



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:49 PM GMT

PDB ID : 1CJ1
Title : GROWTH FACTOR RECEPTOR BINDING PROTEIN SH2 DOMAIN (HUMAN) COMPLEXED WITH A PHOSPHOTYROSYL DERIVATIVE
Authors : Rahuel, J.
Deposited on : 1999-04-21
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

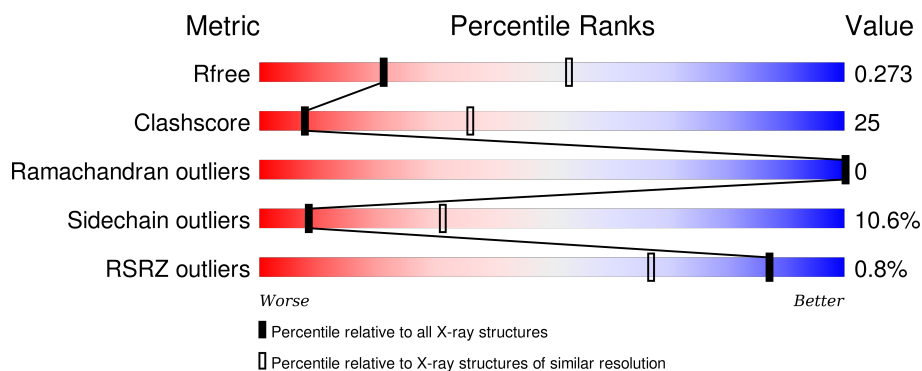
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	96	
1	B	96	
1	C	96	
1	D	96	
1	E	96	

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Mol	Chain	Length	Quality of chain
1	F	96	
1	G	96	
1	H	96	
1	I	96	
1	J	96	
1	K	96	
1	L	96	

2 Entry composition

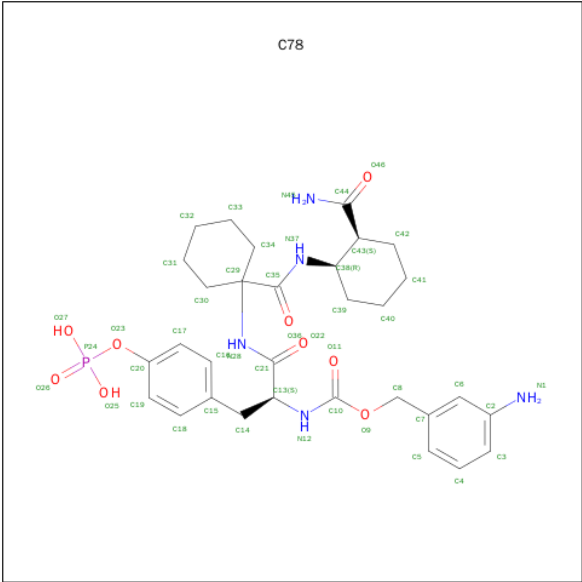
There are 3 unique types of molecules in this entry. The entry contains 10060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	B	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	C	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	D	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	E	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	F	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	G	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	H	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	I	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	J	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	K	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			
1	L	96	Total	C	N	O	S	0	0	0
			792	509	142	140	1			

- Molecule 2 is [1-[1-(6-CARBAMOYL-CYCLOHEX-2-ENYLCARBAMOYL)-CYCLOHEXYLCARBAMOYL]-2-(4-PHOSPHONOOXY-PHENYL)-ETHYL]-CARBAMIC ACID 3-AMINO BENZYLESTER (three-letter code: C78) (formula: C₃₁H₄₂N₅O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	B	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	C	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	D	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	E	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	F	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	G	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	H	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	I	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	J	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	K	1	Total	C	N	O	P	0	0
			46	31	5	9	1		
2	L	1	Total	C	N	O	P	0	0
			46	31	5	9	1		

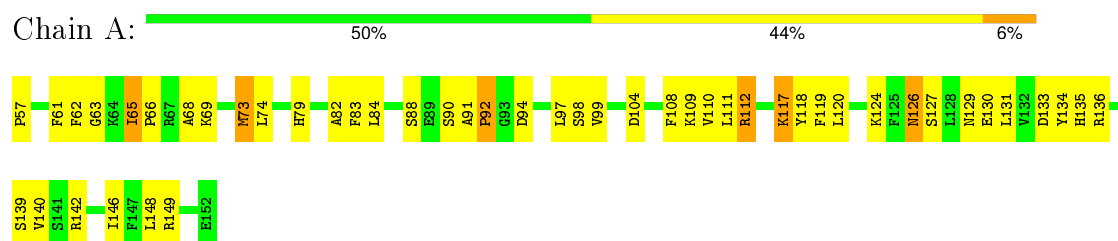
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		

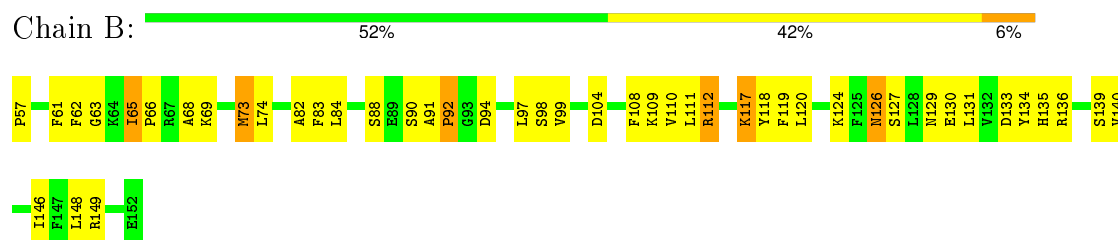
3 Residue-property plots

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

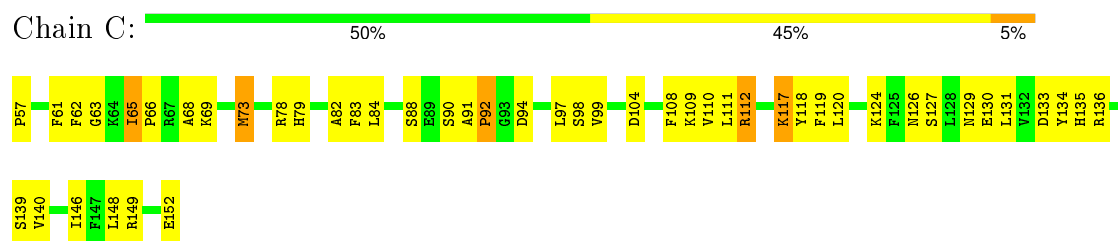
• Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



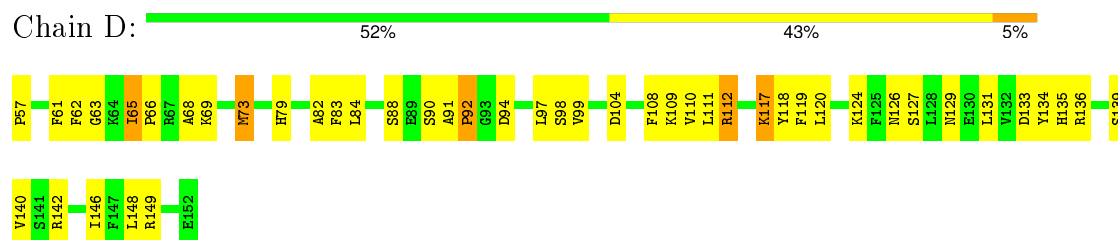
• Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



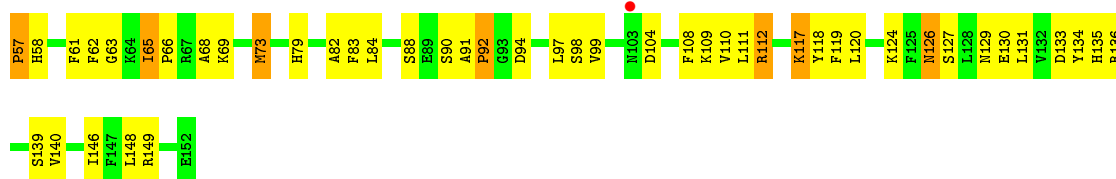
• Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



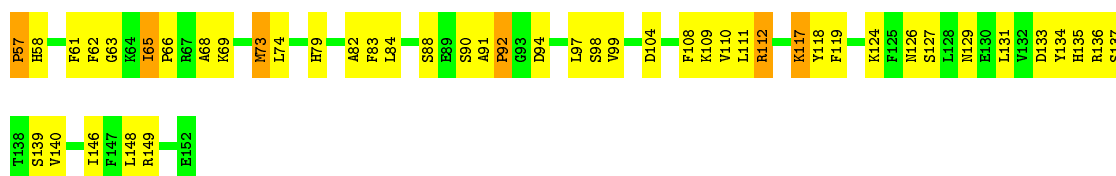
• Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



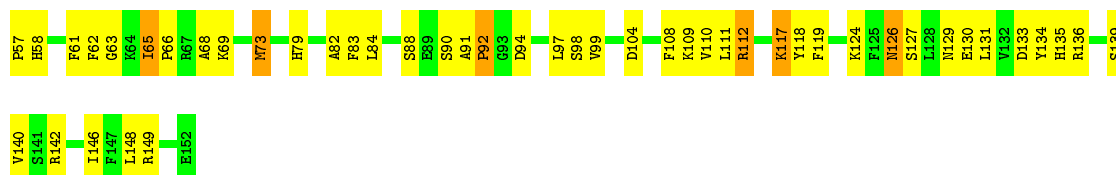
- Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



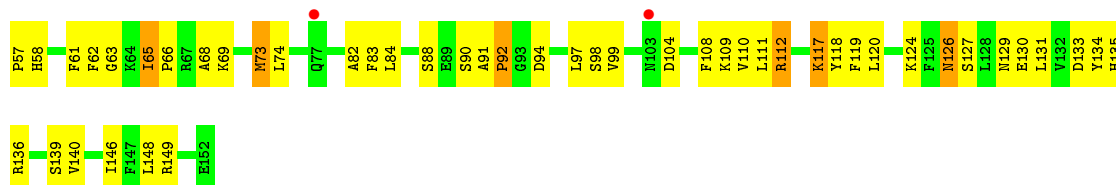
- Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



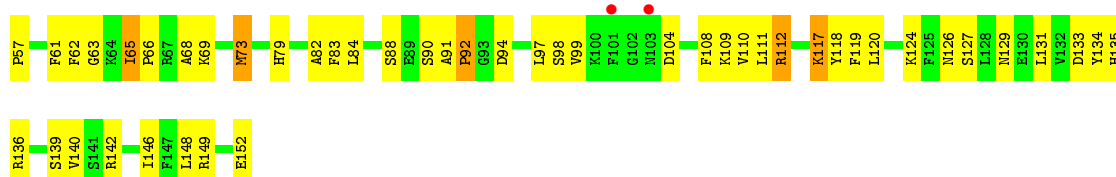
- Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



- Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)

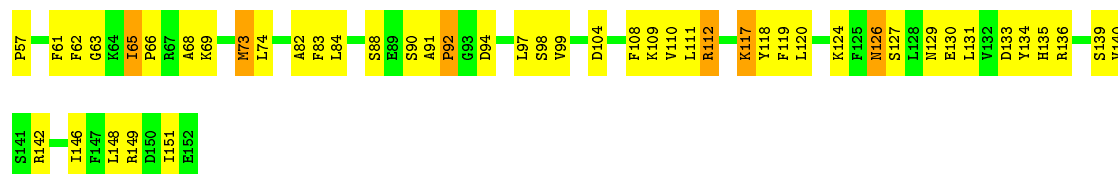


- Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)



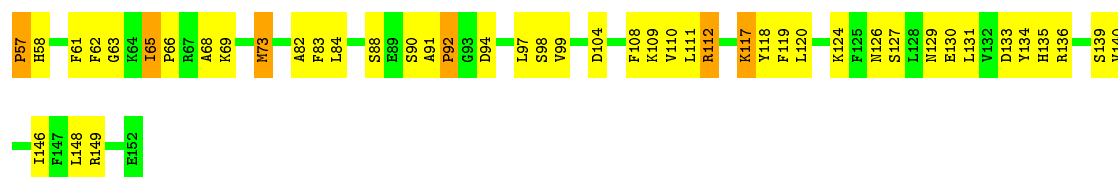
• Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)

Chain J: 



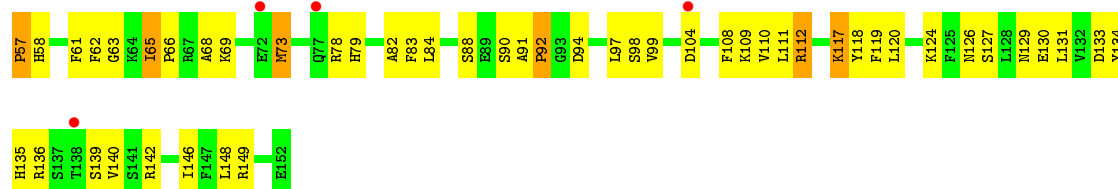
• Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)

Chain K: 



• Molecule 1: PROTEIN (GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2)

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.80 Å 93.30 Å 232.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 3.00 30.05 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (31.00-3.00) 90.0 (30.05-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	20.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.00 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.305 , 0.317 0.261 , 0.273	Depositor DCC
R_{free} test set	1436 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 31892 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10060	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: C78

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	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	B	1.31	3/814 (0.4%)	1.24	3/1094 (0.3%)
1	C	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	D	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	E	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	F	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	G	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	H	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	I	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	J	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	K	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
1	L	1.31	3/814 (0.4%)	1.23	3/1094 (0.3%)
All	All	1.31	36/9768 (0.4%)	1.23	36/13128 (0.3%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	68	ALA	CA-CB	-6.17	1.39	1.52
1	E	68	ALA	CA-CB	-6.17	1.39	1.52
1	H	68	ALA	CA-CB	-6.17	1.39	1.52
1	K	68	ALA	CA-CB	-6.17	1.39	1.52
1	G	68	ALA	CA-CB	-6.16	1.39	1.52
1	C	68	ALA	CA-CB	-6.16	1.39	1.52
1	B	68	ALA	CA-CB	-6.16	1.39	1.52
1	A	68	ALA	CA-CB	-6.16	1.39	1.52
1	D	68	ALA	CA-CB	-6.15	1.39	1.52
1	J	68	ALA	CA-CB	-6.15	1.39	1.52
1	I	68	ALA	CA-CB	-6.13	1.39	1.52
1	F	68	ALA	CA-CB	-6.13	1.39	1.52
1	J	110	VAL	CB-CG2	-5.64	1.41	1.52
1	C	110	VAL	CB-CG2	-5.63	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	110	VAL	CB-CG2	-5.62	1.41	1.52
1	K	110	VAL	CB-CG2	-5.62	1.41	1.52
1	A	110	VAL	CB-CG2	-5.62	1.41	1.52
1	L	110	VAL	CB-CG2	-5.62	1.41	1.52
1	G	110	VAL	CB-CG2	-5.61	1.41	1.52
1	E	110	VAL	CB-CG2	-5.60	1.41	1.52
1	I	110	VAL	CB-CG2	-5.59	1.41	1.52
1	H	110	VAL	CB-CG2	-5.59	1.41	1.52
1	B	110	VAL	CB-CG2	-5.59	1.41	1.52
1	F	110	VAL	CB-CG2	-5.58	1.41	1.52
1	C	73	MET	SD-CE	5.08	2.06	1.77
1	I	73	MET	SD-CE	5.08	2.06	1.77
1	F	73	MET	SD-CE	5.08	2.06	1.77
1	D	73	MET	SD-CE	5.08	2.06	1.77
1	G	73	MET	SD-CE	5.08	2.06	1.77
1	H	73	MET	SD-CE	5.07	2.06	1.77
1	A	73	MET	SD-CE	5.07	2.06	1.77
1	B	73	MET	SD-CE	5.06	2.06	1.77
1	K	73	MET	SD-CE	5.06	2.06	1.77
1	L	73	MET	SD-CE	5.06	2.06	1.77
1	J	73	MET	SD-CE	5.06	2.06	1.77
1	E	73	MET	SD-CE	5.06	2.06	1.77

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	57	PRO	N-CA-CB	7.40	112.19	103.30
1	B	57	PRO	N-CA-CB	7.39	112.17	103.30
1	G	57	PRO	N-CA-CB	7.39	112.17	103.30
1	F	57	PRO	N-CA-CB	7.39	112.17	103.30
1	D	57	PRO	N-CA-CB	7.39	112.16	103.30
1	H	57	PRO	N-CA-CB	7.39	112.16	103.30
1	J	57	PRO	N-CA-CB	7.38	112.16	103.30
1	E	57	PRO	N-CA-CB	7.38	112.15	103.30
1	A	57	PRO	N-CA-CB	7.37	112.15	103.30
1	L	57	PRO	N-CA-CB	7.37	112.14	103.30
1	C	57	PRO	N-CA-CB	7.36	112.13	103.30
1	K	57	PRO	N-CA-CB	7.35	112.12	103.30
1	J	99	VAL	CB-CA-C	-5.98	100.04	111.40
1	K	99	VAL	CB-CA-C	-5.97	100.06	111.40
1	B	99	VAL	CB-CA-C	-5.97	100.06	111.40
1	I	99	VAL	CB-CA-C	-5.97	100.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	99	VAL	CB-CA-C	-5.97	100.06	111.40
1	H	99	VAL	CB-CA-C	-5.96	100.07	111.40
1	A	99	VAL	CB-CA-C	-5.96	100.09	111.40
1	E	99	VAL	CB-CA-C	-5.96	100.09	111.40
1	C	99	VAL	CB-CA-C	-5.95	100.09	111.40
1	G	99	VAL	CB-CA-C	-5.95	100.10	111.40
1	F	99	VAL	CB-CA-C	-5.94	100.11	111.40
1	D	99	VAL	CB-CA-C	-5.93	100.14	111.40
1	G	57	PRO	CA-N-CD	-5.76	103.44	111.50
1	H	57	PRO	CA-N-CD	-5.76	103.44	111.50
1	F	57	PRO	CA-N-CD	-5.75	103.45	111.50
1	D	57	PRO	CA-N-CD	-5.74	103.46	111.50
1	J	57	PRO	CA-N-CD	-5.74	103.47	111.50
1	I	57	PRO	CA-N-CD	-5.73	103.47	111.50
1	E	57	PRO	CA-N-CD	-5.73	103.48	111.50
1	B	57	PRO	CA-N-CD	-5.72	103.48	111.50
1	A	57	PRO	CA-N-CD	-5.72	103.49	111.50
1	K	57	PRO	CA-N-CD	-5.72	103.49	111.50
1	L	57	PRO	CA-N-CD	-5.72	103.50	111.50
1	C	57	PRO	CA-N-CD	-5.69	103.53	111.50

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	792	0	772	46	0
1	B	792	0	772	45	0
1	C	792	0	772	41	2
1	D	792	0	772	39	0
1	E	792	0	772	50	1
1	F	792	0	772	46	1
1	G	792	0	772	44	0
1	H	792	0	772	47	0
1	I	792	0	772	38	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	792	0	772	43	0
1	K	792	0	772	41	0
1	L	792	0	772	47	1
2	A	46	0	40	0	0
2	B	46	0	40	0	0
2	C	46	0	40	0	0
2	D	46	0	40	0	0
2	E	46	0	40	0	0
2	F	46	0	40	0	0
2	G	46	0	40	0	0
2	H	46	0	40	0	0
2	I	46	0	40	0	0
2	J	46	0	40	0	0
2	K	46	0	40	0	0
2	L	46	0	40	0	0
3	A	4	0	0	0	0
All	All	10060	0	9744	497	3

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 25.

All (497) 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:L:73:MET:CE	1:L:73:MET:SD	2.06	1.44
1:G:73:MET:CE	1:G:73:MET:SD	2.06	1.44
1:I:73:MET:SD	1:I:73:MET:CE	2.06	1.44
1:B:73:MET:SD	1:B:73:MET:CE	2.06	1.44
1:K:73:MET:SD	1:K:73:MET:CE	2.06	1.44
1:D:73:MET:SD	1:D:73:MET:CE	2.06	1.44
1:E:73:MET:SD	1:E:73:MET:CE	2.06	1.43
1:F:73:MET:CE	1:F:73:MET:SD	2.06	1.43
1:A:73:MET:SD	1:A:73:MET:CE	2.06	1.43
1:J:73:MET:SD	1:J:73:MET:CE	2.06	1.43
1:H:73:MET:SD	1:H:73:MET:CE	2.06	1.43
1:C:73:MET:CE	1:C:73:MET:SD	2.06	1.43
1:E:73:MET:HB3	1:E:73:MET:CE	1.86	1.05
1:J:73:MET:HB3	1:J:73:MET:CE	1.86	1.05
1:F:73:MET:HB3	1:F:73:MET:CE	1.86	1.05
1:C:73:MET:HB3	1:C:73:MET:CE	1.86	1.05
1:H:73:MET:HB3	1:H:73:MET:CE	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:MET:HB3	1:B:73:MET:CE	1.86	1.04
1:K:73:MET:HB3	1:K:73:MET:CE	1.86	1.04
1:A:73:MET:HB3	1:A:73:MET:CE	1.86	1.04
1:L:73:MET:CE	1:L:73:MET:HB3	1.86	1.04
1:I:73:MET:HB3	1:I:73:MET:CE	1.86	1.03
1:G:73:MET:CE	1:G:73:MET:HB3	1.86	1.03
1:D:73:MET:HB3	1:D:73:MET:CE	1.86	1.03
1:A:73:MET:HE3	1:A:73:MET:HB3	1.48	0.95
1:I:73:MET:HB3	1:I:73:MET:HE3	1.47	0.94
1:G:73:MET:HB3	1:G:73:MET:HE3	1.47	0.94
1:K:57:PRO:HB3	1:L:62:PHE:CZ	2.08	0.88
1:K:62:PHE:CZ	1:L:57:PRO:HB3	2.09	0.88
1:K:57:PRO:HB3	1:L:62:PHE:CE1	2.09	0.87
1:K:73:MET:HB3	1:K:73:MET:HE3	1.55	0.86
1:K:62:PHE:CE1	1:L:57:PRO:HB3	2.12	0.84
1:E:57:PRO:HB3	1:F:62:PHE:CZ	2.12	0.84
1:E:58:HIS:CD2	1:F:63:GLY:HA3	2.12	0.84
1:F:73:MET:HB3	1:F:73:MET:HE3	1.57	0.83
1:L:73:MET:CE	1:L:73:MET:CB	2.57	0.83
1:F:73:MET:CE	1:F:73:MET:CB	2.57	0.83
1:G:73:MET:CB	1:G:73:MET:CE	2.57	0.82
1:I:73:MET:CB	1:I:73:MET:CE	2.57	0.82
1:J:73:MET:CB	1:J:73:MET:CE	2.57	0.82
1:E:73:MET:CB	1:E:73:MET:CE	2.57	0.82
1:K:73:MET:CB	1:K:73:MET:CE	2.57	0.82
1:D:73:MET:HB3	1:D:73:MET:HE3	1.61	0.82
1:A:73:MET:CE	1:A:73:MET:CB	2.57	0.82
1:C:73:MET:CE	1:C:73:MET:CB	2.57	0.81
1:B:73:MET:CB	1:B:73:MET:CE	2.57	0.81
1:D:73:MET:CB	1:D:73:MET:CE	2.57	0.81
1:H:73:MET:CB	1:H:73:MET:CE	2.57	0.81
1:E:57:PRO:HB3	1:F:62:PHE:CE1	2.17	0.78
1:E:62:PHE:CZ	1:F:57:PRO:HB3	2.20	0.77
1:E:73:MET:HB3	1:E:73:MET:HE3	1.65	0.76
1:C:73:MET:HB3	1:C:73:MET:HE3	1.69	0.74
1:D:88:SER:HB3	1:D:91:ALA:O	1.88	0.74
1:L:88:SER:HB3	1:L:91:ALA:O	1.88	0.74
1:F:88:SER:HB3	1:F:91:ALA:O	1.88	0.74
1:E:88:SER:HB3	1:E:91:ALA:O	1.88	0.74
1:C:88:SER:HB3	1:C:91:ALA:O	1.88	0.74
1:A:88:SER:HB3	1:A:91:ALA:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:SER:HB3	1:H:91:ALA:O	1.88	0.73
1:J:88:SER:HB3	1:J:91:ALA:O	1.88	0.73
1:G:88:SER:HB3	1:G:91:ALA:O	1.88	0.73
1:I:88:SER:HB3	1:I:91:ALA:O	1.88	0.73
1:B:88:SER:HB3	1:B:91:ALA:O	1.88	0.72
1:K:88:SER:HB3	1:K:91:ALA:O	1.88	0.72
1:L:73:MET:HE3	1:L:73:MET:HB3	1.69	0.71
1:J:73:MET:HB3	1:J:73:MET:HE2	1.72	0.71
1:B:73:MET:HB3	1:B:73:MET:HE3	1.69	0.70
1:H:73:MET:HB3	1:H:73:MET:HE3	1.72	0.68
1:H:73:MET:HB3	1:H:73:MET:HE2	1.74	0.67
1:J:73:MET:HB3	1:J:73:MET:HE3	1.75	0.66
1:I:131:LEU:HD23	1:I:131:LEU:C	2.16	0.66
1:D:131:LEU:C	1:D:131:LEU:HD23	2.16	0.66
1:H:131:LEU:HD23	1:H:131:LEU:C	2.16	0.66
1:G:131:LEU:C	1:G:131:LEU:HD23	2.16	0.66
1:A:131:LEU:HD23	1:A:131:LEU:C	2.16	0.66
1:J:131:LEU:HD23	1:J:131:LEU:C	2.16	0.66
1:C:131:LEU:C	1:C:131:LEU:HD23	2.16	0.66
1:L:131:LEU:HD23	1:L:131:LEU:C	2.16	0.66
1:E:131:LEU:HD23	1:E:131:LEU:C	2.16	0.65
1:A:126:ASN:HB3	1:B:92:PRO:HB3	1.77	0.65
1:K:131:LEU:HD23	1:K:131:LEU:C	2.16	0.65
1:B:131:LEU:HD23	1:B:131:LEU:C	2.16	0.65
1:F:131:LEU:C	1:F:131:LEU:HD23	2.16	0.65
1:B:73:MET:HB3	1:B:73:MET:HE2	1.77	0.64
1:A:119:PHE:CE1	1:A:124:LYS:HE2	2.32	0.64
1:C:119:PHE:CE1	1:C:124:LYS:HE2	2.32	0.64
1:K:119:PHE:CE1	1:K:124:LYS:HE2	2.32	0.64
1:A:92:PRO:HB3	1:B:126:ASN:HB3	1.79	0.64
1:I:119:PHE:CE1	1:I:124:LYS:HE2	2.32	0.64
1:D:119:PHE:CE1	1:D:124:LYS:HE2	2.32	0.64
1:E:119:PHE:CE1	1:E:124:LYS:HE2	2.32	0.64
1:G:119:PHE:CE1	1:G:124:LYS:HE2	2.32	0.64
1:L:119:PHE:CE1	1:L:124:LYS:HE2	2.32	0.63
1:F:119:PHE:CE1	1:F:124:LYS:HE2	2.32	0.63
1:H:119:PHE:CE1	1:H:124:LYS:HE2	2.32	0.63
1:J:119:PHE:CE1	1:J:124:LYS:HE2	2.32	0.63
1:K:133:ASP:O	1:K:136:ARG:HB2	1.99	0.63
1:I:133:ASP:O	1:I:136:ARG:HB2	1.99	0.63
1:C:133:ASP:O	1:C:136:ARG:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:ASP:O	1:G:136:ARG:HB2	1.99	0.62
1:B:119:PHE:CE1	1:B:124:LYS:HE2	2.32	0.62
1:H:133:ASP:O	1:H:136:ARG:HB2	1.99	0.62
1:L:133:ASP:O	1:L:136:ARG:HB2	1.99	0.62
1:E:133:ASP:O	1:E:136:ARG:HB2	1.99	0.62
1:A:112:ARG:HH21	1:B:112:ARG:NH2	1.97	0.62
1:F:133:ASP:O	1:F:136:ARG:HB2	1.99	0.62
1:J:133:ASP:O	1:J:136:ARG:HB2	1.99	0.62
1:B:133:ASP:O	1:B:136:ARG:HB2	1.99	0.62
1:D:133:ASP:O	1:D:136:ARG:HB2	1.99	0.61
1:A:133:ASP:O	1:A:136:ARG:HB2	1.99	0.61
1:C:73:MET:HB3	1:C:73:MET:HE2	1.77	0.61
1:A:112:ARG:NH2	1:B:112:ARG:NH2	2.48	0.61
1:E:73:MET:HB3	1:E:73:MET:HE2	1.82	0.60
1:A:112:ARG:NH2	1:B:112:ARG:HH21	1.98	0.60
1:K:58:HIS:CD2	1:L:63:GLY:HA3	2.36	0.59
1:L:112:ARG:HG2	1:L:117:LYS:O	2.04	0.58
1:K:112:ARG:HG2	1:K:117:LYS:O	2.04	0.58
1:J:112:ARG:HG2	1:J:117:LYS:O	2.04	0.57
1:H:112:ARG:HG2	1:H:117:LYS:O	2.04	0.57
1:A:112:ARG:HG2	1:A:117:LYS:O	2.04	0.57
1:E:112:ARG:HG2	1:E:117:LYS:O	2.04	0.57
1:L:73:MET:HE2	1:L:73:MET:HB3	1.77	0.57
1:B:69:LYS:O	1:B:73:MET:HG3	2.05	0.57
1:C:112:ARG:HG2	1:C:117:LYS:O	2.04	0.57
1:G:112:ARG:HG2	1:G:117:LYS:O	2.04	0.57
1:I:112:ARG:HG2	1:I:117:LYS:O	2.04	0.57
1:L:69:LYS:O	1:L:73:MET:HG3	2.05	0.56
1:C:69:LYS:O	1:C:73:MET:HG3	2.05	0.56
1:B:112:ARG:HG2	1:B:117:LYS:O	2.04	0.56
1:I:69:LYS:O	1:I:73:MET:HG3	2.05	0.56
1:E:58:HIS:HD2	1:F:63:GLY:HA3	1.65	0.56
1:F:112:ARG:HG2	1:F:117:LYS:O	2.04	0.56
1:K:63:GLY:HA3	1:L:58:HIS:CD2	2.40	0.56
1:G:69:LYS:O	1:G:73:MET:HG3	2.05	0.56
1:K:69:LYS:O	1:K:73:MET:HG3	2.05	0.56
1:E:69:LYS:O	1:E:73:MET:HG3	2.05	0.56
1:J:69:LYS:O	1:J:73:MET:HG3	2.05	0.56
1:D:112:ARG:HG2	1:D:117:LYS:O	2.04	0.56
1:F:69:LYS:O	1:F:73:MET:HG3	2.05	0.56
1:H:69:LYS:O	1:H:73:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LYS:O	1:D:73:MET:HG3	2.05	0.56
1:E:82:ALA:HA	1:E:149:ARG:O	2.06	0.56
1:K:82:ALA:HA	1:K:149:ARG:O	2.06	0.56
1:G:92:PRO:HB3	1:H:126:ASN:HB3	1.88	0.56
1:D:82:ALA:HA	1:D:149:ARG:O	2.06	0.56
1:F:82:ALA:HA	1:F:149:ARG:O	2.06	0.55
1:A:82:ALA:HA	1:A:149:ARG:O	2.06	0.55
1:B:82:ALA:HA	1:B:149:ARG:O	2.06	0.55
1:I:82:ALA:HA	1:I:149:ARG:O	2.06	0.55
1:A:69:LYS:O	1:A:73:MET:HG3	2.05	0.55
1:G:82:ALA:HA	1:G:149:ARG:O	2.06	0.55
1:F:119:PHE:CD1	1:F:124:LYS:HE2	2.42	0.55
1:L:82:ALA:HA	1:L:149:ARG:O	2.06	0.55
1:H:82:ALA:HA	1:H:149:ARG:O	2.06	0.55
1:D:119:PHE:CD1	1:D:124:LYS:HE2	2.42	0.55
1:H:119:PHE:CD1	1:H:124:LYS:HE2	2.42	0.55
1:J:119:PHE:CD1	1:J:124:LYS:HE2	2.42	0.55
1:A:119:PHE:CD1	1:A:124:LYS:HE2	2.42	0.55
1:J:82:ALA:HA	1:J:149:ARG:O	2.06	0.54
1:L:119:PHE:CD1	1:L:124:LYS:HE2	2.42	0.54
1:A:65:ILE:HB	1:A:66:PRO:HD2	1.90	0.54
1:I:65:ILE:HB	1:I:66:PRO:HD2	1.90	0.54
1:C:82:ALA:HA	1:C:149:ARG:O	2.06	0.54
1:K:65:ILE:HB	1:K:66:PRO:HD2	1.90	0.54
1:G:65:ILE:HB	1:G:66:PRO:HD2	1.90	0.54
1:J:73:MET:CB	1:J:73:MET:HE2	2.35	0.54
1:E:65:ILE:HB	1:E:66:PRO:HD2	1.90	0.54
1:C:119:PHE:CD1	1:C:124:LYS:HE2	2.42	0.54
1:I:119:PHE:CD1	1:I:124:LYS:HE2	2.42	0.54
1:E:119:PHE:CD1	1:E:124:LYS:HE2	2.42	0.54
1:G:119:PHE:CD1	1:G:124:LYS:HE2	2.42	0.53
1:B:65:ILE:HB	1:B:66:PRO:HD2	1.90	0.53
1:K:119:PHE:CD1	1:K:124:LYS:HE2	2.42	0.53
1:B:119:PHE:CD1	1:B:124:LYS:HE2	2.42	0.53
1:F:65:ILE:HB	1:F:66:PRO:HD2	1.90	0.53
1:L:65:ILE:HB	1:L:66:PRO:HD2	1.90	0.53
1:D:65:ILE:HB	1:D:66:PRO:HD2	1.90	0.53
1:L:62:PHE:CD1	1:L:62:PHE:N	2.77	0.53
1:A:62:PHE:N	1:A:62:PHE:CD1	2.77	0.53
1:H:65:ILE:HB	1:H:66:PRO:HD2	1.90	0.53
1:I:62:PHE:N	1:I:62:PHE:CD1	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:PHE:CD1	1:G:62:PHE:N	2.77	0.53
1:C:65:ILE:HB	1:C:66:PRO:HD2	1.90	0.53
1:F:91:ALA:O	1:F:94:ASP:HB2	2.09	0.52
1:C:91:ALA:O	1:C:94:ASP:HB2	2.10	0.52
1:G:91:ALA:O	1:G:94:ASP:HB2	2.10	0.52
1:K:91:ALA:O	1:K:94:ASP:HB2	2.10	0.52
1:F:62:PHE:N	1:F:62:PHE:CD1	2.77	0.52
1:I:91:ALA:O	1:I:94:ASP:HB2	2.10	0.52
1:C:62:PHE:N	1:C:62:PHE:CD1	2.77	0.52
1:J:65:ILE:HB	1:J:66:PRO:HD2	1.90	0.52
1:K:62:PHE:N	1:K:62:PHE:CD1	2.77	0.52
1:E:91:ALA:O	1:E:94:ASP:HB2	2.10	0.52
1:D:91:ALA:O	1:D:94:ASP:HB2	2.10	0.52
1:L:91:ALA:O	1:L:94:ASP:HB2	2.09	0.52
1:A:91:ALA:O	1:A:94:ASP:HB2	2.10	0.52
1:G:126:ASN:HB3	1:H:92:PRO:HB3	1.92	0.52
1:J:139:SER:HA	1:J:146:ILE:O	2.11	0.51
1:G:139:SER:HA	1:G:146:ILE:O	2.11	0.51
1:L:139:SER:HA	1:L:146:ILE:O	2.11	0.51
1:I:139:SER:HA	1:I:146:ILE:O	2.10	0.51
1:J:91:ALA:O	1:J:94:ASP:HB2	2.10	0.51
1:B:91:ALA:O	1:B:94:ASP:HB2	2.10	0.51
1:A:139:SER:HA	1:A:146:ILE:O	2.11	0.51
1:E:62:PHE:N	1:E:62:PHE:CD1	2.77	0.51
1:H:139:SER:HA	1:H:146:ILE:O	2.10	0.51
1:F:139:SER:HA	1:F:146:ILE:O	2.11	0.51
1:D:139:SER:HA	1:D:146:ILE:O	2.11	0.51
1:B:62:PHE:N	1:B:62:PHE:CD1	2.77	0.51
1:C:139:SER:HA	1:C:146:ILE:O	2.10	0.51
1:J:62:PHE:CD1	1:J:62:PHE:N	2.77	0.51
1:D:62:PHE:N	1:D:62:PHE:CD1	2.77	0.51
1:H:91:ALA:O	1:H:94:ASP:HB2	2.09	0.51
1:J:112:ARG:NH1	1:J:118:TYR:CE2	2.79	0.51
1:H:112:ARG:NH1	1:H:118:TYR:CE2	2.79	0.51
1:C:112:ARG:NH1	1:C:118:TYR:CE2	2.79	0.51
1:L:112:ARG:NH1	1:L:118:TYR:CE2	2.79	0.51
1:G:112:ARG:NH1	1:G:118:TYR:CE2	2.79	0.51
1:I:112:ARG:NH1	1:I:118:TYR:CE2	2.79	0.51
1:K:139:SER:HA	1:K:146:ILE:O	2.11	0.50
1:E:139:SER:HA	1:E:146:ILE:O	2.11	0.50
1:B:112:ARG:NH1	1:B:118:TYR:CE2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:SER:HA	1:B:146:ILE:O	2.10	0.50
1:A:112:ARG:NH1	1:A:118:TYR:CE2	2.79	0.50
1:E:112:ARG:NH1	1:E:118:TYR:CE2	2.79	0.50
1:D:73:MET:HE2	1:D:73:MET:HB3	1.86	0.50
1:K:112:ARG:NH1	1:K:118:TYR:CE2	2.79	0.50
1:E:84:LEU:C	1:E:84:LEU:HD12	2.32	0.50
1:F:112:ARG:NH1	1:F:118:TYR:CE2	2.79	0.50
1:C:84:LEU:HD12	1:C:84:LEU:C	2.32	0.50
1:B:84:LEU:C	1:B:84:LEU:HD12	2.32	0.50
1:G:58:HIS:CD2	1:H:63:GLY:HA3	2.47	0.50
1:D:112:ARG:NH1	1:D:118:TYR:CE2	2.79	0.50
1:H:62:PHE:CD1	1:H:62:PHE:N	2.77	0.50
1:A:84:LEU:HD12	1:A:84:LEU:C	2.32	0.50
1:D:84:LEU:HD12	1:D:84:LEU:C	2.32	0.49
1:K:84:LEU:C	1:K:84:LEU:HD12	2.32	0.49
1:E:58:HIS:CD2	1:F:63:GLY:CA	2.91	0.49
1:E:62:PHE:CE1	1:F:57:PRO:HB3	2.46	0.49
1:G:84:LEU:HD12	1:G:84:LEU:C	2.32	0.49
1:L:84:LEU:C	1:L:84:LEU:HD12	2.32	0.49
1:I:84:LEU:C	1:I:84:LEU:HD12	2.32	0.49
1:F:84:LEU:C	1:F:84:LEU:HD12	2.32	0.49
1:H:84:LEU:C	1:H:84:LEU:HD12	2.32	0.49
1:J:84:LEU:HD12	1:J:84:LEU:C	2.32	0.49
1:A:142:ARG:HB2	1:A:142:ARG:HE	1.48	0.48
1:E:58:HIS:HD2	1:F:63:GLY:CA	2.26	0.47
1:A:135:HIS:HB2	1:A:148:LEU:CD1	2.45	0.47
1:J:135:HIS:HB2	1:J:148:LEU:CD1	2.45	0.47
1:C:135:HIS:HB2	1:C:148:LEU:CD1	2.45	0.47
1:D:135:HIS:HB2	1:D:148:LEU:CD1	2.45	0.47
1:B:135:HIS:HB2	1:B:148:LEU:CD1	2.45	0.47
1:K:135:HIS:HB2	1:K:148:LEU:CD1	2.45	0.47
1:E:73:MET:HE2	1:E:73:MET:CB	2.44	0.47
1:E:58:HIS:NE2	1:F:63:GLY:HA3	2.29	0.47
1:A:120:LEU:HA	1:A:120:LEU:HD23	1.63	0.46
1:E:135:HIS:HB2	1:E:148:LEU:CD1	2.45	0.46
1:L:135:HIS:HB2	1:L:148:LEU:CD1	2.45	0.46
1:H:135:HIS:HB2	1:H:148:LEU:CD1	2.45	0.46
1:C:118:TYR:HE1	1:C:127:SER:HA	1.81	0.46
1:F:135:HIS:HB2	1:F:148:LEU:CD1	2.45	0.46
1:G:135:HIS:HB2	1:G:148:LEU:CD1	2.45	0.46
1:I:135:HIS:HB2	1:I:148:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:118:TYR:HE1	1:L:127:SER:HA	1.81	0.46
1:H:120:LEU:HA	1:H:120:LEU:HD23	1.63	0.46
1:G:142:ARG:HB2	1:G:142:ARG:HE	1.47	0.46
1:C:73:MET:CB	1:C:73:MET:HE2	2.40	0.46
1:D:118:TYR:HE1	1:D:127:SER:HA	1.81	0.46
1:B:118:TYR:HE1	1:B:127:SER:HA	1.81	0.46
1:H:118:TYR:HE1	1:H:127:SER:HA	1.81	0.46
1:E:118:TYR:HE1	1:E:127:SER:HA	1.81	0.46
1:I:118:TYR:HE1	1:I:127:SER:HA	1.81	0.46
1:A:69:LYS:HD3	1:A:69:LYS:HA	1.84	0.46
1:A:119:PHE:HB3	1:A:124:LYS:HA	1.98	0.46
1:C:119:PHE:HB3	1:C:124:LYS:HA	1.98	0.46
1:I:119:PHE:HB3	1:I:124:LYS:HA	1.98	0.46
1:G:112:ARG:HH21	1:H:112:ARG:NH2	2.14	0.46
1:G:118:TYR:HE1	1:G:127:SER:HA	1.81	0.46
1:F:118:TYR:HE1	1:F:127:SER:HA	1.81	0.46
1:L:73:MET:CB	1:L:73:MET:HE2	2.40	0.46
1:K:119:PHE:HB3	1:K:124:LYS:HA	1.98	0.46
1:G:119:PHE:HB3	1:G:124:LYS:HA	1.98	0.46
1:I:142:ARG:HE	1:I:142:ARG:HB2	1.48	0.46
1:D:119:PHE:HB3	1:D:124:LYS:HA	1.98	0.45
1:J:118:TYR:HE1	1:J:127:SER:HA	1.81	0.45
1:G:112:ARG:NH2	1:H:112:ARG:NH2	2.64	0.45
1:I:61:PHE:CE1	1:I:63:GLY:HA2	2.51	0.45
1:E:61:PHE:CE1	1:E:63:GLY:HA2	2.51	0.45
1:E:119:PHE:HB3	1:E:124:LYS:HA	1.98	0.45
1:H:119:PHE:HB3	1:H:124:LYS:HA	1.98	0.45
1:G:61:PHE:CE1	1:G:63:GLY:HA2	2.51	0.45
1:A:61:PHE:CE1	1:A:63:GLY:HA2	2.51	0.45
1:K:118:TYR:HE1	1:K:127:SER:HA	1.81	0.45
1:C:120:LEU:HD23	1:C:120:LEU:HA	1.63	0.45
1:F:61:PHE:CE1	1:F:63:GLY:HA2	2.51	0.45
1:J:119:PHE:HB3	1:J:124:LYS:HA	1.98	0.45
1:D:61:PHE:CE1	1:D:63:GLY:HA2	2.51	0.45
1:B:119:PHE:HB3	1:B:124:LYS:HA	1.98	0.45
1:L:69:LYS:HA	1:L:69:LYS:HD3	1.84	0.45
1:K:61:PHE:CE1	1:K:63:GLY:HA2	2.51	0.45
1:H:61:PHE:CE1	1:H:63:GLY:HA2	2.51	0.45
1:C:61:PHE:CE1	1:C:63:GLY:HA2	2.51	0.45
1:G:69:LYS:HD3	1:G:69:LYS:HA	1.84	0.45
1:L:119:PHE:HB3	1:L:124:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ARG:NH2	1:H:112:ARG:HH21	2.14	0.45
1:F:119:PHE:HB3	1:F:124:LYS:HA	1.98	0.45
1:L:142:ARG:HE	1:L:142:ARG:HB2	1.48	0.45
1:J:61:PHE:CE1	1:J:63:GLY:HA2	2.51	0.45
1:A:118:TYR:HE1	1:A:127:SER:HA	1.81	0.44
1:L:61:PHE:CE1	1:L:63:GLY:HA2	2.51	0.44
1:F:73:MET:HB3	1:F:73:MET:HE2	1.91	0.44
1:B:61:PHE:CE1	1:B:63:GLY:HA2	2.51	0.44
1:D:120:LEU:HD23	1:D:120:LEU:HA	1.63	0.44
1:I:69:LYS:HA	1:I:69:LYS:HD3	1.84	0.44
1:I:92:PRO:HB3	1:J:126:ASN:HB3	2.00	0.44
1:B:108:PHE:CD1	1:B:108:PHE:N	2.86	0.44
1:J:120:LEU:HD23	1:J:120:LEU:HA	1.63	0.44
1:F:83:PHE:N	1:F:83:PHE:CD1	2.86	0.44
1:I:108:PHE:CD1	1:I:108:PHE:N	2.86	0.43
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.90	0.43
1:E:120:LEU:HD23	1:E:120:LEU:HA	1.63	0.43
1:E:83:PHE:CD1	1:E:83:PHE:N	2.86	0.43
1:G:108:PHE:N	1:G:108:PHE:CD1	2.86	0.43
1:L:83:PHE:CD1	1:L:83:PHE:N	2.87	0.43
1:B:73:MET:CB	1:B:73:MET:HE2	2.40	0.43
1:K:120:LEU:HD23	1:K:120:LEU:HA	1.63	0.43
1:D:142:ARG:HB2	1:D:142:ARG:HE	1.48	0.43
1:I:112:ARG:HA	1:I:117:LYS:O	2.19	0.43
1:F:108:PHE:CD1	1:F:108:PHE:N	2.86	0.43
1:H:73:MET:CB	1:H:73:MET:HE2	2.37	0.43
1:L:112:ARG:HA	1:L:117:LYS:O	2.19	0.43
1:G:112:ARG:HA	1:G:117:LYS:O	2.19	0.43
1:H:112:ARG:HA	1:H:117:LYS:O	2.19	0.43
1:C:83:PHE:CD1	1:C:83:PHE:N	2.86	0.43
1:E:108:PHE:N	1:E:108:PHE:CD1	2.86	0.43
1:B:90:SER:C	1:B:92:PRO:HD3	2.39	0.43
1:B:112:ARG:HA	1:B:117:LYS:O	2.19	0.43
1:L:90:SER:C	1:L:92:PRO:HD3	2.39	0.43
1:C:90:SER:C	1:C:92:PRO:HD3	2.39	0.43
1:J:112:ARG:CZ	1:J:118:TYR:CE2	3.02	0.43
1:H:112:ARG:CZ	1:H:118:TYR:CE2	3.02	0.43
1:G:90:SER:C	1:G:92:PRO:HD3	2.39	0.43
1:J:90:SER:C	1:J:92:PRO:HD3	2.39	0.43
1:K:90:SER:C	1:K:92:PRO:HD3	2.39	0.43
1:A:83:PHE:N	1:A:83:PHE:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:CD1	1:A:108:PHE:N	2.86	0.43
1:A:97:LEU:HD12	1:A:98:SER:N	2.34	0.43
1:A:90:SER:C	1:A:92:PRO:HD3	2.39	0.43
1:A:112:ARG:CZ	1:A:118:TYR:CE2	3.02	0.43
1:E:112:ARG:HA	1:E:117:LYS:O	2.19	0.43
1:F:112:ARG:HA	1:F:117:LYS:O	2.19	0.43
1:D:112:ARG:HA	1:D:117:LYS:O	2.19	0.43
1:I:134:TYR:C	1:I:134:TYR:CD1	2.92	0.43
1:H:74:LEU:HA	1:H:74:LEU:HD23	1.90	0.43
1:J:111:LEU:N	1:J:111:LEU:HD22	2.34	0.43
1:E:63:GLY:HA3	1:F:58:HIS:CD2	2.54	0.43
1:A:118:TYR:CE1	1:A:127:SER:HA	2.54	0.43
1:I:112:ARG:CZ	1:I:118:TYR:CE2	3.02	0.43
1:H:90:SER:C	1:H:92:PRO:HD3	2.39	0.43
1:G:134:TYR:CD1	1:G:134:TYR:C	2.92	0.43
1:I:90:SER:C	1:I:92:PRO:HD3	2.39	0.43
1:B:111:LEU:HD22	1:B:111:LEU:N	2.34	0.43
1:J:112:ARG:HA	1:J:117:LYS:O	2.19	0.43
1:G:112:ARG:CZ	1:G:118:TYR:CE2	3.02	0.43
1:H:118:TYR:CE1	1:H:127:SER:HA	2.54	0.43
1:E:112:ARG:CZ	1:E:118:TYR:CE2	3.02	0.43
1:K:108:PHE:N	1:K:108:PHE:CD1	2.86	0.43
1:F:111:LEU:N	1:F:111:LEU:HD22	2.34	0.43
1:H:97:LEU:HD12	1:H:98:SER:N	2.34	0.43
1:B:69:LYS:HD3	1:B:69:LYS:HA	1.84	0.42
1:D:69:LYS:HA	1:D:69:LYS:HD3	1.84	0.42
1:J:118:TYR:CE1	1:J:127:SER:HA	2.54	0.42
1:I:118:TYR:CE1	1:I:127:SER:HA	2.54	0.42
1:C:134:TYR:CD1	1:C:134:TYR:C	2.93	0.42
1:D:134:TYR:C	1:D:134:TYR:CD1	2.92	0.42
1:E:90:SER:C	1:E:92:PRO:HD3	2.39	0.42
1:G:111:LEU:N	1:G:111:LEU:HD22	2.34	0.42
1:B:118:TYR:CE1	1:B:127:SER:HA	2.54	0.42
1:G:118:TYR:CE1	1:G:127:SER:HA	2.54	0.42
1:C:112:ARG:HA	1:C:117:LYS:O	2.19	0.42
1:C:112:ARG:CZ	1:C:118:TYR:CE2	3.02	0.42
1:D:112:ARG:CZ	1:D:118:TYR:CE2	3.02	0.42
1:A:134:TYR:C	1:A:134:TYR:CD1	2.92	0.42
1:L:134:TYR:C	1:L:134:TYR:CD1	2.92	0.42
1:H:111:LEU:N	1:H:111:LEU:HD22	2.34	0.42
1:I:111:LEU:N	1:I:111:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PHE:CD1	1:D:108:PHE:N	2.86	0.42
1:J:83:PHE:CD1	1:J:83:PHE:N	2.86	0.42
1:F:97:LEU:HD12	1:F:98:SER:N	2.34	0.42
1:L:130:GLU:O	1:L:131:LEU:C	2.58	0.42
1:L:118:TYR:CE1	1:L:127:SER:HA	2.54	0.42
1:B:134:TYR:CD1	1:B:134:TYR:C	2.92	0.42
1:J:97:LEU:HD12	1:J:98:SER:N	2.34	0.42
1:D:90:SER:C	1:D:92:PRO:HD3	2.39	0.42
1:G:83:PHE:N	1:G:83:PHE:CD1	2.86	0.42
1:C:111:LEU:HD22	1:C:111:LEU:N	2.34	0.42
1:D:111:LEU:N	1:D:111:LEU:HD22	2.34	0.42
1:H:108:PHE:N	1:H:108:PHE:CD1	2.86	0.42
1:E:111:LEU:HD22	1:E:111:LEU:N	2.34	0.42
1:L:111:LEU:N	1:L:111:LEU:HD22	2.34	0.42
1:C:118:TYR:CE1	1:C:127:SER:HA	2.54	0.42
1:F:118:TYR:CE1	1:F:127:SER:HA	2.54	0.42
1:C:108:PHE:CD1	1:C:108:PHE:N	2.86	0.42
1:H:83:PHE:CD1	1:H:83:PHE:N	2.86	0.42
1:I:83:PHE:N	1:I:83:PHE:CD1	2.86	0.42
1:K:111:LEU:N	1:K:111:LEU:HD22	2.34	0.42
1:K:83:PHE:N	1:K:83:PHE:CD1	2.86	0.42
1:B:97:LEU:HD12	1:B:98:SER:N	2.34	0.42
1:E:118:TYR:CE1	1:E:127:SER:HA	2.54	0.42
1:H:134:TYR:C	1:H:134:TYR:CD1	2.92	0.42
1:E:97:LEU:HD12	1:E:98:SER:N	2.34	0.42
1:J:108:PHE:CD1	1:J:108:PHE:N	2.86	0.42
1:B:112:ARG:CZ	1:B:118:TYR:CE2	3.02	0.42
1:K:112:ARG:CZ	1:K:118:TYR:CE2	3.02	0.42
1:K:134:TYR:CD1	1:K:134:TYR:C	2.93	0.42
1:G:63:GLY:HA3	1:H:58:HIS:CD2	2.55	0.42
1:L:97:LEU:HD12	1:L:98:SER:N	2.34	0.42
1:D:83:PHE:N	1:D:83:PHE:CD1	2.86	0.42
1:C:130:GLU:O	1:C:131:LEU:C	2.58	0.42
1:D:118:TYR:CE1	1:D:127:SER:HA	2.54	0.42
1:E:134:TYR:CD1	1:E:134:TYR:C	2.92	0.42
1:K:97:LEU:HD12	1:K:98:SER:N	2.34	0.42
1:A:74:LEU:HA	1:A:74:LEU:HD23	1.90	0.42
1:L:112:ARG:CZ	1:L:118:TYR:CE2	3.02	0.42
1:E:134:TYR:HD1	1:E:135:HIS:CD2	2.38	0.42
1:L:108:PHE:N	1:L:108:PHE:CD1	2.86	0.42
1:I:97:LEU:HD12	1:I:98:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LEU:HD12	1:C:98:SER:N	2.34	0.42
1:D:73:MET:HE2	1:D:73:MET:CB	2.47	0.42
1:H:130:GLU:O	1:H:131:LEU:C	2.58	0.42
1:A:130:GLU:O	1:A:131:LEU:C	2.58	0.42
1:A:112:ARG:HA	1:A:117:LYS:O	2.19	0.42
1:G:134:TYR:HD1	1:G:135:HIS:CD2	2.38	0.42
1:D:97:LEU:HD12	1:D:98:SER:N	2.34	0.42
1:A:111:LEU:N	1:A:111:LEU:HD22	2.34	0.42
1:G:97:LEU:HD12	1:G:98:SER:N	2.34	0.42
1:K:112:ARG:HA	1:K:117:LYS:O	2.19	0.41
1:F:112:ARG:CZ	1:F:118:TYR:CE2	3.02	0.41
1:J:134:TYR:C	1:J:134:TYR:CD1	2.92	0.41
1:H:69:LYS:HA	1:H:69:LYS:HD3	1.84	0.41
1:D:134:TYR:HD1	1:D:135:HIS:CD2	2.38	0.41
1:K:134:TYR:HD1	1:K:135:HIS:CD2	2.38	0.41
1:I:134:TYR:HD1	1:I:135:HIS:CD2	2.38	0.41
1:B:134:TYR:HD1	1:B:135:HIS:CD2	2.38	0.41
1:B:135:HIS:HB2	1:B:148:LEU:HD12	2.03	0.41
1:K:135:HIS:HB2	1:K:148:LEU:HD12	2.03	0.41
1:F:134:TYR:CD1	1:F:134:TYR:C	2.92	0.41
1:C:69:LYS:HD3	1:C:69:LYS:HA	1.84	0.41
1:K:118:TYR:CE1	1:K:127:SER:HA	2.54	0.41
1:E:79:HIS:HB2	1:E:149:ARG:HD3	2.03	0.41
1:C:79:HIS:HB2	1:C:149:ARG:HD3	2.03	0.41
1:A:135:HIS:HB2	1:A:148:LEU:HD12	2.03	0.41
1:C:135:HIS:HB2	1:C:148:LEU:HD12	2.03	0.41
1:F:90:SER:C	1:F:92:PRO:HD3	2.39	0.41
1:E:135:HIS:HB2	1:E:148:LEU:HD12	2.03	0.41
1:L:134:TYR:HD1	1:L:135:HIS:CD2	2.38	0.41
1:H:134:TYR:HD1	1:H:135:HIS:CD2	2.38	0.41
1:E:61:PHE:CG	1:F:61:PHE:CG	3.08	0.41
1:J:134:TYR:HD1	1:J:135:HIS:CD2	2.38	0.41
1:I:79:HIS:HB2	1:I:149:ARG:HD3	2.03	0.41
1:J:130:GLU:O	1:J:131:LEU:C	2.58	0.41
1:F:79:HIS:HB2	1:F:149:ARG:HD3	2.03	0.41
1:G:79:HIS:HB2	1:G:149:ARG:HD3	2.03	0.41
1:G:135:HIS:HB2	1:G:148:LEU:HD12	2.03	0.41
1:B:83:PHE:N	1:B:83:PHE:CD1	2.86	0.41
1:E:130:GLU:O	1:E:131:LEU:C	2.58	0.41
1:K:130:GLU:O	1:K:131:LEU:C	2.58	0.41
1:B:130:GLU:O	1:B:131:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:HIS:HB2	1:L:149:ARG:HD3	2.03	0.41
1:C:134:TYR:HD1	1:C:135:HIS:CD2	2.38	0.41
1:J:142:ARG:HB2	1:J:142:ARG:HE	1.48	0.41
1:B:120:LEU:HA	1:B:120:LEU:HD23	1.63	0.41
1:J:74:LEU:HD23	1:J:74:LEU:HA	1.90	0.41
1:L:135:HIS:HB2	1:L:148:LEU:HD12	2.03	0.41
1:C:62:PHE:N	1:C:62:PHE:HD1	2.19	0.40
1:J:62:PHE:HD1	1:J:62:PHE:N	2.20	0.40
1:H:62:PHE:N	1:H:62:PHE:HD1	2.20	0.40
1:J:135:HIS:HB2	1:J:148:LEU:HD12	2.02	0.40
1:L:120:LEU:HD23	1:L:120:LEU:HA	1.63	0.40
1:L:62:PHE:N	1:L:62:PHE:HD1	2.20	0.40
1:A:79:HIS:HB2	1:A:149:ARG:HD3	2.03	0.40
1:D:84:LEU:HD12	1:D:84:LEU:O	2.21	0.40
1:J:84:LEU:HD12	1:J:84:LEU:O	2.21	0.40
1:A:134:TYR:HD1	1:A:135:HIS:CD2	2.38	0.40
1:J:151:ILE:H	1:J:151:ILE:HG22	1.56	0.40
1:E:62:PHE:N	1:E:62:PHE:HD1	2.20	0.40
1:G:130:GLU:O	1:G:131:LEU:C	2.58	0.40
1:D:79:HIS:HB2	1:D:149:ARG:HD3	2.03	0.40
1:F:134:TYR:HD1	1:F:135:HIS:CD2	2.38	0.40
1:I:135:HIS:HB2	1:I:148:LEU:HD12	2.03	0.40
1:B:84:LEU:O	1:B:84:LEU:HD12	2.21	0.40
1:H:135:HIS:HB2	1:H:148:LEU:HD12	2.03	0.40
1:I:120:LEU:HD23	1:I:120:LEU:HA	1.63	0.40
1:F:74:LEU:HD23	1:F:74:LEU:HA	1.90	0.40
1:A:62:PHE:N	1:A:62:PHE:HD1	2.20	0.40
1:C:84:LEU:HD12	1:C:84:LEU:O	2.22	0.40
1:A:84:LEU:HD12	1:A:84:LEU:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:NH2	1:F:137:SER:O[4_566]	2.04	0.16
1:C:152:GLU:OE2	1:I:152:GLU:OE2[2_564]	2.07	0.13
1:E:126:ASN:OD1	1:L:78:ARG:NH2[2_565]	2.19	0.01

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	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	B	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	C	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	D	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	E	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	F	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	G	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	H	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	I	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	J	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	K	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
1	L	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
All	All	1128/1152 (98%)	1056 (94%)	72 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	B	85/85 (100%)	76 (89%)	9 (11%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	D	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	E	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	F	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	G	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	H	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	I	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	J	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	K	85/85 (100%)	76 (89%)	9 (11%)	8	31
1	L	85/85 (100%)	76 (89%)	9 (11%)	8	31
All	All	1020/1020 (100%)	912 (89%)	108 (11%)	8	31

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	92	PRO
1	A	104	ASP
1	A	109	LYS
1	A	112	ARG
1	A	117	LYS
1	A	126	ASN
1	A	129	ASN
1	A	140	VAL
1	B	65	ILE
1	B	92	PRO
1	B	104	ASP
1	B	109	LYS
1	B	112	ARG
1	B	117	LYS
1	B	126	ASN
1	B	129	ASN
1	B	140	VAL
1	C	65	ILE
1	C	92	PRO
1	C	104	ASP
1	C	109	LYS
1	C	112	ARG

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Mol	Chain	Res	Type
1	C	117	LYS
1	C	126	ASN
1	C	129	ASN
1	C	140	VAL
1	D	65	ILE
1	D	92	PRO
1	D	104	ASP
1	D	109	LYS
1	D	112	ARG
1	D	117	LYS
1	D	126	ASN
1	D	129	ASN
1	D	140	VAL
1	E	65	ILE
1	E	92	PRO
1	E	104	ASP
1	E	109	LYS
1	E	112	ARG
1	E	117	LYS
1	E	126	ASN
1	E	129	ASN
1	E	140	VAL
1	F	65	ILE
1	F	92	PRO
1	F	104	ASP
1	F	109	LYS
1	F	112	ARG
1	F	117	LYS
1	F	126	ASN
1	F	129	ASN
1	F	140	VAL
1	G	65	ILE
1	G	92	PRO
1	G	104	ASP
1	G	109	LYS
1	G	112	ARG
1	G	117	LYS
1	G	126	ASN
1	G	129	ASN
1	G	140	VAL
1	H	65	ILE
1	H	92	PRO

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Mol	Chain	Res	Type
1	H	104	ASP
1	H	109	LYS
1	H	112	ARG
1	H	117	LYS
1	H	126	ASN
1	H	129	ASN
1	H	140	VAL
1	I	65	ILE
1	I	92	PRO
1	I	104	ASP
1	I	109	LYS
1	I	112	ARG
1	I	117	LYS
1	I	126	ASN
1	I	129	ASN
1	I	140	VAL
1	J	65	ILE
1	J	92	PRO
1	J	104	ASP
1	J	109	LYS
1	J	112	ARG
1	J	117	LYS
1	J	126	ASN
1	J	129	ASN
1	J	140	VAL
1	K	65	ILE
1	K	92	PRO
1	K	104	ASP
1	K	109	LYS
1	K	112	ARG
1	K	117	LYS
1	K	126	ASN
1	K	129	ASN
1	K	140	VAL
1	L	65	ILE
1	L	92	PRO
1	L	104	ASP
1	L	109	LYS
1	L	112	ARG
1	L	117	LYS
1	L	126	ASN
1	L	129	ASN

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Mol	Chain	Res	Type
1	L	140	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	58	HIS
1	F	58	HIS
1	K	58	HIS
1	L	58	HIS

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	C78	A	155	-	48,49,49	2.00	10 (20%)	68,69,69	1.96	11 (16%)
2	C78	B	156	-	48,49,49	2.00	10 (20%)	68,69,69	1.96	11 (16%)
2	C78	C	157	-	48,49,49	2.00	11 (22%)	68,69,69	1.96	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C78	D	158	-	48,49,49	1.99	10 (20%)	68,69,69	1.96	11 (16%)
2	C78	E	159	-	48,49,49	2.00	10 (20%)	68,69,69	1.96	11 (16%)
2	C78	F	160	-	48,49,49	1.99	11 (22%)	68,69,69	1.96	11 (16%)
2	C78	G	161	-	48,49,49	2.00	10 (20%)	68,69,69	1.96	11 (16%)
2	C78	H	162	-	48,49,49	2.00	10 (20%)	68,69,69	1.96	11 (16%)
2	C78	I	163	-	48,49,49	1.99	10 (20%)	68,69,69	1.97	11 (16%)
2	C78	J	164	-	48,49,49	2.00	10 (20%)	68,69,69	1.97	11 (16%)
2	C78	K	165	-	48,49,49	2.00	11 (22%)	68,69,69	1.96	11 (16%)
2	C78	L	166	-	48,49,49	1.99	10 (20%)	68,69,69	1.96	11 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C78	A	155	-	-	0/41/62/62	0/4/4/4
2	C78	B	156	-	-	0/41/62/62	0/4/4/4
2	C78	C	157	-	-	0/41/62/62	0/4/4/4
2	C78	D	158	-	-	0/41/62/62	0/4/4/4
2	C78	E	159	-	-	0/41/62/62	0/4/4/4
2	C78	F	160	-	-	0/41/62/62	0/4/4/4
2	C78	G	161	-	-	0/41/62/62	0/4/4/4
2	C78	H	162	-	-	0/41/62/62	0/4/4/4
2	C78	I	163	-	-	0/41/62/62	0/4/4/4
2	C78	J	164	-	-	0/41/62/62	0/4/4/4
2	C78	K	165	-	-	0/41/62/62	0/4/4/4
2	C78	L	166	-	-	0/41/62/62	0/4/4/4

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	156	C78	C40-C39	-6.91	1.34	1.53
2	G	161	C78	C40-C39	-6.90	1.34	1.53
2	L	166	C78	C40-C39	-6.88	1.34	1.53
2	J	164	C78	C40-C39	-6.88	1.34	1.53
2	K	165	C78	C40-C39	-6.88	1.34	1.53
2	H	162	C78	C40-C39	-6.88	1.34	1.53
2	A	155	C78	C40-C39	-6.87	1.34	1.53
2	D	158	C78	C40-C39	-6.87	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	159	C78	C40-C39	-6.87	1.34	1.53
2	F	160	C78	C40-C39	-6.87	1.34	1.53
2	C	157	C78	C40-C39	-6.86	1.34	1.53
2	I	163	C78	C40-C39	-6.85	1.34	1.53
2	B	156	C78	C34-C29	-5.45	1.46	1.54
2	G	161	C78	C34-C29	-5.44	1.46	1.54
2	J	164	C78	C34-C29	-5.41	1.46	1.54
2	K	165	C78	C34-C29	-5.39	1.46	1.54
2	A	155	C78	C34-C29	-5.38	1.46	1.54
2	E	159	C78	C34-C29	-5.37	1.46	1.54
2	F	160	C78	C34-C29	-5.36	1.46	1.54
2	H	162	C78	C34-C29	-5.35	1.46	1.54
2	C	157	C78	C34-C29	-5.35	1.46	1.54
2	D	158	C78	C34-C29	-5.33	1.46	1.54
2	I	163	C78	C34-C29	-5.33	1.46	1.54
2	L	166	C78	C34-C29	-5.33	1.46	1.54
2	C	157	C78	C30-C29	-3.66	1.48	1.54
2	F	160	C78	C30-C29	-3.64	1.48	1.54
2	E	159	C78	C30-C29	-3.63	1.48	1.54
2	H	162	C78	C30-C29	-3.62	1.48	1.54
2	L	166	C78	C30-C29	-3.61	1.48	1.54
2	G	161	C78	C30-C29	-3.60	1.48	1.54
2	D	158	C78	C30-C29	-3.60	1.48	1.54
2	I	163	C78	C30-C29	-3.59	1.48	1.54
2	A	155	C78	C30-C29	-3.59	1.48	1.54
2	B	156	C78	C30-C29	-3.58	1.48	1.54
2	J	164	C78	C30-C29	-3.57	1.48	1.54
2	H	162	C78	C39-C38	-3.56	1.46	1.53
2	K	165	C78	C30-C29	-3.56	1.48	1.54
2	B	156	C78	C39-C38	-3.55	1.46	1.53
2	E	159	C78	C39-C38	-3.55	1.46	1.53
2	I	163	C78	C39-C38	-3.55	1.46	1.53
2	J	164	C78	C39-C38	-3.55	1.46	1.53
2	F	160	C78	C39-C38	-3.53	1.46	1.53
2	A	155	C78	C39-C38	-3.53	1.46	1.53
2	G	161	C78	C39-C38	-3.53	1.46	1.53
2	C	157	C78	C39-C38	-3.52	1.46	1.53
2	D	158	C78	C39-C38	-3.51	1.46	1.53
2	L	166	C78	C39-C38	-3.51	1.46	1.53
2	K	165	C78	C39-C38	-3.51	1.46	1.53
2	D	158	C78	C29-C35	-3.25	1.47	1.54
2	H	162	C78	C29-C35	-3.22	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	161	C78	C29-C35	-3.22	1.47	1.54
2	B	156	C78	C29-C35	-3.22	1.47	1.54
2	J	164	C78	C29-C35	-3.22	1.47	1.54
2	E	159	C78	C29-C35	-3.22	1.47	1.54
2	A	155	C78	C29-C35	-3.21	1.47	1.54
2	I	163	C78	C29-C35	-3.21	1.47	1.54
2	C	157	C78	C29-C35	-3.20	1.47	1.54
2	F	160	C78	C29-C35	-3.20	1.47	1.54
2	L	166	C78	C29-C35	-3.20	1.47	1.54
2	K	165	C78	C29-C35	-3.19	1.47	1.54
2	L	166	C78	C4-C3	-2.68	1.33	1.38
2	K	165	C78	C4-C3	-2.67	1.33	1.38
2	B	156	C78	C4-C3	-2.65	1.33	1.38
2	G	161	C78	C4-C3	-2.65	1.33	1.38
2	J	164	C78	C4-C3	-2.65	1.33	1.38
2	E	159	C78	C4-C3	-2.64	1.33	1.38
2	D	158	C78	C4-C3	-2.64	1.33	1.38
2	A	155	C78	C4-C3	-2.63	1.33	1.38
2	C	157	C78	C4-C3	-2.63	1.33	1.38
2	F	160	C78	C4-C3	-2.63	1.33	1.38
2	I	163	C78	C4-C3	-2.63	1.33	1.38
2	H	162	C78	C4-C3	-2.61	1.33	1.38
2	J	164	C78	C41-C42	-2.27	1.47	1.53
2	C	157	C78	C41-C42	-2.26	1.47	1.53
2	I	163	C78	C41-C42	-2.26	1.47	1.53
2	G	161	C78	C41-C42	-2.26	1.47	1.53
2	D	158	C78	C41-C42	-2.25	1.47	1.53
2	A	155	C78	C41-C42	-2.25	1.47	1.53
2	B	156	C78	C41-C42	-2.25	1.47	1.53
2	H	162	C78	C41-C42	-2.24	1.47	1.53
2	E	159	C78	C41-C42	-2.24	1.47	1.53
2	L	166	C78	C41-C42	-2.24	1.47	1.53
2	K	165	C78	C41-C42	-2.23	1.47	1.53
2	F	160	C78	C41-C42	-2.23	1.47	1.53
2	F	160	C78	C6-C7	-2.01	1.35	1.39
2	K	165	C78	C6-C7	-2.00	1.35	1.39
2	C	157	C78	C6-C7	-2.00	1.35	1.39
2	H	162	C78	O9-C10	2.78	1.40	1.35
2	F	160	C78	O9-C10	2.81	1.40	1.35
2	G	161	C78	O9-C10	2.81	1.40	1.35
2	L	166	C78	O9-C10	2.82	1.40	1.35
2	J	164	C78	O9-C10	2.82	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	163	C78	O9-C10	2.82	1.40	1.35
2	A	155	C78	O9-C10	2.83	1.40	1.35
2	C	157	C78	O9-C10	2.83	1.40	1.35
2	D	158	C78	O9-C10	2.83	1.40	1.35
2	E	159	C78	O9-C10	2.83	1.40	1.35
2	B	156	C78	O9-C10	2.84	1.40	1.35
2	K	165	C78	O9-C10	2.84	1.40	1.35
2	F	160	C78	O23-C20	3.05	1.47	1.40
2	H	162	C78	O23-C20	3.06	1.47	1.40
2	B	156	C78	O23-C20	3.06	1.47	1.40
2	G	161	C78	O23-C20	3.06	1.47	1.40
2	L	166	C78	O23-C20	3.07	1.47	1.40
2	D	158	C78	O23-C20	3.07	1.47	1.40
2	I	163	C78	O23-C20	3.07	1.47	1.40
2	A	155	C78	O23-C20	3.07	1.47	1.40
2	C	157	C78	O23-C20	3.07	1.47	1.40
2	E	159	C78	O23-C20	3.07	1.47	1.40
2	K	165	C78	O23-C20	3.08	1.48	1.40
2	J	164	C78	O23-C20	3.11	1.48	1.40
2	I	163	C78	C17-C16	3.47	1.45	1.38
2	F	160	C78	C17-C16	3.48	1.45	1.38
2	L	166	C78	C17-C16	3.49	1.45	1.38
2	K	165	C78	C17-C16	3.49	1.45	1.38
2	E	159	C78	C17-C16	3.50	1.45	1.38
2	A	155	C78	C17-C16	3.52	1.45	1.38
2	D	158	C78	C17-C16	3.52	1.45	1.38
2	G	161	C78	C17-C16	3.53	1.45	1.38
2	B	156	C78	C17-C16	3.53	1.45	1.38
2	H	162	C78	C17-C16	3.54	1.45	1.38
2	C	157	C78	C17-C16	3.54	1.45	1.38
2	J	164	C78	C17-C16	3.54	1.45	1.38

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	164	C78	C39-C38-N37	-6.02	100.82	110.80
2	K	165	C78	C39-C38-N37	-6.01	100.83	110.80
2	F	160	C78	C39-C38-N37	-6.01	100.83	110.80
2	A	155	C78	C39-C38-N37	-6.01	100.84	110.80
2	L	166	C78	C39-C38-N37	-6.01	100.84	110.80
2	C	157	C78	C39-C38-N37	-6.00	100.84	110.80
2	I	163	C78	C39-C38-N37	-6.00	100.85	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	159	C78	C39-C38-N37	-6.00	100.85	110.80
2	G	161	C78	C39-C38-N37	-6.00	100.85	110.80
2	D	158	C78	C39-C38-N37	-6.00	100.85	110.80
2	H	162	C78	C39-C38-N37	-5.98	100.88	110.80
2	B	156	C78	C39-C38-N37	-5.98	100.88	110.80
2	G	161	C78	O36-C35-C29	-5.05	113.13	120.97
2	K	165	C78	O36-C35-C29	-5.05	113.14	120.97
2	J	164	C78	O36-C35-C29	-5.05	113.14	120.97
2	H	162	C78	O36-C35-C29	-5.04	113.15	120.97
2	C	157	C78	O36-C35-C29	-5.04	113.15	120.97
2	D	158	C78	O36-C35-C29	-5.03	113.16	120.97
2	A	155	C78	O36-C35-C29	-5.03	113.16	120.97
2	B	156	C78	O36-C35-C29	-5.03	113.17	120.97
2	F	160	C78	O36-C35-C29	-5.02	113.18	120.97
2	I	163	C78	O36-C35-C29	-5.02	113.18	120.97
2	L	166	C78	O36-C35-C29	-5.02	113.19	120.97
2	E	159	C78	O36-C35-C29	-5.01	113.20	120.97
2	G	161	C78	C33-C34-C29	-4.54	106.28	112.45
2	F	160	C78	C33-C34-C29	-4.54	106.28	112.45
2	I	163	C78	C33-C34-C29	-4.54	106.28	112.45
2	L	166	C78	C33-C34-C29	-4.53	106.30	112.45
2	J	164	C78	C33-C34-C29	-4.53	106.30	112.45
2	K	165	C78	C33-C34-C29	-4.52	106.31	112.45
2	H	162	C78	C33-C34-C29	-4.52	106.31	112.45
2	E	159	C78	C33-C34-C29	-4.52	106.31	112.45
2	A	155	C78	C33-C34-C29	-4.52	106.31	112.45
2	B	156	C78	C33-C34-C29	-4.51	106.32	112.45
2	D	158	C78	C33-C34-C29	-4.51	106.32	112.45
2	C	157	C78	C33-C34-C29	-4.49	106.35	112.45
2	D	158	C78	C34-C29-N28	-2.66	104.58	109.61
2	C	157	C78	C34-C29-N28	-2.64	104.61	109.61
2	J	164	C78	C34-C29-N28	-2.64	104.62	109.61
2	I	163	C78	C34-C29-N28	-2.64	104.62	109.61
2	H	162	C78	C34-C29-N28	-2.63	104.63	109.61
2	L	166	C78	C34-C29-N28	-2.63	104.64	109.61
2	F	160	C78	C34-C29-N28	-2.63	104.64	109.61
2	A	155	C78	C34-C29-N28	-2.62	104.65	109.61
2	K	165	C78	C34-C29-N28	-2.61	104.67	109.61
2	E	159	C78	C34-C29-N28	-2.61	104.67	109.61
2	B	156	C78	C34-C29-N28	-2.61	104.67	109.61
2	G	161	C78	C34-C29-N28	-2.59	104.71	109.61
2	H	162	C78	C38-C43-C44	2.07	113.69	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	163	C78	C38-C43-C44	2.08	113.71	110.88
2	B	156	C78	C38-C43-C44	2.08	113.71	110.88
2	J	164	C78	C38-C43-C44	2.09	113.72	110.88
2	E	159	C78	C38-C43-C44	2.10	113.73	110.88
2	G	161	C78	C38-C43-C44	2.10	113.73	110.88
2	K	165	C78	C38-C43-C44	2.11	113.74	110.88
2	A	155	C78	C38-C43-C44	2.11	113.74	110.88
2	F	160	C78	C38-C43-C44	2.12	113.75	110.88
2	C	157	C78	C38-C43-C44	2.12	113.75	110.88
2	L	166	C78	C38-C43-C44	2.13	113.76	110.88
2	D	158	C78	C38-C43-C44	2.15	113.79	110.88
2	E	159	C78	C29-C35-N37	3.08	122.23	116.55
2	F	160	C78	C29-C35-N37	3.08	122.24	116.55
2	K	165	C78	C29-C35-N37	3.09	122.24	116.55
2	L	166	C78	C29-C35-N37	3.09	122.24	116.55
2	C	157	C78	C29-C35-N37	3.09	122.25	116.55
2	H	162	C78	C29-C35-N37	3.09	122.25	116.55
2	A	155	C78	C29-C35-N37	3.10	122.27	116.55
2	D	158	C78	C29-C35-N37	3.11	122.28	116.55
2	I	163	C78	C29-C35-N37	3.11	122.28	116.55
2	B	156	C78	C29-C35-N37	3.11	122.29	116.55
2	G	161	C78	C29-C35-N37	3.13	122.31	116.55
2	J	164	C78	C29-C35-N37	3.13	122.32	116.55
2	L	166	C78	C34-C29-C30	3.65	113.87	109.28
2	C	157	C78	C34-C29-C30	3.66	113.88	109.28
2	K	165	C78	C34-C29-C30	3.66	113.88	109.28
2	E	159	C78	C34-C29-C30	3.66	113.89	109.28
2	I	163	C78	C34-C29-C30	3.67	113.90	109.28
2	A	155	C78	C34-C29-C30	3.67	113.90	109.28
2	H	162	C78	C34-C29-C30	3.67	113.90	109.28
2	D	158	C78	C34-C29-C30	3.67	113.90	109.28
2	B	156	C78	C34-C29-C30	3.68	113.91	109.28
2	G	161	C78	C34-C29-C30	3.68	113.91	109.28
2	F	160	C78	C34-C29-C30	3.68	113.91	109.28
2	J	164	C78	C34-C29-C30	3.70	113.93	109.28
2	G	161	C78	C39-C38-C43	3.74	115.73	111.19
2	D	158	C78	C39-C38-C43	3.75	115.74	111.19
2	C	157	C78	C39-C38-C43	3.76	115.75	111.19
2	K	165	C78	C39-C38-C43	3.77	115.76	111.19
2	J	164	C78	C39-C38-C43	3.77	115.77	111.19
2	L	166	C78	C39-C38-C43	3.78	115.78	111.19
2	E	159	C78	C39-C38-C43	3.79	115.79	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	155	C78	C39-C38-C43	3.79	115.80	111.19
2	B	156	C78	C39-C38-C43	3.81	115.81	111.19
2	I	163	C78	C39-C38-C43	3.81	115.81	111.19
2	H	162	C78	C39-C38-C43	3.82	115.83	111.19
2	F	160	C78	C39-C38-C43	3.82	115.83	111.19
2	B	156	C78	C30-C29-N28	4.40	117.93	109.61
2	D	158	C78	C30-C29-N28	4.42	117.97	109.61
2	J	164	C78	C30-C29-N28	4.42	117.97	109.61
2	G	161	C78	C30-C29-N28	4.42	117.97	109.61
2	E	159	C78	C30-C29-N28	4.43	117.98	109.61
2	A	155	C78	C30-C29-N28	4.43	117.98	109.61
2	K	165	C78	C30-C29-N28	4.44	118.00	109.61
2	H	162	C78	C30-C29-N28	4.44	118.00	109.61
2	F	160	C78	C30-C29-N28	4.44	118.01	109.61
2	C	157	C78	C30-C29-N28	4.44	118.01	109.61
2	L	166	C78	C30-C29-N28	4.45	118.03	109.61
2	I	163	C78	C30-C29-N28	4.46	118.04	109.61
2	F	160	C78	C40-C39-C38	5.03	118.89	111.51
2	B	156	C78	C40-C39-C38	5.03	118.90	111.51
2	H	162	C78	C40-C39-C38	5.03	118.90	111.51
2	L	166	C78	C40-C39-C38	5.04	118.91	111.51
2	K	165	C78	C40-C39-C38	5.04	118.91	111.51
2	I	163	C78	C40-C39-C38	5.04	118.91	111.51
2	A	155	C78	C40-C39-C38	5.05	118.92	111.51
2	J	164	C78	C40-C39-C38	5.05	118.93	111.51
2	D	158	C78	C40-C39-C38	5.06	118.94	111.51
2	E	159	C78	C40-C39-C38	5.07	118.95	111.51
2	G	161	C78	C40-C39-C38	5.07	118.95	111.51
2	C	157	C78	C40-C39-C38	5.07	118.96	111.51
2	E	159	C78	C41-C40-C39	6.19	124.41	111.44
2	C	157	C78	C41-C40-C39	6.20	124.43	111.44
2	J	164	C78	C41-C40-C39	6.21	124.45	111.44
2	A	155	C78	C41-C40-C39	6.21	124.46	111.44
2	G	161	C78	C41-C40-C39	6.21	124.46	111.44
2	D	158	C78	C41-C40-C39	6.21	124.47	111.44
2	I	163	C78	C41-C40-C39	6.22	124.47	111.44
2	F	160	C78	C41-C40-C39	6.22	124.47	111.44
2	L	166	C78	C41-C40-C39	6.22	124.48	111.44
2	H	162	C78	C41-C40-C39	6.22	124.48	111.44
2	K	165	C78	C41-C40-C39	6.23	124.50	111.44
2	B	156	C78	C41-C40-C39	6.23	124.50	111.44

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, 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	96/96 (100%)	-0.44	0 100 100	2, 20, 60, 105	0
1	B	96/96 (100%)	-0.40	0 100 100	2, 20, 60, 105	0
1	C	96/96 (100%)	-0.47	0 100 100	2, 20, 60, 105	0
1	D	96/96 (100%)	-0.51	0 100 100	2, 20, 60, 105	0
1	E	96/96 (100%)	-0.31	1 (1%) 84 60	2, 20, 60, 105	0
1	F	96/96 (100%)	-0.42	0 100 100	2, 20, 60, 105	0
1	G	96/96 (100%)	-0.38	0 100 100	2, 20, 60, 105	0
1	H	96/96 (100%)	-0.27	2 (2%) 67 36	2, 20, 60, 105	0
1	I	96/96 (100%)	0.13	2 (2%) 67 36	2, 20, 60, 105	0
1	J	96/96 (100%)	-0.37	0 100 100	2, 20, 60, 105	0
1	K	96/96 (100%)	-0.18	0 100 100	2, 20, 60, 105	0
1	L	96/96 (100%)	0.31	4 (4%) 40 16	2, 20, 60, 105	0
All	All	1152/1152 (100%)	-0.28	9 (0%) 87 67	2, 20, 64, 105	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	103	ASN	3.9
1	L	77	GLN	3.1
1	I	101	PHE	2.9
1	H	103	ASN	2.2
1	H	77	GLN	2.2
1	E	103	ASN	2.2
1	L	104	ASP	2.1
1	L	72	GLU	2.0
1	L	138	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	C78	E	159	46/46	0.90	0.22	1.07	2,13,50,50	0
2	C78	D	158	46/46	0.95	0.18	0.34	2,13,50,50	0
2	C78	C	157	46/46	0.95	0.19	0.11	2,13,50,50	0
2	C78	A	155	46/46	0.95	0.18	0.09	2,13,50,50	0
2	C78	G	161	46/46	0.94	0.16	-0.12	2,13,50,50	0
2	C78	K	165	46/46	0.93	0.18	-0.14	2,13,50,50	0
2	C78	F	160	46/46	0.96	0.17	-0.16	2,13,50,50	0
2	C78	B	156	46/46	0.96	0.17	-0.18	2,13,50,50	0
2	C78	H	162	46/46	0.94	0.17	-0.26	2,13,50,50	0
2	C78	I	163	46/46	0.93	0.19	-0.53	2,13,50,50	0
2	C78	L	166	46/46	0.92	0.18	-0.63	2,13,50,50	0
2	C78	J	164	46/46	0.95	0.14	-1.15	2,13,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.