



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:55 AM UTC

PDB ID : 3L3S / pdb_00003l3s
Title : Crystal structure of an enoyl-CoA hydrotase/isomerase family protein from *Silicibacter pomeroyi*
Authors : Eswaramoorthy, S.; Silberstein, M.; Burley, S.K.; Swaminathan, S.; New York
SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-12-17
Resolution : 2.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

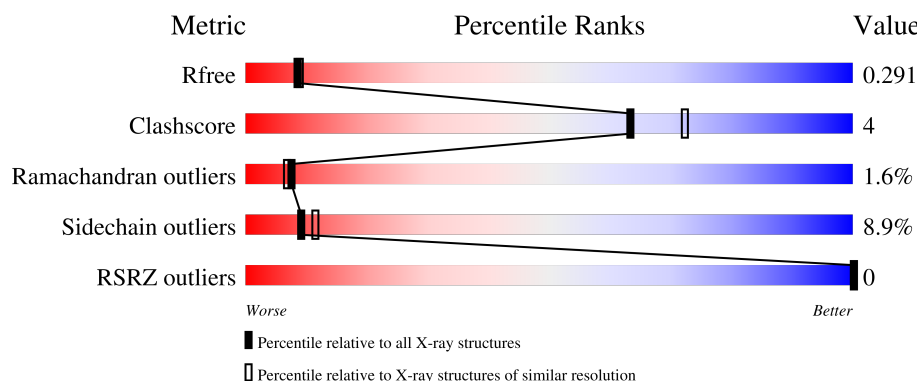
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	263	
1	B	263	
1	C	263	
1	D	263	
1	E	263	

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Mol	Chain	Length	Quality of chain
1	F	263	 74%11% • 12%
1	G	263	 71%14% • 11%
1	H	263	 73%12% • 12%
1	I	263	 74%13% • 11%
1	J	263	 72%15% • 11%
1	K	263	 71%14% • 12%
1	L	263	 68%15% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20649 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 Enoyl-CoA hydratase/isomerase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	Se	0	0	0
			1711	1077	311	310	6	7			
1	B	234	Total	C	N	O	S	Se	0	0	0
			1721	1086	312	310	6	7			
1	C	234	Total	C	N	O	S	Se	0	0	0
			1722	1085	310	314	6	7			
1	D	232	Total	C	N	O	S	Se	0	0	0
			1710	1079	308	310	6	7			
1	E	231	Total	C	N	O	S	Se	0	0	0
			1697	1072	307	305	6	7			
1	F	231	Total	C	N	O	S	Se	0	0	0
			1701	1074	307	307	6	7			
1	G	233	Total	C	N	O	S	Se	0	0	0
			1710	1079	309	309	6	7			
1	H	232	Total	C	N	O	S	Se	0	0	0
			1706	1077	308	308	6	7			
1	I	234	Total	C	N	O	S	Se	0	0	0
			1718	1083	310	312	6	7			
1	J	233	Total	C	N	O	S	Se	0	0	0
			1710	1079	309	309	6	7			
1	K	232	Total	C	N	O	S	Se	0	0	0
			1707	1076	308	310	6	7			
1	L	231	Total	C	N	O	S	Se	0	0	0
			1702	1073	307	309	6	7			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MSE	-	expression tag	UNP Q5LQZ3
A	3	SER	-	expression tag	UNP Q5LQZ3
A	4	LEU	-	expression tag	UNP Q5LQZ3
A	257	GLU	-	expression tag	UNP Q5LQZ3
A	258	GLY	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	259	HIS	-	expression tag	UNP Q5LQZ3
A	260	HIS	-	expression tag	UNP Q5LQZ3
A	261	HIS	-	expression tag	UNP Q5LQZ3
A	262	HIS	-	expression tag	UNP Q5LQZ3
A	263	HIS	-	expression tag	UNP Q5LQZ3
A	264	HIS	-	expression tag	UNP Q5LQZ3
B	2	MSE	-	expression tag	UNP Q5LQZ3
B	3	SER	-	expression tag	UNP Q5LQZ3
B	4	LEU	-	expression tag	UNP Q5LQZ3
B	257	GLU	-	expression tag	UNP Q5LQZ3
B	258	GLY	-	expression tag	UNP Q5LQZ3
B	259	HIS	-	expression tag	UNP Q5LQZ3
B	260	HIS	-	expression tag	UNP Q5LQZ3
B	261	HIS	-	expression tag	UNP Q5LQZ3
B	262	HIS	-	expression tag	UNP Q5LQZ3
B	263	HIS	-	expression tag	UNP Q5LQZ3
B	264	HIS	-	expression tag	UNP Q5LQZ3
C	2	MSE	-	expression tag	UNP Q5LQZ3
C	3	SER	-	expression tag	UNP Q5LQZ3
C	4	LEU	-	expression tag	UNP Q5LQZ3
C	257	GLU	-	expression tag	UNP Q5LQZ3
C	258	GLY	-	expression tag	UNP Q5LQZ3
C	259	HIS	-	expression tag	UNP Q5LQZ3
C	260	HIS	-	expression tag	UNP Q5LQZ3
C	261	HIS	-	expression tag	UNP Q5LQZ3
C	262	HIS	-	expression tag	UNP Q5LQZ3
C	263	HIS	-	expression tag	UNP Q5LQZ3
C	264	HIS	-	expression tag	UNP Q5LQZ3
D	2	MSE	-	expression tag	UNP Q5LQZ3
D	3	SER	-	expression tag	UNP Q5LQZ3
D	4	LEU	-	expression tag	UNP Q5LQZ3
D	257	GLU	-	expression tag	UNP Q5LQZ3
D	258	GLY	-	expression tag	UNP Q5LQZ3
D	259	HIS	-	expression tag	UNP Q5LQZ3
D	260	HIS	-	expression tag	UNP Q5LQZ3
D	261	HIS	-	expression tag	UNP Q5LQZ3
D	262	HIS	-	expression tag	UNP Q5LQZ3
D	263	HIS	-	expression tag	UNP Q5LQZ3
D	264	HIS	-	expression tag	UNP Q5LQZ3
E	2	MSE	-	expression tag	UNP Q5LQZ3
E	3	SER	-	expression tag	UNP Q5LQZ3
E	4	LEU	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	257	GLU	-	expression tag	UNP Q5LQZ3
E	258	GLY	-	expression tag	UNP Q5LQZ3
E	259	HIS	-	expression tag	UNP Q5LQZ3
E	260	HIS	-	expression tag	UNP Q5LQZ3
E	261	HIS	-	expression tag	UNP Q5LQZ3
E	262	HIS	-	expression tag	UNP Q5LQZ3
E	263	HIS	-	expression tag	UNP Q5LQZ3
E	264	HIS	-	expression tag	UNP Q5LQZ3
F	2	MSE	-	expression tag	UNP Q5LQZ3
F	3	SER	-	expression tag	UNP Q5LQZ3
F	4	LEU	-	expression tag	UNP Q5LQZ3
F	257	GLU	-	expression tag	UNP Q5LQZ3
F	258	GLY	-	expression tag	UNP Q5LQZ3
F	259	HIS	-	expression tag	UNP Q5LQZ3
F	260	HIS	-	expression tag	UNP Q5LQZ3
F	261	HIS	-	expression tag	UNP Q5LQZ3
F	262	HIS	-	expression tag	UNP Q5LQZ3
F	263	HIS	-	expression tag	UNP Q5LQZ3
F	264	HIS	-	expression tag	UNP Q5LQZ3
G	2	MSE	-	expression tag	UNP Q5LQZ3
G	3	SER	-	expression tag	UNP Q5LQZ3
G	4	LEU	-	expression tag	UNP Q5LQZ3
G	257	GLU	-	expression tag	UNP Q5LQZ3
G	258	GLY	-	expression tag	UNP Q5LQZ3
G	259	HIS	-	expression tag	UNP Q5LQZ3
G	260	HIS	-	expression tag	UNP Q5LQZ3
G	261	HIS	-	expression tag	UNP Q5LQZ3
G	262	HIS	-	expression tag	UNP Q5LQZ3
G	263	HIS	-	expression tag	UNP Q5LQZ3
G	264	HIS	-	expression tag	UNP Q5LQZ3
H	2	MSE	-	expression tag	UNP Q5LQZ3
H	3	SER	-	expression tag	UNP Q5LQZ3
H	4	LEU	-	expression tag	UNP Q5LQZ3
H	257	GLU	-	expression tag	UNP Q5LQZ3
H	258	GLY	-	expression tag	UNP Q5LQZ3
H	259	HIS	-	expression tag	UNP Q5LQZ3
H	260	HIS	-	expression tag	UNP Q5LQZ3
H	261	HIS	-	expression tag	UNP Q5LQZ3
H	262	HIS	-	expression tag	UNP Q5LQZ3
H	263	HIS	-	expression tag	UNP Q5LQZ3
H	264	HIS	-	expression tag	UNP Q5LQZ3
I	2	MSE	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	3	SER	-	expression tag	UNP Q5LQZ3
I	4	LEU	-	expression tag	UNP Q5LQZ3
I	257	GLU	-	expression tag	UNP Q5LQZ3
I	258	GLY	-	expression tag	UNP Q5LQZ3
I	259	HIS	-	expression tag	UNP Q5LQZ3
I	260	HIS	-	expression tag	UNP Q5LQZ3
I	261	HIS	-	expression tag	UNP Q5LQZ3
I	262	HIS	-	expression tag	UNP Q5LQZ3
I	263	HIS	-	expression tag	UNP Q5LQZ3
I	264	HIS	-	expression tag	UNP Q5LQZ3
J	2	MSE	-	expression tag	UNP Q5LQZ3
J	3	SER	-	expression tag	UNP Q5LQZ3
J	4	LEU	-	expression tag	UNP Q5LQZ3
J	257	GLU	-	expression tag	UNP Q5LQZ3
J	258	GLY	-	expression tag	UNP Q5LQZ3
J	259	HIS	-	expression tag	UNP Q5LQZ3
J	260	HIS	-	expression tag	UNP Q5LQZ3
J	261	HIS	-	expression tag	UNP Q5LQZ3
J	262	HIS	-	expression tag	UNP Q5LQZ3
J	263	HIS	-	expression tag	UNP Q5LQZ3
J	264	HIS	-	expression tag	UNP Q5LQZ3
K	2	MSE	-	expression tag	UNP Q5LQZ3
K	3	SER	-	expression tag	UNP Q5LQZ3
K	4	LEU	-	expression tag	UNP Q5LQZ3
K	257	GLU	-	expression tag	UNP Q5LQZ3
K	258	GLY	-	expression tag	UNP Q5LQZ3
K	259	HIS	-	expression tag	UNP Q5LQZ3
K	260	HIS	-	expression tag	UNP Q5LQZ3
K	261	HIS	-	expression tag	UNP Q5LQZ3
K	262	HIS	-	expression tag	UNP Q5LQZ3
K	263	HIS	-	expression tag	UNP Q5LQZ3
K	264	HIS	-	expression tag	UNP Q5LQZ3
L	2	MSE	-	expression tag	UNP Q5LQZ3
L	3	SER	-	expression tag	UNP Q5LQZ3
L	4	LEU	-	expression tag	UNP Q5LQZ3
L	257	GLU	-	expression tag	UNP Q5LQZ3
L	258	GLY	-	expression tag	UNP Q5LQZ3
L	259	HIS	-	expression tag	UNP Q5LQZ3
L	260	HIS	-	expression tag	UNP Q5LQZ3
L	261	HIS	-	expression tag	UNP Q5LQZ3
L	262	HIS	-	expression tag	UNP Q5LQZ3
L	263	HIS	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	264	HIS	-	expression tag	UNP Q5LQZ3

- Molecule 2 is water.

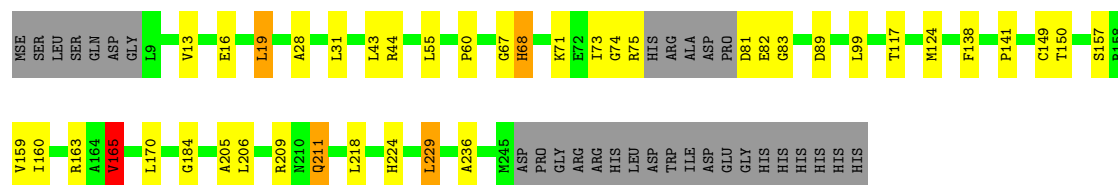
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	20	Total O 20 20	0	0
2	C	19	Total O 19 19	0	0
2	D	16	Total O 16 16	0	0
2	E	14	Total O 14 14	0	0
2	F	20	Total O 20 20	0	0
2	G	8	Total O 8 8	0	0
2	H	9	Total O 9 9	0	0
2	I	6	Total O 6 6	0	0
2	J	3	Total O 3 3	0	0
2	K	10	Total O 10 10	0	0
2	L	4	Total O 4 4	0	0

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.

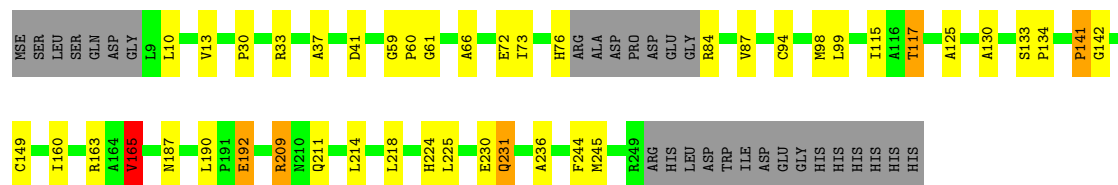
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain A: 



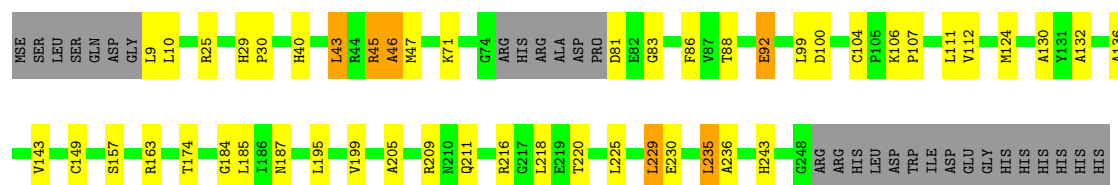
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain B: 



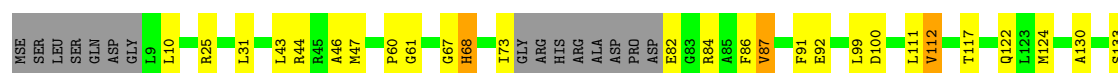
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain C: 



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain D: 

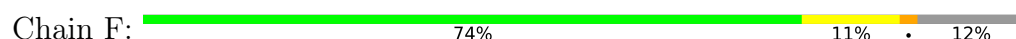




- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



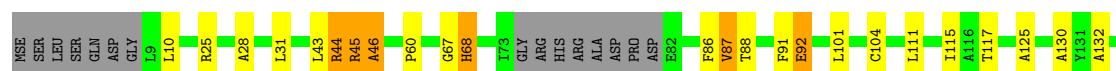
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



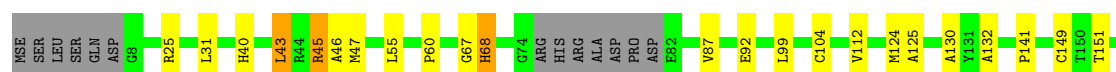
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein





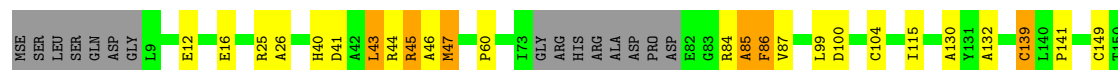
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain J: 72% 15% 11%



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain K: 71% 14% 12%



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain L: 68% 15% 12%



HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.40Å 124.28Å 147.00Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	50.00 – 2.32 50.00 – 2.32	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.32) 75.1 (50.00-2.32)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.294 0.262 , 0.291	Depositor DCC
R_{free} test set	5005 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 18.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20649	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.66	0/1725	1.19	9/2335 (0.4%)
1	B	0.65	0/1737	1.20	13/2354 (0.6%)
1	C	0.68	0/1737	1.19	9/2353 (0.4%)
1	D	0.66	0/1725	1.19	9/2337 (0.4%)
1	E	0.68	0/1712	1.21	10/2320 (0.4%)
1	F	0.67	0/1716	1.20	12/2325 (0.5%)
1	G	0.69	0/1725	1.24	13/2337 (0.6%)
1	H	0.66	0/1721	1.22	15/2332 (0.6%)
1	I	0.68	0/1733	1.22	11/2347 (0.5%)
1	J	0.67	0/1725	1.15	7/2337 (0.3%)
1	K	0.68	0/1722	1.21	18/2333 (0.8%)
1	L	0.70	0/1717	1.20	10/2326 (0.4%)
All	All	0.67	0/20695	1.20	136/28036 (0.5%)

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	211	GLN	N-CA-C	11.15	123.44	111.28
1	I	211	GLN	N-CA-C	11.11	123.39	111.28
1	K	211	GLN	N-CA-C	10.93	122.77	111.07
1	F	211	GLN	N-CA-C	10.81	122.64	111.07
1	J	211	GLN	N-CA-C	10.78	123.03	111.28
1	E	211	GLN	N-CA-C	10.63	122.87	111.28
1	L	211	GLN	N-CA-C	10.57	122.80	111.28
1	C	211	GLN	N-CA-C	10.36	122.57	111.28
1	B	211	GLN	N-CA-C	10.32	122.11	111.07
1	A	211	GLN	N-CA-C	10.22	122.42	111.28
1	G	211	GLN	N-CA-C	9.54	122.55	111.11
1	D	211	GLN	N-CA-C	9.18	121.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	45	ARG	N-CA-C	-8.97	98.43	110.55
1	I	45	ARG	N-CA-C	-8.89	97.70	110.59
1	B	72	GLU	N-CA-C	8.60	122.54	108.52
1	G	45	ARG	N-CA-C	-8.20	96.19	109.96
1	C	45	ARG	N-CA-C	-8.01	97.54	110.20
1	C	236	ALA	N-CA-C	7.92	119.92	111.28
1	H	236	ALA	N-CA-C	7.87	119.94	111.36
1	H	141	PRO	N-CA-C	7.76	122.75	114.68
1	B	236	ALA	N-CA-C	7.69	119.66	111.28
1	G	236	ALA	N-CA-C	7.33	119.35	111.36
1	F	84	ARG	N-CA-C	7.10	120.05	111.82
1	E	45	ARG	N-CA-C	-6.98	97.87	109.46
1	B	142	GLY	N-CA-C	6.98	121.08	112.64
1	G	28	ALA	N-CA-C	6.90	119.64	111.71
1	E	165	VAL	CB-CA-C	-6.88	102.85	112.14
1	I	159	VAL	CB-CA-C	6.82	117.85	111.30
1	F	236	ALA	N-CA-C	6.78	119.68	111.82
1	I	236	ALA	N-CA-C	6.77	118.74	111.36
1	D	165	VAL	CB-CA-C	-6.65	103.05	112.22
1	E	192	GLU	N-CA-C	6.62	119.06	111.11
1	A	141	PRO	N-CA-C	6.50	121.44	114.68
1	B	192	GLU	N-CA-C	6.50	120.79	112.34
1	K	139	CYS	N-CA-C	6.50	118.94	109.07
1	F	45	ARG	N-CA-C	-6.48	97.97	108.41
1	K	47	MSE	N-CA-C	-6.45	105.23	113.23
1	B	165	VAL	CB-CA-C	-6.44	103.33	112.22
1	E	60	PRO	N-CA-C	6.43	121.44	111.21
1	B	61	GLY	N-CA-C	6.37	124.08	112.37
1	J	139	CYS	N-CA-C	6.30	119.00	109.23
1	E	236	ALA	N-CA-C	6.30	119.13	111.82
1	A	236	ALA	N-CA-C	6.21	118.13	111.36
1	H	142	GLY	N-CA-C	6.21	120.16	112.64
1	K	45	ARG	N-CA-C	-6.17	100.51	110.32
1	D	61	GLY	N-CA-C	6.17	122.59	112.84
1	H	165	VAL	CB-CA-C	-6.14	103.75	112.22
1	B	30	PRO	N-CA-C	6.13	120.81	111.19
1	A	71	LYS	N-CA-C	-6.06	103.32	111.87
1	H	44	ARG	N-CA-C	-6.02	104.28	111.69
1	G	115	ILE	N-CA-C	6.01	116.83	108.89
1	L	85	ALA	N-CA-C	-6.00	102.45	110.55
1	B	59	GLY	N-CA-C	-5.99	100.12	112.34
1	B	133	SER	N-CA-C	-5.98	103.13	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	165	VAL	CB-CA-C	-5.98	104.19	112.02
1	G	60	PRO	N-CA-C	5.95	120.56	111.34
1	L	45	ARG	N-CA-C	-5.93	100.33	109.76
1	D	133	SER	N-CA-C	-5.93	102.63	110.40
1	L	72	GLU	N-CA-C	5.92	119.21	110.46
1	H	139	CYS	N-CA-C	5.90	118.26	108.99
1	G	132	ALA	N-CA-C	5.90	118.66	109.52
1	F	195	LEU	N-CA-C	5.86	117.35	110.97
1	A	229	LEU	N-CA-C	5.83	118.14	111.02
1	H	115	ILE	N-CA-C	5.82	116.95	108.58
1	C	136	ALA	N-CA-C	5.80	118.89	110.42
1	F	142	GLY	N-CA-C	5.80	119.65	112.64
1	K	151	THR	CA-C-N	-5.80	113.84	119.87
1	K	151	THR	C-N-CA	-5.80	113.84	119.87
1	G	142	GLY	N-CA-C	5.78	119.63	112.64
1	E	132	ALA	N-CA-C	5.75	118.43	109.52
1	K	165	VAL	CB-CA-C	-5.74	104.30	112.22
1	L	140	LEU	CA-C-N	5.66	126.41	120.12
1	L	140	LEU	C-N-CA	5.66	126.41	120.12
1	G	195	LEU	N-CA-C	5.65	117.11	111.07
1	H	229	LEU	N-CA-C	5.62	117.86	111.11
1	D	236	ALA	N-CA-C	5.59	117.46	111.36
1	K	162	ARG	N-CA-C	5.57	117.79	111.11
1	G	30	PRO	N-CA-C	5.56	119.82	111.14
1	C	195	LEU	N-CA-C	5.54	117.75	111.11
1	F	28	ALA	N-CA-C	5.51	118.21	111.82
1	F	112	VAL	N-CA-C	5.50	115.78	107.80
1	A	60	PRO	N-CA-C	5.50	119.95	111.21
1	B	141	PRO	N-CA-C	5.49	123.78	112.47
1	C	229	LEU	N-CA-C	5.49	117.70	111.11
1	H	132	ALA	N-CA-C	5.47	117.49	109.24
1	D	60	PRO	N-CA-C	5.46	119.66	111.14
1	A	165	VAL	CB-CA-C	-5.46	104.69	112.22
1	K	236	ALA	N-CA-C	5.43	119.07	112.23
1	F	60	PRO	N-CA-C	5.40	119.51	111.41
1	H	28	ALA	N-CA-C	5.38	119.01	112.23
1	K	202	LEU	N-CA-C	-5.38	106.39	113.12
1	G	139	CYS	N-CA-C	5.38	117.44	108.99
1	I	151	THR	CA-C-N	-5.37	114.24	120.04
1	I	151	THR	C-N-CA	-5.37	114.24	120.04
1	D	139	CYS	N-CA-C	5.34	116.97	108.79
1	A	73	ILE	N-CA-C	-5.34	107.27	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	85	ALA	N-CA-C	-5.33	102.38	110.28
1	I	60	PRO	N-CA-C	5.33	119.69	111.21
1	H	60	PRO	N-CA-C	5.32	119.67	111.21
1	J	165	VAL	CB-CA-C	-5.30	103.68	112.26
1	K	104	CYS	CA-C-N	5.30	125.11	119.28
1	K	104	CYS	C-N-CA	5.30	125.11	119.28
1	J	117	THR	N-CA-C	5.29	118.08	109.24
1	F	132	ALA	N-CA-C	5.27	117.69	109.52
1	F	159	VAL	CB-CA-C	5.27	116.62	110.88
1	B	60	PRO	N-CA-C	5.20	119.48	111.21
1	K	132	ALA	N-CA-C	5.19	116.88	109.14
1	E	47	MSE	N-CA-C	-5.18	105.70	112.23
1	C	104	CYS	CA-C-N	5.15	124.82	119.56
1	C	104	CYS	C-N-CA	5.15	124.82	119.56
1	L	151	THR	CA-C-N	-5.15	113.40	119.84
1	L	151	THR	C-N-CA	-5.15	113.40	119.84
1	K	60	PRO	N-CA-C	5.15	119.56	111.38
1	J	60	PRO	N-CA-C	5.14	119.56	111.38
1	E	195	LEU	N-CA-C	5.14	117.29	111.02
1	D	142	GLY	N-CA-C	5.14	119.10	112.83
1	K	115	ILE	N-CA-C	5.13	115.96	108.58
1	K	179	TRP	N-CA-C	-5.13	105.38	111.69
1	G	165	VAL	CB-CA-C	-5.12	103.97	112.26
1	G	229	LEU	N-CA-C	5.12	117.25	111.11
1	C	83	GLY	N-CA-C	-5.10	108.08	115.27
1	J	236	ALA	N-CA-C	5.08	117.94	111.69
1	A	28	ALA	N-CA-C	5.08	118.74	112.54
1	J	136	ALA	N-CA-C	5.08	117.06	109.59
1	L	165	VAL	CB-CA-C	-5.07	105.44	112.24
1	F	139	CYS	N-CA-C	5.07	116.77	109.07
1	K	187	ASN	N-CA-C	5.06	117.92	111.69
1	B	115	ILE	N-CA-C	5.06	115.56	108.89
1	I	104	CYS	CA-C-N	5.04	124.83	119.28
1	I	104	CYS	C-N-CA	5.04	124.83	119.28
1	E	229	LEU	N-CA-C	5.04	117.43	111.33
1	D	112	VAL	N-CA-C	5.03	115.00	107.51
1	H	104	CYS	CA-C-N	5.02	124.80	119.28
1	H	104	CYS	C-N-CA	5.02	124.80	119.28
1	L	139	CYS	N-CA-C	5.01	115.76	108.14
1	I	132	ALA	N-CA-C	5.00	117.27	109.52

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	1711	0	1729	11	0
1	B	1721	0	1737	15	0
1	C	1722	0	1738	24	0
1	D	1710	0	1732	12	0
1	E	1697	0	1721	12	0
1	F	1701	0	1726	11	0
1	G	1710	0	1731	17	0
1	H	1706	0	1728	22	0
1	I	1718	0	1737	11	0
1	J	1710	0	1731	12	0
1	K	1707	0	1722	23	0
1	L	1702	0	1720	20	0
2	A	5	0	0	0	0
2	B	20	0	0	1	0
2	C	19	0	0	2	0
2	D	16	0	0	0	0
2	E	14	0	0	0	0
2	F	20	0	0	1	0
2	G	8	0	0	0	0
2	H	9	0	0	0	0
2	I	6	0	0	0	0
2	J	3	0	0	0	0
2	K	10	0	0	0	0
2	L	4	0	0	0	0
All	All	20649	0	20752	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (163) 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:130:ALA:H	1:F:187:ASN:HD22	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ALA:H	1:B:187:ASN:HD22	1.35	0.71
1:H:44:ARG:HH22	1:K:44:ARG:HH22	1.40	0.69
1:D:130:ALA:H	1:D:187:ASN:HD22	1.39	0.68
1:I:130:ALA:H	1:I:187:ASN:HD22	1.41	0.68
1:E:9:LEU:HD23	1:E:25:ARG:H	1.59	0.68
1:L:130:ALA:H	1:L:187:ASN:ND2	1.91	0.67
1:D:130:ALA:H	1:D:187:ASN:ND2	1.93	0.66
1:K:209:ARG:HH11	1:K:209:ARG:HG3	1.60	0.66
1:B:130:ALA:H	1:B:187:ASN:ND2	1.94	0.66
1:K:139:CYS:HB2	1:K:174:THR:HG22	1.78	0.65
1:H:44:ARG:NH2	1:K:44:ARG:HH22	1.94	0.64
1:G:130:ALA:H	1:G:187:ASN:HD22	1.44	0.64
1:J:73:ILE:HG22	1:J:74:GLY:H	1.63	0.64
1:A:184:GLY:O	1:B:163:ARG:HG3	1.98	0.63
1:B:209:ARG:HD3	1:C:143:VAL:HB	1.81	0.63
1:L:26:ALA:HB1	1:L:27:PRO:HA	1.81	0.62
1:E:130:ALA:H	1:E:187:ASN:HD22	1.48	0.61
1:J:9:LEU:HD23	1:J:25:ARG:H	1.67	0.60
1:C:130:ALA:H	1:C:187:ASN:HD22	1.49	0.59
1:E:26:ALA:HB1	1:E:27:PRO:HD2	1.83	0.59
1:C:130:ALA:H	1:C:187:ASN:ND2	2.01	0.59
1:A:170:LEU:HD21	1:C:218:LEU:HD12	1.85	0.58
1:K:209:ARG:HH11	1:K:209:ARG:CG	2.16	0.57
1:C:111:LEU:HD13	1:C:199:VAL:HG21	1.86	0.57
1:I:130:ALA:H	1:I:187:ASN:ND2	2.01	0.57
1:D:111:LEU:HD13	1:D:199:VAL:HG21	1.88	0.56
1:D:170:LEU:HD21	1:F:218:LEU:HD12	1.86	0.56
1:H:111:LEU:HD13	1:H:199:VAL:HG21	1.88	0.56
1:J:130:ALA:H	1:J:187:ASN:HD22	1.54	0.56
1:A:31:LEU:HB2	1:A:68:HIS:H	1.72	0.55
1:G:209:ARG:HH11	1:G:209:ARG:HG3	1.71	0.55
1:H:44:ARG:NH1	1:K:44:ARG:HH22	2.05	0.54
1:K:160:ILE:HG13	1:K:165:VAL:HG22	1.88	0.54
1:L:130:ALA:H	1:L:187:ASN:HD22	1.53	0.53
1:G:85:ALA:O	1:G:86:PHE:HB3	2.07	0.53
1:H:44:ARG:HH12	1:K:44:ARG:HH22	1.55	0.53
1:A:150:THR:HG23	2:C:268:HOH:O	2.09	0.52
1:G:130:ALA:H	1:G:187:ASN:ND2	2.06	0.52
1:L:161:GLY:O	1:L:165:VAL:HG23	2.09	0.52
1:E:111:LEU:HD13	1:E:199:VAL:HG21	1.91	0.52
1:D:205:ALA:O	1:D:209:ARG:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:HIS:HE2	1:B:84:ARG:N	2.08	0.51
1:F:130:ALA:H	1:F:187:ASN:ND2	2.05	0.51
1:G:160:ILE:HG13	1:G:165:VAL:HG22	1.92	0.51
1:C:216:ARG:NH1	1:C:243:HIS:ND1	2.59	0.51
1:K:152:PRO:O	1:K:156:VAL:HG23	2.11	0.51
1:B:160:ILE:HG13	1:B:165:VAL:HG22	1.92	0.50
1:L:98:MSE:HG3	1:L:122:GLN:NE2	2.27	0.50
1:L:88:THR:O	1:L:92:GLU:HB2	2.12	0.50
1:H:44:ARG:CZ	1:K:44:ARG:HH22	2.25	0.50
1:J:209:ARG:HH11	1:J:209:ARG:HG3	1.78	0.49
1:C:124:MSE:HE1	1:C:185:LEU:HG	1.94	0.49
1:G:149:OCS:HB2	1:G:152:PRO:HG2	1.94	0.49
1:F:174:THR:HG23	2:F:267:HOH:O	2.12	0.49
1:G:209:ARG:HH11	1:G:209:ARG:CG	2.24	0.49
1:H:130:ALA:H	1:H:187:ASN:HD22	1.59	0.49
1:K:85:ALA:O	1:K:86:PHE:HB3	2.13	0.49
1:K:245:MSE:HE2	1:L:82:GLU:HG3	1.93	0.49
1:L:139:CYS:HB3	1:L:174:THR:HA	1.93	0.49
1:B:13:VAL:HG22	2:B:274:HOH:O	2.14	0.48
1:E:31:LEU:HB2	1:E:68:HIS:H	1.77	0.48
1:A:160:ILE:HG13	1:A:165:VAL:HG22	1.95	0.48
1:L:26:ALA:HB2	1:L:29:HIS:H	1.77	0.48
1:G:115:ILE:HG12	1:G:117:THR:HG22	1.95	0.48
1:L:149:OCS:OD2	1:L:152:PRO:HG3	2.13	0.48
1:B:125:ALA:HA	1:C:163:ARG:NH2	2.29	0.48
1:D:31:LEU:HB2	1:D:68:HIS:H	1.79	0.48
1:H:44:ARG:HH22	1:K:44:ARG:NH2	2.09	0.48
1:G:163:ARG:HH21	1:I:125:ALA:HA	1.79	0.47
1:B:66:ALA:HA	1:B:117:THR:HG23	1.95	0.47
1:K:130:ALA:H	1:K:187:ASN:HD22	1.61	0.47
1:A:81:ASP:O	1:A:83:GLY:N	2.43	0.47
1:C:45:ARG:O	1:C:46:ALA:HB3	2.15	0.47
1:C:220:THR:HG23	1:C:235:LEU:HD22	1.96	0.47
1:F:31:LEU:HB2	1:F:68:HIS:H	1.80	0.47
1:J:88:THR:O	1:J:92:GLU:HB2	2.15	0.47
1:C:205:ALA:O	1:C:209:ARG:HG2	2.15	0.47
1:C:209:ARG:HH11	1:C:209:ARG:HG3	1.79	0.47
1:C:45:ARG:O	1:C:46:ALA:CB	2.63	0.47
1:H:31:LEU:HB2	1:H:68:HIS:H	1.80	0.47
1:H:44:ARG:HH12	1:K:44:ARG:NH2	2.12	0.47
1:J:124:MSE:SE	1:J:138:PHE:HE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:ALA:O	1:J:209:ARG:HG2	2.15	0.46
1:B:225:LEU:HD21	1:C:157:SER:HB2	1.98	0.46
1:E:160:ILE:HG13	1:E:165:VAL:HG22	1.97	0.46
1:I:45:ARG:O	1:I:46:ALA:HB3	2.15	0.46
1:H:139:CYS:HB2	1:H:174:THR:HG22	1.96	0.46
1:L:26:ALA:HB1	1:L:27:PRO:CA	2.44	0.46
1:D:82:GLU:HG2	1:D:84:ARG:H	1.79	0.46
1:L:160:ILE:HG13	1:L:165:VAL:HG22	1.98	0.46
1:G:241:VAL:HG13	1:H:87:VAL:HG12	1.99	0.45
1:J:112:VAL:HG21	1:J:124:MSE:SE	2.66	0.45
1:H:45:ARG:O	1:H:46:ALA:HB3	2.17	0.45
1:I:205:ALA:O	1:I:209:ARG:HG2	2.16	0.45
1:A:157:SER:HB2	1:C:225:LEU:HD21	1.98	0.44
1:H:43:LEU:HD11	1:H:101:LEU:HD13	1.98	0.44
1:G:122:GLN:HB2	1:G:152:PRO:HB3	1.99	0.44
1:H:88:THR:O	1:H:92:GLU:HB2	2.18	0.44
1:E:45:ARG:O	1:E:46:ALA:CB	2.65	0.44
1:K:43:LEU:O	1:K:47:MSE:HB2	2.17	0.44
1:C:112:VAL:O	1:C:132:ALA:HA	2.18	0.44
1:H:130:ALA:H	1:H:187:ASN:ND2	2.16	0.44
1:E:42:ALA:O	1:E:45:ARG:O	2.36	0.44
1:F:45:ARG:O	1:F:46:ALA:CB	2.66	0.44
1:C:29:HIS:N	1:C:30:PRO:HD3	2.33	0.44
1:C:43:LEU:O	1:C:47:MSE:HB2	2.18	0.44
1:G:45:ARG:O	1:G:46:ALA:CB	2.65	0.44
1:L:133:SER:HB3	1:L:195:LEU:HD22	1.99	0.43
1:A:163:ARG:HG3	1:C:184:GLY:O	2.17	0.43
1:C:112:VAL:HG21	1:C:124:MSE:SE	2.67	0.43
1:I:43:LEU:O	1:I:45:ARG:O	2.36	0.43
1:G:228:PRO:HD2	1:G:231:GLN:OE1	2.19	0.43
1:D:124:MSE:HE1	1:D:185:LEU:HG	2.01	0.43
1:F:42:ALA:O	1:F:45:ARG:O	2.37	0.43
1:I:112:VAL:HG21	1:I:124:MSE:SE	2.69	0.43
1:J:94:CYS:O	1:J:98:MSE:HG2	2.19	0.43
1:L:220:THR:HG23	1:L:235:LEU:HD13	2.00	0.43
1:L:209:ARG:HG3	1:L:209:ARG:HH11	1.83	0.43
1:G:209:ARG:HD2	1:H:143:VAL:O	2.18	0.43
1:E:236:ALA:HB1	1:F:150:THR:HG22	2.00	0.42
1:B:231:GLN:HA	1:B:231:GLN:HE21	1.84	0.42
1:F:88:THR:O	1:F:92:GLU:HB2	2.19	0.42
1:B:33:ARG:HH12	1:B:37:ALA:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ARG:HE	1:G:162:ARG:HB2	1.66	0.42
1:A:205:ALA:O	1:A:209:ARG:HG2	2.19	0.42
1:C:71:LYS:H	1:C:71:LYS:HG3	1.76	0.42
1:D:112:VAL:HG21	1:D:124:MSE:SE	2.69	0.42
1:I:31:LEU:HB2	1:I:68:HIS:H	1.85	0.42
1:J:245:MSE:HG2	1:K:84:ARG:NH2	2.35	0.42
1:K:45:ARG:O	1:K:46:ALA:HB3	2.19	0.42
1:L:45:ARG:O	1:L:46:ALA:CB	2.68	0.42
1:B:244:PHE:O	1:B:245:MSE:HE2	2.20	0.42
1:D:87:VAL:HG13	1:D:91:PHE:CE2	2.54	0.42
1:K:41:ASP:HB3	1:K:45:ARG:HH21	1.84	0.42
1:B:94:CYS:O	1:B:98:MSE:HG2	2.19	0.42
1:F:95:SER:O	1:F:99:LEU:HB2	2.19	0.41
1:A:124:MSE:SE	1:A:138:PHE:HE1	2.53	0.41
1:E:149:OCS:OD2	1:E:152:PRO:HG2	2.20	0.41
1:F:46:ALA:HB1	1:F:52:VAL:HG11	2.01	0.41
1:E:9:LEU:HD23	1:E:25:ARG:N	2.32	0.41
1:J:142:GLY:N	1:J:149:OCS:OD3	2.52	0.41
1:D:122:GLN:HB2	1:D:152:PRO:HB3	2.01	0.41
1:I:164:ALA:O	1:I:168:MSE:HG3	2.20	0.41
1:G:71:LYS:HE3	1:G:86:PHE:HZ	1.84	0.41
1:C:81:ASP:N	2:C:282:HOH:O	2.53	0.41
1:H:87:VAL:HG13	1:H:91:PHE:CE2	2.56	0.41
1:H:44:ARG:NH2	1:K:44:ARG:HH12	2.19	0.41
1:K:224:HIS:HB2	1:K:232:ALA:HB1	2.03	0.41
1:A:19:LEU:HB3	1:A:55:LEU:HD23	2.02	0.41
1:C:88:THR:O	1:C:92:GLU:HB2	2.21	0.41
1:C:106:LYS:HA	1:C:107:PRO:HD3	1.98	0.41
1:H:160:ILE:HG13	1:H:165:VAL:HG22	2.02	0.41
1:K:159:VAL:HG13	1:L:163:ARG:HG3	2.02	0.41
1:L:25:ARG:CG	1:L:26:ALA:H	2.34	0.41
1:L:66:ALA:HA	1:L:117:THR:HG23	2.03	0.40
1:E:71:LYS:NZ	1:E:86:PHE:HZ	2.18	0.40
1:H:125:ALA:HA	1:I:163:ARG:NH2	2.36	0.40
1:J:12:GLU:HB2	1:J:19:LEU:HD11	2.03	0.40
1:B:134:PRO:HG2	1:H:174:THR:OG1	2.22	0.40
1:D:137:ARG:HH21	1:D:176:ASP:HB3	1.85	0.40
1:K:187:ASN:HB3	1:L:167:GLU:OE2	2.22	0.40
1:G:170:LEU:HD21	1:I:218:LEU:HD12	2.04	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	227/263 (86%)	214 (94%)	9 (4%)	4 (2%)	6	5
1	B	229/263 (87%)	221 (96%)	8 (4%)	0	100	100
1	C	229/263 (87%)	216 (94%)	11 (5%)	2 (1%)	14	16
1	D	227/263 (86%)	216 (95%)	7 (3%)	4 (2%)	6	5
1	E	226/263 (86%)	216 (96%)	5 (2%)	5 (2%)	5	4
1	F	226/263 (86%)	217 (96%)	6 (3%)	3 (1%)	9	10
1	G	228/263 (87%)	218 (96%)	6 (3%)	4 (2%)	6	5
1	H	227/263 (86%)	218 (96%)	5 (2%)	4 (2%)	6	5
1	I	229/263 (87%)	218 (95%)	9 (4%)	2 (1%)	14	16
1	J	228/263 (87%)	213 (93%)	10 (4%)	5 (2%)	5	4
1	K	227/263 (86%)	214 (94%)	9 (4%)	4 (2%)	6	5
1	L	226/263 (86%)	208 (92%)	11 (5%)	7 (3%)	3	2
All	All	2729/3156 (86%)	2589 (95%)	96 (4%)	44 (2%)	7	7

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	D	86	PHE
1	G	46	ALA
1	G	86	PHE
1	K	86	PHE
1	L	46	ALA
1	C	46	ALA
1	E	26	ALA
1	E	46	ALA
1	E	67	GLY
1	F	46	ALA
1	G	26	ALA

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Mol	Chain	Res	Type
1	H	68	HIS
1	H	86	PHE
1	I	68	HIS
1	J	46	ALA
1	J	68	HIS
1	L	28	ALA
1	A	68	HIS
1	C	86	PHE
1	D	68	HIS
1	E	68	HIS
1	G	25	ARG
1	L	26	ALA
1	F	67	GLY
1	F	68	HIS
1	H	46	ALA
1	H	67	GLY
1	J	26	ALA
1	K	25	ARG
1	A	67	GLY
1	D	46	ALA
1	I	67	GLY
1	J	73	ILE
1	K	16	GLU
1	L	148	PHE
1	E	25	ARG
1	L	16	GLU
1	L	27	PRO
1	D	67	GLY
1	K	26	ALA
1	L	17	GLY
1	A	74	GLY
1	J	67	GLY

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	168/188 (89%)	152 (90%)	16 (10%)	8	10
1	B	169/188 (90%)	153 (90%)	16 (10%)	8	10
1	C	170/188 (90%)	158 (93%)	12 (7%)	13	18
1	D	169/188 (90%)	154 (91%)	15 (9%)	9	11
1	E	167/188 (89%)	151 (90%)	16 (10%)	8	10
1	F	168/188 (89%)	157 (94%)	11 (6%)	15	21
1	G	168/188 (89%)	150 (89%)	18 (11%)	6	7
1	H	168/188 (89%)	156 (93%)	12 (7%)	13	18
1	I	169/188 (90%)	153 (90%)	16 (10%)	8	10
1	J	168/188 (89%)	152 (90%)	16 (10%)	8	10
1	K	168/188 (89%)	154 (92%)	14 (8%)	10	13
1	L	168/188 (89%)	151 (90%)	17 (10%)	7	8
All	All	2020/2256 (90%)	1841 (91%)	179 (9%)	9	11

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	16	GLU
1	A	19	LEU
1	A	43	LEU
1	A	44	ARG
1	A	75	ARG
1	A	89	ASP
1	A	99	LEU
1	A	117	THR
1	A	159	VAL
1	A	165	VAL
1	A	206	LEU
1	A	211	GLN
1	A	218	LEU
1	A	224	HIS
1	A	229	LEU
1	B	10	LEU
1	B	41	ASP
1	B	73	ILE
1	B	87	VAL
1	B	99	LEU
1	B	117	THR

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Mol	Chain	Res	Type
1	B	141	PRO
1	B	165	VAL
1	B	190	LEU
1	B	192	GLU
1	B	209	ARG
1	B	214	LEU
1	B	218	LEU
1	B	224	HIS
1	B	230	GLU
1	B	231	GLN
1	C	9	LEU
1	C	10	LEU
1	C	25	ARG
1	C	40	HIS
1	C	43	LEU
1	C	92	GLU
1	C	99	LEU
1	C	100	ASP
1	C	174	THR
1	C	229	LEU
1	C	230	GLU
1	C	235	LEU
1	D	10	LEU
1	D	25	ARG
1	D	43	LEU
1	D	44	ARG
1	D	47	MSE
1	D	73	ILE
1	D	87	VAL
1	D	92	GLU
1	D	99	LEU
1	D	100	ASP
1	D	117	THR
1	D	137	ARG
1	D	143	VAL
1	D	165	VAL
1	D	229	LEU
1	E	10	LEU
1	E	43	LEU
1	E	92	GLU
1	E	99	LEU
1	E	100	ASP

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Mol	Chain	Res	Type
1	E	112	VAL
1	E	117	THR
1	E	141	PRO
1	E	165	VAL
1	E	190	LEU
1	E	192	GLU
1	E	206	LEU
1	E	214	LEU
1	E	218	LEU
1	E	224	HIS
1	E	229	LEU
1	F	40	HIS
1	F	43	LEU
1	F	71	LYS
1	F	92	GLU
1	F	99	LEU
1	F	100	ASP
1	F	117	THR
1	F	141	PRO
1	F	159	VAL
1	F	224	HIS
1	F	229	LEU
1	G	10	LEU
1	G	40	HIS
1	G	43	LEU
1	G	47	MSE
1	G	87	VAL
1	G	99	LEU
1	G	100	ASP
1	G	117	THR
1	G	165	VAL
1	G	190	LEU
1	G	202	LEU
1	G	209	ARG
1	G	214	LEU
1	G	218	LEU
1	G	224	HIS
1	G	229	LEU
1	G	235	LEU
1	G	245	MSE
1	H	10	LEU
1	H	25	ARG

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Mol	Chain	Res	Type
1	H	87	VAL
1	H	92	GLU
1	H	117	THR
1	H	141	PRO
1	H	165	VAL
1	H	202	LEU
1	H	214	LEU
1	H	224	HIS
1	H	229	LEU
1	H	235	LEU
1	I	25	ARG
1	I	40	HIS
1	I	43	LEU
1	I	47	MSE
1	I	55	LEU
1	I	87	VAL
1	I	92	GLU
1	I	99	LEU
1	I	141	PRO
1	I	159	VAL
1	I	165	VAL
1	I	190	LEU
1	I	192	GLU
1	I	214	LEU
1	I	231	GLN
1	I	235	LEU
1	J	10	LEU
1	J	40	HIS
1	J	43	LEU
1	J	47	MSE
1	J	72	GLU
1	J	92	GLU
1	J	99	LEU
1	J	100	ASP
1	J	165	VAL
1	J	190	LEU
1	J	202	LEU
1	J	216	ARG
1	J	218	LEU
1	J	224	HIS
1	J	235	LEU
1	J	245	MSE

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Mol	Chain	Res	Type
1	K	12	GLU
1	K	40	HIS
1	K	43	LEU
1	K	87	VAL
1	K	99	LEU
1	K	100	ASP
1	K	141	PRO
1	K	165	VAL
1	K	192	GLU
1	K	209	ARG
1	K	216	ARG
1	K	229	LEU
1	K	235	LEU
1	K	245	MSE
1	L	10	LEU
1	L	16	GLU
1	L	22	THR
1	L	39	LEU
1	L	99	LEU
1	L	100	ASP
1	L	111	LEU
1	L	117	THR
1	L	124	MSE
1	L	174	THR
1	L	190	LEU
1	L	192	GLU
1	L	202	LEU
1	L	224	HIS
1	L	229	LEU
1	L	231	GLN
1	L	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	198	HIS
1	A	231	GLN
1	B	122	GLN
1	B	187	ASN
1	B	198	HIS
1	B	231	GLN

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Mol	Chain	Res	Type
1	C	144	GLN
1	C	187	ASN
1	C	231	GLN
1	D	122	GLN
1	D	187	ASN
1	E	144	GLN
1	E	187	ASN
1	E	231	GLN
1	F	144	GLN
1	F	187	ASN
1	F	231	GLN
1	G	187	ASN
1	H	144	GLN
1	H	187	ASN
1	I	144	GLN
1	I	187	ASN
1	J	68	HIS
1	J	187	ASN
1	J	211	GLN
1	K	40	HIS
1	K	58	HIS
1	K	144	GLN
1	K	187	ASN
1	K	211	GLN
1	L	40	HIS
1	L	122	GLN
1	L	187	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	$\# Z > 2$
1	OCS	L	149	1	6,8,9	2.09	3 (50%)	7,11,13	3.34	2 (28%)
1	OCS	G	149	1	6,8,9	2.21	2 (33%)	7,11,13	2.91	3 (42%)
1	OCS	J	149	1	6,8,9	2.34	2 (33%)	7,11,13	3.29	3 (42%)
1	OCS	F	149	1	6,8,9	2.35	2 (33%)	7,11,13	2.75	3 (42%)
1	OCS	D	149	1	6,8,9	2.38	3 (50%)	7,11,13	2.60	3 (42%)
1	OCS	C	149	1	6,8,9	2.44	2 (33%)	7,11,13	3.08	5 (71%)
1	OCS	H	149	1	6,8,9	2.62	2 (33%)	7,11,13	3.17	4 (57%)
1	OCS	K	149	1	6,8,9	2.41	2 (33%)	7,11,13	2.96	3 (42%)
1	OCS	I	149	1	6,8,9	2.06	2 (33%)	7,11,13	2.76	3 (42%)
1	OCS	A	149	1	6,8,9	2.69	3 (50%)	7,11,13	2.74	3 (42%)
1	OCS	E	149	1	6,8,9	2.34	2 (33%)	7,11,13	2.49	3 (42%)
1	OCS	B	149	1	6,8,9	2.54	2 (33%)	7,11,13	2.97	5 (71%)

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
1	OCS	L	149	1	-	4/4/7/9	-
1	OCS	G	149	1	-	4/4/7/9	-
1	OCS	J	149	1	-	2/4/7/9	-
1	OCS	F	149	1	-	3/4/7/9	-
1	OCS	D	149	1	-	4/4/7/9	-
1	OCS	C	149	1	-	3/4/7/9	-
1	OCS	H	149	1	-	2/4/7/9	-
1	OCS	K	149	1	-	4/4/7/9	-
1	OCS	I	149	1	-	4/4/7/9	-
1	OCS	A	149	1	-	3/4/7/9	-
1	OCS	E	149	1	-	4/4/7/9	-
1	OCS	B	149	1	-	3/4/7/9	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	149	OCS	OD3-SG	-5.08	1.30	1.45
1	A	149	OCS	OD3-SG	-4.73	1.31	1.45
1	J	149	OCS	OD3-SG	-4.61	1.32	1.45
1	B	149	OCS	OD3-SG	-4.25	1.33	1.45
1	G	149	OCS	OD3-SG	-4.20	1.33	1.45
1	F	149	OCS	OD3-SG	-4.09	1.33	1.45
1	E	149	OCS	OD3-SG	-3.93	1.34	1.45
1	C	149	OCS	OD1-SG	-3.92	1.34	1.45
1	B	149	OCS	OD1-SG	-3.90	1.34	1.45
1	K	149	OCS	OD3-SG	-3.88	1.34	1.45
1	C	149	OCS	OD3-SG	-3.87	1.34	1.45
1	K	149	OCS	OD1-SG	-3.77	1.34	1.45
1	D	149	OCS	OD3-SG	-3.77	1.34	1.45
1	A	149	OCS	OD1-SG	-3.67	1.34	1.45
1	E	149	OCS	OD1-SG	-3.67	1.34	1.45
1	H	149	OCS	OD1-SG	-3.60	1.35	1.45
1	I	149	OCS	OD3-SG	-3.60	1.35	1.45
1	F	149	OCS	OD1-SG	-3.42	1.35	1.45
1	D	149	OCS	OD1-SG	-3.41	1.35	1.45
1	L	149	OCS	OD3-SG	-3.28	1.35	1.45
1	I	149	OCS	OD1-SG	-3.13	1.36	1.45
1	J	149	OCS	OD1-SG	-3.03	1.36	1.45
1	G	149	OCS	OD1-SG	-2.72	1.37	1.45
1	L	149	OCS	CB-CA	-2.66	1.51	1.53
1	D	149	OCS	CB-CA	-2.41	1.51	1.53
1	L	149	OCS	OD1-SG	-2.37	1.38	1.45
1	A	149	OCS	CB-CA	-2.28	1.52	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	149	OCS	OD1-SG-CB	-5.96	97.86	106.76
1	J	149	OCS	OD1-SG-CB	-5.94	97.89	106.76
1	L	149	OCS	OD2-SG-CB	5.67	116.92	105.97
1	H	149	OCS	OD1-SG-CB	-5.28	98.87	106.76
1	K	149	OCS	OD1-SG-CB	-5.25	98.91	106.76
1	G	149	OCS	OD1-SG-CB	-5.24	98.93	106.76
1	H	149	OCS	OD2-SG-CB	5.08	115.79	105.97
1	J	149	OCS	OD2-SG-CB	4.90	115.44	105.97
1	A	149	OCS	OD1-SG-CB	-4.68	99.77	106.76
1	B	149	OCS	OD1-SG-CB	-4.59	99.90	106.76
1	K	149	OCS	OD2-SG-CB	4.49	114.64	105.97
1	I	149	OCS	OD2-SG-CB	4.48	114.63	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	149	OCS	OD1-SG-CB	-4.43	100.14	106.76
1	D	149	OCS	OD1-SG-CB	-4.38	100.22	106.76
1	C	149	OCS	OD2-SG-CB	4.35	114.38	105.97
1	A	149	OCS	OD2-SG-CB	4.30	114.28	105.97
1	C	149	OCS	OD1-SG-CB	-4.30	100.34	106.76
1	C	149	OCS	CA-CB-SG	-4.11	107.50	113.61
1	B	149	OCS	OD2-SG-CB	4.07	113.84	105.97
1	F	149	OCS	OD1-SG-CB	-3.97	100.83	106.76
1	F	149	OCS	OD2-SG-CB	3.90	113.51	105.97
1	E	149	OCS	OD2-SG-CB	3.90	113.50	105.97
1	G	149	OCS	OD2-SG-CB	3.88	113.45	105.97
1	F	149	OCS	CA-CB-SG	-3.87	107.86	113.61
1	E	149	OCS	OD1-SG-CB	-3.85	101.01	106.76
1	D	149	OCS	OD2-SG-CB	3.63	112.98	105.97
1	G	149	OCS	OD3-SG-CB	3.16	111.48	106.76
1	B	149	OCS	OD3-SG-CB	3.14	111.44	106.76
1	J	149	OCS	CA-CB-SG	3.09	118.20	113.61
1	K	149	OCS	OD3-SG-CB	2.80	110.94	106.76
1	D	149	OCS	OD3-SG-CB	2.76	110.87	106.76
1	H	149	OCS	OD2-SG-OD1	-2.55	105.01	111.40
1	E	149	OCS	OD2-SG-OD3	-2.47	105.22	111.40
1	B	149	OCS	CA-CB-SG	-2.37	110.09	113.61
1	B	149	OCS	OD2-SG-OD1	-2.14	106.05	111.40
1	I	149	OCS	OD2-SG-OD3	-2.13	106.06	111.40
1	H	149	OCS	CA-CB-SG	2.09	116.71	113.61
1	C	149	OCS	OD2-SG-OD3	-2.07	106.21	111.40
1	A	149	OCS	OD3-SG-CB	2.02	109.78	106.76
1	C	149	OCS	OD3-SG-CB	2.01	109.76	106.76

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	149	OCS	CA-CB-SG-OD2
1	B	149	OCS	CA-CB-SG-OD2
1	C	149	OCS	CA-CB-SG-OD2
1	D	149	OCS	N-CA-CB-SG
1	D	149	OCS	CA-CB-SG-OD2
1	E	149	OCS	N-CA-CB-SG
1	E	149	OCS	CA-CB-SG-OD1
1	E	149	OCS	CA-CB-SG-OD2
1	E	149	OCS	CA-CB-SG-OD3

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Mol	Chain	Res	Type	Atoms
1	F	149	OCS	CA-CB-SG-OD1
1	F	149	OCS	CA-CB-SG-OD2
1	G	149	OCS	N-CA-CB-SG
1	G	149	OCS	CA-CB-SG-OD2
1	H	149	OCS	CA-CB-SG-OD2
1	I	149	OCS	N-CA-CB-SG
1	I	149	OCS	CA-CB-SG-OD1
1	I	149	OCS	CA-CB-SG-OD2
1	I	149	OCS	CA-CB-SG-OD3
1	J	149	OCS	CA-CB-SG-OD2
1	K	149	OCS	N-CA-CB-SG
1	K	149	OCS	CA-CB-SG-OD2
1	L	149	OCS	N-CA-CB-SG
1	L	149	OCS	CA-CB-SG-OD1
1	L	149	OCS	CA-CB-SG-OD2
1	A	149	OCS	CA-CB-SG-OD3
1	B	149	OCS	CA-CB-SG-OD3
1	C	149	OCS	CA-CB-SG-OD3
1	D	149	OCS	CA-CB-SG-OD3
1	F	149	OCS	CA-CB-SG-OD3
1	G	149	OCS	CA-CB-SG-OD3
1	K	149	OCS	CA-CB-SG-OD3
1	L	149	OCS	CA-CB-SG-OD3
1	A	149	OCS	CA-CB-SG-OD1
1	C	149	OCS	CA-CB-SG-OD1
1	D	149	OCS	CA-CB-SG-OD1
1	H	149	OCS	CA-CB-SG-OD3
1	J	149	OCS	CA-CB-SG-OD3
1	K	149	OCS	CA-CB-SG-OD1
1	G	149	OCS	CA-CB-SG-OD1
1	B	149	OCS	CA-CB-SG-OD1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	149	OCS	1	0
1	G	149	OCS	1	0
1	J	149	OCS	1	0
1	E	149	OCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/263 (85%)	-1.18	0 100 100	14, 36, 52, 62	0
1	B	226/263 (85%)	-1.28	0 100 100	15, 28, 46, 55	0
1	C	226/263 (85%)	-1.30	0 100 100	15, 30, 47, 56	0
1	D	224/263 (85%)	-1.20	0 100 100	15, 33, 49, 59	0
1	E	223/263 (84%)	-1.23	0 100 100	18, 34, 49, 58	0
1	F	223/263 (84%)	-1.25	0 100 100	17, 31, 45, 58	0
1	G	225/263 (85%)	-1.16	0 100 100	20, 35, 51, 66	0
1	H	224/263 (85%)	-1.10	0 100 100	20, 40, 54, 65	0
1	I	226/263 (85%)	-1.15	0 100 100	16, 38, 52, 59	0
1	J	225/263 (85%)	-1.10	0 100 100	20, 38, 53, 59	0
1	K	224/263 (85%)	-0.98	0 100 100	21, 46, 60, 66	0
1	L	223/263 (84%)	-0.94	0 100 100	21, 50, 61, 63	0
All	All	2693/3156 (85%)	-1.15	0 100 100	14, 36, 55, 66	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OCS	L	149	9/10	0.98	0.04	46,48,51,51	0
1	OCS	B	149	9/10	0.99	0.06	32,35,41,42	0
1	OCS	D	149	9/10	0.99	0.05	29,32,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OCS	E	149	9/10	0.99	0.05	30,30,39,40	0
1	OCS	F	149	9/10	0.99	0.03	30,32,38,38	0
1	OCS	G	149	9/10	0.99	0.03	25,33,42,43	0
1	OCS	H	149	9/10	0.99	0.04	34,34,38,40	0
1	OCS	I	149	9/10	0.99	0.02	34,36,45,46	0
1	OCS	J	149	9/10	0.99	0.03	36,37,46,46	0
1	OCS	K	149	9/10	0.99	0.03	35,36,40,40	0
1	OCS	A	149	9/10	0.99	0.03	25,28,32,33	0
1	OCS	C	149	9/10	1.00	0.02	22,23,35,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.