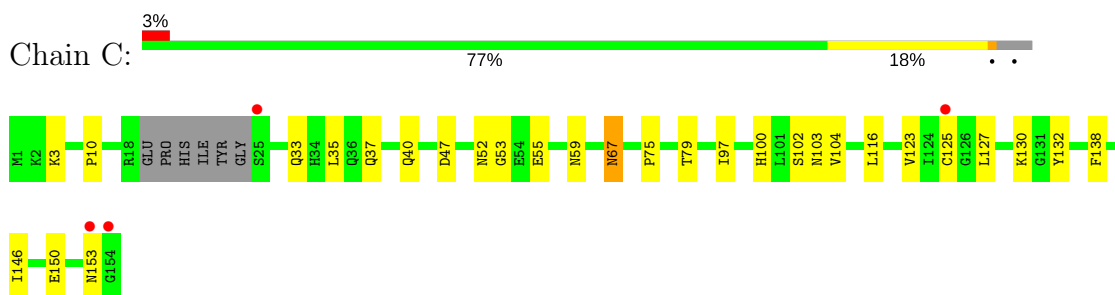
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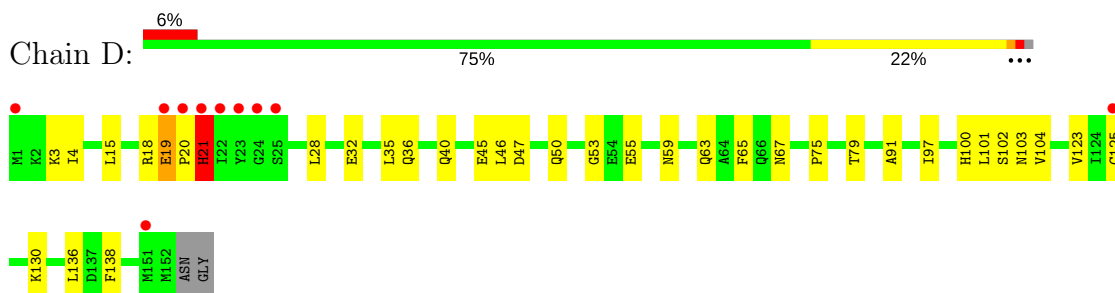
#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

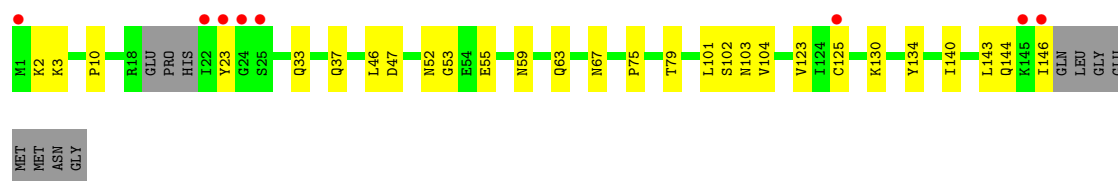


#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

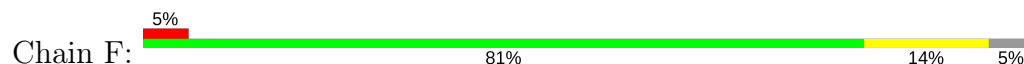


#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE





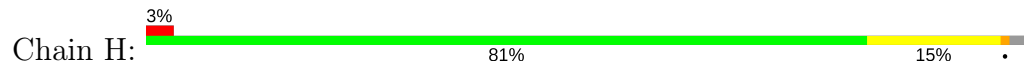
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



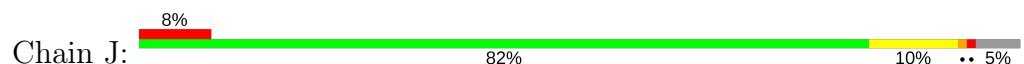
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



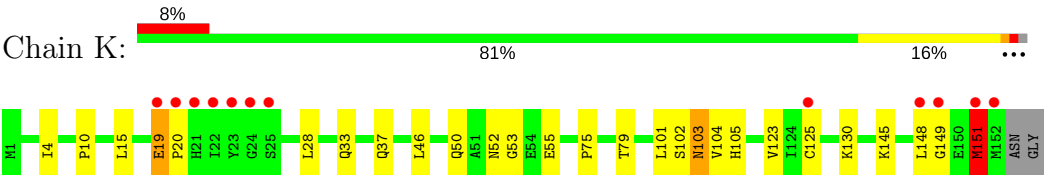
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



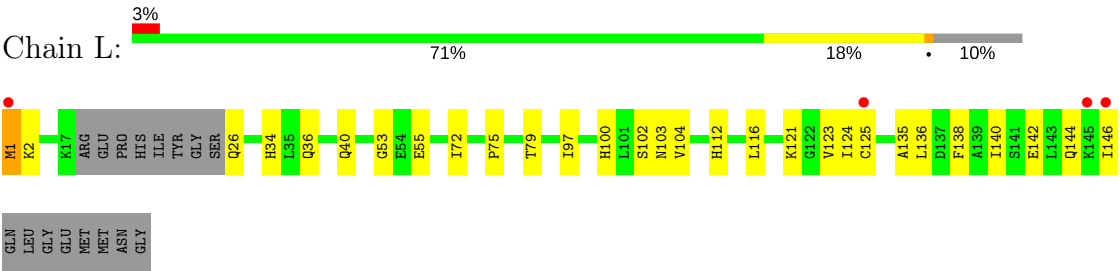
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.09Å 131.33Å 161.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 14.99 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-1.70) 98.5 (14.99-1.71)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.88 (at 1.71Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.178 , 0.199 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: TRS, 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	0.40	0/1189	0.63	0/1609
1	B	0.40	0/1118	0.64	0/1511
1	C	0.39	0/1190	0.62	0/1606
1	D	0.39	0/1228	0.61	0/1661
1	E	0.38	0/1160	0.61	0/1567
1	F	0.38	0/1174	0.63	0/1585
1	G	0.40	0/1135	0.61	0/1533
1	H	0.44	3/1190 (0.3%)	0.60	3/1606 (0.2%)
1	I	0.42	0/1144	0.66	0/1545
1	J	0.44	1/1189 (0.1%)	0.65	0/1609
1	K	0.39	0/1228	0.64	0/1661
1	L	0.39	0/1118	0.63	0/1511
All	All	0.40	4/14063 (0.0%)	0.63	3/19004 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	2	LYS	C-N	6.11	1.48	1.34
1	H	125[A]	CYS	CB-SG	5.27	1.91	1.82
1	H	125[B]	CYS	CB-SG	5.27	1.91	1.82
1	H	125[C]	CYS	CB-SG	5.27	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	125[A]	CYS	N-CA-CB	5.34	120.22	110.60
1	H	125[B]	CYS	N-CA-CB	5.34	120.22	110.60
1	H	125[C]	CYS	N-CA-CB	5.34	120.22	110.60

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	1156	0	1141	39	0
1	B	1089	0	1079	28	0
1	C	1161	0	1149	29	0
1	D	1195	0	1178	37	0
1	E	1130	0	1120	26	0
1	F	1145	0	1134	36	0
1	G	1106	0	1097	34	0
1	H	1161	0	1149	26	0
1	I	1115	0	1103	48	0
1	J	1156	0	1141	22	0
1	K	1195	0	1178	31	0
1	L	1089	0	1079	31	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
2	F	20	0	0	0	0
2	G	5	0	0	0	0
2	H	20	0	0	0	0
2	I	5	0	0	0	0
2	J	15	0	0	0	0
2	K	15	0	0	0	0
2	L	10	0	0	0	0
3	B	8	0	12	0	0
3	E	8	0	12	0	0
3	H	8	0	12	0	0
3	K	8	0	12	0	0
4	A	195	0	0	7	0
4	B	204	0	0	7	0
4	C	216	0	0	4	0
4	D	203	0	0	4	0
4	E	162	0	0	1	0
4	F	216	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	156	0	0	3	0
4	H	199	0	0	5	0
4	I	179	0	0	14	0
4	J	152	0	0	3	0
4	K	199	0	0	3	0
4	L	181	0	0	6	0
All	All	16147	0	13596	345	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (345) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125[B]:CYS:CB	1:F:125[B]:CYS:SG	2.30	1.19
1:F:125[C]:CYS:SG	1:F:125[C]:CYS:CB	2.32	1.17
1:I:79:THR:HG21	1:I:100:HIS:HE1	1.10	1.10
1:D:19:GLU:HB3	1:D:20:PRO:HD3	1.35	1.07
1:G:75:PRO:HG2	1:G:79:THR:CG2	1.89	1.02
1:G:75:PRO:CG	1:G:79:THR:HG22	1.89	1.01
1:I:79:THR:HG21	1:I:100:HIS:CE1	1.96	0.99
1:I:75:PRO:HG2	1:I:79:THR:HG22	1.02	0.99
1:B:125[A]:CYS:SG	1:H:123:VAL:HB	2.03	0.99
1:A:125[A]:CYS:SG	1:D:123:VAL:HB	2.04	0.98
1:G:79:THR:HG21	1:G:100:HIS:CE1	1.98	0.97
1:G:76:GLY:O	1:G:79:THR:HG23	1.66	0.95
1:G:75:PRO:HG2	1:G:79:THR:HG22	0.95	0.93
1:F:123:VAL:HB	1:I:125[A]:CYS:SG	2.09	0.92
1:C:125[A]:CYS:SG	1:L:123:VAL:HB	2.09	0.92
1:I:76:GLY:O	1:I:79:THR:HG23	1.69	0.92
1:L:103:ASN:HA	1:L:125[B]:CYS:SG	2.10	0.92
1:K:19:GLU:HB2	1:K:20:PRO:HD3	1.52	0.90
1:F:125[A]:CYS:SG	1:I:123:VAL:HB	2.12	0.90
1:A:75:PRO:HG2	1:A:79:THR:OG1	1.71	0.89
1:G:103:ASN:HA	1:G:125[B]:CYS:SG	2.12	0.89
1:A:103:ASN:HA	1:A:125[B]:CYS:SG	2.12	0.89
1:C:123:VAL:HB	1:L:125[A]:CYS:SG	2.13	0.89
1:I:75:PRO:HG2	1:I:79:THR:CG2	1.98	0.87
1:J:19:GLU:OE2	1:J:19:GLU:HA	1.73	0.87
1:E:123:VAL:HB	1:K:125[A]:CYS:SG	2.14	0.86
1:I:75:PRO:CG	1:I:79:THR:HG22	1.98	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:THR:HG21	1:G:100:HIS:HE1	1.36	0.85
1:B:103:ASN:HA	1:B:125[B]:CYS:SG	2.17	0.85
1:G:125[A]:CYS:SG	1:J:123:VAL:HB	2.17	0.83
1:J:21:HIS:HB3	4:J:2152:HOH:O	1.77	0.83
1:K:103:ASN:HA	1:K:125[C]:CYS:SG	2.19	0.82
1:C:103:ASN:HA	1:C:125[C]:CYS:SG	2.20	0.81
1:J:102:SER:O	1:J:125[C]:CYS:SG	2.39	0.80
1:E:102:SER:O	1:E:125[B]:CYS:SG	2.40	0.79
1:E:125[A]:CYS:SG	1:K:123:VAL:HB	2.23	0.79
1:I:103:ASN:HA	1:I:125[B]:CYS:SG	2.23	0.79
1:G:123:VAL:HB	1:J:125[A]:CYS:SG	2.22	0.79
1:L:102:SER:O	1:L:125[B]:CYS:SG	2.41	0.79
1:A:2:LYS:HD3	1:A:143:LEU:HB3	1.65	0.79
1:J:104:VAL:HG13	1:J:125[C]:CYS:SG	2.24	0.76
1:F:102:SER:O	1:F:125[B]:CYS:SG	2.43	0.76
1:J:19:GLU:O	1:J:21:HIS:N	2.18	0.76
1:A:123:VAL:HB	1:D:125[A]:CYS:SG	2.24	0.76
1:D:102:SER:O	1:D:125[B]:CYS:SG	2.44	0.76
1:B:102:SER:O	1:B:125[B]:CYS:SG	2.44	0.75
1:D:19:GLU:HB3	1:D:20:PRO:CD	2.16	0.75
1:A:123:VAL:HG12	1:A:125[C]:CYS:SG	2.27	0.75
1:H:102:SER:O	1:H:125[A]:CYS:SG	2.44	0.74
1:K:102:SER:O	1:K:125[C]:CYS:SG	2.45	0.74
1:L:100:HIS:HD2	1:L:125[C]:CYS:SG	2.10	0.74
1:F:103:ASN:HA	1:F:125[B]:CYS:SG	2.28	0.74
1:A:100:HIS:HD2	1:A:125[C]:CYS:SG	2.11	0.73
1:D:103:ASN:HA	1:D:125[B]:CYS:SG	2.28	0.73
1:A:40:GLN:HG3	4:A:2050:HOH:O	1.89	0.73
1:J:100:HIS:HB2	1:J:125[C]:CYS:SG	2.29	0.73
1:I:145:LYS:HE3	4:I:2171:HOH:O	1.89	0.73
1:A:18:ARG:H	1:A:18:ARG:HD3	1.52	0.72
1:I:102:SER:O	1:I:125[B]:CYS:SG	2.46	0.72
1:G:102:SER:O	1:G:125[B]:CYS:SG	2.48	0.72
1:I:100:HIS:HD2	1:I:125[C]:CYS:SG	2.12	0.72
1:A:18:ARG:H	1:A:18:ARG:CD	2.03	0.72
1:I:145:LYS:HG3	4:I:2178:HOH:O	1.89	0.71
1:B:100:HIS:HD2	1:B:125[C]:CYS:SG	2.13	0.71
1:B:123:VAL:HG12	1:B:125[C]:CYS:SG	2.31	0.70
1:F:123:VAL:HG12	1:F:125[C]:CYS:SG	2.32	0.70
1:J:123:VAL:HG12	1:J:125[B]:CYS:SG	2.31	0.70
1:C:102:SER:O	1:C:125[C]:CYS:SG	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:GLN:O	1:D:40:GLN:HG3	1.93	0.68
1:F:59:ASN:O	1:F:63:GLN:HG3	1.94	0.68
1:G:3:LYS:HD2	1:G:47:ASP:OD2	1.94	0.68
1:A:18:ARG:N	1:A:18:ARG:HD3	2.08	0.68
1:J:59:ASN:O	1:J:63:GLN:HG3	1.92	0.68
1:F:100:HIS:HD2	1:F:125[C]:CYS:SG	2.16	0.67
1:L:144:GLN:C	1:L:146:ILE:H	1.97	0.67
1:A:100:HIS:ND1	4:A:2136:HOH:O	2.26	0.67
1:H:123:VAL:HG12	1:H:125[B]:CYS:SG	2.35	0.67
1:I:123:VAL:HG12	1:I:125[C]:CYS:SG	2.35	0.67
1:A:102:SER:O	1:A:125[B]:CYS:SG	2.52	0.66
1:F:2:LYS:HG3	1:F:143:LEU:HD13	1.76	0.66
1:F:2:LYS:HE3	1:F:147:GLN:HG2	1.79	0.65
1:L:100:HIS:CD2	1:L:125[C]:CYS:SG	2.90	0.65
1:A:21:HIS:HE1	1:A:30:ASP:OD2	1.80	0.65
1:D:59:ASN:O	1:D:63:GLN:HG3	1.97	0.64
1:G:75:PRO:HG3	1:G:116:LEU:HD12	1.79	0.64
1:J:1:MET:O	1:J:2:LYS:O	2.16	0.64
1:C:35:LEU:HD11	1:C:132:TYR:HB3	1.79	0.64
1:B:2:LYS:HB3	1:B:44:TYR:CD1	2.33	0.64
1:K:19:GLU:CB	1:K:20:PRO:HD3	2.26	0.63
1:A:17:LYS:HE2	4:A:2021:HOH:O	2.00	0.62
1:I:140:ILE:O	1:I:144:GLN:HG3	2.00	0.62
1:C:146:ILE:O	1:C:150:GLU:HG3	2.00	0.61
1:C:104:VAL:N	1:C:125[C]:CYS:SG	2.70	0.61
1:H:2:LYS:HE2	4:H:2077:HOH:O	2.00	0.61
1:I:146:ILE:HD11	4:I:2079:HOH:O	2.00	0.61
1:K:19:GLU:HB2	1:K:20:PRO:CD	2.28	0.61
1:L:34:HIS:HD2	4:L:2026:HOH:O	1.83	0.61
1:F:123:VAL:CB	1:I:125[A]:CYS:SG	2.88	0.60
1:L:121:LYS:HE2	1:L:142:GLU:OE2	2.01	0.60
1:I:75:PRO:HG3	1:I:116:LEU:HD12	1.81	0.60
1:K:104:VAL:N	1:K:125[C]:CYS:SG	2.72	0.60
1:A:17:LYS:HE3	4:B:2140:HOH:O	2.01	0.59
1:E:103:ASN:HA	1:E:125[B]:CYS:SG	2.42	0.59
1:A:3:LYS:HE2	1:A:45:GLU:OE2	2.01	0.59
1:E:123:VAL:HG12	1:E:125[C]:CYS:SG	2.43	0.59
1:A:143:LEU:O	1:A:146:ILE:HG12	2.02	0.59
1:A:100:HIS:CD2	1:A:125[C]:CYS:SG	2.96	0.59
1:G:100:HIS:HD2	1:G:125[C]:CYS:SG	2.25	0.58
1:C:40:GLN:NE2	4:C:2071:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LEU:HD11	1:D:101:LEU:HD11	1.84	0.58
1:B:140:ILE:O	1:B:144:GLN:HG3	2.03	0.58
1:D:104:VAL:N	1:D:125[B]:CYS:SG	2.72	0.58
1:B:125[A]:CYS:SG	1:H:123:VAL:CB	2.87	0.58
1:B:104:VAL:N	1:B:125[B]:CYS:SG	2.74	0.58
1:I:37:GLN:HG2	4:I:2055:HOH:O	2.03	0.58
1:L:144:GLN:C	1:L:146:ILE:N	2.55	0.57
1:D:123:VAL:HG12	1:D:125[C]:CYS:SG	2.45	0.56
1:E:75:PRO:HG2	1:E:79:THR:HB	1.87	0.56
1:E:53:GLY:HA3	1:F:55:GLU:HB2	1.87	0.56
1:I:104:VAL:O	4:I:2126:HOH:O	2.18	0.56
1:I:25:SER:O	1:I:26:GLN:O	2.24	0.56
1:C:3:LYS:HD2	1:C:47:ASP:OD2	2.06	0.56
1:J:19:GLU:OE2	1:J:19:GLU:CA	2.51	0.56
1:K:149:GLY:C	1:K:151:MET:H	2.08	0.56
1:I:25:SER:N	4:I:2031:HOH:O	2.38	0.56
1:G:100:HIS:HB2	1:G:125[C]:CYS:SG	2.45	0.55
1:B:1:MET:HG2	4:B:2002:HOH:O	2.06	0.55
1:G:100:HIS:CD2	1:G:125[C]:CYS:SG	2.99	0.55
1:L:140:ILE:O	1:L:144:GLN:HG3	2.06	0.55
1:L:36:GLN:O	1:L:40:GLN:HG3	2.07	0.55
1:F:2:LYS:HG2	1:F:143:LEU:HB3	1.88	0.55
1:D:75:PRO:HG2	1:D:79:THR:HB	1.87	0.55
1:F:125[A]:CYS:SG	1:I:123:VAL:CB	2.92	0.55
1:I:112:HIS:CD2	4:I:2126:HOH:O	2.60	0.55
1:B:123:VAL:HB	1:H:125[C]:CYS:SG	2.47	0.55
1:H:100:HIS:HB2	1:H:125[A]:CYS:SG	2.46	0.54
1:K:103:ASN:C	1:K:103:ASN:HD22	2.10	0.54
1:B:52:ASN:HD22	1:C:59:ASN:HD21	1.55	0.54
1:F:75:PRO:HG2	1:F:116:LEU:HD12	1.90	0.54
1:G:104:VAL:N	1:G:125[B]:CYS:SG	2.78	0.54
1:B:40:GLN:HG3	4:B:2083:HOH:O	2.08	0.54
1:H:104:VAL:HG12	4:H:2140:HOH:O	2.08	0.54
1:B:53:GLY:HA3	1:C:55:GLU:HB2	1.89	0.53
1:C:75:PRO:HG2	1:C:79:THR:HB	1.89	0.53
1:H:36:GLN:O	1:H:40:GLN:HG3	2.07	0.53
1:F:104:VAL:N	1:F:125[B]:CYS:SG	2.72	0.53
1:D:45:GLU:HB3	4:D:2083:HOH:O	2.08	0.53
1:A:18:ARG:N	1:A:18:ARG:CD	2.69	0.53
1:I:79:THR:CG2	1:I:100:HIS:HE1	2.01	0.53
1:L:124:ILE:O	1:L:125[C]:CYS:SG	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:GLN:O	1:G:40:GLN:HG3	2.09	0.53
1:E:140:ILE:O	1:E:144:GLN:HG3	2.09	0.53
1:B:28:LEU:HD23	4:B:2008:HOH:O	2.08	0.52
1:E:104:VAL:HG13	1:E:125[B]:CYS:SG	2.49	0.52
1:E:104:VAL:N	1:E:125[B]:CYS:SG	2.74	0.52
1:E:140:ILE:HG22	1:E:144:GLN:HE21	1.75	0.52
1:G:33:GLN:O	1:G:37:GLN:HG3	2.10	0.52
1:H:2:LYS:HE2	4:H:2178:HOH:O	2.10	0.52
1:I:107:ARG:C	4:I:2126:HOH:O	2.48	0.52
1:A:2:LYS:CD	1:A:143:LEU:HB3	2.35	0.52
1:F:1:MET:HG3	1:F:2:LYS:H	1.75	0.52
1:I:2:LYS:HE3	4:I:2175:HOH:O	2.10	0.52
1:I:104:VAL:N	1:I:125[B]:CYS:SG	2.73	0.52
1:F:2:LYS:HE3	1:F:147:GLN:CG	2.40	0.51
1:H:53:GLY:HA3	1:I:55:GLU:HB2	1.93	0.51
1:B:100:HIS:CD2	1:B:125[C]:CYS:SG	3.01	0.51
1:D:19:GLU:O	1:D:21:HIS:N	2.41	0.51
1:F:143:LEU:O	1:F:147:GLN:HG3	2.11	0.51
1:I:100:HIS:CD2	1:I:125[C]:CYS:SG	2.99	0.51
1:G:116:LEU:HG	4:G:2094:HOH:O	2.10	0.51
1:A:125[A]:CYS:SG	1:D:123:VAL:CB	2.89	0.51
1:A:2:LYS:HE3	1:A:143:LEU:O	2.11	0.51
1:I:141:SER:O	1:I:145:LYS:HG2	2.11	0.51
1:I:26:GLN:HG2	4:I:2034:HOH:O	2.11	0.51
1:K:75:PRO:HG2	1:K:79:THR:HB	1.92	0.51
1:J:123:VAL:CG1	1:J:125[B]:CYS:SG	2.99	0.50
1:B:130:LYS:HG2	4:B:2189:HOH:O	2.11	0.50
1:C:125[A]:CYS:SG	1:L:123:VAL:CB	2.93	0.50
1:F:3:LYS:HD2	1:F:47:ASP:OD2	2.12	0.50
1:I:40:GLN:HG3	4:I:2073:HOH:O	2.11	0.50
1:B:3:LYS:HD3	4:B:2125:HOH:O	2.10	0.50
1:H:100:HIS:HD2	1:H:125[B]:CYS:SG	2.35	0.50
1:E:2:LYS:HD3	1:E:143:LEU:HB3	1.94	0.50
1:D:65:PHE:CE2	1:F:18:ARG:HG3	2.47	0.50
1:I:130:LYS:HE3	1:I:134:TYR:OH	2.11	0.50
1:K:19:GLU:HG2	4:L:2105:HOH:O	2.11	0.50
1:A:123:VAL:CG1	1:A:125[C]:CYS:SG	2.99	0.49
1:I:123:VAL:CG1	1:I:125[C]:CYS:SG	3.00	0.49
1:J:55:GLU:HB2	1:L:53:GLY:HA3	1.93	0.49
1:E:3:LYS:HD3	1:E:47:ASP:OD2	2.12	0.49
1:K:53:GLY:HA3	1:L:55:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LYS:HD2	1:D:47:ASP:OD2	2.11	0.49
1:K:145:LYS:HE2	4:K:2186:HOH:O	2.11	0.49
1:H:97:ILE:HD11	1:H:138:PHE:CD2	2.48	0.49
1:J:28:LEU:HD21	1:J:50:GLN:HG3	1.94	0.49
1:J:53:GLY:HA3	1:K:55:GLU:HB2	1.94	0.49
1:A:55:GLU:HB2	1:C:53:GLY:HA3	1.94	0.49
1:E:33:GLN:O	1:E:37:GLN:HG3	2.13	0.49
1:I:18:ARG:O	1:I:19:GLU:C	2.50	0.49
1:J:75:PRO:HG2	1:J:79:THR:HB	1.95	0.49
1:H:123:VAL:CG1	1:H:125[B]:CYS:SG	3.01	0.49
1:A:123:VAL:CB	1:D:125[A]:CYS:SG	2.98	0.48
1:I:33:GLN:NE2	4:I:2047:HOH:O	2.44	0.48
1:E:123:VAL:CB	1:K:125[A]:CYS:SG	2.97	0.48
1:K:149:GLY:C	1:K:151:MET:N	2.66	0.48
1:E:59:ASN:O	1:E:63:GLN:HG3	2.13	0.48
1:I:3:LYS:HG3	1:I:45:GLU:HG3	1.94	0.48
1:L:26:GLN:N	4:L:2029:HOH:O	2.45	0.48
1:G:130:LYS:HG3	4:G:2143:HOH:O	2.14	0.48
1:B:3:LYS:HD2	1:B:67:ASN:O	2.14	0.48
1:C:55:GLU:CD	4:C:2105:HOH:O	2.51	0.48
1:C:97:ILE:HD11	1:C:138:PHE:CD2	2.48	0.48
1:D:19:GLU:HA	4:D:2023:HOH:O	2.13	0.48
1:F:123:VAL:CG1	1:F:125[C]:CYS:SG	3.00	0.47
1:H:147:GLN:HG3	4:H:2178:HOH:O	2.14	0.47
1:C:123:VAL:HB	1:L:125[A]:CYS:HG	1.75	0.47
1:I:25:SER:O	1:I:26:GLN:C	2.50	0.47
1:B:52:ASN:HD22	1:C:59:ASN:ND2	2.11	0.47
1:D:55:GLU:HB2	1:F:53:GLY:HA3	1.95	0.47
1:B:125[A]:CYS:HG	1:H:123:VAL:HB	1.78	0.47
1:I:97:ILE:HD11	1:I:138:PHE:CD2	2.49	0.47
1:C:130:LYS:HG3	4:C:2185:HOH:O	2.14	0.47
1:A:37:GLN:HG2	4:A:2048:HOH:O	2.15	0.47
1:K:15:LEU:HD21	1:K:101:LEU:CD1	2.44	0.47
1:C:33:GLN:O	1:C:37:GLN:HG3	2.15	0.47
1:L:1:MET:CB	4:L:2067:HOH:O	2.62	0.47
1:F:123:VAL:HB	1:I:125[A]:CYS:HG	1.77	0.47
1:G:104:VAL:HG12	4:G:2115:HOH:O	2.15	0.47
1:H:146:ILE:O	1:H:150:GLU:HG3	2.15	0.47
1:K:148:LEU:HD23	1:K:148:LEU:C	2.35	0.47
1:D:53:GLY:HA3	1:E:55:GLU:HB2	1.96	0.46
1:I:2:LYS:O	1:I:45:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:103:ASN:CA	1:L:125[B]:CYS:SG	2.94	0.46
1:C:123:VAL:HG12	1:C:125[B]:CYS:SG	2.55	0.46
1:K:151:MET:HA	1:K:151:MET:CE	2.46	0.46
1:F:147:GLN:O	1:F:150:GLU:HG2	2.15	0.46
1:H:104:VAL:HG13	1:H:125[A]:CYS:SG	2.55	0.46
1:A:53:GLY:HA3	1:B:55:GLU:HB2	1.97	0.46
1:L:144:GLN:O	1:L:146:ILE:N	2.49	0.46
1:B:103:ASN:CA	1:B:125[B]:CYS:SG	2.97	0.46
1:G:55:GLU:HB2	1:I:53:GLY:HA3	1.98	0.46
1:G:97:ILE:HD11	1:G:138:PHE:CD2	2.51	0.46
1:L:75:PRO:HG2	1:L:116:LEU:HD12	1.99	0.45
1:F:1:MET:CG	1:F:2:LYS:N	2.77	0.45
1:J:100:HIS:CB	1:J:125[C]:CYS:SG	3.03	0.45
1:L:97:ILE:HD13	1:L:135:ALA:HA	1.98	0.45
1:A:2:LYS:HZ1	1:A:146:ILE:HG13	1.82	0.45
1:G:130:LYS:HE3	1:G:134:TYR:OH	2.16	0.45
1:K:28:LEU:HD21	1:K:50:GLN:HG3	1.98	0.45
1:G:103:ASN:CA	1:G:125[B]:CYS:SG	2.95	0.45
1:D:130:LYS:HG2	4:D:2182:HOH:O	2.17	0.45
1:B:1:MET:O	1:B:3:LYS:HG3	2.17	0.45
1:F:1:MET:HG3	1:F:2:LYS:N	2.31	0.44
1:L:79:THR:OG1	1:L:100:HIS:HE1	2.00	0.44
1:L:104:VAL:HG12	4:L:2141:HOH:O	2.17	0.44
1:A:21:HIS:CE1	1:A:30:ASP:OD2	2.66	0.44
1:D:97:ILE:HD11	1:D:138:PHE:CD2	2.52	0.44
1:H:130:LYS:HE3	1:H:133:ASP:OD1	2.18	0.44
1:A:36:GLN:NE2	4:A:2048:HOH:O	2.44	0.44
1:A:141:SER:O	1:A:145:LYS:HG3	2.18	0.44
1:A:47:ASP:HB3	4:A:2106:HOH:O	2.17	0.44
1:L:2:LYS:NZ	4:L:2001:HOH:O	2.51	0.44
1:D:18:ARG:NH2	4:D:2020:HOH:O	2.50	0.44
1:C:100:HIS:HD2	1:C:125[B]:CYS:SG	2.41	0.44
1:J:28:LEU:CD2	1:J:50:GLN:HG3	2.48	0.44
1:D:28:LEU:O	1:D:32:GLU:HG3	2.18	0.43
1:G:53:GLY:HA3	1:H:55:GLU:HB2	1.99	0.43
1:H:79:THR:HG23	1:H:80:HIS:CE1	2.53	0.43
1:L:104:VAL:N	1:L:125[B]:CYS:SG	2.86	0.43
1:G:79:THR:CG2	1:G:100:HIS:HE1	2.18	0.43
1:C:103:ASN:CA	1:C:125[C]:CYS:SG	2.99	0.43
1:C:10:PRO:HA	1:C:52:ASN:OD1	2.19	0.43
4:C:2067:HOH:O	1:L:112:HIS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125[A]:CYS:SG	1:K:123:VAL:CB	3.02	0.43
1:D:91:ALA:O	1:F:18:ARG:HD3	2.18	0.43
1:G:1:MET:C	1:G:1:MET:SD	2.97	0.43
1:K:103:ASN:CA	1:K:125[C]:CYS:SG	2.99	0.43
1:B:1:MET:O	1:B:2:LYS:C	2.56	0.43
1:E:130:LYS:HE3	1:E:134:TYR:OH	2.17	0.43
1:H:140:ILE:O	1:H:144:GLN:HG3	2.18	0.43
1:K:46:LEU:C	1:K:46:LEU:HD23	2.38	0.43
1:H:143:LEU:O	1:H:147:GLN:HG3	2.18	0.43
1:E:123:VAL:CG1	1:E:125[C]:CYS:SG	3.07	0.43
1:K:10:PRO:HA	1:K:52:ASN:OD1	2.18	0.43
1:G:3:LYS:HE2	1:G:67:ASN:O	2.19	0.43
1:G:139:ALA:O	1:G:143:LEU:HG	2.19	0.43
1:E:10:PRO:HA	1:E:52:ASN:OD1	2.20	0.42
1:L:123:VAL:HG12	1:L:125[C]:CYS:SG	2.58	0.42
1:A:103:ASN:CA	1:A:125[B]:CYS:SG	2.96	0.42
1:E:23:TYR:CE2	1:E:101:LEU:HB3	2.53	0.42
1:E:46:LEU:HD23	1:E:46:LEU:C	2.40	0.42
1:K:130:LYS:HG3	4:K:2171:HOH:O	2.19	0.42
1:C:3:LYS:HE2	1:C:67:ASN:O	2.19	0.42
1:H:75:PRO:HG2	1:H:116:LEU:HD12	2.01	0.42
1:K:33:GLN:O	1:K:37:GLN:HG3	2.19	0.42
1:A:35:LEU:HD11	1:A:132:TYR:HB3	2.01	0.42
1:C:75:PRO:HG3	1:C:116:LEU:HD12	2.02	0.42
1:D:100:HIS:HD2	1:D:125[C]:CYS:SG	2.43	0.42
1:D:35:LEU:HG	1:D:136:LEU:HD22	2.02	0.42
1:L:72:ILE:HD11	1:L:136:LEU:HA	2.02	0.42
1:D:4:ILE:O	1:D:46:LEU:HA	2.20	0.42
1:A:104:VAL:HG12	4:A:2146:HOH:O	2.19	0.41
1:B:26:GLN:N	4:B:2039:HOH:O	2.52	0.41
1:D:28:LEU:CD2	1:D:50:GLN:HG3	2.50	0.41
1:F:130:LYS:HE3	1:I:141:SER:CB	2.50	0.41
1:G:28:LEU:HD21	1:G:50:GLN:HG3	2.03	0.41
1:E:2:LYS:CD	1:E:143:LEU:HB3	2.49	0.41
1:J:28:LEU:HD23	4:J:2002:HOH:O	2.21	0.41
1:A:104:VAL:N	1:A:125[B]:CYS:SG	2.83	0.41
1:F:1:MET:CG	1:F:2:LYS:H	2.33	0.41
1:C:127:LEU:HD22	1:L:138:PHE:CD2	2.56	0.41
1:D:3:LYS:HE2	1:D:67:ASN:O	2.21	0.41
1:D:46:LEU:HD23	1:D:46:LEU:C	2.41	0.41
1:K:4:ILE:O	1:K:46:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:OG1	1:A:100:HIS:HE1	2.03	0.41
1:D:65:PHE:CZ	1:F:18:ARG:HG3	2.56	0.41
1:A:17:LYS:HB3	1:A:18:ARG:H	1.68	0.41
1:B:123:VAL:CG1	1:B:125[C]:CYS:SG	3.03	0.41
1:C:153:ASN:HA	1:C:153:ASN:HD22	1.64	0.41
1:D:103:ASN:CA	1:D:125[B]:CYS:SG	3.06	0.41
1:H:2:LYS:HG2	4:H:2186:HOH:O	2.20	0.41
1:J:18:ARG:NH1	4:J:2024:HOH:O	2.46	0.41
1:K:104:VAL:HG12	4:K:2131:HOH:O	2.21	0.41
1:G:15:LEU:HD11	1:G:101:LEU:HD11	2.03	0.40
1:I:103:ASN:CA	1:I:125[B]:CYS:SG	3.02	0.40
1:I:26:GLN:N	4:I:2037:HOH:O	2.39	0.40
1:E:146:ILE:HG13	4:E:2158:HOH:O	2.20	0.40
1:K:103:ASN:ND2	1:K:105:HIS:H	2.20	0.40
1:D:104:VAL:HG13	1:D:125[B]:CYS:SG	2.61	0.40
1:D:123:VAL:CG1	1:D:125[C]:CYS:SG	3.09	0.40
1:F:75:PRO:CG	1:F:116:LEU:HD12	2.52	0.40
1:G:46:LEU:C	1:G:46:LEU:HD23	2.41	0.40
1:I:104:VAL:HG12	4:I:2124:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	146/154 (95%)	139 (95%)	7 (5%)	0	100	100
1	B	136/154 (88%)	133 (98%)	2 (2%)	1 (1%)	25	9
1	C	146/154 (95%)	144 (99%)	2 (1%)	0	100	100
1	D	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	25	9
1	E	141/154 (92%)	139 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	144/154 (94%)	142 (99%)	2 (1%)	0	100	100
1	G	138/154 (90%)	136 (99%)	2 (1%)	0	100	100
1	H	146/154 (95%)	144 (99%)	2 (1%)	0	100	100
1	I	139/154 (90%)	135 (97%)	3 (2%)	1 (1%)	25	9
1	J	146/154 (95%)	142 (97%)	3 (2%)	1 (1%)	25	9
1	K	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	14	2
1	L	136/154 (88%)	133 (98%)	3 (2%)	0	100	100
All	All	1722/1848 (93%)	1680 (98%)	36 (2%)	6 (0%)	38	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	26	GLN
1	D	21	HIS
1	J	2	LYS
1	K	151	MET
1	K	19	GLU
1	B	2	LYS

### 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	125/129 (97%)	124 (99%)	1 (1%)	85	78
1	B	118/129 (92%)	117 (99%)	1 (1%)	85	78
1	C	126/129 (98%)	125 (99%)	1 (1%)	85	78
1	D	129/129 (100%)	127 (98%)	2 (2%)	68	53
1	E	122/129 (95%)	121 (99%)	1 (1%)	85	78
1	F	124/129 (96%)	124 (100%)	0	100	100
1	G	120/129 (93%)	119 (99%)	1 (1%)	85	78
1	H	126/129 (98%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	121/129 (94%)	120 (99%)	1 (1%)	85	78
1	J	125/129 (97%)	122 (98%)	3 (2%)	54	35
1	K	129/129 (100%)	127 (98%)	2 (2%)	68	53
1	L	118/129 (92%)	117 (99%)	1 (1%)	85	78
All	All	1483/1548 (96%)	1469 (99%)	14 (1%)	80	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	B	1	MET
1	C	67	ASN
1	D	19	GLU
1	D	21	HIS
1	E	67	ASN
1	G	1	MET
1	I	26	GLN
1	J	19	GLU
1	J	21	HIS
1	J	35	LEU
1	K	103	ASN
1	K	151	MET
1	L	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	36	GLN
1	A	37	GLN
1	A	40	GLN
1	A	42	GLN
1	A	100	HIS
1	A	144	GLN
1	B	26	GLN
1	B	33	GLN
1	B	40	GLN
1	B	100	HIS
1	C	33	GLN
1	C	37	GLN

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Mol	Chain	Res	Type
1	C	59	ASN
1	C	63	GLN
1	C	67	ASN
1	C	144	GLN
1	C	153	ASN
1	D	21	HIS
1	D	26	GLN
1	D	33	GLN
1	D	66	GLN
1	D	144	GLN
1	E	26	GLN
1	E	40	GLN
1	E	63	GLN
1	E	67	ASN
1	E	144	GLN
1	F	26	GLN
1	F	100	HIS
1	F	144	GLN
1	F	147	GLN
1	G	33	GLN
1	G	100	HIS
1	G	112	HIS
1	G	144	GLN
1	H	13	ASN
1	H	26	GLN
1	H	33	GLN
1	H	37	GLN
1	H	66	GLN
1	H	112	HIS
1	I	40	GLN
1	I	66	GLN
1	I	67	ASN
1	I	100	HIS
1	I	112	HIS
1	J	33	GLN
1	J	37	GLN
1	J	40	GLN
1	J	144	GLN
1	K	33	GLN
1	K	37	GLN
1	K	40	GLN
1	K	66	GLN

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Mol	Chain	Res	Type
1	K	103	ASN
1	K	144	GLN
1	L	26	GLN
1	L	34	HIS
1	L	67	ASN
1	L	100	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	1147	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	A	1148	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	B	1147	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	B	1148	-	4,4,4	0.35	0	6,6,6	0.05	0
3	TRS	B	1149	-	7,7,7	1.64	2 (28%)	9,9,9	2.22	4 (44%)
2	SO4	C	1154	-	4,4,4	0.30	0	6,6,6	0.08	0
2	SO4	C	1155	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	C	1156	-	4,4,4	0.32	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	D	1152	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	D	1153	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	D	1154	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	E	1147	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	E	1148	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	E	1149	-	4,4,4	0.34	0	6,6,6	0.10	0
3	TRS	E	1150	-	7,7,7	1.61	1 (14%)	9,9,9	2.29	4 (44%)
2	SO4	F	1152	-	4,4,4	0.33	0	6,6,6	0.18	0
2	SO4	F	1153	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	F	1154	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	F	1155	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	G	1147	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	H	1154	-	4,4,4	0.39	0	6,6,6	0.17	0
2	SO4	H	1155	-	4,4,4	0.31	0	6,6,6	0.07	0
2	SO4	H	1156	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	H	1157	-	4,4,4	0.34	0	6,6,6	0.10	0
3	TRS	H	1158	-	7,7,7	1.49	1 (14%)	9,9,9	2.18	4 (44%)
2	SO4	I	1147	-	4,4,4	0.34	0	6,6,6	0.10	0
2	SO4	J	1147	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	J	1148	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	J	1149	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	K	1152	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	K	1153	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	K	1154	-	4,4,4	0.33	0	6,6,6	0.07	0
3	TRS	K	1155	-	7,7,7	1.54	1 (14%)	9,9,9	2.16	4 (44%)
2	SO4	L	1147	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	L	1148	-	4,4,4	0.32	0	6,6,6	0.11	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	A	1147	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1148	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1147	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1148	-	-	0/0/0/0	0/0/0/0
3	TRS	B	1149	-	-	0/9/9/9	0/0/0/0
2	SO4	C	1154	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1155	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1156	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	1152	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1153	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1154	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1147	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1148	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1149	-	-	0/0/0/0	0/0/0/0
3	TRS	E	1150	-	-	0/9/9/9	0/0/0/0
2	SO4	F	1152	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1153	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1154	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1155	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1147	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1154	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1155	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1156	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1157	-	-	0/0/0/0	0/0/0/0
3	TRS	H	1158	-	-	0/9/9/9	0/0/0/0
2	SO4	I	1147	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1147	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1148	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1149	-	-	0/0/0/0	0/0/0/0
2	SO4	K	1152	-	-	0/0/0/0	0/0/0/0
2	SO4	K	1153	-	-	0/0/0/0	0/0/0/0
2	SO4	K	1154	-	-	0/0/0/0	0/0/0/0
3	TRS	K	1155	-	-	0/9/9/9	0/0/0/0
2	SO4	L	1147	-	-	0/0/0/0	0/0/0/0
2	SO4	L	1148	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1149	TRS	C-N	-2.10	1.42	1.49
3	H	1158	TRS	C1-C	2.28	1.58	1.52
3	K	1155	TRS	C1-C	2.30	1.58	1.52
3	E	1150	TRS	C1-C	2.36	1.58	1.52
3	B	1149	TRS	C1-C	2.44	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1158	TRS	C2-C-C1	-2.66	103.54	111.06
3	E	1150	TRS	C2-C-C1	-2.65	103.55	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1155	TRS	C2-C-C1	-2.64	103.57	111.06
3	B	1149	TRS	C2-C-C1	-2.59	103.71	111.06
3	B	1149	TRS	O1-C1-C	-2.51	103.20	110.47
3	E	1150	TRS	O1-C1-C	-2.42	103.46	110.47
3	K	1155	TRS	O1-C1-C	-2.15	104.24	110.47
3	H	1158	TRS	O1-C1-C	-2.15	104.25	110.47
3	H	1158	TRS	C3-C-N	3.02	114.14	107.73
3	K	1155	TRS	C3-C-N	3.06	114.24	107.73
3	B	1149	TRS	C3-C-N	3.07	114.25	107.73
3	E	1150	TRS	C3-C-N	3.28	114.70	107.73
3	H	1158	TRS	C2-C-N	3.80	115.81	107.73
3	E	1150	TRS	C2-C-N	3.81	115.82	107.73
3	K	1155	TRS	C2-C-N	3.85	115.91	107.73
3	B	1149	TRS	C2-C-N	3.93	116.07	107.73

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	146/154 (94%)	-0.16	11 (7%) 15 18	11, 18, 49, 66	0
1	B	138/154 (89%)	-0.37	4 (2%) 52 58	10, 16, 33, 62	0
1	C	148/154 (96%)	-0.30	4 (2%) 55 60	11, 20, 38, 74	0
1	D	152/154 (98%)	-0.00	10 (6%) 19 22	13, 21, 56, 73	0
1	E	143/154 (92%)	-0.01	8 (5%) 25 28	14, 23, 48, 73	0
1	F	146/154 (94%)	-0.30	8 (5%) 26 29	12, 18, 40, 70	0
1	G	140/154 (90%)	-0.10	6 (4%) 36 41	13, 22, 45, 69	0
1	H	148/154 (96%)	-0.17	5 (3%) 46 52	13, 21, 37, 72	0
1	I	141/154 (91%)	-0.25	6 (4%) 36 41	12, 18, 39, 67	0
1	J	146/154 (94%)	0.11	12 (8%) 12 15	15, 25, 52, 71	0
1	K	152/154 (98%)	-0.06	12 (7%) 13 16	15, 21, 50, 74	0
1	L	138/154 (89%)	-0.24	4 (2%) 52 58	14, 18, 36, 70	0
All	All	1738/1848 (94%)	-0.15	90 (5%) 28 31	10, 20, 45, 74	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	GLY	11.3
1	L	146	ILE	10.7
1	H	154	GLY	10.6
1	A	23	TYR	8.9
1	K	152	MET	8.7
1	F	1	MET	8.4
1	L	1	MET	8.2
1	D	20	PRO	8.1
1	B	1	MET	7.9
1	E	146	ILE	7.6
1	I	146	ILE	7.5

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Mol	Chain	Res	Type	RSRZ
1	J	146	ILE	7.4
1	D	22	ILE	7.3
1	J	19	GLU	7.3
1	D	21	HIS	7.3
1	D	23	TYR	7.2
1	I	25	SER	7.0
1	J	1	MET	6.8
1	E	1	MET	6.8
1	G	1	MET	6.8
1	K	19	GLU	6.6
1	A	146	ILE	6.5
1	K	151	MET	6.5
1	E	24	GLY	6.3
1	G	146	ILE	6.2
1	J	22	ILE	6.1
1	K	23	TYR	6.1
1	A	22	ILE	6.0
1	E	23	TYR	5.8
1	D	19	GLU	5.8
1	I	1	MET	5.8
1	B	146	ILE	5.6
1	J	21	HIS	5.4
1	F	152	MET	5.4
1	E	22	ILE	5.2
1	C	153	ASN	4.8
1	G	18	ARG	4.1
1	A	1	MET	4.1
1	A	125[A]	CYS	4.0
1	L	145	LYS	4.0
1	H	25	SER	3.9
1	J	20	PRO	3.9
1	D	1	MET	3.8
1	F	151	MET	3.8
1	H	153	ASN	3.8
1	K	22	ILE	3.7
1	E	125[A]	CYS	3.7
1	J	23	TYR	3.6
1	J	125[A]	CYS	3.6
1	I	125[A]	CYS	3.6
1	A	18	ARG	3.5
1	F	150	GLU	3.5
1	B	125[A]	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	25	SER	3.4
1	A	19	GLU	3.4
1	D	151	MET	3.3
1	G	25	SER	3.3
1	D	25	SER	3.2
1	E	25	SER	3.2
1	K	125[A]	CYS	3.1
1	H	125[A]	CYS	3.1
1	A	24	GLY	3.0
1	K	24	GLY	3.0
1	F	25	SER	3.0
1	E	145	LYS	2.8
1	F	125[A]	CYS	2.8
1	D	125[A]	CYS	2.7
1	L	125[A]	CYS	2.7
1	D	24	GLY	2.7
1	K	20	PRO	2.7
1	J	25	SER	2.7
1	J	145	LYS	2.6
1	I	19	GLU	2.6
1	G	145	LYS	2.6
1	K	21	HIS	2.5
1	B	145	LYS	2.5
1	A	20	PRO	2.4
1	G	125[A]	CYS	2.4
1	K	148	LEU	2.2
1	C	25	SER	2.2
1	F	18	ARG	2.2
1	H	18	ARG	2.2
1	A	25	SER	2.2
1	A	145	LYS	2.2
1	C	125[A]	CYS	2.2
1	J	24	GLY	2.2
1	I	145	LYS	2.1
1	K	149	GLY	2.1
1	J	2	LYS	2.0
1	F	149	GLY	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 carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
3	TRS	B	1149	8/8	0.96	0.09	5.51	14,15,16,17	0
3	TRS	E	1150	8/8	0.94	0.08	3.32	14,16,19,19	0
2	SO4	F	1155	5/5	0.80	0.37	3.21	41,55,67,68	0
2	SO4	H	1157	5/5	0.85	0.32	3.04	50,60,67,70	0
3	TRS	K	1155	8/8	0.96	0.08	2.88	16,18,19,22	0
2	SO4	C	1156	5/5	0.95	0.24	2.53	35,44,55,57	0
3	TRS	H	1158	8/8	0.96	0.07	1.25	15,16,18,19	0
2	SO4	K	1154	5/5	0.99	0.09	0.74	28,29,37,47	0
2	SO4	B	1147	5/5	0.98	0.07	0.74	18,21,36,38	0
2	SO4	A	1148	5/5	0.97	0.07	0.39	21,29,36,38	0
2	SO4	F	1154	5/5	0.89	0.23	0.23	31,33,41,49	0
2	SO4	J	1149	5/5	0.95	0.20	-0.02	39,40,46,52	0
2	SO4	K	1153	5/5	0.96	0.17	-0.13	41,42,46,46	0
2	SO4	J	1147	5/5	0.97	0.09	-0.24	22,27,31,32	0
2	SO4	D	1152	5/5	0.98	0.06	-0.47	17,27,33,43	0
2	SO4	G	1147	5/5	0.99	0.07	-0.48	23,27,39,44	0
2	SO4	D	1154	5/5	0.94	0.15	-0.49	53,56,60,66	0
2	SO4	C	1154	5/5	0.99	0.06	-0.50	18,23,29,33	0
2	SO4	E	1149	5/5	0.97	0.13	-0.55	39,42,49,50	0
2	SO4	H	1155	5/5	0.99	0.07	-0.59	19,25,38,40	0
2	SO4	K	1152	5/5	0.98	0.06	-0.59	24,25,30,33	0
2	SO4	I	1147	5/5	0.99	0.06	-0.60	22,29,38,39	0
2	SO4	E	1147	5/5	0.99	0.04	-0.84	20,24,28,29	0
2	SO4	F	1152	5/5	0.99	0.04	-0.98	15,17,19,22	0
2	SO4	A	1147	5/5	1.00	0.04	-1.13	13,13,16,20	0
2	SO4	L	1148	5/5	0.99	0.06	-1.20	25,27,38,46	0
2	SO4	L	1147	5/5	1.00	0.05	-1.28	17,18,20,25	0
2	SO4	H	1154	5/5	1.00	0.04	-1.43	15,16,18,23	0
2	SO4	F	1153	5/5	0.99	0.05	-1.80	17,25,35,47	0
2	SO4	D	1153	5/5	0.91	0.24	-	43,52,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	E	1148	5/5	0.95	0.27	-	33,47,55,56	0
2	SO4	H	1156	5/5	0.97	0.23	-	33,34,54,55	0
2	SO4	B	1148	5/5	0.92	0.27	-	57,58,71,74	0
2	SO4	C	1155	5/5	0.92	0.22	-	31,36,49,53	0
2	SO4	J	1148	5/5	0.95	0.28	-	46,53,65,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.