



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 09:18 AM BST

PDB ID : 2DD4  
Title : Thiocyanate hydrolase (SCNase) from Thiobacillus thioparus recombinant apo-enzyme  
Authors : Arakawa, T.; Kawano, Y.; Kataoka, S.; Katayama, Y.; Kamiya, N.; Yohda, M.; Odaka, M.  
Deposited on : 2006-01-19  
Resolution : 2.06 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 : 2.13.1  
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) : 2.13.1

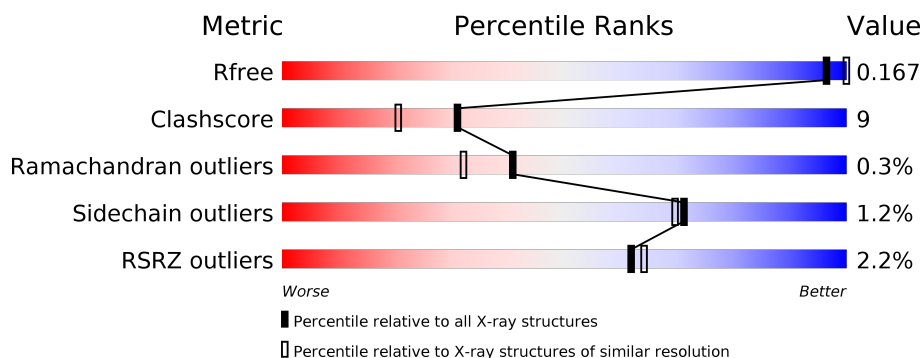
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	126	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	D	126	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>6%</div> </div> </div>
1	G	126	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
1	J	126	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
2	B	157	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>
2	E	157	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	157	<div><div></div><div>3%</div><div>83%</div><div>15%</div><div>••</div></div>
2	K	157	<div><div></div><div>4%</div><div>76%</div><div>19%</div><div>••</div></div>
3	C	243	<div><div></div><div>%</div><div>73%</div><div>16%</div><div>11%</div></div>
3	F	243	<div><div></div><div>2%</div><div>68%</div><div>19%</div><div>•11%</div></div>
3	I	243	<div><div></div><div>%</div><div>74%</div><div>15%</div><div>11%</div></div>
3	L	243	<div><div></div><div>2%</div><div>70%</div><div>18%</div><div>•11%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18077 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 Thiocyanate hydrolase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			958	609	159	186	4			
1	D	119	Total	C	N	O	S	0	0	0
			965	614	160	187	4			
1	G	120	Total	C	N	O	S	0	0	0
			974	620	162	188	4			
1	J	120	Total	C	N	O	S	0	0	0
			974	620	162	188	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O66187
D	1	MET	-	initiating methionine	UNP O66187
G	1	MET	-	initiating methionine	UNP O66187
J	1	MET	-	initiating methionine	UNP O66187

- Molecule 2 is a protein called Thiocyanate hydrolase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1232	778	222	226	6			
2	E	151	Total	C	N	O	S	0	0	0
			1226	775	221	224	6			
2	H	156	Total	C	N	O	S	0	0	0
			1262	796	228	232	6			
2	K	152	Total	C	N	O	S	0	0	0
			1232	778	222	226	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP O66186
E	1	MET	-	initiating methionine	UNP O66186
H	1	MET	-	initiating methionine	UNP O66186
K	1	MET	-	initiating methionine	UNP O66186

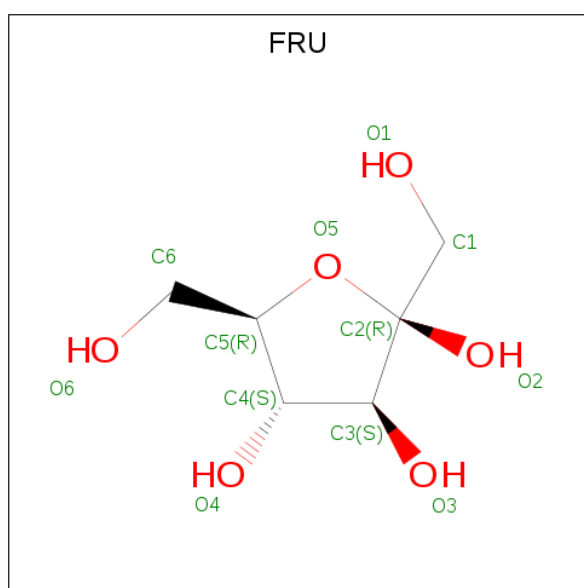
- Molecule 3 is a protein called Thiocyanate hydrolase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1721	1098	304	311	8			
3	F	216	Total	C	N	O	S	0	0	0
			1712	1093	303	308	8			
3	I	217	Total	C	N	O	S	0	0	0
			1721	1098	304	311	8			
3	L	216	Total	C	N	O	S	0	0	0
			1712	1093	303	308	8			

There are 4 discrepancies between the modelled and reference sequences:

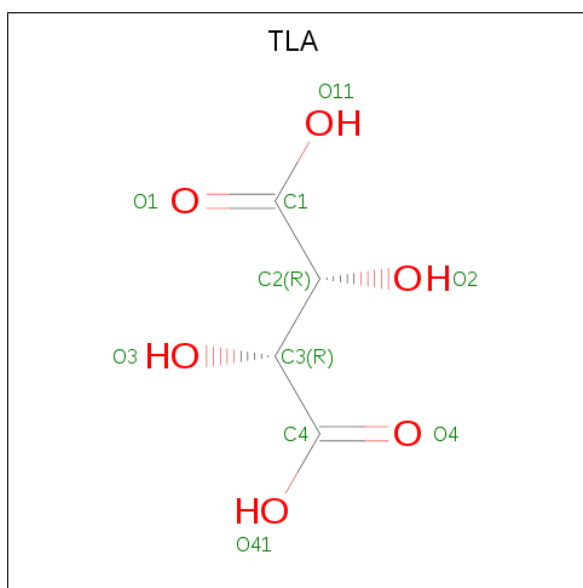
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP O66188
F	1	MET	-	initiating methionine	UNP O66188
I	1	MET	-	initiating methionine	UNP O66188
L	1	MET	-	initiating methionine	UNP O66188

- Molecule 4 is beta-D-fructofuranose (three-letter code: FRU) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 6 6	0	0
4	B	1	Total C O 12 6 6	0	0
4	C	1	Total C O 12 6 6	0	0
4	H	1	Total C O 12 6 6	0	0
4	H	1	Total C O 12 6 6	0	0
4	H	1	Total C O 12 6 6	0	0
4	K	1	Total C O 12 6 6	0	0
4	K	1	Total C O 12 6 6	0	0

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 4 6	0	0
5	C	1	Total C O 10 4 6	0	0
5	F	1	Total C O 10 4 6	0	0
5	F	1	Total C O 10 4 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			10	4	6		
5	I	1	Total	C	O	0	0
			10	4	6		
5	L	1	Total	C	O	0	0
			10	4	6		
5	L	1	Total	C	O	0	0
			10	4	6		

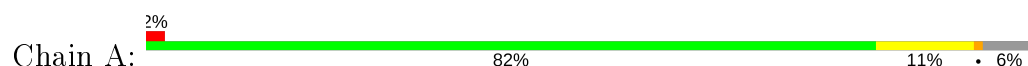
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	182	Total	O	0	0
			182	182		
6	C	257	Total	O	0	0
			257	257		
6	D	123	Total	O	0	0
			123	123		
6	E	166	Total	O	0	0
			166	166		
6	F	209	Total	O	0	0
			209	209		
6	G	122	Total	O	0	0
			122	122		
6	H	185	Total	O	0	0
			185	185		
6	I	281	Total	O	0	0
			281	281		
6	J	132	Total	O	0	0
			132	132		
6	K	183	Total	O	0	0
			183	183		
6	L	252	Total	O	0	0
			252	252		

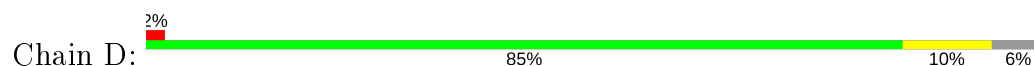
### 3 Residue-property plots

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.

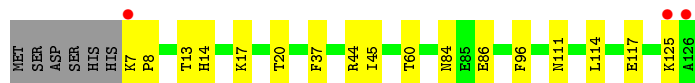
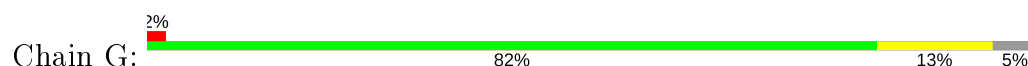
- Molecule 1: Thiocyanate hydrolase alpha subunit



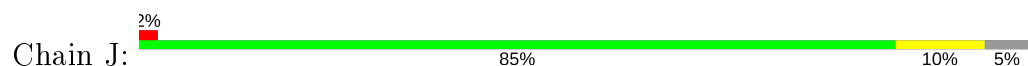
- Molecule 1: Thiocyanate hydrolase alpha subunit



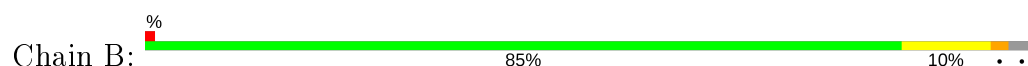
- Molecule 1: Thiocyanate hydrolase alpha subunit



- Molecule 1: Thiocyanate hydrolase alpha subunit



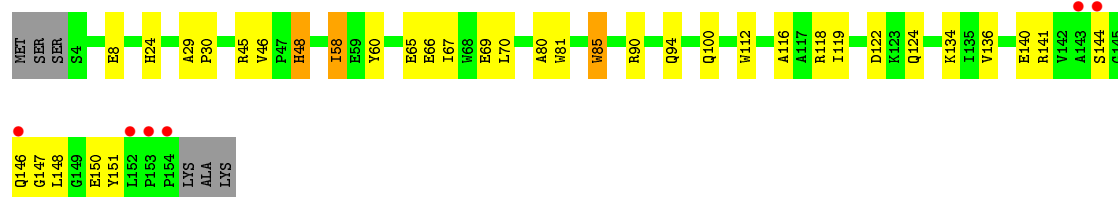
- Molecule 2: Thiocyanate hydrolase beta subunit




- Molecule 2: Thiocyanate hydrolase beta subunit



Chain E:  4% 73% 21% . .

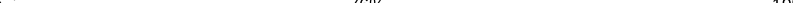


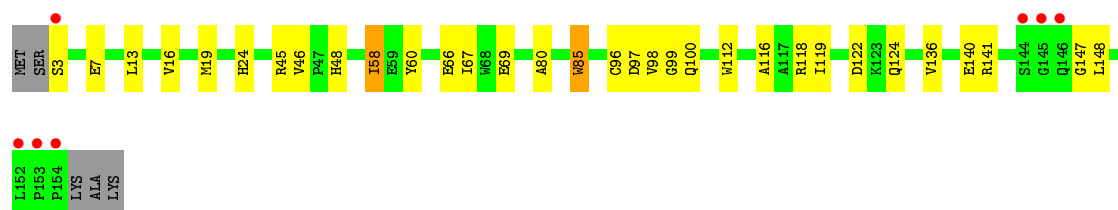
- Molecule 2: Thiocyanate hydrolase beta subunit

Chain H: 

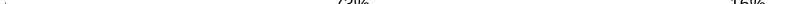


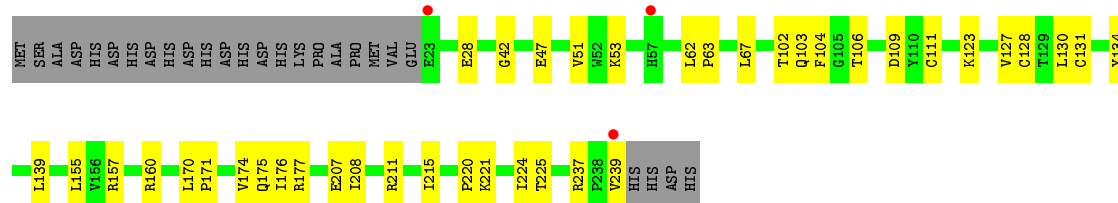
- Molecule 2: Thiocyanate hydrolase beta subunit

Chain K: 



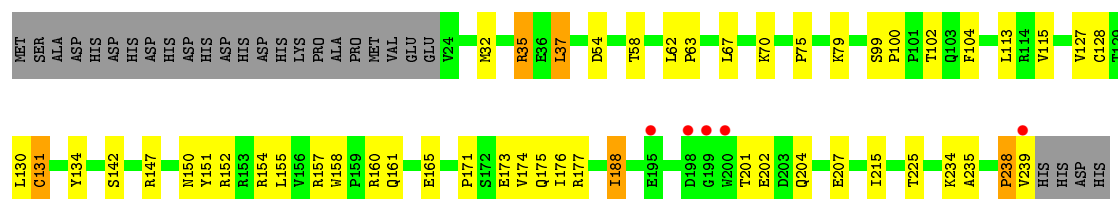
- Molecule 3: Thiocyanate hydrolase gamma subunit

Chain C:  73% 16% 11%

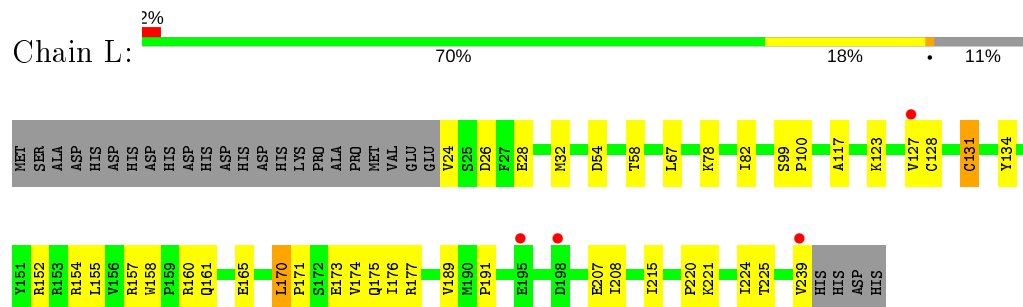


- Molecule 3: Thiocyanate hydrolase gamma subunit

Chain F:  2% 68% 19% 11%



- Molecule 3: Thiocyanate hydrolase gamma subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.31Å 175.60Å 114.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.95 – 2.06 32.95 – 2.06	Depositor EDS
% Data completeness (in resolution range)	96.3 (32.95-2.06) 97.0 (32.95-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.56 (at 2.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.165 , 0.193 0.163 , 0.167	Depositor DCC
$R_{free}$ test set	10298 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.0	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.34	0/983	0.61	0/1331
1	D	0.33	0/991	0.60	0/1342
1	G	0.32	0/1000	0.59	0/1354
1	J	0.34	0/1000	0.60	0/1354
2	B	0.30	0/1264	0.58	0/1720
2	E	0.30	0/1258	0.57	0/1712
2	H	0.31	0/1294	0.58	0/1757
2	K	0.31	0/1264	0.59	0/1720
3	C	0.29	0/1765	0.60	0/2410
3	F	0.29	0/1756	0.60	0/2398
3	I	0.29	0/1765	0.61	0/2410
3	L	0.29	0/1756	0.61	0/2398
All	All	0.31	0/16096	0.60	0/21906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	958	0	906	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	965	0	914	12	0
1	G	974	0	926	18	0
1	J	974	0	926	13	0
2	B	1232	0	1198	20	0
2	E	1226	0	1193	31	0
2	H	1262	0	1234	22	0
2	K	1232	0	1198	29	0
3	C	1721	0	1739	41	0
3	F	1712	0	1733	50	0
3	I	1721	0	1739	29	0
3	L	1712	0	1733	38	0
4	B	24	0	24	2	0
4	C	12	0	12	1	0
4	H	36	0	36	6	0
4	K	24	0	24	4	0
5	C	20	0	8	1	0
5	F	20	0	8	1	0
5	I	20	0	8	1	0
5	L	20	0	8	1	0
6	A	120	0	0	3	0
6	B	182	0	0	1	0
6	C	257	0	0	3	0
6	D	123	0	0	1	0
6	E	166	0	0	2	0
6	F	209	0	0	2	0
6	G	122	0	0	1	0
6	H	185	0	0	1	0
6	I	281	0	0	2	0
6	J	132	0	0	2	0
6	K	183	0	0	0	0
6	L	252	0	0	2	0
All	All	18077	0	15567	287	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 (287) 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)
3:F:113:LEU:HD11	3:F:188:ILE:HD12	1.36	1.05
3:I:82:ILE:HD11	3:I:117:ALA:HB2	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:HE21	1:A:26:GLN:H	1.08	0.97
3:F:115:VAL:HG22	3:F:188:ILE:HD11	1.47	0.94
1:D:45:ILE:HD11	1:D:96:PHE:HZ	1.32	0.93
1:D:45:ILE:HD11	1:D:96:PHE:CZ	2.09	0.86
1:G:45:ILE:HD11	1:G:96:PHE:HZ	1.41	0.85
3:C:208:ILE:HD13	3:C:220:PRO:HB2	1.61	0.83
3:I:208:ILE:HD13	3:I:220:PRO:HB2	1.58	0.82
2:K:58:ILE:HD11	2:K:60:TYR:CE1	2.15	0.82
2:E:58:ILE:HD11	2:E:60:TYR:CE1	2.15	0.81
3:F:131:CYS:O	3:F:152:ARG:HD3	1.81	0.79
3:L:208:ILE:HD13	3:L:220:PRO:HB2	1.66	0.77
3:C:139:LEU:HD13	3:C:139:LEU:O	1.85	0.76
1:A:26:GLN:NE2	1:A:26:GLN:H	1.81	0.76
2:B:119:ILE:HD13	2:B:119:ILE:O	1.87	0.75
3:C:237:ARG:HB2	3:C:237:ARG:NH1	2.00	0.75
3:F:35:ARG:CB	3:F:35:ARG:HH21	1.99	0.75
3:L:131:CYS:O	3:L:152:ARG:HD3	1.88	0.74
3:L:142:SER:OG	3:L:147:ARG:HD3	1.89	0.73
3:L:175:GLN:HE22	3:L:177:ARG:HH21	1.35	0.73
1:G:45:ILE:HD11	1:G:96:PHE:CZ	2.22	0.73
3:F:175:GLN:HE22	3:F:177:ARG:HH11	1.37	0.73
2:B:67:ILE:HD13	3:C:239:VAL:HA	1.70	0.72
3:I:175:GLN:HE22	3:I:177:ARG:HH21	1.35	0.72
2:H:3:SER:O	2:H:7:GLU:HG3	1.89	0.72
3:C:237:ARG:HB2	3:C:237:ARG:HH11	1.53	0.72
3:C:175:GLN:HE22	3:C:177:ARG:HH11	1.35	0.71
3:I:66:ARG:HD2	3:I:202:GLU:OE2	1.91	0.70
3:F:127:VAL:HB	3:F:155:LEU:HD23	1.74	0.70
2:H:119:ILE:HD11	2:H:123:LYS:HD2	1.73	0.70
3:F:142:SER:OG	3:F:147:ARG:HD3	1.91	0.70
3:I:82:ILE:CD1	3:I:117:ALA:HB2	2.20	0.69
3:F:201:THR:HG23	3:F:204:GLN:NE2	2.08	0.69
2:B:3:SER:O	2:B:7:GLU:HG3	1.92	0.69
2:E:24:HIS:ND1	2:K:24:HIS:HD2	1.89	0.69
1:G:45:ILE:HD12	1:G:60:THR:HB	1.75	0.68
1:A:117:GLU:C	1:A:118:ILE:HD12	2.13	0.68
1:A:68:VAL:HG21	6:A:268:HOH:O	1.93	0.68
3:C:160:ARG:NH2	3:C:176:ILE:HD13	2.09	0.68
2:B:119:ILE:HD11	2:B:123:LYS:HD2	1.77	0.67
2:B:66:GLU:HB2	2:B:69:GLU:HG3	1.75	0.67
3:L:127:VAL:HB	3:L:155:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:102:VAL:HG21	4:H:3006:FRU:O1	1.94	0.66
2:E:66:GLU:HB2	2:E:69:GLU:HG3	1.76	0.66
3:L:82:ILE:HD11	3:L:117:ALA:HB2	1.78	0.66
3:L:221:LYS:HE3	3:L:224:ILE:HD12	1.78	0.65
1:A:26:GLN:N	1:A:26:GLN:HE21	1.88	0.65
4:H:3007:FRU:H12	6:H:3017:HOH:O	1.95	0.65
2:E:58:ILE:H	2:E:58:ILE:HD13	1.61	0.64
3:L:82:ILE:CD1	3:L:117:ALA:HB2	2.26	0.64
3:C:237:ARG:CB	3:C:237:ARG:HH11	2.10	0.64
2:H:42:ALA:HB1	2:K:19:MET:HE2	1.80	0.64
3:F:134:TYR:CE1	3:F:215:ILE:HD11	2.33	0.64
3:C:160:ARG:CZ	3:C:176:ILE:HD13	2.28	0.63
2:K:66:GLU:HB2	2:K:69:GLU:HG3	1.80	0.62
1:D:111:ASN:O	3:F:175:GLN:HG3	1.98	0.62
2:K:3:SER:O	2:K:7:GLU:HG3	1.99	0.62
4:B:3008:FRU:H12	2:K:99:GLY:HA2	1.80	0.62
2:E:150:GLU:HG2	6:F:4652:HOH:O	1.98	0.62
1:G:37:PHE:CD1	1:G:125:LYS:HE3	2.35	0.61
1:A:111:ASN:O	3:C:175:GLN:HG3	2.01	0.61
2:K:136:VAL:O	2:K:140:GLU:HG3	2.01	0.61
1:G:111:ASN:O	3:I:175:GLN:HG3	2.00	0.61
2:B:150:GLU:HG2	6:C:3652:HOH:O	2.00	0.61
3:C:134:TYR:CZ	3:C:139:LEU:HD12	2.35	0.60
1:G:37:PHE:HD1	1:G:125:LYS:HE3	1.66	0.60
3:C:134:TYR:CE2	3:C:139:LEU:HD12	2.37	0.60
2:B:67:ILE:CD1	3:C:239:VAL:HA	2.31	0.60
1:D:45:ILE:CD1	1:D:60:THR:HB	2.31	0.60
3:I:127:VAL:HB	3:I:155:LEU:HD23	1.83	0.60
3:C:28:GLU:OE2	3:C:237:ARG:NH1	2.35	0.59
2:K:58:ILE:HD12	3:L:150:ASN:CG	2.22	0.59
2:H:66:GLU:HB2	2:H:69:GLU:HG3	1.83	0.59
3:I:102:THR:O	3:I:103:GLN:HB2	2.01	0.59
3:F:188:ILE:H	3:F:188:ILE:HD13	1.68	0.59
1:A:26:GLN:HE22	3:C:111:CYS:HB2	1.67	0.58
2:K:58:ILE:H	2:K:58:ILE:HD13	1.68	0.58
3:C:127:VAL:HG22	3:C:128:CYS:N	2.19	0.58
2:H:119:ILE:HD13	2:H:119:ILE:O	2.04	0.58
2:E:148:LEU:CD1	3:F:32:MET:HG3	2.33	0.58
1:J:56:THR:HG23	1:J:118:ILE:HD12	1.85	0.58
3:F:188:ILE:N	3:F:188:ILE:HD13	2.19	0.58
2:K:98:VAL:HA	4:K:3005:FRU:O2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:124:GLN:HE21	1:G:84:ASN:ND2	2.02	0.57
1:A:84:ASN:ND2	2:K:124:GLN:HE21	2.02	0.57
2:K:13:LEU:HB2	4:K:3003:FRU:H12	1.86	0.57
2:B:45:ARG:HH11	2:B:100:GLN:HE22	1.51	0.57
4:H:3004:FRU:H3	3:L:157:ARG:HH12	1.70	0.57
1:G:45:ILE:CD1	1:G:60:THR:HB	2.34	0.57
3:L:123:LYS:HG2	3:L:170:LEU:CD1	2.34	0.56
2:E:134:LYS:HE3	3:F:37:LEU:HD13	1.87	0.56
2:H:45:ARG:HH11	2:H:100:GLN:HE22	1.53	0.56
2:B:45:ARG:NH1	2:B:100:GLN:HE22	2.04	0.56
3:F:35:ARG:HH21	3:F:35:ARG:HB3	1.69	0.56
3:I:127:VAL:HG22	3:I:128:CYS:N	2.21	0.55
2:H:42:ALA:HB1	2:K:19:MET:CE	2.36	0.55
1:J:125:LYS:HG3	6:J:236:HOH:O	2.05	0.55
1:J:111:ASN:O	3:L:175:GLN:HG3	2.06	0.55
3:F:35:ARG:HH21	3:F:35:ARG:HB2	1.72	0.54
2:B:84:VAL:CG1	2:B:119:ILE:HD12	2.37	0.54
3:C:134:TYR:OH	3:C:139:LEU:HD12	2.08	0.54
2:E:58:ILE:HD12	3:F:150:ASN:CG	2.28	0.54
3:F:154:ARG:NH2	3:F:165:GLU:OE2	2.35	0.54
1:A:116:THR:HG23	1:A:118:ILE:HD11	1.89	0.54
3:C:42:GLY:HA2	6:C:3621:HOH:O	2.08	0.54
2:E:90:ARG:HH11	2:E:94:GLN:HE22	1.56	0.54
3:C:102:THR:O	3:C:103:GLN:HB2	2.07	0.53
3:C:224:ILE:HD12	3:C:224:ILE:N	2.24	0.53
2:E:58:ILE:N	2:E:58:ILE:HD13	2.24	0.53
6:C:3640:HOH:O	3:F:161:GLN:HG2	2.07	0.53
1:A:86:GLU:H	1:A:86:GLU:CD	2.10	0.53
2:H:45:ARG:NH1	2:H:100:GLN:HE22	2.07	0.53
3:L:207:GLU:HG2	3:L:225:THR:CG2	2.39	0.53
3:L:173:GLU:H	3:L:173:GLU:CD	2.12	0.53
2:E:148:LEU:HD11	3:F:32:MET:HG3	1.91	0.53
1:J:99:LYS:HE3	6:J:215:HOH:O	2.09	0.53
3:F:239:VAL:O	3:F:239:VAL:HG13	2.09	0.53
3:I:207:GLU:HG2	3:I:225:THR:CG2	2.38	0.53
3:L:221:LYS:HB2	3:L:224:ILE:HD12	1.91	0.53
3:C:123:LYS:HG3	3:C:170:LEU:HD21	1.92	0.52
3:L:123:LYS:HG2	3:L:170:LEU:HD11	1.89	0.52
3:L:221:LYS:HE3	3:L:224:ILE:CD1	2.40	0.52
3:F:175:GLN:HE22	3:F:177:ARG:NH1	2.06	0.52
2:K:46:VAL:HG12	2:K:96:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:VAL:HB	3:C:155:LEU:HD23	1.92	0.51
3:F:238:PRO:O	3:F:239:VAL:HG12	2.11	0.51
1:A:118:ILE:HD12	1:A:118:ILE:N	2.26	0.51
2:H:118:ARG:NH1	4:H:3006:FRU:H62	2.26	0.51
2:K:45:ARG:HH11	2:K:100:GLN:HE22	1.59	0.51
2:B:124:GLN:HE21	1:J:84:ASN:ND2	2.08	0.51
3:L:134:TYR:CE1	3:L:215:ILE:HD11	2.45	0.51
2:H:85:TRP:CE3	2:H:119:ILE:HG13	2.46	0.51
3:L:189:VAL:O	3:L:191:PRO:HD3	2.10	0.51
3:C:157:ARG:HH12	4:C:3001:FRU:C6	2.23	0.51
2:E:81:TRP:CD1	3:F:102:THR:HG22	2.46	0.50
1:G:13:THR:HB	1:G:17:LYS:HE2	1.93	0.50
1:J:86:GLU:CD	1:J:86:GLU:H	2.15	0.50
3:F:127:VAL:HG22	3:F:128:CYS:N	2.26	0.50
2:E:118:ARG:HG3	2:E:122:ASP:OD2	2.11	0.50
1:D:45:ILE:HD12	1:D:60:THR:HB	1.93	0.50
3:I:207:GLU:HG2	3:I:225:THR:HG22	1.94	0.50
3:L:207:GLU:HG2	3:L:225:THR:HG22	1.94	0.50
3:F:134:TYR:HE1	3:F:215:ILE:HD11	1.76	0.50
1:G:117:GLU:HG3	6:I:5523:HOH:O	2.12	0.50
1:J:92:TYR:HB2	1:J:94:ILE:HD11	1.94	0.50
2:E:67:ILE:HA	2:E:70:LEU:HD12	1.94	0.49
1:G:13:THR:CB	1:G:17:LYS:HE2	2.42	0.49
3:L:127:VAL:HG22	3:L:128:CYS:N	2.27	0.49
3:C:207:GLU:HG2	3:C:225:THR:CG2	2.42	0.49
1:D:20:THR:HA	3:F:104:PHE:HB3	1.94	0.49
3:I:208:ILE:HD12	3:I:208:ILE:C	2.32	0.49
3:I:208:ILE:HD13	3:I:220:PRO:CB	2.35	0.49
2:K:45:ARG:NH1	2:K:100:GLN:HE22	2.11	0.49
3:F:160:ARG:NH2	3:F:176:ILE:HD13	2.27	0.49
2:B:116:ALA:O	2:B:119:ILE:HG22	2.13	0.49
2:E:136:VAL:O	2:E:140:GLU:HG3	2.13	0.49
1:D:86:GLU:CD	1:D:86:GLU:H	2.17	0.48
6:E:258:HOH:O	3:F:234:LYS:HE2	2.12	0.48
3:I:54:ASP:O	3:I:58:THR:HG23	2.13	0.48
2:E:116:ALA:O	2:E:119:ILE:HG22	2.13	0.48
2:E:144:SER:OG	2:E:146:GLN:HG3	2.13	0.48
3:C:175:GLN:HE22	3:C:177:ARG:NH1	2.08	0.48
1:G:13:THR:OG1	1:G:17:LYS:HE2	2.14	0.48
1:A:79:ASP:HB3	1:A:84:ASN:O	2.13	0.48
2:H:98:VAL:O	4:H:3006:FRU:H11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:HA	6:A:184:HOH:O	2.14	0.48
2:B:67:ILE:HG12	3:C:237:ARG:O	2.14	0.48
2:B:112:TRP:CZ2	5:C:3401:TLA:H3	2.48	0.48
3:F:99:SER:HB2	3:F:100:PRO:HD3	1.96	0.48
3:C:47:GLU:O	3:C:51:VAL:HG23	2.14	0.47
2:E:112:TRP:CZ2	5:F:4401:TLA:H3	2.49	0.47
1:D:53:TYR:HA	2:E:46:VAL:HG11	1.95	0.47
1:J:94:ILE:N	1:J:94:ILE:HD12	2.29	0.47
2:K:16:VAL:HA	2:K:19:MET:HE2	1.96	0.47
3:F:62:LEU:HB3	3:F:63:PRO:HD3	1.96	0.47
3:F:102:THR:HB	3:F:104:PHE:CE2	2.50	0.47
3:F:239:VAL:HG22	3:F:239:VAL:O	2.14	0.47
2:K:118:ARG:HG3	2:K:122:ASP:OD2	2.15	0.47
1:A:44:ARG:NH1	1:A:44:ARG:HB2	2.30	0.47
3:F:207:GLU:HG2	3:F:225:THR:CG2	2.45	0.47
3:I:118:ASP:OD1	3:I:124:HIS:HD2	1.98	0.47
2:K:148:LEU:HG	3:L:32:MET:HG3	1.97	0.47
6:E:165:HOH:O	2:K:24:HIS:HE1	1.98	0.47
2:E:90:ARG:HH11	2:E:94:GLN:NE2	2.12	0.46
2:K:58:ILE:N	2:K:58:ILE:HD13	2.29	0.46
2:H:112:TRP:CZ2	5:I:5401:TLA:H3	2.50	0.46
3:C:139:LEU:HD11	3:C:211:ARG:HG3	1.96	0.46
1:A:34:LYS:HD3	6:A:1424:HOH:O	2.16	0.46
3:F:235:ALA:HB3	3:F:238:PRO:HB3	1.97	0.46
3:L:24:VAL:HG13	3:L:28:GLU:HB2	1.96	0.46
2:K:116:ALA:O	2:K:119:ILE:HG22	2.16	0.46
3:F:173:GLU:CD	3:F:173:GLU:H	2.19	0.46
3:L:171:PRO:HB2	3:L:174:VAL:HG23	1.98	0.46
1:J:79:ASP:HB3	1:J:84:ASN:O	2.15	0.45
3:L:154:ARG:NH2	3:L:165:GLU:OE2	2.41	0.45
3:F:113:LEU:HD11	3:F:188:ILE:CD1	2.26	0.45
2:H:118:ARG:NH1	4:H:3006:FRU:C6	2.80	0.45
3:C:134:TYR:CE1	3:C:215:ILE:HD11	2.51	0.45
3:I:161:GLN:HE21	3:L:165:GLU:HG3	1.81	0.45
3:L:99:SER:HB2	3:L:100:PRO:HD3	1.99	0.45
1:D:84:ASN:HB3	1:D:86:GLU:OE1	2.17	0.45
3:L:171:PRO:HB3	3:L:173:GLU:OE2	2.17	0.45
3:L:54:ASP:O	3:L:58:THR:HG23	2.16	0.45
2:B:71:ASN:HD21	3:C:53:LYS:NZ	2.15	0.45
1:G:14:HIS:HE1	6:G:161:HOH:O	1.99	0.45
2:K:97:ASP:O	4:K:3005:FRU:H12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:58:ILE:HD12	3:L:150:ASN:ND2	2.32	0.44
3:C:102:THR:HB	3:C:104:PHE:CE2	2.53	0.44
3:C:134:TYR:OH	3:C:139:LEU:CD1	2.66	0.44
3:C:171:PRO:HB2	3:C:174:VAL:HG23	1.98	0.44
3:I:157:ARG:HD3	3:I:158:TRP:CH2	2.52	0.44
1:D:12:ARG:HD2	6:F:4559:HOH:O	2.18	0.44
3:F:67:LEU:C	3:F:67:LEU:HD23	2.38	0.44
3:I:189:VAL:O	3:I:191:PRO:HD3	2.18	0.44
2:H:142:VAL:HG21	3:I:29:ILE:HD11	1.98	0.44
1:A:10:TRP:CZ3	1:J:8:PRO:HG2	2.53	0.44
3:C:221:LYS:HB2	3:C:224:ILE:HD13	2.00	0.44
3:I:23:GLU:HG2	3:I:23:GLU:O	2.17	0.44
1:D:79:ASP:HA	6:D:137:HOH:O	2.17	0.44
2:B:37:HIS:HD2	3:L:26:ASP:OD2	2.01	0.44
2:H:84:VAL:CG1	2:H:119:ILE:HD12	2.48	0.43
2:B:37:HIS:HE1	2:E:8:GLU:OE2	2.00	0.43
3:F:35:ARG:NH2	3:F:35:ARG:HB3	2.33	0.43
2:H:2:SER:OG	2:H:5:ILE:HG12	2.17	0.43
2:K:141:ARG:HG2	2:K:147:GLY:O	2.19	0.43
6:I:5603:HOH:O	3:L:161:GLN:HG2	2.18	0.43
2:B:119:ILE:HD13	2:B:119:ILE:C	2.39	0.43
3:F:115:VAL:CG2	3:F:188:ILE:HD11	2.34	0.43
2:K:80:ALA:HA	2:K:85:TRP:O	2.18	0.43
3:L:67:LEU:HD23	3:L:67:LEU:C	2.39	0.42
3:C:106:THR:OG1	3:C:109:ASP:HB2	2.20	0.42
1:D:13:THR:HB	1:D:17:LYS:HE3	2.00	0.42
3:F:75:PRO:O	3:F:79:LYS:HG3	2.19	0.42
2:H:46:VAL:HG12	2:H:96:CYS:SG	2.60	0.42
3:F:157:ARG:HD3	3:F:158:TRP:CH2	2.54	0.42
3:I:131:CYS:O	3:I:152:ARG:HD2	2.20	0.42
3:I:142:SER:HA	3:I:143:PRO:HD3	1.92	0.42
2:K:46:VAL:CG1	2:K:96:CYS:SG	3.08	0.42
3:F:207:GLU:HG2	3:F:225:THR:HG22	2.01	0.42
2:E:141:ARG:HG2	2:E:147:GLY:O	2.20	0.42
2:E:148:LEU:CD1	2:E:151:TYR:HD2	2.32	0.42
2:H:152:LEU:HD12	2:H:153:PRO:HD2	2.01	0.42
2:E:45:ARG:HH11	2:E:100:GLN:HE22	1.68	0.42
3:L:82:ILE:HD12	3:L:117:ALA:HB2	1.99	0.42
3:F:54:ASP:O	3:F:58:THR:HG23	2.19	0.42
1:A:9:VAL:HG12	1:J:8:PRO:HB3	2.02	0.42
2:E:46:VAL:HG23	2:E:46:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:70:LYS:HG2	3:F:202:GLU:OE1	2.20	0.42
2:K:67:ILE:HA	3:L:239:VAL:HG22	2.02	0.42
2:E:80:ALA:HA	2:E:85:TRP:O	2.20	0.41
1:A:118:ILE:CG2	1:A:122:TYR:HB2	2.51	0.41
3:F:151:TYR:CZ	3:F:155:LEU:HD22	2.56	0.41
1:G:7:LYS:N	1:G:8:PRO:CD	2.83	0.41
1:J:117:GLU:HG3	6:L:6513:HOH:O	2.20	0.41
2:B:48:HIS:HB2	3:C:130:LEU:O	2.20	0.41
2:K:112:TRP:CZ2	5:L:6401:TLA:H2	2.55	0.41
2:B:80:ALA:HA	2:B:85:TRP:O	2.20	0.41
3:C:207:GLU:HG2	3:C:225:THR:HG22	2.02	0.41
2:E:45:ARG:NH1	2:E:100:GLN:HE22	2.18	0.41
1:G:114:LEU:HD23	1:G:114:LEU:C	2.40	0.41
1:G:20:THR:HA	3:I:104:PHE:HB3	2.02	0.41
2:H:48:HIS:HB2	3:I:130:LEU:O	2.21	0.41
4:B:3002:FRU:H12	6:B:3054:HOH:O	2.20	0.41
3:F:160:ARG:CZ	3:F:176:ILE:HD13	2.51	0.41
3:I:99:SER:HB2	3:I:100:PRO:HD3	2.03	0.41
3:C:208:ILE:HD12	3:C:208:ILE:C	2.41	0.41
2:E:29:ALA:N	2:E:30:PRO:HD3	2.36	0.41
3:F:171:PRO:HB2	3:F:174:VAL:HG23	2.02	0.41
3:F:201:THR:HG23	3:F:204:GLN:HE21	1.81	0.41
1:G:44:ARG:NH1	1:G:44:ARG:HB2	2.35	0.41
2:H:2:SER:O	2:H:6:ARG:HG2	2.21	0.41
3:L:157:ARG:HD3	3:L:158:TRP:CH2	2.55	0.41
1:A:84:ASN:HD22	1:J:7:LYS:NZ	2.19	0.41
3:C:62:LEU:HB2	3:C:63:PRO:HD3	2.02	0.41
3:C:67:LEU:C	3:C:67:LEU:HD23	2.41	0.41
2:H:80:ALA:HA	2:H:85:TRP:O	2.21	0.41
3:I:161:GLN:HG2	6:L:6744:HOH:O	2.21	0.41
3:L:78:LYS:O	3:L:82:ILE:HG12	2.21	0.40
2:E:65:GLU:OE2	2:E:70:LEU:CD2	2.69	0.40
2:E:48:HIS:HB2	3:F:130:LEU:O	2.21	0.40
3:I:67:LEU:HD23	3:I:67:LEU:C	2.41	0.40
1:G:86:GLU:CD	1:G:86:GLU:H	2.23	0.40
3:I:62:LEU:HB2	3:I:63:PRO:HD3	2.02	0.40
3:C:127:VAL:CG2	3:C:128:CYS:N	2.84	0.40
3:I:157:ARG:NH1	4:K:3003:FRU:O1	2.37	0.40
3:L:160:ARG:NE	3:L:176:ILE:HD12	2.36	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	116/126 (92%)	109 (94%)	7 (6%)	0	100	100
1	D	117/126 (93%)	111 (95%)	6 (5%)	0	100	100
1	G	118/126 (94%)	115 (98%)	3 (2%)	0	100	100
1	J	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
2	B	150/157 (96%)	147 (98%)	3 (2%)	0	100	100
2	E	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
2	H	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
2	K	150/157 (96%)	146 (97%)	4 (3%)	0	100	100
3	C	215/243 (88%)	206 (96%)	8 (4%)	1 (0%)	29	19
3	F	214/243 (88%)	205 (96%)	7 (3%)	2 (1%)	17	8
3	I	215/243 (88%)	206 (96%)	8 (4%)	1 (0%)	29	19
3	L	214/243 (88%)	205 (96%)	8 (4%)	1 (0%)	29	19
All	All	1930/2104 (92%)	1859 (96%)	66 (3%)	5 (0%)	41	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	131	CYS
3	F	131	CYS
3	I	131	CYS
3	L	131	CYS
3	F	238	PRO

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/108 (93%)	98 (98%)	2 (2%)	55	51
1	D	101/108 (94%)	101 (100%)	0	100	100
1	G	102/108 (94%)	102 (100%)	0	100	100
1	J	102/108 (94%)	102 (100%)	0	100	100
2	B	130/134 (97%)	127 (98%)	3 (2%)	50	45
2	E	129/134 (96%)	126 (98%)	3 (2%)	50	45
2	H	133/134 (99%)	129 (97%)	4 (3%)	41	35
2	K	130/134 (97%)	127 (98%)	3 (2%)	50	45
3	C	190/214 (89%)	190 (100%)	0	100	100
3	F	189/214 (88%)	186 (98%)	3 (2%)	62	59
3	I	190/214 (89%)	189 (100%)	1 (0%)	88	89
3	L	189/214 (88%)	188 (100%)	1 (0%)	88	89
All	All	1685/1824 (92%)	1665 (99%)	20 (1%)	71	69

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	125	LYS
2	B	48	HIS
2	B	85	TRP
2	B	119	ILE
2	E	48	HIS
2	E	58	ILE
2	E	85	TRP
3	F	35	ARG
3	F	37	LEU
3	F	188	ILE
2	H	39	LEU
2	H	48	HIS
2	H	85	TRP
2	H	119	ILE
3	I	181	SER
2	K	48	HIS
2	K	58	ILE
2	K	85	TRP

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Mol	Chain	Res	Type
3	L	170	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	84	ASN
1	A	111	ASN
2	B	37	HIS
2	B	71	ASN
2	B	100	GLN
3	C	175	GLN
3	C	236	ASN
2	E	61	HIS
2	E	94	GLN
2	E	100	GLN
2	E	146	GLN
3	F	49	HIS
3	F	175	GLN
3	F	204	GLN
1	G	14	HIS
1	G	84	ASN
2	H	61	HIS
2	H	100	GLN
3	I	112	ASN
3	I	124	HIS
3	I	169	GLN
3	I	175	GLN
1	J	84	ASN
1	J	87	ASN
2	K	12	HIS
2	K	24	HIS
2	K	100	GLN
3	L	112	ASN
3	L	175	GLN

### 5.3.3 RNA ⓘ

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](#)

16 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$
5	TLA	L	6501	-	3,9,9	0.99	0	6,12,12	1.10	1 (16%)
4	FRU	B	3008	-	11,12,12	2.41	4 (36%)	10,18,18	5.70	3 (30%)
5	TLA	C	3501	-	3,9,9	0.87	0	6,12,12	1.10	1 (16%)
4	FRU	K	3005	-	11,12,12	1.67	2 (18%)	10,18,18	1.97	3 (30%)
4	FRU	H	3007	-	11,12,12	1.77	2 (18%)	10,18,18	1.82	3 (30%)
4	FRU	C	3001	-	11,12,12	1.67	2 (18%)	10,18,18	1.88	2 (20%)
5	TLA	L	6401	-	3,9,9	0.98	0	6,12,12	1.02	1 (16%)
4	FRU	K	3003	-	11,12,12	1.48	2 (18%)	10,18,18	1.91	2 (20%)
5	TLA	F	4401	-	3,9,9	0.87	0	6,12,12	1.06	1 (16%)
5	TLA	I	5401	-	3,9,9	1.06	0	6,12,12	1.01	0
5	TLA	C	3401	-	3,9,9	0.91	0	6,12,12	1.05	1 (16%)
5	TLA	F	4501	-	3,9,9	0.76	0	6,12,12	1.16	1 (16%)
4	FRU	B	3002	-	11,12,12	1.41	2 (18%)	10,18,18	1.80	2 (20%)
5	TLA	I	5501	-	3,9,9	0.88	0	6,12,12	1.09	1 (16%)
4	FRU	H	3004	-	11,12,12	1.49	2 (18%)	10,18,18	1.84	2 (20%)
4	FRU	H	3006	-	11,12,12	1.39	1 (9%)	10,18,18	2.08	2 (20%)

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
5	TLA	L	6501	-	-	0/4/12/12	-
4	FRU	B	3008	-	-	3/5/24/24	0/1/1/1
5	TLA	C	3501	-	-	0/4/12/12	-
4	FRU	K	3005	-	-	2/5/24/24	0/1/1/1
4	FRU	H	3007	-	-	0/5/24/24	0/1/1/1
4	FRU	C	3001	-	-	0/5/24/24	0/1/1/1
5	TLA	L	6401	-	-	0/4/12/12	-
4	FRU	K	3003	-	-	2/5/24/24	0/1/1/1
5	TLA	F	4401	-	-	0/4/12/12	-
5	TLA	I	5401	-	-	0/4/12/12	-
5	TLA	C	3401	-	-	0/4/12/12	-
5	TLA	F	4501	-	-	0/4/12/12	-
4	FRU	B	3002	-	-	2/5/24/24	0/1/1/1
5	TLA	I	5501	-	-	0/4/12/12	-
4	FRU	H	3004	-	-	2/5/24/24	0/1/1/1
4	FRU	H	3006	-	-	0/5/24/24	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3008	FRU	C1-C2	5.29	1.60	1.52
4	H	3007	FRU	C1-C2	4.61	1.59	1.52
4	C	3001	FRU	C1-C2	4.45	1.59	1.52
4	K	3005	FRU	C1-C2	4.41	1.59	1.52
4	H	3004	FRU	C1-C2	3.72	1.58	1.52
4	K	3003	FRU	C1-C2	3.64	1.58	1.52
4	H	3006	FRU	C1-C2	3.59	1.58	1.52
4	B	3008	FRU	C4-C5	-3.52	1.44	1.53
4	B	3002	FRU	C1-C2	3.44	1.57	1.52
4	B	3008	FRU	O5-C2	3.43	1.48	1.43
4	H	3007	FRU	O5-C5	3.11	1.50	1.43
4	K	3005	FRU	O5-C5	2.59	1.49	1.43
4	B	3002	FRU	O5-C5	2.58	1.49	1.43
4	B	3008	FRU	O5-C5	2.54	1.49	1.43
4	H	3004	FRU	O5-C5	2.52	1.49	1.43
4	C	3001	FRU	O5-C5	2.48	1.49	1.43
4	K	3003	FRU	O5-C5	2.45	1.49	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3008	FRU	O2-C2-O5	-17.18	76.33	109.50
4	H	3006	FRU	O2-C2-O5	5.51	120.14	109.50
4	K	3005	FRU	O2-C2-O5	4.66	118.50	109.50
4	K	3003	FRU	O2-C2-O5	4.56	118.31	109.50
4	C	3001	FRU	O2-C2-O5	4.37	117.95	109.50
4	B	3002	FRU	O2-C2-O5	4.29	117.79	109.50
4	H	3004	FRU	O2-C2-O5	4.22	117.66	109.50
4	H	3007	FRU	O2-C2-O5	4.07	117.36	109.50
4	B	3008	FRU	O5-C5-C6	3.07	117.39	108.85
4	B	3008	FRU	O3-C3-C4	-2.87	103.42	113.32
4	H	3007	FRU	C6-C5-C4	-2.56	108.91	115.09
4	K	3003	FRU	C6-C5-C4	-2.51	109.02	115.09
4	C	3001	FRU	C6-C5-C4	-2.41	109.29	115.09
4	B	3002	FRU	C6-C5-C4	-2.33	109.46	115.09
4	H	3004	FRU	C6-C5-C4	-2.32	109.49	115.09
4	K	3005	FRU	C6-C5-C4	-2.31	109.51	115.09
5	F	4501	TLA	C4-C3-C2	-2.31	108.14	113.11
4	H	3006	FRU	C6-C5-C4	-2.21	109.76	115.09
5	C	3501	TLA	C4-C3-C2	-2.15	108.48	113.11
5	L	6501	TLA	C4-C3-C2	-2.10	108.60	113.11
4	K	3005	FRU	O5-C5-C6	2.09	114.67	108.85
5	L	6401	TLA	C4-C3-C2	-2.08	108.63	113.11
5	I	5501	TLA	C4-C3-C2	-2.05	108.69	113.11
4	H	3007	FRU	O5-C5-C6	2.04	114.52	108.85
5	F	4401	TLA	C4-C3-C2	-2.03	108.74	113.11
5	C	3401	TLA	C4-C3-C2	-2.00	108.79	113.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3008	FRU	O1-C1-C2-O5
4	K	3003	FRU	O5-C5-C6-O6
4	H	3004	FRU	O5-C5-C6-O6
4	H	3004	FRU	C4-C5-C6-O6
4	B	3008	FRU	O5-C5-C6-O6
4	K	3003	FRU	C4-C5-C6-O6
4	B	3002	FRU	C4-C5-C6-O6
4	B	3008	FRU	C4-C5-C6-O6
4	K	3005	FRU	O5-C5-C6-O6
4	B	3002	FRU	O5-C5-C6-O6
4	K	3005	FRU	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3008	FRU	1	0
4	K	3005	FRU	2	0
4	H	3007	FRU	1	0
4	C	3001	FRU	1	0
5	L	6401	TLA	1	0
4	K	3003	FRU	2	0
5	F	4401	TLA	1	0
5	I	5401	TLA	1	0
5	C	3401	TLA	1	0
4	B	3002	FRU	1	0
4	H	3004	FRU	1	0
4	H	3006	FRU	4	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	118/126 (93%)	-0.21	3 (2%) 57 60	8, 14, 28, 34	0
1	D	119/126 (94%)	-0.24	2 (1%) 70 71	8, 13, 29, 36	0
1	G	120/126 (95%)	-0.19	3 (2%) 57 60	9, 15, 29, 43	0
1	J	120/126 (95%)	-0.34	2 (1%) 70 71	7, 12, 29, 38	0
2	B	152/157 (96%)	-0.48	1 (0%) 87 88	7, 11, 24, 33	0
2	E	151/157 (96%)	-0.38	6 (3%) 38 40	6, 12, 31, 41	0
2	H	156/157 (99%)	-0.38	4 (2%) 56 59	7, 11, 23, 60	0
2	K	152/157 (96%)	-0.37	7 (4%) 32 33	5, 11, 29, 37	0
3	C	217/243 (89%)	-0.26	3 (1%) 75 76	7, 14, 25, 46	0
3	F	216/243 (88%)	-0.03	5 (2%) 60 63	7, 16, 30, 43	0
3	I	217/243 (89%)	-0.36	3 (1%) 75 76	8, 12, 21, 42	0
3	L	216/243 (88%)	-0.29	4 (1%) 66 68	7, 11, 23, 34	0
All	All	1954/2104 (92%)	-0.29	43 (2%) 62 64	5, 13, 27, 60	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	239	VAL	8.9
2	H	157	LYS	8.3
2	H	156	ALA	6.6
2	H	2	SER	5.2
2	H	3	SER	4.8
3	C	239	VAL	4.0
2	K	3	SER	3.7
3	I	23	GLU	3.6
1	A	126	ALA	3.6
3	C	23	GLU	3.4
3	L	239	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	9	VAL	2.8
1	J	126	ALA	2.8
2	E	146	GLN	2.8
3	F	198	ASP	2.7
1	D	126	ALA	2.7
2	K	144	SER	2.6
2	K	153	PRO	2.6
2	K	154	PRO	2.6
1	A	125	LYS	2.5
3	F	195	GLU	2.5
2	E	144	SER	2.4
2	K	146	GLN	2.4
2	K	145	GLY	2.4
1	J	34	LYS	2.3
1	G	126	ALA	2.3
1	G	7	LYS	2.3
3	I	239	VAL	2.2
2	E	143	ALA	2.2
3	L	198	ASP	2.2
2	K	152	LEU	2.2
3	F	199	GLY	2.2
2	E	153	PRO	2.1
1	G	125	LYS	2.1
3	I	229	LYS	2.1
2	E	152	LEU	2.1
2	E	154	PRO	2.1
3	C	57	HIS	2.1
1	D	34	LYS	2.1
3	F	200	TRP	2.1
2	B	3	SER	2.0
3	L	127	VAL	2.0
3	L	195	GLU	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, 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( $\text{\AA}^2$ )	Q<0.9
4	FRU	H	3007	12/12	0.60	0.38	35,38,40,40	0
4	FRU	K	3003	12/12	0.62	0.34	43,45,49,50	0
4	FRU	H	3006	12/12	0.64	0.40	39,45,48,49	0
4	FRU	B	3008	12/12	0.66	0.34	32,37,40,41	0
4	FRU	K	3005	12/12	0.70	0.30	29,34,36,39	0
4	FRU	B	3002	12/12	0.72	0.32	29,37,40,40	0
4	FRU	H	3004	12/12	0.73	0.30	29,37,41,42	0
4	FRU	C	3001	12/12	0.79	0.26	32,36,37,41	0
5	TLA	I	5501	10/10	0.93	0.23	20,24,28,30	0
5	TLA	C	3501	10/10	0.94	0.19	16,22,29,29	0
5	TLA	F	4501	10/10	0.94	0.17	18,23,27,29	0
5	TLA	L	6501	10/10	0.95	0.16	15,21,26,28	0
5	TLA	C	3401	10/10	0.97	0.10	14,17,19,22	0
5	TLA	I	5401	10/10	0.97	0.11	13,16,19,21	0
5	TLA	F	4401	10/10	0.98	0.10	13,16,18,20	0
5	TLA	L	6401	10/10	0.98	0.11	13,15,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.