



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:27 PM BST

PDB ID : 3VYG  
Title : Crystal structure of Thiocyanate hydrolase mutant R136W  
Authors : Yamanaka, Y.; Sato, M.; Arakawa, T.; Namima, S.; Hori, S.; Ohtaki, A.;  
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Deposited on : 2012-09-25  
Resolution : 1.72 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  
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

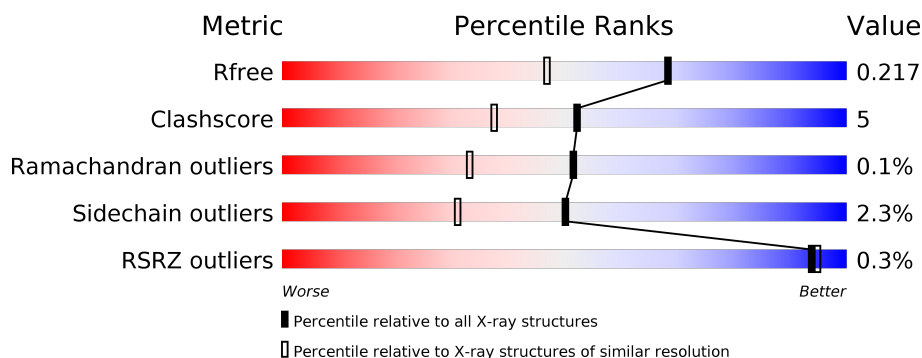
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 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>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	D	126	<div> <div>80%</div> <div>12%</div> <div>• 6%</div> </div>
1	G	126	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	J	126	<div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
2	B	157	<div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
2	E	157	<div> <div>76%</div> <div>18%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	157	<div><div></div><div>81%15%<div><div></div><div></div><div></div></div></div></div>
2	K	157	<div>%<div><div></div><div>77%18%<div><div></div><div></div><div></div></div></div></div></div>
3	C	243	<div><div></div><div>77%11%<div><div></div><div></div><div></div></div></div></div>
3	F	243	<div><div></div><div>79%10%11%</div></div>
3	I	243	<div><div></div><div>74%13%<div><div></div><div></div><div></div></div></div></div>
3	L	243	<div><div></div><div>74%12%<div><div></div><div></div><div></div></div></div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17343 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	15	0	0
			974	620	162	188	4			
1	D	119	Total	C	N	O	S	10	1	0
			973	620	161	188	4			
1	G	120	Total	C	N	O	S	16	1	0
			982	626	163	189	4			
1	J	120	Total	C	N	O	S	8	1	0
			981	625	163	189	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	2	0
			1244	787	224	227	6			
2	E	151	Total	C	N	O	S	0	3	0
			1248	790	226	226	6			
2	H	151	Total	C	N	O	S	0	0	0
			1226	775	221	224	6			
2	K	151	Total	C	N	O	S	0	0	0
			1224	773	221	224	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	10	2	0
			1743	1114	306	315	8			
3	F	217	Total	C	N	O	S	0	2	0
			1744	1113	306	317	8			
3	I	217	Total	C	N	O	S	7	0	0
			1727	1103	302	314	8			
3	L	217	Total	C	N	O	S	17	1	0
			1733	1107	303	315	8			

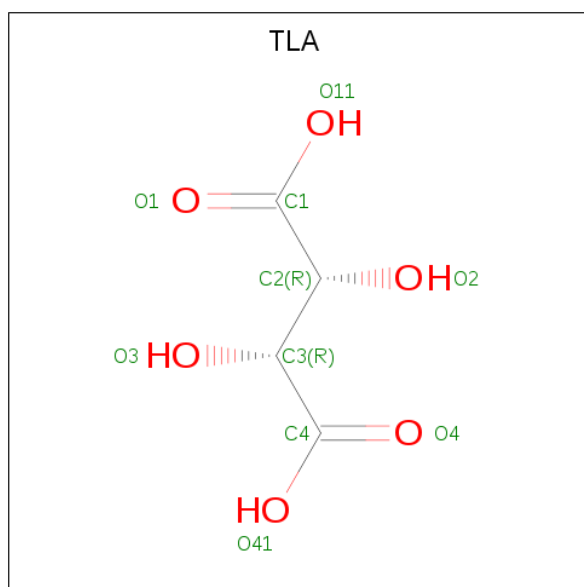
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	136	TRP	ARG	ENGINEERED MUTATION	UNP O66188
F	136	TRP	ARG	ENGINEERED MUTATION	UNP O66188
I	136	TRP	ARG	ENGINEERED MUTATION	UNP O66188
L	136	TRP	ARG	ENGINEERED MUTATION	UNP O66188

- Molecule 4 is COBALT (III) ION (three-letter code: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total Co 1 1	0	0
4	L	1	Total Co 1 1	0	0
4	C	1	Total Co 1 1	0	0
4	F	1	Total Co 1 1	0	0

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



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

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

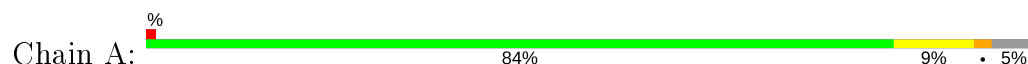
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	129	Total	O	0	0
			129	129		
6	C	214	Total	O	0	0
			214	214		
6	D	78	Total	O	0	0
			78	78		
6	E	128	Total	O	0	0
			128	128		
6	F	189	Total	O	0	0
			189	189		
6	G	84	Total	O	0	0
			84	84		
6	H	107	Total	O	0	0
			107	107		
6	I	148	Total	O	0	0
			148	148		
6	J	90	Total	O	0	0
			90	90		
6	K	109	Total	O	0	0
			109	109		
6	L	153	Total	O	0	0
			153	153		

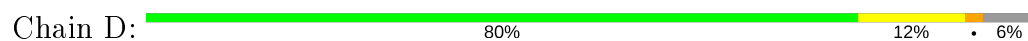
### 3 Residue-property plots [i](#)

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.

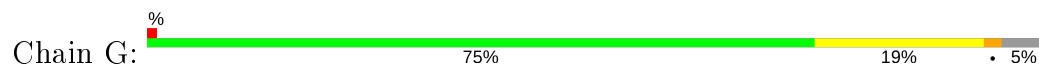
- Molecule 1: Thiocyanate hydrolase subunit alpha



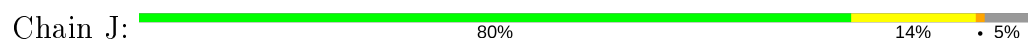
- Molecule 1: Thiocyanate hydrolase subunit alpha



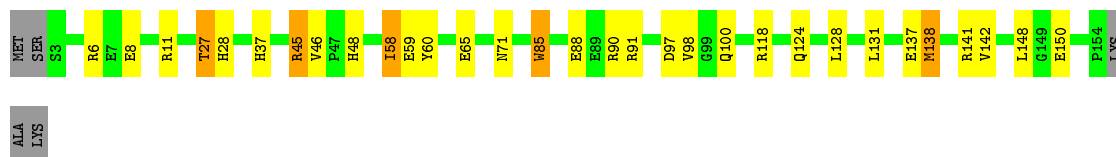
- Molecule 1: Thiocyanate hydrolase subunit alpha



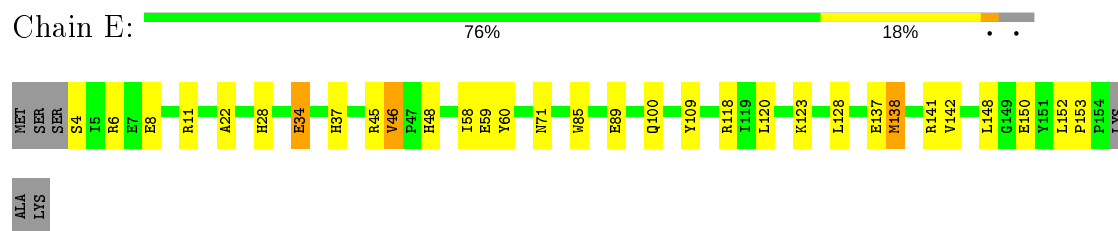
- Molecule 1: Thiocyanate hydrolase subunit alpha



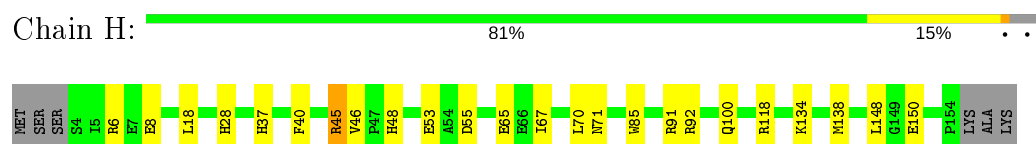
- Molecule 2: Thiocyanate hydrolase subunit beta



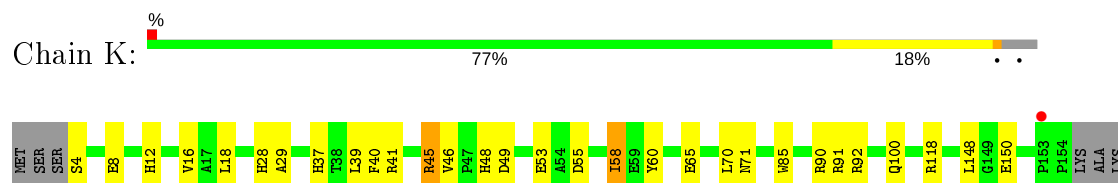
- Molecule 2: Thiocyanate hydrolase subunit beta



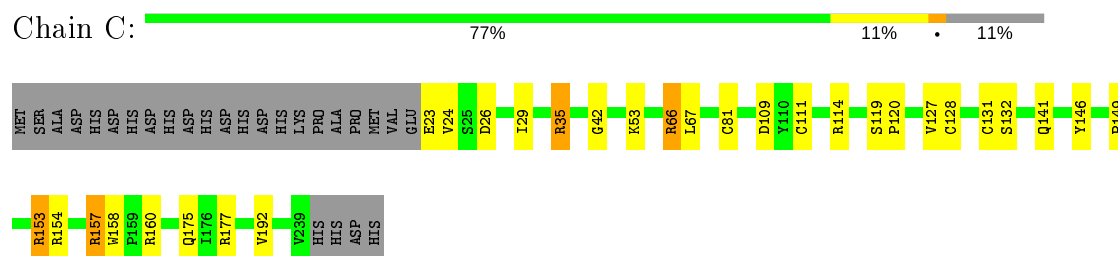
- Molecule 2: Thiocyanate hydrolase subunit beta



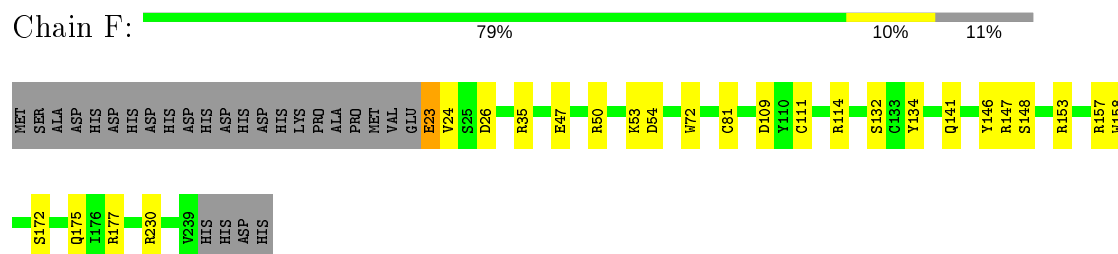
- Molecule 2: Thiocyanate hydrolase subunit beta



- Molecule 3: Thiocyanate hydrolase subunit gamma



- Molecule 3: Thiocyanate hydrolase subunit gamma



- Molecule 3: Thiocyanate hydrolase subunit gamma







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.45Å 172.40Å 172.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.96 – 1.72 33.96 – 1.72	Depositor EDS
% Data completeness (in resolution range)	96.5 (33.96-1.72) 96.2 (33.96-1.72)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.52 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.187 , 0.218 0.188 , 0.217	Depositor DCC
$R_{free}$ test set	17284 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.447 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: CSO, CSD, 3CO, TLA

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	1.46	4/1000 (0.4%)	1.15	3/1354 (0.2%)
1	D	1.48	5/999 (0.5%)	1.17	5/1353 (0.4%)
1	G	1.52	7/1008 (0.7%)	1.36	13/1365 (1.0%)
1	J	1.51	7/1007 (0.7%)	1.32	7/1364 (0.5%)
2	B	1.41	8/1279 (0.6%)	1.35	14/1741 (0.8%)
2	E	1.40	6/1283 (0.5%)	1.27	7/1746 (0.4%)
2	H	1.36	2/1258 (0.2%)	1.27	7/1712 (0.4%)
2	K	1.39	5/1256 (0.4%)	1.22	13/1709 (0.8%)
3	C	1.48	5/1776 (0.3%)	1.30	12/2425 (0.5%)
3	F	1.49	6/1777 (0.3%)	1.26	9/2426 (0.4%)
3	I	1.40	7/1757 (0.4%)	1.26	13/2400 (0.5%)
3	L	1.50	12/1766 (0.7%)	1.22	13/2412 (0.5%)
All	All	1.45	74/16166 (0.5%)	1.26	116/22007 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	50	ARG	CD-NE	-12.79	1.24	1.46
3	L	79	LYS	CD-CE	-10.39	1.25	1.51
1	D	34	LYS	CB-CG	8.68	1.75	1.52
3	F	81	CYS	CB-SG	-8.04	1.68	1.82
3	C	81	CYS	CB-SG	-7.89	1.68	1.82
2	B	59	GLU	CD-OE2	7.81	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	89	GLU	CG-CD	7.60	1.63	1.51
1	J	32	ALA	CA-CB	7.35	1.67	1.52
1	G	89	GLU	CG-CD	7.29	1.62	1.51
2	E	59	GLU	CD-OE2	7.19	1.33	1.25
3	L	158	TRP	CE3-CZ3	6.91	1.50	1.38
2	B	85	TRP	CB-CG	6.79	1.62	1.50
1	G	125	LYS	CB-CG	-6.78	1.34	1.52
3	L	187	TYR	CD1-CE1	6.75	1.49	1.39
1	D	104	GLU	CG-CD	6.56	1.61	1.51
3	C	146	TYR	CE1-CZ	6.45	1.47	1.38
2	K	16	VAL	CA-CB	6.36	1.68	1.54
3	I	158	TRP	CE3-CZ3	6.33	1.49	1.38
3	I	173	GLU	CD-OE1	6.28	1.32	1.25
1	A	125	LYS	CB-CG	-6.18	1.35	1.52
3	L	134	TYR	CE1-CZ	6.12	1.46	1.38
3	F	148	SER	CA-CB	6.11	1.62	1.52
2	E	34	GLU	CG-CD	6.10	1.61	1.51
1	G	120	GLU	CG-CD	6.03	1.60	1.51
1	D	17	LYS	CD-CE	-6.02	1.36	1.51
2	K	92	ARG	CZ-NH1	5.99	1.40	1.33
3	F	132	SER	CB-OG	5.88	1.49	1.42
1	A	93	SER	CB-OG	5.84	1.49	1.42
3	C	23	GLU	CB-CG	-5.83	1.41	1.52
2	E	150	GLU	CD-OE2	5.78	1.32	1.25
3	F	230	ARG	CG-CD	5.73	1.66	1.51
1	J	59	TYR	CD2-CE2	5.72	1.48	1.39
1	G	102	TRP	CD2-CE2	5.71	1.48	1.41
2	H	92	ARG	CZ-NH1	5.68	1.40	1.33
3	L	127	VAL	CA-CB	5.64	1.66	1.54
3	I	162	VAL	CB-CG2	5.62	1.64	1.52
3	L	109	ASP	CG-OD2	5.60	1.38	1.25
2	B	98	VAL	CB-CG1	5.58	1.64	1.52
3	C	192	VAL	CB-CG2	-5.58	1.41	1.52
2	E	109	TYR	CG-CD2	5.56	1.46	1.39
3	I	230	ARG	CG-CD	5.54	1.65	1.51
1	A	34	LYS	CB-CG	5.51	1.67	1.52
3	C	149	PRO	N-CA	-5.49	1.38	1.47
2	K	150	GLU	CG-CD	5.48	1.60	1.51
2	K	40	PHE	CE1-CZ	5.48	1.47	1.37
1	G	92	TYR	CD2-CE2	5.47	1.47	1.39
3	L	109	ASP	CB-CG	5.47	1.63	1.51
3	I	27	PHE	CE2-CZ	5.46	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	109	PHE	CE1-CZ	5.45	1.47	1.37
1	J	7	LYS	CB-CG	-5.43	1.37	1.52
2	B	150	GLU	CD-OE1	5.42	1.31	1.25
3	I	44	PHE	CE1-CZ	5.40	1.47	1.37
2	E	150	GLU	CD-OE1	5.40	1.31	1.25
1	J	86	GLU	CG-CD	5.40	1.60	1.51
1	D	93	SER	CB-OG	5.39	1.49	1.42
2	H	40	PHE	CE1-CZ	5.37	1.47	1.37
1	J	55	ARG	CZ-NH1	5.36	1.40	1.33
1	D	9	VAL	CA-CB	5.35	1.66	1.54
3	L	76	GLU	CG-CD	5.35	1.59	1.51
1	G	59	TYR	CE1-CZ	-5.33	1.31	1.38
2	B	46	VAL	CB-CG2	-5.32	1.41	1.52
3	F	146	TYR	CE1-CZ	5.29	1.45	1.38
3	L	114	ARG	CZ-NH1	5.27	1.40	1.33
2	K	29	ALA	CA-CB	5.22	1.63	1.52
2	E	89	GLU	CG-CD	5.20	1.59	1.51
2	B	150	GLU	CD-OE2	5.19	1.31	1.25
3	I	160	ARG	CG-CD	-5.19	1.39	1.51
2	B	65	GLU	CD-OE2	5.18	1.31	1.25
3	F	72	TRP	CE3-CZ3	5.13	1.47	1.38
3	L	156	VAL	CB-CG2	5.12	1.63	1.52
1	A	102	TRP	CG-CD1	-5.07	1.29	1.36
3	L	27	PHE	CE2-CZ	5.07	1.47	1.37
1	G	59	TYR	CD1-CE1	5.04	1.47	1.39
2	B	88	GLU	CG-CD	5.01	1.59	1.51

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	138	MET	CG-SD-CE	-13.02	79.36	100.20
2	H	91	ARG	NE-CZ-NH2	-11.13	114.73	120.30
3	I	109	ASP	CB-CG-OD2	10.79	128.01	118.30
3	L	109	ASP	CB-CG-OD2	10.70	127.93	118.30
2	E	138	MET	CG-SD-CE	-10.55	83.32	100.20
3	I	186	ARG	NE-CZ-NH1	10.17	125.39	120.30
2	B	11	ARG	NE-CZ-NH1	9.59	125.09	120.30
2	H	45	ARG	NE-CZ-NH2	-9.53	115.53	120.30
3	I	109	ASP	CB-CG-OD1	-9.36	109.88	118.30
2	H	118	ARG	NE-CZ-NH2	-9.34	115.63	120.30
3	L	50	ARG	CG-CD-NE	8.52	129.69	111.80
2	B	91	ARG	NE-CZ-NH2	-8.45	116.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	6	ARG	NE-CZ-NH2	-8.45	116.08	120.30
2	B	118	ARG	NE-CZ-NH2	-8.32	116.14	120.30
3	C	153	ARG	NE-CZ-NH2	-8.15	116.22	120.30
2	K	45	ARG	NE-CZ-NH2	-8.14	116.23	120.30
3	I	74	ASP	CB-CG-OD1	8.00	125.50	118.30
1	D	12	ARG	NE-CZ-NH2	7.99	124.29	120.30
1	J	73	GLU	OE1-CD-OE2	7.87	132.75	123.30
1	D	12	ARG	NE-CZ-NH1	-7.71	116.44	120.30
3	L	79	LYS	CG-CD-CE	7.60	134.70	111.90
1	G	11	ASP	CB-CG-OD2	-7.55	111.50	118.30
3	I	230	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	G	73	GLU	OE1-CD-OE2	7.35	132.12	123.30
2	B	46	VAL	CG1-CB-CG2	-7.32	99.18	110.90
2	H	55	ASP	CB-CG-OD1	7.28	124.86	118.30
3	C	66[A]	ARG	NE-CZ-NH2	-7.27	116.66	120.30
3	C	66[B]	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	A	69	ARG	NE-CZ-NH2	-7.25	116.67	120.30
2	K	91	ARG	NE-CZ-NH2	-7.21	116.70	120.30
3	C	23	GLU	CB-CG-CD	-7.18	94.81	114.20
2	B	11	ARG	NE-CZ-NH2	-7.17	116.71	120.30
3	L	186	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	J	55	ARG	NE-CZ-NH2	-7.11	116.75	120.30
3	I	186	ARG	NE-CZ-NH2	-6.87	116.86	120.30
3	C	160	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	G	29	LYS	CD-CE-NZ	-6.84	95.98	111.70
3	F	114	ARG	NE-CZ-NH1	6.78	123.69	120.30
3	I	152	ARG	NE-CZ-NH2	-6.67	116.97	120.30
2	H	45	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	K	118	ARG	NE-CZ-NH2	-6.66	116.97	120.30
3	I	66	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	D	79	ASP	CB-CG-OD1	6.62	124.26	118.30
3	C	109	ASP	CB-CG-OD1	-6.62	112.35	118.30
3	L	198	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	79	ASP	CB-CG-OD1	6.56	124.20	118.30
3	L	160	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	G	121	ARG	NE-CZ-NH2	-6.55	117.03	120.30
2	E	118	ARG	NE-CZ-NH2	-6.54	117.03	120.30
3	F	114	ARG	NE-CZ-NH2	-6.54	117.03	120.30
3	C	157	ARG	NE-CZ-NH2	-6.52	117.04	120.30
3	L	170	LEU	CB-CG-CD1	6.46	121.99	111.00
1	G	11	ASP	CB-CG-OD1	6.43	124.09	118.30
3	I	74	ASP	CB-CG-OD2	-6.42	112.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	41	ARG	NE-CZ-NH2	-6.39	117.10	120.30
2	B	45	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	C	35	ARG	NE-CZ-NH1	-6.37	117.11	120.30
3	C	109	ASP	CB-CG-OD2	6.34	124.00	118.30
3	F	146	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	E	6	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	B	118	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	E	120	LEU	CB-CG-CD2	6.25	121.63	111.00
3	I	237	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	G	55	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	D	125	LYS	CA-CB-CG	6.13	126.89	113.40
3	L	153	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	J	42	ARG	NE-CZ-NH1	-6.11	117.24	120.30
2	K	90	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	34	LYS	CA-CB-CG	-6.09	100.01	113.40
3	F	109	ASP	CB-CG-OD2	6.05	123.75	118.30
2	B	6	ARG	NE-CZ-NH1	-6.04	117.28	120.30
3	L	74	ASP	CB-CG-OD1	5.96	123.66	118.30
2	K	45	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	K	55	ASP	CB-CG-OD1	5.94	123.65	118.30
1	G	46	LYS	CD-CE-NZ	-5.89	98.16	111.70
2	E	46	VAL	CG1-CB-CG2	-5.82	101.59	110.90
3	F	54	ASP	CB-CG-OD1	5.73	123.46	118.30
3	L	109	ASP	CB-CG-OD1	-5.73	113.14	118.30
3	F	35	ARG	NE-CZ-NH1	-5.71	117.44	120.30
2	K	18	LEU	CB-CG-CD1	-5.70	101.30	111.00
2	K	118	ARG	CG-CD-NE	-5.69	99.86	111.80
3	F	146	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
1	G	116	THR	CA-CB-CG2	-5.59	104.58	112.40
3	C	154	ARG	NE-CZ-NH2	5.55	123.07	120.30
3	C	114	ARG	NE-CZ-NH2	-5.53	117.53	120.30
3	I	170	LEU	CA-CB-CG	-5.50	102.66	115.30
3	C	160	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	72	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	G	51	LEU	CB-CG-CD2	-5.44	101.76	111.00
2	K	49	ASP	CB-CG-OD1	5.42	123.18	118.30
3	L	230	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	L	152	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	105	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
2	K	90	ARG	NE-CZ-NH1	5.35	122.97	120.30
3	I	170	LEU	CB-CG-CD1	5.33	120.06	111.00
2	H	18	LEU	CB-CG-CD1	-5.24	102.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	F	134	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	B	131	LEU	CB-CG-CD2	-5.23	102.11	111.00
2	B	27	THR	OG1-CB-CG2	-5.21	98.01	110.00
1	G	12	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	J	78	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	G	107	ASP	CB-CG-OD2	-5.17	113.65	118.30
2	K	39	LEU	CB-CG-CD1	-5.17	102.21	111.00
3	I	86	VAL	CG1-CB-CG2	-5.15	102.66	110.90
2	B	90	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	J	46	LYS	CD-CE-NZ	-5.12	99.92	111.70
2	B	128	LEU	CB-CG-CD2	-5.12	102.29	111.00
3	F	147	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	J	12	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	17	LYS	CG-CD-CE	5.08	127.12	111.90
1	J	11	ASP	CB-CG-OD1	5.05	122.85	118.30
2	E	118	ARG	CG-CD-NE	-5.05	101.20	111.80
3	L	238	PRO	N-CA-C	5.04	125.20	112.10
2	K	45	ARG	CB-CG-CD	5.01	124.63	111.60
2	B	97	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	4	SER	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	974	0	926	17	0
1	D	973	0	924	17	0
1	G	982	0	936	14	0
1	J	981	0	934	10	0
2	B	1244	0	1211	22	0
2	E	1248	0	1222	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1226	0	1193	19	0
2	K	1224	0	1186	24	0
3	C	1743	0	1755	16	0
3	F	1744	0	1750	11	0
3	I	1727	0	1732	30	0
3	L	1733	0	1740	16	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
5	C	10	0	4	0	0
5	F	10	0	4	0	0
5	I	10	0	4	0	0
5	L	10	0	4	0	0
6	A	71	0	0	1	0
6	B	129	0	0	0	0
6	C	214	0	0	3	0
6	D	78	0	0	0	0
6	E	128	0	0	2	0
6	F	189	0	0	0	0
6	G	84	0	0	1	0
6	H	107	0	0	3	0
6	I	148	0	0	4	0
6	J	90	0	0	0	0
6	K	109	0	0	5	0
6	L	153	0	0	2	0
All	All	17343	0	15525	170	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 5.

All (170) 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:I:47:GLU:HG2	3:I:50:ARG:NH2	1.40	1.32
2:K:65:GLU:OE1	2:K:70:LEU:HB2	1.17	1.27
2:B:137:GLU:OE1	2:B:141:ARG:HD2	1.35	1.22
2:B:137:GLU:OE1	2:B:141:ARG:CD	1.97	1.11
1:D:10:TRP:HZ3	6:H:283:HOH:O	1.36	1.08
2:E:137:GLU:OE1	2:E:141[A]:ARG:HD2	1.53	1.07
3:I:66:ARG:HH11	3:I:66:ARG:HG3	1.04	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TRP:HZ3	6:K:297:HOH:O	1.44	0.98
2:K:65:GLU:OE1	2:K:70:LEU:CB	2.12	0.97
2:K:45:ARG:HD3	6:K:307:HOH:O	1.65	0.97
2:E:58:ILE:HD11	2:E:60:TYR:CE1	2.02	0.95
3:I:66:ARG:NH1	3:I:66:ARG:HG3	1.73	0.94
2:E:137:GLU:OE1	2:E:141[A]:ARG:CD	2.17	0.92
3:I:66:ARG:CG	3:I:66:ARG:HH11	1.83	0.92
1:G:26:GLN:H	1:G:26:GLN:HE21	1.18	0.90
1:A:26:GLN:HE21	1:A:26:GLN:H	1.19	0.90
3:I:47:GLU:CG	3:I:50:ARG:HH21	1.87	0.88
2:K:4:SER:N	6:K:274:HOH:O	2.09	0.86
3:I:47:GLU:HG2	3:I:50:ARG:HH21	1.07	0.86
1:D:26:GLN:H	1:D:26:GLN:HE21	1.24	0.85
2:H:45:ARG:HD3	6:H:306:HOH:O	1.77	0.85
1:J:26:GLN:HE21	1:J:26:GLN:H	1.24	0.84
3:I:47:GLU:CG	3:I:50:ARG:NH2	2.35	0.82
1:G:26:GLN:HE22	3:I:111:CYS:HB2	1.44	0.81
1:J:26:GLN:HE22	3:L:111:CYS:HB2	1.46	0.79
2:E:58:ILE:HD12	2:E:58:ILE:O	1.83	0.78
1:A:26:GLN:HE22	3:C:111:CYS:HB2	1.47	0.78
1:A:38:ASN:ND2	6:A:269:HOH:O	2.17	0.77
3:I:66:ARG:CG	3:I:66:ARG:NH1	2.42	0.75
1:D:26:GLN:HE22	3:F:111:CYS:HB2	1.49	0.75
3:L:175:GLN:HE22	3:L:177:ARG:HH11	1.33	0.74
3:I:175:GLN:HE22	3:I:177:ARG:HH11	1.34	0.74
3:C:153:ARG:HH12	2:K:28:HIS:CD2	2.07	0.73
2:E:28:HIS:CD2	3:I:153:ARG:HH12	2.06	0.73
2:K:45:ARG:HH11	2:K:100:GLN:HE22	1.37	0.72
1:A:7:LYS:NZ	1:J:84:ASN:HD22	1.88	0.72
2:H:138:MET:HE2	3:I:33:ALA:HA	1.72	0.72
2:B:58:ILE:HD11	2:B:60:TYR:CE1	2.29	0.68
3:F:153:ARG:HH12	2:H:28:HIS:CD2	2.11	0.68
2:H:45:ARG:HH11	2:H:100:GLN:HE22	1.42	0.67
2:B:28:HIS:CD2	3:L:153:ARG:HH12	2.12	0.67
2:K:58:ILE:HD11	2:K:60:TYR:CE1	2.31	0.66
3:C:175:GLN:HE22	3:C:177:ARG:HH11	1.44	0.65
2:B:138:MET:SD	2:B:148:LEU:HD11	2.37	0.65
2:B:45:ARG:HH11	2:B:100:GLN:HE22	1.45	0.65
1:A:7:LYS:HZ2	1:J:84:ASN:HD22	1.44	0.64
2:B:137:GLU:OE1	2:B:141:ARG:HD3	1.96	0.64
3:F:175:GLN:HE22	3:F:177:ARG:HH11	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:28:HIS:HD2	3:I:153:ARG:HH12	1.46	0.62
3:C:153:ARG:HH12	2:K:28:HIS:HD2	1.48	0.62
2:B:37:HIS:HE1	2:H:8:GLU:OE1	1.82	0.62
2:H:71:ASN:HD21	3:I:53:LYS:NZ	1.98	0.61
3:F:153:ARG:HH12	2:H:28:HIS:HD2	1.47	0.61
1:A:10:TRP:CZ3	6:K:297:HOH:O	2.32	0.61
2:K:58:ILE:HD11	2:K:60:TYR:CZ	2.36	0.61
2:B:58:ILE:HD13	2:B:58:ILE:O	2.01	0.60
1:A:7:LYS:HD2	2:B:124:GLN:NE2	2.17	0.60
1:D:83:GLY:O	1:G:7:LYS:HE2	2.03	0.59
2:E:11:ARG:HD3	6:K:279:HOH:O	2.03	0.59
2:E:8:GLU:OE2	2:K:37:HIS:HE1	1.86	0.59
1:G:26:GLN:H	1:G:26:GLN:NE2	1.94	0.59
2:B:71:ASN:HD21	3:C:53:LYS:NZ	2.00	0.59
1:D:86:GLU:OE2	1:G:7:LYS:NZ	2.34	0.59
2:K:71:ASN:HD21	3:L:53:LYS:NZ	2.01	0.58
3:I:76:GLU:HG3	6:I:547:HOH:O	2.04	0.58
2:B:142:VAL:HG21	3:C:24:VAL:HG21	1.84	0.58
2:K:45:ARG:NH1	2:K:100:GLN:HE22	2.02	0.58
3:C:66[A]:ARG:HD3	6:C:583:HOH:O	2.04	0.57
2:B:45:ARG:NH1	2:B:100:GLN:HE22	2.03	0.57
2:E:142:VAL:HG21	3:F:24:VAL:HG21	1.86	0.57
2:K:45:ARG:HH11	2:K:100:GLN:NE2	2.03	0.56
3:I:230:ARG:HB2	3:I:231:PRO:HD2	1.87	0.56
2:B:8:GLU:OE2	2:H:37:HIS:HE1	1.88	0.56
3:C:29[A]:ILE:HD11	6:C:555:HOH:O	2.05	0.56
2:H:45:ARG:HG3	2:H:45:ARG:O	2.05	0.55
2:H:65:GLU:OE1	2:H:70:LEU:HB2	2.06	0.55
3:F:47[B]:GLU:HB2	3:F:50:ARG:NH2	2.21	0.55
2:E:71:ASN:HD21	3:F:53:LYS:NZ	2.05	0.55
3:I:47:GLU:HG2	3:I:50:ARG:HH22	1.58	0.55
1:D:86:GLU:OE2	1:G:7:LYS:HE3	2.07	0.54
2:E:138:MET:SD	2:E:148:LEU:HD11	2.47	0.54
3:L:75:PRO:HD3	6:L:552:HOH:O	2.08	0.53
2:K:58:ILE:O	2:K:58:ILE:HD13	2.06	0.53
1:D:8:PRO:HG3	1:G:10:TRP:CZ3	2.43	0.53
2:H:45:ARG:NH1	2:H:100:GLN:HE22	2.07	0.53
2:K:58:ILE:N	2:K:58:ILE:CD1	2.71	0.53
1:A:7:LYS:HD2	2:B:124:GLN:HE22	1.73	0.53
1:D:26:GLN:HE21	1:D:26:GLN:N	2.01	0.52
2:E:37:HIS:HE1	2:K:8:GLU:OE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:ARG:HH11	2:E:100:GLN:HE22	1.57	0.52
1:A:26:GLN:N	1:A:26:GLN:HE21	1.97	0.52
2:E:58:ILE:CD1	2:E:60:TYR:CE1	2.84	0.52
2:E:46:VAL:HG23	2:E:46:VAL:O	2.10	0.51
1:J:26:GLN:NE2	1:J:26:GLN:H	2.03	0.51
1:D:26:GLN:H	1:D:26:GLN:NE2	2.03	0.51
1:G:12:ARG:HD3	6:G:249:HOH:O	2.10	0.51
2:H:148:LEU:HG	3:I:32:MET:HG3	1.93	0.51
1:A:8:PRO:HG3	1:J:10:TRP:CZ3	2.44	0.51
3:L:230:ARG:HB2	3:L:231:PRO:HD2	1.92	0.51
6:E:251:HOH:O	2:K:12:HIS:HE1	1.92	0.51
3:C:119:SER:HB2	3:C:120:PRO:CD	2.41	0.50
3:I:99:SER:N	3:I:100:PRO:CD	2.74	0.50
2:B:28:HIS:HD2	3:L:153:ARG:HH12	1.54	0.50
1:D:86:GLU:OE2	1:G:7:LYS:CE	2.60	0.50
2:H:134:LYS:HD2	2:H:138:MET:CE	2.42	0.49
2:H:134:LYS:HD2	2:H:138:MET:HE1	1.94	0.49
3:F:26:ASP:OD2	2:H:37:HIS:HD2	1.94	0.49
2:H:45:ARG:HH11	2:H:100:GLN:NE2	2.07	0.49
1:D:10:TRP:CZ3	6:H:283:HOH:O	2.27	0.48
3:C:42:GLY:HA2	6:C:578:HOH:O	2.13	0.48
1:D:10:TRP:CZ3	2:E:123:LYS:HE2	2.49	0.48
2:E:152:LEU:HD12	2:E:153:PRO:HD2	1.96	0.48
1:D:108:THR:HG22	3:F:172:SER:HB2	1.96	0.48
2:E:137:GLU:OE1	2:E:141[A]:ARG:CG	2.62	0.48
2:K:53:GLU:HB2	3:L:153:ARG:HG2	1.96	0.48
3:I:100:PRO:HG3	6:I:494:HOH:O	2.15	0.47
3:L:99:SER:N	3:L:100:PRO:CD	2.77	0.47
2:B:45:ARG:HH11	2:B:100:GLN:NE2	2.12	0.47
2:H:67:ILE:HD12	3:I:237:ARG:HG2	1.97	0.47
2:E:37:HIS:HD2	3:I:26:ASP:OD2	1.98	0.47
3:C:157:ARG:HD3	3:C:158:TRP:CH2	2.50	0.47
3:I:96:TRP:O	3:I:105:GLY:HA2	2.15	0.47
2:B:58:ILE:CD1	2:B:58:ILE:N	2.78	0.46
3:F:23:GLU:HG3	3:F:24:VAL:N	2.30	0.46
3:I:76:GLU:CG	6:I:547:HOH:O	2.61	0.46
2:K:45:ARG:O	2:K:45:ARG:HG3	2.09	0.46
3:L:100:PRO:HG3	6:L:453:HOH:O	2.14	0.46
1:A:10:TRP:CZ3	1:J:8:PRO:HG3	2.50	0.46
2:B:58:ILE:CD1	2:B:58:ILE:H	2.28	0.46
3:C:26:ASP:OD2	2:K:37:HIS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HZ1	1:J:84:ASN:ND2	2.14	0.45
1:G:26:GLN:HE21	1:G:26:GLN:N	2.00	0.45
3:I:157:ARG:HD3	3:I:158:TRP:CH2	2.52	0.45
2:E:58:ILE:CD1	2:E:60:TYR:CD1	3.00	0.45
2:E:45:ARG:O	2:E:45:ARG:HG3	2.15	0.44
2:E:34:GLU:HG3	6:E:324:HOH:O	2.16	0.44
2:E:58:ILE:HD12	2:E:58:ILE:C	2.38	0.44
3:I:76:GLU:CB	6:I:547:HOH:O	2.64	0.44
1:D:10:TRP:CZ3	1:G:8:PRO:HG3	2.53	0.44
2:B:27:THR:HG23	2:E:22:ALA:HA	1.99	0.44
2:K:148:LEU:HG	3:L:32:MET:HG3	1.98	0.43
2:K:71:ASN:HD21	3:L:53:LYS:HZ1	1.65	0.43
3:L:175:GLN:NE2	3:L:177:ARG:HH11	2.09	0.43
1:A:99:LYS:HG2	1:A:100:ASP:N	2.32	0.43
3:L:157:ARG:HD3	3:L:158:TRP:CH2	2.54	0.43
2:H:71:ASN:HD21	3:I:53:LYS:HZ2	1.65	0.43
2:E:58:ILE:O	2:E:58:ILE:CD1	2.61	0.43
3:L:207:GLU:HG2	3:L:225:THR:CG2	2.49	0.43
2:K:58:ILE:HD12	2:K:58:ILE:N	2.34	0.42
1:A:26:GLN:NE2	1:A:26:GLN:H	2.01	0.42
1:D:79:ASP:HB3	1:D:84:ASN:O	2.18	0.42
2:B:58:ILE:HD13	2:B:58:ILE:H	1.85	0.42
3:L:96:TRP:O	3:L:105:GLY:HA2	2.19	0.42
3:F:157:ARG:HD3	3:F:158:TRP:CH2	2.54	0.42
1:A:79:ASP:HB3	1:A:84:ASN:O	2.20	0.42
3:C:127:VAL:HG22	3:C:128:CYS:N	2.35	0.42
3:C:35:ARG:HD2	3:C:35:ARG:HH11	1.64	0.42
2:K:58:ILE:H	2:K:58:ILE:CD1	2.32	0.42
3:I:136:TRP:CH2	3:I:141:GLN:HB2	2.54	0.41
1:A:8:PRO:HG3	1:J:10:TRP:CH2	2.56	0.41
1:J:26:GLN:HE21	1:J:26:GLN:N	2.04	0.41
2:B:71:ASN:HD21	3:C:53:LYS:HZ2	1.68	0.41
1:D:10:TRP:CE3	1:G:8:PRO:HG3	2.56	0.41
2:E:58:ILE:C	2:E:58:ILE:CD1	2.89	0.41
2:H:53:GLU:HB2	3:I:153:ARG:HG2	2.01	0.41
2:E:128:LEU:HA	2:E:128:LEU:HD12	1.85	0.41
3:C:67:LEU:HD23	3:C:67:LEU:C	2.42	0.40
1:D:94[A]:ILE:O	1:D:115:GLU:HA	2.21	0.40
1:G:111:ASN:O	3:I:175:GLN:HG3	2.21	0.40
1:G:58:THR:HA	1:G:61:ARG:HG2	2.03	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	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
1	D	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
1	G	119/126 (94%)	114 (96%)	5 (4%)	0	100	100
1	J	119/126 (94%)	115 (97%)	4 (3%)	0	100	100
2	B	152/157 (97%)	147 (97%)	5 (3%)	0	100	100
2	E	152/157 (97%)	148 (97%)	4 (3%)	0	100	100
2	H	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
2	K	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
3	C	215/243 (88%)	206 (96%)	8 (4%)	1 (0%)	29	13
3	F	215/243 (88%)	209 (97%)	6 (3%)	0	100	100
3	I	213/243 (88%)	207 (97%)	6 (3%)	0	100	100
3	L	214/243 (88%)	209 (98%)	5 (2%)	0	100	100
All	All	1933/2104 (92%)	1874 (97%)	58 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	132	SER

### 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	102/108 (94%)	100 (98%)	2 (2%)	55	37
1	D	102/108 (94%)	99 (97%)	3 (3%)	42	22
1	G	103/108 (95%)	101 (98%)	2 (2%)	57	39
1	J	103/108 (95%)	100 (97%)	3 (3%)	42	22
2	B	131/134 (98%)	128 (98%)	3 (2%)	50	31
2	E	132/134 (98%)	130 (98%)	2 (2%)	65	49
2	H	129/134 (96%)	125 (97%)	4 (3%)	40	19
2	K	128/134 (96%)	124 (97%)	4 (3%)	40	19
3	C	190/212 (90%)	189 (100%)	1 (0%)	88	83
3	F	190/212 (90%)	188 (99%)	2 (1%)	73	62
3	I	188/212 (89%)	180 (96%)	8 (4%)	29	10
3	L	189/212 (89%)	183 (97%)	6 (3%)	39	18
All	All	1687/1816 (93%)	1647 (98%)	40 (2%)	50	29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	99	LYS
2	B	48	HIS
2	B	58	ILE
2	B	85	TRP
3	C	141	GLN
1	D	26	GLN
1	D	44	ARG
1	D	125	LYS
2	E	48	HIS
2	E	85	TRP
3	F	23	GLU
3	F	141	GLN
1	G	18	MET
1	G	26	GLN
2	H	46	VAL
2	H	48	HIS
2	H	85	TRP
2	H	150	GLU
3	I	47	GLU
3	I	50	ARG
3	I	66	ARG

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Mol	Chain	Res	Type
3	I	107	PRO
3	I	170	LEU
3	I	198	ASP
3	I	229	LYS
3	I	239	VAL
1	J	18	MET
1	J	26	GLN
1	J	34	LYS
2	K	46	VAL
2	K	48	HIS
2	K	58	ILE
2	K	85	TRP
3	L	109	ASP
3	L	141[A]	GLN
3	L	141[B]	GLN
3	L	170	LEU
3	L	198	ASP
3	L	239	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	38	ASN
1	A	111	ASN
2	B	28	HIS
2	B	37	HIS
2	B	71	ASN
2	B	100	GLN
2	B	124	GLN
3	C	103	GLN
3	C	141	GLN
3	C	175	GLN
1	D	26	GLN
1	D	84	ASN
1	D	111	ASN
2	E	28	HIS
2	E	37	HIS
2	E	71	ASN
2	E	100	GLN
2	E	124	GLN
3	F	103	GLN

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Mol	Chain	Res	Type
3	F	175	GLN
1	G	26	GLN
1	G	111	ASN
2	H	28	HIS
2	H	37	HIS
2	H	71	ASN
2	H	100	GLN
3	I	175	GLN
1	J	26	GLN
1	J	84	ASN
1	J	111	ASN
2	K	12	HIS
2	K	28	HIS
2	K	37	HIS
2	K	71	ASN
2	K	100	GLN
2	K	124	GLN
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 ⓘ

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
3	CSO	L	133	3,4	3,6,7	1.10	0	0,6,8	0.00	-
3	CSO	C	133	3,4	3,6,7	1.11	0	0,6,8	0.00	-
3	CSD	I	131	3,4	3,7,8	0.23	0	1,8,10	1.49	0
3	CSO	I	133	3,4	3,6,7	1.42	0	0,6,8	0.00	-
3	CSD	C	131	3,4	3,7,8	0.98	0	1,8,10	2.43	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CSO	F	133	3,4	3,6,7	1.02	0	0,6,8	0.00	-
3	CSD	F	131	3,4	3,7,8	1.13	0	1,8,10	0.80	0
3	CSD	L	131	3,4	3,7,8	0.85	0	1,8,10	1.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CSO	L	133	3,4	-	0/1/5/7	-
3	CSO	C	133	3,4	-	0/1/5/7	-
3	CSD	I	131	3,4	-	0/2/6/8	-
3	CSO	I	133	3,4	-	0/1/5/7	-
3	CSD	C	131	3,4	-	0/2/6/8	-
3	CSO	F	133	3,4	-	0/1/5/7	-
3	CSD	F	131	3,4	-	0/2/6/8	-
3	CSD	L	131	3,4	-	0/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	131	CSD	OD1-SG-CB	-2.43	100.91	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	TLA	F	302	-	3,9,9	0.89	0	6,12,12	1.04	0
5	TLA	I	302	-	3,9,9	0.67	0	6,12,12	1.09	0
5	TLA	L	302	-	3,9,9	0.47	0	6,12,12	1.36	2 (33%)
5	TLA	C	302	-	3,9,9	0.74	0	6,12,12	1.04	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
5	TLA	F	302	-	-	0/4/12/12	-
5	TLA	I	302	-	-	0/4/12/12	-
5	TLA	L	302	-	-	0/4/12/12	-
5	TLA	C	302	-	-	0/4/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	TLA	C1-C2-C3	-2.19	108.40	113.11
5	L	302	TLA	C4-C3-C2	-2.11	108.57	113.11

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	120/126 (95%)	-0.27	1 (0%) 86 89	13, 20, 30, 38	4 (3%)
1	D	119/126 (94%)	-0.29	0 100 100	14, 20, 30, 37	3 (2%)
1	G	120/126 (95%)	-0.30	1 (0%) 86 89	12, 16, 29, 43	5 (4%)
1	J	120/126 (95%)	-0.32	0 100 100	11, 16, 29, 36	2 (1%)
2	B	152/157 (96%)	-0.31	0 100 100	12, 16, 30, 39	0
2	E	151/157 (96%)	-0.32	0 100 100	12, 16, 31, 37	0
2	H	151/157 (96%)	-0.24	0 100 100	12, 19, 39, 48	0
2	K	151/157 (96%)	-0.15	1 (0%) 87 90	12, 18, 39, 50	0
3	C	215/243 (88%)	-0.30	0 100 100	12, 17, 28, 37	4 (1%)
3	F	215/243 (88%)	-0.32	0 100 100	12, 17, 28, 45	0
3	I	215/243 (88%)	-0.23	1 (0%) 91 92	13, 19, 35, 49	2 (0%)
3	L	215/243 (88%)	-0.17	1 (0%) 91 92	12, 19, 35, 53	5 (2%)
All	All	1944/2104 (92%)	-0.26	5 (0%) 94 95	11, 18, 33, 53	25 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	239	VAL	6.8
1	G	126	ALA	3.0
3	I	239	VAL	2.3
1	A	126	ALA	2.3
2	K	153	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CSO	F	133	7/8	0.96	0.10	13,15,20,31	1
3	CSO	C	133	7/8	0.97	0.09	13,14,20,29	1
3	CSO	I	133	7/8	0.97	0.09	12,14,21,32	1
3	CSO	L	133	7/8	0.97	0.09	13,14,21,33	1
3	CSD	C	131	8/9	0.98	0.07	12,15,18,18	2
3	CSD	I	131	8/9	0.98	0.09	12,16,17,18	2
3	CSD	L	131	8/9	0.98	0.07	12,15,17,17	2
3	CSD	F	131	8/9	0.99	0.07	12,15,18,19	2

### 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(Å <sup>2</sup> )	Q<0.9
5	TLA	C	302	10/10	0.94	0.11	18,27,34,37	0
5	TLA	I	302	10/10	0.95	0.08	18,21,30,32	0
5	TLA	F	302	10/10	0.95	0.08	20,24,34,35	0
5	TLA	L	302	10/10	0.96	0.09	20,22,28,32	0
4	3CO	F	301	1/1	0.98	0.08	12,12,12,12	1
4	3CO	I	301	1/1	0.99	0.10	13,13,13,13	1
4	3CO	C	301	1/1	0.99	0.09	12,12,12,12	1
4	3CO	L	301	1/1	1.00	0.08	13,13,13,13	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.