



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:37 PM UTC

PDB ID : 3RCC / pdb_00003rcc
Title : Crystal Structure of the Streptococcus agalactiae Sortase A
Authors : Khare, B.; Narayana, S.V.L.
Deposited on : 2011-03-30
Resolution : 3.10 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
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

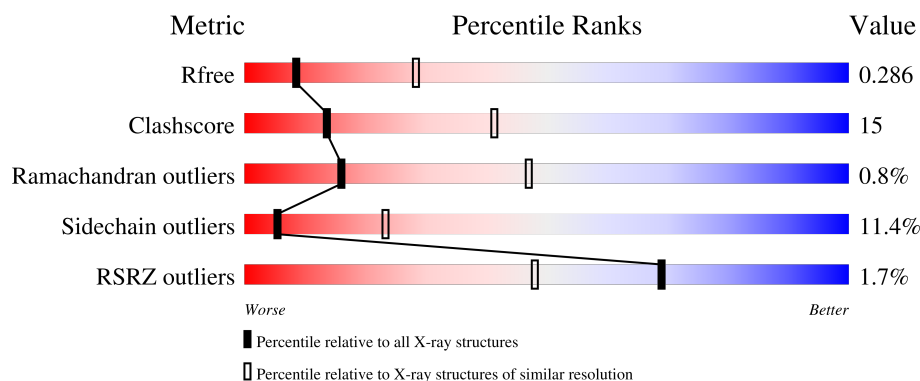
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	160	46% 31% • 19%
1	B	160	2% 48% 27% • 22%
1	C	160	49% 28% • 19%
1	D	160	2% 60% 19% • 19%
1	E	160	54% 22% 8% 16%

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Mol	Chain	Length	Quality of chain
1	F	160	
1	G	160	
1	H	160	
1	I	160	
1	J	160	
1	K	160	
1	L	160	
1	M	160	
1	N	160	
1	O	160	
1	P	160	
1	Q	160	
1	R	160	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17807 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 Sortase SrtA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			976	623	161	188	4			
1	B	124	Total	C	N	O	S	0	0	0
			938	601	155	178	4			
1	C	129	Total	C	N	O	S	0	0	0
			973	621	161	187	4			
1	D	129	Total	C	N	O	S	0	0	0
			981	628	161	188	4			
1	E	134	Total	C	N	O	S	0	0	0
			1011	645	166	196	4			
1	F	132	Total	C	N	O	S	0	0	0
			992	632	164	192	4			
1	G	132	Total	C	N	O	S	0	0	0
			992	632	164	192	4			
1	H	130	Total	C	N	O	S	0	0	0
			982	626	162	190	4			
1	I	131	Total	C	N	O	S	0	0	0
			983	627	163	189	4			
1	J	129	Total	C	N	O	S	0	0	0
			980	626	161	189	4			
1	K	129	Total	C	N	O	S	0	0	0
			974	621	161	188	4			
1	L	127	Total	C	N	O	S	0	0	0
			960	613	159	184	4			
1	M	128	Total	C	N	O	S	0	0	0
			964	616	159	185	4			
1	N	137	Total	C	N	O	S	0	0	0
			1031	656	169	202	4			
1	O	131	Total	C	N	O	S	0	0	0
			984	627	163	190	4			
1	P	132	Total	C	N	O	S	0	0	0
			1003	640	164	195	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	133	Total	C	N	O	S	0	0	0
			1009	643	165	197	4			
1	R	125	Total	C	N	O	S	0	0	0
			947	605	157	181	4			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	expression tag	UNP Q8DZY1
A	58	ASN	-	expression tag	UNP Q8DZY1
A	59	ALA	-	expression tag	UNP Q8DZY1
B	57	SER	-	expression tag	UNP Q8DZY1
B	58	ASN	-	expression tag	UNP Q8DZY1
B	59	ALA	-	expression tag	UNP Q8DZY1
C	57	SER	-	expression tag	UNP Q8DZY1
C	58	ASN	-	expression tag	UNP Q8DZY1
C	59	ALA	-	expression tag	UNP Q8DZY1
D	57	SER	-	expression tag	UNP Q8DZY1
D	58	ASN	-	expression tag	UNP Q8DZY1
D	59	ALA	-	expression tag	UNP Q8DZY1
E	57	SER	-	expression tag	UNP Q8DZY1
E	58	ASN	-	expression tag	UNP Q8DZY1
E	59	ALA	-	expression tag	UNP Q8DZY1
F	57	SER	-	expression tag	UNP Q8DZY1
F	58	ASN	-	expression tag	UNP Q8DZY1
F	59	ALA	-	expression tag	UNP Q8DZY1
G	57	SER	-	expression tag	UNP Q8DZY1
G	58	ASN	-	expression tag	UNP Q8DZY1
G	59	ALA	-	expression tag	UNP Q8DZY1
H	57	SER	-	expression tag	UNP Q8DZY1
H	58	ASN	-	expression tag	UNP Q8DZY1
H	59	ALA	-	expression tag	UNP Q8DZY1
I	57	SER	-	expression tag	UNP Q8DZY1
I	58	ASN	-	expression tag	UNP Q8DZY1
I	59	ALA	-	expression tag	UNP Q8DZY1
J	57	SER	-	expression tag	UNP Q8DZY1
J	58	ASN	-	expression tag	UNP Q8DZY1
J	59	ALA	-	expression tag	UNP Q8DZY1
K	57	SER	-	expression tag	UNP Q8DZY1
K	58	ASN	-	expression tag	UNP Q8DZY1
K	59	ALA	-	expression tag	UNP Q8DZY1
L	57	SER	-	expression tag	UNP Q8DZY1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	58	ASN	-	expression tag	UNP Q8DZY1
L	59	ALA	-	expression tag	UNP Q8DZY1
M	57	SER	-	expression tag	UNP Q8DZY1
M	58	ASN	-	expression tag	UNP Q8DZY1
M	59	ALA	-	expression tag	UNP Q8DZY1
N	57	SER	-	expression tag	UNP Q8DZY1
N	58	ASN	-	expression tag	UNP Q8DZY1
N	59	ALA	-	expression tag	UNP Q8DZY1
O	57	SER	-	expression tag	UNP Q8DZY1
O	58	ASN	-	expression tag	UNP Q8DZY1
O	59	ALA	-	expression tag	UNP Q8DZY1
P	57	SER	-	expression tag	UNP Q8DZY1
P	58	ASN	-	expression tag	UNP Q8DZY1
P	59	ALA	-	expression tag	UNP Q8DZY1
Q	57	SER	-	expression tag	UNP Q8DZY1
Q	58	ASN	-	expression tag	UNP Q8DZY1
Q	59	ALA	-	expression tag	UNP Q8DZY1
R	57	SER	-	expression tag	UNP Q8DZY1
R	58	ASN	-	expression tag	UNP Q8DZY1
R	59	ALA	-	expression tag	UNP Q8DZY1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total 5 Zn 5	0	0
2	B	6	Total 6 Zn 6	0	0
2	C	5	Total 5 Zn 5	0	0
2	D	4	Total 4 Zn 4	0	0
2	E	4	Total 4 Zn 4	0	0
2	F	2	Total 2 Zn 2	0	0
2	G	7	Total 7 Zn 7	0	0
2	H	4	Total 4 Zn 4	0	0
2	I	4	Total 4 Zn 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	3	Total 3	Zn 3	0	0
2	K	3	Total 3	Zn 3	0	0
2	L	2	Total 2	Zn 2	0	0
2	M	6	Total 6	Zn 6	0	0
2	N	4	Total 4	Zn 4	0	0
2	O	4	Total 4	Zn 4	0	0
2	P	4	Total 4	Zn 4	0	0
2	Q	4	Total 4	Zn 4	0	0
2	R	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	4	Total 4	O 4	0	0
3	C	3	Total 3	O 3	0	0
3	D	1	Total 1	O 1	0	0
3	E	3	Total 3	O 3	0	0
3	F	5	Total 5	O 5	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	I	5	Total 5	O 5	0	0
3	J	2	Total 2	O 2	0	0

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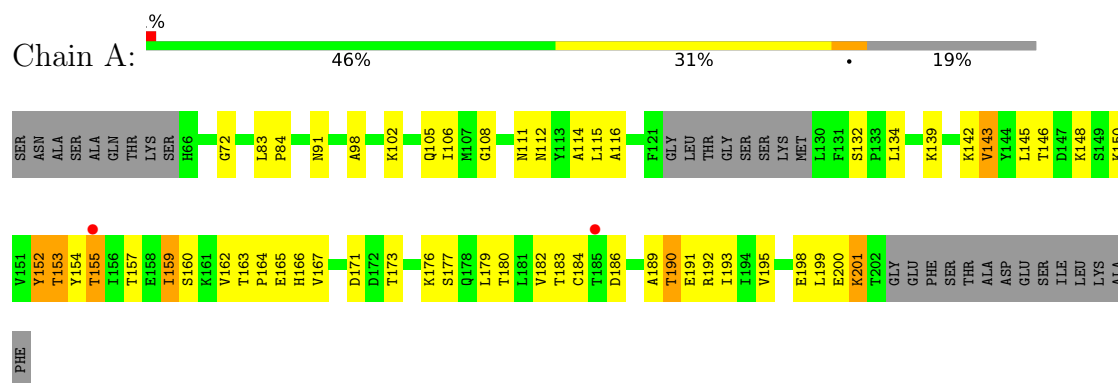
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	5	Total 5	O 5	0	0
3	L	4	Total 4	O 4	0	0
3	M	3	Total 3	O 3	0	0
3	N	4	Total 4	O 4	0	0
3	O	1	Total 1	O 1	0	0
3	P	4	Total 4	O 4	0	0
3	Q	3	Total 3	O 3	0	0
3	R	3	Total 3	O 3	0	0

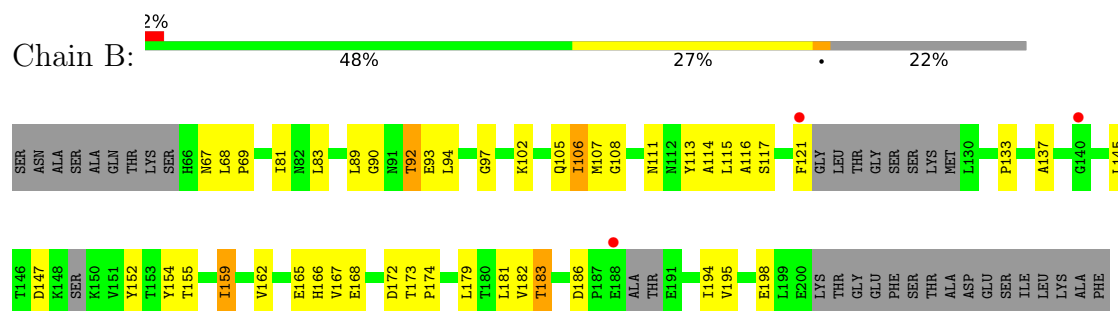
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

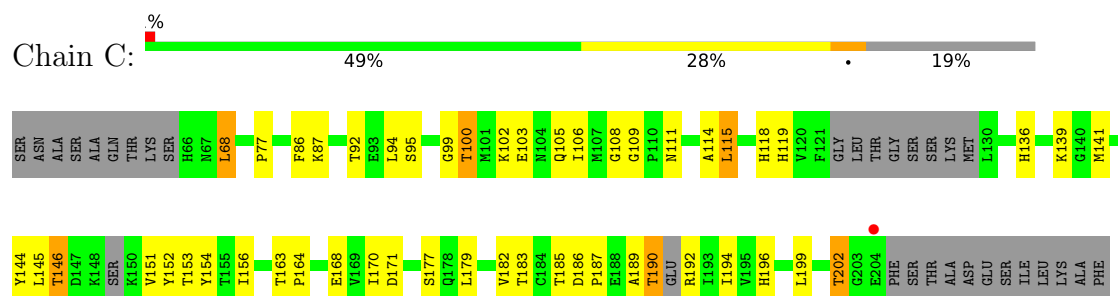
• Molecule 1: Sortase SrtA



• Molecule 1: Sortase SrtA

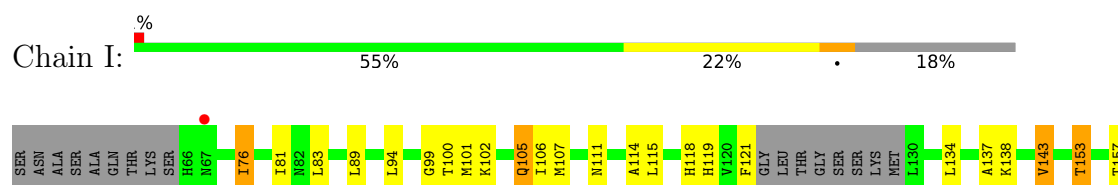


• Molecule 1: Sortase SrtA

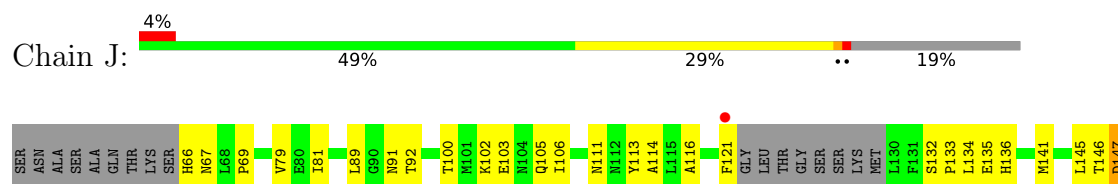


• Molecule 1: Sortase SrtA

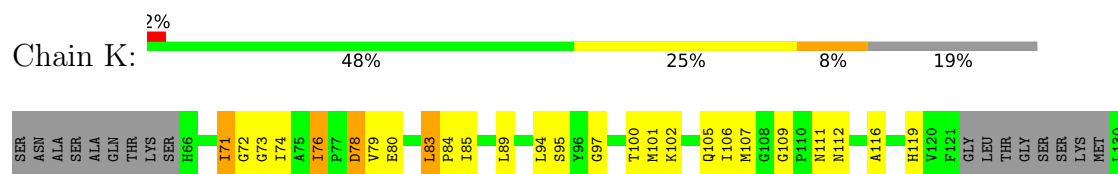




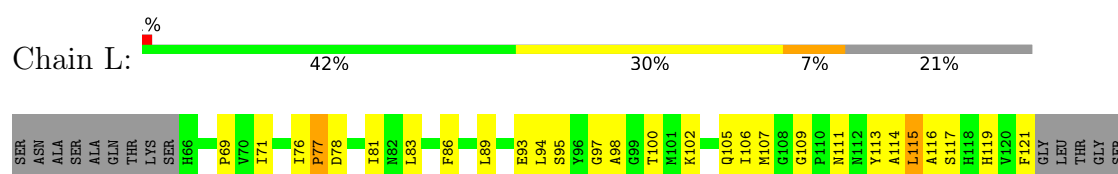
• Molecule 1: Sortase SrtA



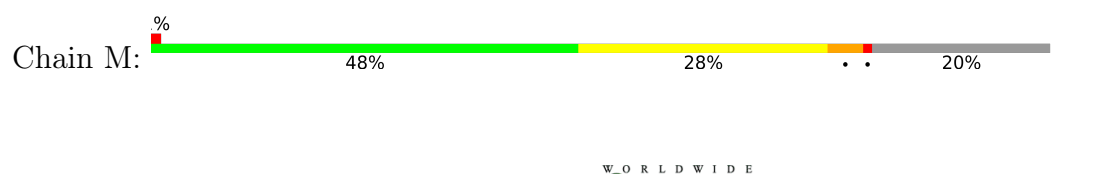
• Molecule 1: Sortase SrtA

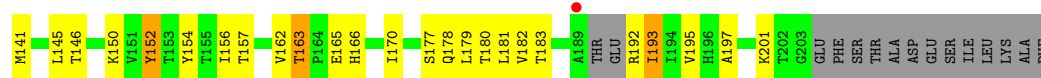


• Molecule 1: Sortase SrtA

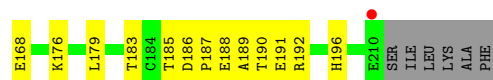


• Molecule 1: Sortase SrtA

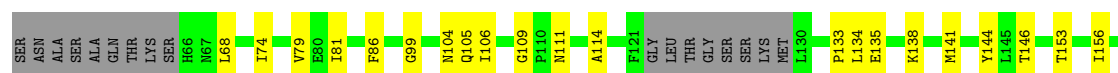




• Molecule 1: Sortase SrtA



• Molecule 1: Sortase SrtA



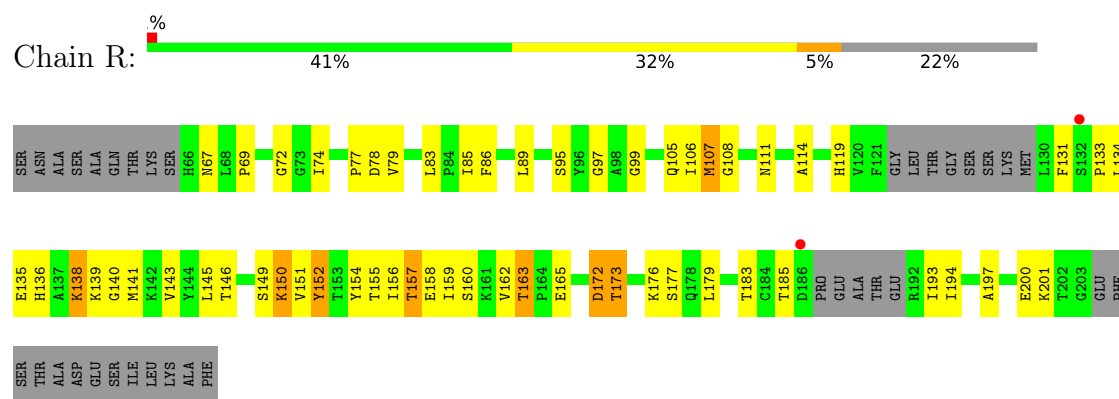
• Molecule 1: Sortase SrtA



• Molecule 1: Sortase SrtA



• Molecule 1: Sortase SrtA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	237.67Å 167.76Å 97.54Å 90.00° 93.55° 90.00°	Depositor
Resolution (Å)	39.23 – 3.10 39.23 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.23-3.10) 99.3 (39.23-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.232 , 0.299 0.225 , 0.286	Depositor DCC
R_{free} test set	3482 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17807	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: ZN

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	0.93	1/996 (0.1%)	1.13	4/1355 (0.3%)
1	B	0.83	0/956	1.09	3/1298 (0.2%)
1	C	0.81	0/991	0.99	0/1345
1	D	1.01	2/1000 (0.2%)	1.09	2/1356 (0.1%)
1	E	0.91	1/1030 (0.1%)	1.11	8/1398 (0.6%)
1	F	0.99	1/1012 (0.1%)	1.08	2/1377 (0.1%)
1	G	0.83	0/1012	0.98	2/1377 (0.1%)
1	H	0.95	1/1001 (0.1%)	1.09	5/1360 (0.4%)
1	I	0.82	0/1002	0.99	3/1362 (0.2%)
1	J	0.90	0/998	1.14	3/1352 (0.2%)
1	K	0.94	0/993	1.15	7/1349 (0.5%)
1	L	1.02	0/979	1.13	6/1329 (0.5%)
1	M	0.89	0/983	1.07	6/1335 (0.4%)
1	N	0.91	0/1052	1.02	4/1431 (0.3%)
1	O	0.95	0/1004	1.06	4/1366 (0.3%)
1	P	0.96	0/1024	1.07	2/1392 (0.1%)
1	Q	1.26	7/1030 (0.7%)	1.22	10/1400 (0.7%)
1	R	0.91	0/965	1.05	3/1309 (0.2%)
All	All	0.94	13/18028 (0.1%)	1.08	74/24491 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	182	VAL	CA-CB	-8.25	1.44	1.54
1	Q	194	ILE	CA-CB	-6.89	1.46	1.54
1	D	90	GLY	C-O	-6.30	1.17	1.23
1	H	190	THR	CA-CB	5.88	1.59	1.52
1	F	151	VAL	CA-CB	-5.64	1.47	1.54
1	A	155	THR	CA-CB	5.63	1.61	1.53
1	E	182	VAL	CA-CB	-5.54	1.47	1.54
1	D	131	PHE	N-CA	5.41	1.52	1.46
1	Q	194	ILE	C-O	-5.23	1.18	1.24
1	Q	205	PHE	CA-C	-5.20	1.46	1.52
1	Q	193	ILE	C-O	-5.17	1.18	1.24
1	Q	181	LEU	C-O	-5.06	1.18	1.24
1	Q	182	VAL	C-O	-5.03	1.18	1.24

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	SER	CA-C-N	-9.49	109.13	119.19
1	A	132	SER	C-N-CA	-9.49	109.13	119.19
1	Q	185	THR	N-CA-C	8.13	119.92	111.14
1	B	186	ASP	CA-C-N	-7.99	109.85	119.84
1	B	186	ASP	C-N-CA	-7.99	109.85	119.84
1	Q	202	THR	N-CA-C	-7.82	103.49	112.87
1	N	189	ALA	N-CA-C	7.53	120.59	110.35
1	M	163	THR	CA-C-N	-7.25	112.23	119.56
1	M	163	THR	C-N-CA	-7.25	112.23	119.56
1	E	162	VAL	N-CA-C	7.00	118.56	108.48
1	O	104	ASN	N-CA-C	6.95	118.78	110.44
1	O	162	VAL	N-CA-C	6.88	118.38	108.48
1	H	173	THR	CA-C-N	6.78	126.81	119.90
1	H	173	THR	C-N-CA	6.78	126.81	119.90
1	J	163	THR	CA-C-N	-6.70	112.79	119.56
1	J	163	THR	C-N-CA	-6.70	112.79	119.56
1	M	201	LYS	N-CA-C	6.67	118.93	107.93
1	E	105	GLN	N-CA-C	6.55	118.89	107.49
1	J	153	THR	N-CA-C	6.26	118.62	108.41
1	L	193	ILE	N-CA-C	6.24	116.85	107.80
1	I	170	ILE	N-CA-C	6.24	117.46	111.91
1	R	72	GLY	N-CA-C	6.13	118.41	110.45
1	E	73	GLY	N-CA-C	6.12	121.27	110.80
1	Q	192	ARG	N-CA-C	-6.12	99.02	109.24
1	N	185	THR	N-CA-C	6.11	117.74	111.14
1	L	163	THR	CA-C-N	-6.04	113.75	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	163	THR	C-N-CA	-6.04	113.75	120.45
1	A	72	GLY	N-CA-C	5.98	119.23	110.80
1	I	105	GLN	N-CA-C	5.95	118.07	108.32
1	D	151	VAL	CB-CA-C	-5.93	103.67	110.73
1	H	72	GLY	N-CA-C	5.91	118.56	110.58
1	E	173	THR	CA-C-N	5.91	127.22	119.84
1	E	173	THR	C-N-CA	5.91	127.22	119.84
1	P	163	THR	CA-C-N	-5.80	113.78	119.64
1	P	163	THR	C-N-CA	-5.80	113.78	119.64
1	O	109	GLY	CA-C-N	5.76	127.04	119.84
1	O	109	GLY	C-N-CA	5.76	127.04	119.84
1	B	162	VAL	N-CA-C	5.67	116.91	108.46
1	M	72	GLY	N-CA-C	5.62	118.72	110.80
1	M	106	ILE	N-CA-C	5.61	116.02	108.17
1	H	83	LEU	CA-C-N	5.60	125.61	119.89
1	H	83	LEU	C-N-CA	5.60	125.61	119.89
1	D	71	ILE	N-CA-C	5.60	117.56	112.29
1	F	187	PRO	N-CA-C	-5.58	106.26	113.57
1	L	162	VAL	N-CA-C	5.56	116.48	108.48
1	N	163	THR	CA-C-N	-5.51	114.09	120.04
1	N	163	THR	C-N-CA	-5.51	114.09	120.04
1	G	109	GLY	CA-C-N	5.48	126.69	119.84
1	G	109	GLY	C-N-CA	5.48	126.69	119.84
1	L	83	LEU	CA-C-N	5.45	125.38	119.76
1	L	83	LEU	C-N-CA	5.45	125.38	119.76
1	K	76	ILE	CA-C-N	5.44	125.09	119.05
1	K	76	ILE	C-N-CA	5.44	125.09	119.05
1	E	193	ILE	N-CA-C	5.44	115.69	107.80
1	K	186	ASP	CA-C-N	-5.39	114.11	119.56
1	K	186	ASP	C-N-CA	-5.39	114.11	119.56
1	Q	109	GLY	CA-C-N	5.36	126.54	119.84
1	Q	109	GLY	C-N-CA	5.36	126.54	119.84
1	F	73	GLY	N-CA-C	5.34	118.92	110.96
1	M	170	ILE	N-CA-C	5.31	117.32	112.43
1	K	72	GLY	N-CA-C	5.29	118.25	110.80
1	A	201	LYS	N-CA-C	5.15	117.55	108.75
1	Q	131	PHE	CB-CA-C	-5.12	101.30	109.75
1	R	119	HIS	N-CA-C	5.10	117.93	109.46
1	Q	83	LEU	CA-C-N	-5.08	114.75	120.14
1	Q	83	LEU	C-N-CA	-5.08	114.75	120.14
1	E	163	THR	CA-C-N	-5.08	113.81	119.19
1	E	163	THR	C-N-CA	-5.08	113.81	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	133	PRO	N-CA-C	-5.08	107.12	114.18
1	R	193	ILE	CB-CA-C	-5.04	103.99	110.84
1	K	83	LEU	N-CA-C	5.04	117.50	109.64
1	I	76	ILE	CB-CA-C	-5.03	106.30	111.08
1	Q	147	ASP	CA-C-N	-5.03	113.90	120.44
1	Q	147	ASP	C-N-CA	-5.03	113.90	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	204	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	976	0	957	41	0
1	B	938	0	920	29	0
1	C	973	0	957	28	0
1	D	981	0	966	20	0
1	E	1011	0	989	27	0
1	F	992	0	969	22	0
1	G	992	0	969	18	0
1	H	982	0	964	33	0
1	I	983	0	962	26	0
1	J	980	0	967	35	0
1	K	974	0	961	36	0
1	L	960	0	945	43	0
1	M	964	0	950	37	0
1	N	1031	0	1004	18	0
1	O	984	0	966	19	0
1	P	1003	0	983	27	0
1	Q	1009	0	988	37	0
1	R	947	0	938	39	0
2	A	5	0	0	0	0
2	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	2	0	0	0	0
2	G	7	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
2	M	6	0	0	0	0
2	N	4	0	0	0	0
2	O	4	0	0	0	0
2	P	4	0	0	0	0
2	Q	4	0	0	0	0
2	R	2	0	0	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	1	0
3	E	3	0	0	0	0
3	F	5	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	5	0	0	0	0
3	J	2	0	0	0	0
3	K	5	0	0	0	0
3	L	4	0	0	0	0
3	M	3	0	0	2	0
3	N	4	0	0	0	0
3	O	1	0	0	0	0
3	P	4	0	0	0	0
3	Q	3	0	0	0	0
3	R	3	0	0	0	0
All	All	17807	0	17355	512	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 15.

All (512) 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:Q:159:ILE:HD13	1:Q:195:VAL:HG22	1.26	1.07
1:J:146:THR:HG22	1:J:151:VAL:HG22	1.34	1.05
1:C:106:ILE:H	1:C:111:ASN:HD21	1.02	1.00
1:I:190:THR:O	1:I:192:ARG:N	1.97	0.97
1:M:106:ILE:H	1:M:111:ASN:HD21	1.14	0.95
1:B:97:GLY:O	1:B:117:SER:HB2	1.64	0.95
1:R:152:TYR:HD1	1:R:152:TYR:H	1.07	0.94
1:R:106:ILE:H	1:R:111:ASN:HD21	1.08	0.93
1:F:105:GLN:HE22	1:F:114:ALA:H	0.98	0.93
1:D:105:GLN:NE2	1:D:114:ALA:H	1.67	0.92
1:L:158:GLU:HG2	1:L:159:ILE:O	1.70	0.92
1:I:186:ASP:HB2	1:I:189:ALA:HB3	1.49	0.92
1:L:145:LEU:HD11	1:L:179:LEU:HD13	1.52	0.91
1:Q:146:THR:HG22	1:Q:151:VAL:HG13	1.52	0.91
1:A:183:THR:O	1:A:192:ARG:HB2	1.71	0.90
1:I:106:ILE:H	1:I:111:ASN:HD21	1.20	0.90
1:I:105:GLN:HE22	1:I:114:ALA:H	1.20	0.88
1:N:105:GLN:NE2	1:N:114:ALA:H	1.73	0.87
1:C:141:MET:HB2	1:C:156:ILE:HD12	1.55	0.86
1:G:106:ILE:H	1:G:111:ASN:HD21	1.21	0.86
1:H:145:LEU:HD11	1:H:179:LEU:HD13	1.56	0.85
1:M:183:THR:HG22	1:M:193:ILE:O	1.76	0.85
1:N:105:GLN:HE22	1:N:114:ALA:H	1.23	0.84
1:Q:183:THR:HG22	1:Q:183:THR:O	1.75	0.84
1:R:145:LEU:HD11	1:R:179:LEU:HD13	1.59	0.84
1:D:105:GLN:HE22	1:D:114:ALA:H	1.25	0.84
1:J:111:ASN:HB2	1:J:172:ASP:OD1	1.78	0.84
1:H:145:LEU:HD12	1:H:154:TYR:CE1	2.13	0.83
1:A:186:ASP:HB3	1:A:189:ALA:HB3	1.59	0.83
1:C:106:ILE:H	1:C:111:ASN:ND2	1.76	0.83
1:J:146:THR:CG2	1:J:151:VAL:HG22	2.09	0.83
1:R:134:LEU:HD12	1:R:183:THR:HG21	1.61	0.82
1:C:190:THR:O	1:C:192:ARG:N	2.12	0.82
1:F:105:GLN:NE2	1:F:114:ALA:H	1.77	0.81
1:J:183:THR:HG22	1:J:193:ILE:O	1.79	0.80
1:L:145:LEU:HD12	1:L:154:TYR:CE1	2.16	0.80
1:H:105:GLN:HE22	1:H:114:ALA:H	1.26	0.80
1:A:159:ILE:HD13	1:A:195:VAL:HG22	1.63	0.80
1:R:152:TYR:N	1:R:152:TYR:CD1	2.46	0.80
1:Q:186:ASP:HB3	1:Q:189:ALA:HB2	1.65	0.79
1:P:86:PHE:CD1	1:P:93:GLU:HB3	2.18	0.78
1:I:106:ILE:H	1:I:111:ASN:ND2	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:183:THR:O	1:Q:183:THR:CG2	2.30	0.78
1:A:106:ILE:H	1:A:111:ASN:HD21	1.32	0.77
1:R:152:TYR:HD1	1:R:152:TYR:N	1.80	0.77
1:C:145:LEU:HD11	1:C:179:LEU:HD13	1.68	0.75
1:E:105:GLN:NE2	1:E:114:ALA:H	1.84	0.75
1:J:79:VAL:HG23	1:J:81:ILE:HG13	1.67	0.75
1:J:106:ILE:H	1:J:111:ASN:HD21	1.33	0.75
1:J:182:VAL:HG22	1:J:194:ILE:HD12	1.69	0.74
1:E:105:GLN:HE22	1:E:114:ALA:H	1.36	0.73
1:P:159:ILE:HD13	1:P:195:VAL:HG22	1.68	0.73
1:C:105:GLN:HE22	1:C:114:ALA:H	1.35	0.73
1:R:106:ILE:H	1:R:111:ASN:ND2	1.85	0.73
1:H:186:ASP:OD1	1:H:187:PRO:O	2.07	0.73
1:P:105:GLN:HE22	1:P:114:ALA:H	1.34	0.73
1:J:105:GLN:NE2	1:J:114:ALA:H	1.88	0.72
1:Q:147:ASP:C	1:Q:147:ASP:OD1	2.30	0.72
1:F:105:GLN:HE22	1:F:114:ALA:N	1.82	0.72
1:Q:159:ILE:CD1	1:Q:195:VAL:HG22	2.13	0.72
1:P:105:GLN:NE2	1:P:114:ALA:H	1.86	0.72
1:J:147:ASP:O	1:J:149:SER:N	2.22	0.71
1:R:67:ASN:O	1:R:69:PRO:HD3	1.90	0.71
1:A:105:GLN:NE2	1:A:114:ALA:H	1.89	0.71
1:H:106:ILE:H	1:H:111:ASN:HD21	1.39	0.71
1:I:105:GLN:NE2	1:I:114:ALA:H	1.88	0.71
1:Q:89:LEU:HD13	1:R:136:HIS:HB3	1.72	0.71
1:B:105:GLN:HE22	1:B:114:ALA:H	1.38	0.71
1:L:121:PHE:HD2	1:L:133:PRO:HG3	1.55	0.71
1:P:186:ASP:HB2	1:P:189:ALA:HB2	1.71	0.71
1:A:108:GLY:HA3	1:A:152:TYR:CD1	2.25	0.70
1:O:105:GLN:NE2	1:O:114:ALA:H	1.89	0.70
1:M:181:LEU:HB3	1:M:195:VAL:HB	1.74	0.70
1:M:78:ASP:HB3	1:M:141:MET:HE2	1.74	0.69
1:B:105:GLN:HE22	1:B:114:ALA:N	1.90	0.69
1:A:153:THR:HB	1:A:201:LYS:O	1.93	0.69
1:R:173:THR:HB	1:R:176:LYS:HB2	1.75	0.68
1:E:186:ASP:HB3	1:E:189:ALA:H	1.59	0.68
1:Q:179:LEU:HD23	1:Q:197:ALA:HB3	1.75	0.67
1:A:177:SER:OG	1:A:199:LEU:HB3	1.93	0.67
1:P:66:HIS:NE2	1:Q:80:GLU:OE1	2.25	0.67
1:K:182:VAL:HG22	1:K:194:ILE:HD12	1.77	0.67
1:F:83:LEU:HD21	1:F:121:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:186:ASP:CG	1:N:187:PRO:HD2	2.20	0.66
1:Q:146:THR:CG2	1:Q:151:VAL:HG13	2.24	0.66
1:L:98:ALA:HB1	1:L:115:LEU:CD2	2.25	0.66
1:M:179:LEU:HB3	1:M:197:ALA:HB3	1.77	0.65
1:K:74:ILE:CG2	1:K:83:LEU:HB2	2.26	0.65
1:H:78:ASP:HB2	1:H:141:MET:HE2	1.78	0.65
1:I:94:LEU:HD13	1:I:118:HIS:CE1	2.32	0.65
1:A:186:ASP:CB	1:A:189:ALA:HB3	2.26	0.65
1:F:168:GLU:OE2	1:F:196:HIS:HE1	1.79	0.65
1:P:202:THR:OG1	1:P:203:GLY:N	2.28	0.65
1:Q:186:ASP:OD1	1:Q:187:PRO:N	2.30	0.64
1:B:89:LEU:HD13	1:C:136:HIS:HB3	1.79	0.64
1:O:106:ILE:H	1:O:111:ASN:HD21	1.43	0.64
1:A:91:ASN:HD21	1:B:133:PRO:HA	1.61	0.64
3:D:401:HOH:O	1:E:135:GLU:HG2	1.97	0.64
1:A:142:LYS:NZ	1:A:200:GLU:OE1	2.31	0.64
1:F:147:ASP:CG	1:F:147:ASP:O	2.41	0.63
1:C:145:LEU:HD12	1:C:154:TYR:CE1	2.34	0.63
1:L:76:ILE:HG12	1:L:143:VAL:HG13	1.81	0.63
1:L:102:LYS:NZ	1:L:105:GLN:HE21	1.97	0.63
1:P:105:GLN:HE22	1:P:114:ALA:N	1.97	0.63
1:G:136:HIS:HB3	1:L:89:LEU:HD13	1.79	0.62
1:L:111:ASN:OD1	1:L:111:ASN:N	2.30	0.62
1:A:164:PRO:HG3	1:A:190:THR:HG23	1.81	0.62
1:O:79:VAL:HG23	1:O:81:ILE:HG13	1.81	0.62
1:H:78:ASP:CB	1:H:141:MET:HE2	2.29	0.62
1:H:106:ILE:H	1:H:111:ASN:ND2	1.96	0.62
1:J:176:LYS:HD3	1:J:178:GLN:NE2	2.15	0.62
1:I:106:ILE:N	1:I:111:ASN:HD21	1.94	0.62
1:J:66:HIS:NE2	1:K:80:GLU:OE1	2.26	0.62
1:I:153:THR:HB	1:I:201:LYS:O	2.00	0.62
1:K:186:ASP:HB2	1:K:189:ALA:HB3	1.82	0.62
1:L:98:ALA:CB	1:L:115:LEU:CD2	2.78	0.62
1:E:119:HIS:NE2	1:E:121:PHE:CZ	2.65	0.61
1:M:152:TYR:CD1	1:M:152:TYR:N	2.67	0.61
1:L:94:LEU:CD2	1:L:116:ALA:O	2.48	0.61
1:O:186:ASP:HB3	1:O:189:ALA:HB3	1.82	0.61
1:K:94:LEU:HD23	1:K:116:ALA:O	2.01	0.61
1:N:75:ALA:HA	1:N:81:ILE:O	2.00	0.61
1:A:166:HIS:O	1:A:192:ARG:NH2	2.32	0.61
1:C:106:ILE:N	1:C:111:ASN:HD21	1.85	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:TYR:CD2	1:D:153:THR:HG22	2.36	0.61
1:E:91:ASN:HB2	1:F:133:PRO:HB3	1.83	0.61
1:K:89:LEU:HD21	1:K:101:MET:HA	1.82	0.61
1:A:145:LEU:HD12	1:A:154:TYR:CE1	2.36	0.60
1:Q:91:ASN:HB2	1:R:133:PRO:HB3	1.82	0.60
1:E:201:LYS:H	1:E:201:LYS:HD3	1.66	0.60
1:L:105:GLN:HE22	1:L:114:ALA:H	1.50	0.60
1:B:145:LEU:HD11	1:B:179:LEU:HD13	1.84	0.60
1:N:186:ASP:OD2	1:N:188:GLU:CB	2.50	0.60
1:F:145:LEU:HD11	1:F:179:LEU:HD22	1.84	0.60
1:C:153:THR:O	1:C:199:LEU:HD12	2.02	0.60
1:A:145:LEU:HD11	1:A:179:LEU:HD13	1.84	0.59
1:M:110:PRO:HA	1:M:177:SER:OG	2.02	0.59
1:I:186:ASP:HB2	1:I:189:ALA:CB	2.26	0.59
1:Q:183:THR:HG22	1:Q:193:ILE:H	1.68	0.59
1:P:102:LYS:HE2	1:P:105:GLN:HE21	1.66	0.59
1:I:89:LEU:HD13	1:J:136:HIS:HB3	1.85	0.59
1:R:135:GLU:HB3	1:R:136:HIS:HD2	1.68	0.59
1:K:71:ILE:HD12	1:K:71:ILE:O	2.02	0.59
1:A:152:TYR:CD2	1:A:152:TYR:N	2.70	0.59
1:B:111:ASN:HB2	1:B:172:ASP:OD1	2.01	0.59
1:G:186:ASP:HB3	1:G:189:ALA:HB3	1.85	0.59
1:D:141:MET:HB2	1:D:156:ILE:HD12	1.85	0.58
1:K:112:ASN:HB2	1:K:172:ASP:HA	1.84	0.58
1:M:81:ILE:CD1	1:M:134:LEU:CD2	2.82	0.58
1:M:105:GLN:NE2	1:M:114:ALA:H	2.02	0.58
1:F:152:TYR:CD1	1:F:152:TYR:N	2.71	0.58
1:I:99:GLY:O	1:I:115:LEU:HA	2.03	0.58
1:F:181:LEU:HB3	1:F:195:VAL:HB	1.85	0.58
1:I:83:LEU:HD21	1:I:119:HIS:CD2	2.39	0.58
1:G:181:LEU:HB3	1:G:195:VAL:HB	1.86	0.57
1:I:159:ILE:CD1	1:I:195:VAL:HG22	2.33	0.57
1:R:150:LYS:HB3	1:R:152:TYR:CE1	2.39	0.57
1:H:202:THR:OG1	1:H:203:GLY:N	2.37	0.57
1:O:134:LEU:CD1	1:O:183:THR:HG21	2.34	0.57
1:Q:105:GLN:HE22	1:Q:114:ALA:H	1.51	0.57
1:D:179:LEU:HD23	1:D:197:ALA:HB3	1.86	0.57
1:O:168:GLU:OE2	1:O:196:HIS:HE1	1.87	0.57
1:Q:167:VAL:O	1:Q:167:VAL:HG23	2.05	0.57
1:M:145:LEU:HD11	1:M:179:LEU:HD13	1.87	0.56
1:B:105:GLN:NE2	1:B:114:ALA:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:VAL:HG22	1:C:194:ILE:HD12	1.87	0.56
1:M:105:GLN:HE22	1:M:114:ALA:H	1.52	0.56
1:Q:147:ASP:OD1	1:Q:148:LYS:N	2.38	0.56
1:M:106:ILE:H	1:M:111:ASN:ND2	1.94	0.56
1:K:186:ASP:CB	1:K:189:ALA:H	2.18	0.56
1:M:106:ILE:HD12	1:M:111:ASN:ND2	2.19	0.56
1:B:154:TYR:HA	1:B:198:GLU:O	2.06	0.56
1:D:106:ILE:HD12	1:D:106:ILE:N	2.21	0.56
1:G:186:ASP:HB3	1:G:189:ALA:CB	2.36	0.56
1:K:186:ASP:HB2	1:K:189:ALA:H	1.69	0.56
1:I:102:LYS:NZ	1:I:172:ASP:OD1	2.39	0.56
1:B:137:ALA:HB3	1:B:159:ILE:HD12	1.88	0.55
1:R:140:GLY:HA2	1:R:155:THR:HG23	1.86	0.55
1:B:106:ILE:H	1:B:111:ASN:HD21	1.55	0.55
1:K:152:TYR:N	1:K:152:TYR:CD1	2.75	0.55
1:M:133:PRO:C	1:M:135:GLU:H	2.15	0.55
1:N:107:MET:HG3	1:N:145:LEU:HD13	1.88	0.55
1:H:141:MET:HB2	1:H:156:ILE:HD12	1.88	0.54
1:J:105:GLN:HE22	1:J:114:ALA:H	1.55	0.54
1:J:105:GLN:NE2	1:J:114:ALA:N	2.54	0.54
1:R:138:LYS:HB2	1:R:141:MET:HE3	1.88	0.54
1:B:81:ILE:HD11	1:B:133:PRO:HB2	1.89	0.54
1:B:108:GLY:HA3	1:B:152:TYR:CD2	2.42	0.54
1:H:153:THR:O	1:H:199:LEU:HD12	2.07	0.54
1:H:145:LEU:HD12	1:H:154:TYR:HE1	1.71	0.54
1:H:168:GLU:OE2	1:H:196:HIS:HE1	1.90	0.54
1:I:89:LEU:HD21	1:I:101:MET:HG2	1.89	0.54
1:N:89:LEU:HD21	1:N:101:MET:HG2	1.89	0.54
1:K:76:ILE:HG12	1:K:143:VAL:HG22	1.90	0.54
1:F:147:ASP:O	1:F:148:LYS:CB	2.51	0.54
1:H:106:ILE:N	1:H:111:ASN:HD21	2.06	0.54
1:H:185:THR:HG23	1:H:186:ASP:H	1.73	0.54
1:M:81:ILE:CD1	1:M:134:LEU:HD23	2.38	0.54
1:P:81:ILE:HD11	1:P:133:PRO:HB2	1.89	0.54
1:Q:159:ILE:HD13	1:Q:195:VAL:CG2	2.19	0.54
1:N:137:ALA:C	1:N:138:LYS:HG2	2.33	0.53
1:H:161:LYS:HG2	1:H:193:ILE:HG12	1.90	0.53
1:Q:105:GLN:NE2	1:Q:114:ALA:H	2.07	0.53
1:O:74:ILE:HG23	1:O:74:ILE:O	2.08	0.53
1:I:76:ILE:HG12	1:I:143:VAL:HG13	1.90	0.53
1:N:186:ASP:OD1	1:N:187:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:186:ASP:OD1	1:Q:188:GLU:N	2.30	0.53
1:E:75:ALA:HA	1:E:81:ILE:O	2.08	0.53
1:M:136:HIS:HB3	1:R:89:LEU:HD13	1.91	0.53
1:Q:201:LYS:C	1:Q:203:GLY:N	2.61	0.53
1:G:80:GLU:OE2	1:L:93:GLU:OE1	2.27	0.53
1:F:168:GLU:OE2	1:F:196:HIS:CE1	2.62	0.53
1:L:98:ALA:CB	1:L:115:LEU:HD22	2.39	0.53
1:L:98:ALA:HB1	1:L:115:LEU:HD22	1.90	0.53
1:R:143:VAL:HB	1:R:154:TYR:HB2	1.91	0.53
1:I:119:HIS:HD2	1:I:121:PHE:CZ	2.27	0.52
1:M:139:LYS:HA	1:M:156:ILE:HG22	1.90	0.52
1:N:106:ILE:H	1:N:111:ASN:HD21	1.55	0.52
1:D:108:GLY:HA2	1:D:154:TYR:OH	2.10	0.52
1:M:107:MET:O	1:M:152:TYR:CE2	2.62	0.52
1:R:179:LEU:HB3	1:R:197:ALA:HB3	1.92	0.52
1:J:145:LEU:HD12	1:J:154:TYR:CE1	2.44	0.52
1:K:107:MET:HE1	1:K:146:THR:O	2.10	0.52
1:H:78:ASP:N	1:H:78:ASP:OD1	2.41	0.52
1:K:83:LEU:HD13	1:K:97:GLY:HA2	1.92	0.52
1:L:98:ALA:HB1	1:L:115:LEU:HD23	1.90	0.51
1:R:107:MET:O	1:R:152:TYR:CE2	2.63	0.51
1:R:111:ASN:HA	1:R:172:ASP:HB3	1.91	0.51
1:K:199:LEU:HD11	1:K:202:THR:HB	1.92	0.51
1:Q:201:LYS:C	1:Q:203:GLY:H	2.17	0.51
1:Q:146:THR:HG22	1:Q:151:VAL:CG1	2.35	0.51
1:C:105:GLN:NE2	1:C:114:ALA:H	2.04	0.51
1:M:134:LEU:HD13	1:M:195:VAL:CG2	2.41	0.51
1:A:134:LEU:HB3	1:A:193:ILE:HG21	1.93	0.51
1:D:106:ILE:H	1:D:111:ASN:HD21	1.59	0.51
1:G:102:LYS:HD3	1:G:105:GLN:NE2	2.26	0.51
1:L:102:LYS:HZ3	1:L:105:GLN:HE21	1.57	0.51
1:J:146:THR:HG22	1:J:151:VAL:CG2	2.25	0.51
1:E:90:GLY:O	1:E:93:GLU:HB2	2.11	0.51
1:F:188:GLU:O	1:F:190:THR:HG23	2.11	0.51
1:A:162:VAL:HG11	1:A:166:HIS:CD2	2.46	0.51
1:L:186:ASP:HB2	1:L:187:PRO:HD3	1.93	0.51
1:R:83:LEU:HD22	1:R:97:GLY:HA2	1.93	0.51
1:M:81:ILE:CD1	1:M:134:LEU:HD21	2.41	0.50
1:N:161:LYS:HD3	1:N:191:GLU:OE2	2.11	0.50
1:M:121:PHE:CD2	1:M:133:PRO:HG3	2.46	0.50
1:J:204:GLU:OE2	1:J:204:GLU:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:TYR:N	1:M:152:TYR:HD1	2.10	0.50
1:P:89:LEU:HD13	1:Q:136:HIS:HB3	1.93	0.50
1:Q:115:LEU:O	1:Q:181:LEU:HD12	2.11	0.50
1:C:68:LEU:HB3	1:C:86:PHE:CE2	2.47	0.50
1:C:99:GLY:O	1:C:115:LEU:HA	2.11	0.50
1:E:146:THR:HG22	1:E:151:VAL:HG13	1.93	0.50
1:D:111:ASN:OD1	1:D:111:ASN:N	2.43	0.50
1:J:89:LEU:HD13	1:K:136:HIS:HB3	1.94	0.50
1:J:141:MET:HB2	1:J:156:ILE:HD12	1.92	0.50
1:J:168:GLU:OE2	1:J:196:HIS:HE1	1.95	0.50
1:A:116:ALA:HA	1:A:182:VAL:O	2.11	0.50
1:D:144:TYR:CE2	1:D:153:THR:HG22	2.46	0.50
1:M:99:GLY:O	1:M:115:LEU:HA	2.12	0.50
1:F:147:ASP:O	1:F:147:ASP:OD1	2.29	0.50
1:R:105:GLN:HE22	1:R:114:ALA:H	1.59	0.49
1:A:143:VAL:HB	1:A:154:TYR:HB2	1.93	0.49
1:G:102:LYS:HD3	1:G:105:GLN:HE21	1.77	0.49
1:N:162:VAL:HG11	1:N:166:HIS:CD2	2.46	0.49
1:G:145:LEU:HD11	1:G:179:LEU:HD13	1.95	0.49
1:N:167:VAL:HG23	1:N:167:VAL:O	2.12	0.49
1:F:150:LYS:HB3	1:F:203:GLY:O	2.12	0.49
1:H:74:ILE:HD12	1:H:145:LEU:HD21	1.94	0.49
1:N:145:LEU:HD12	1:N:154:TYR:CE1	2.48	0.49
1:E:201:LYS:H	1:E:201:LYS:CD	2.25	0.49
1:H:102:LYS:HD3	1:H:105:GLN:NE2	2.27	0.49
1:R:74:ILE:HG23	1:R:83:LEU:HB2	1.93	0.49
1:A:150:LYS:HE3	1:A:152:TYR:OH	2.12	0.49
1:K:74:ILE:HG22	1:K:83:LEU:HB2	1.95	0.49
1:P:179:LEU:HD23	1:P:197:ALA:HB3	1.94	0.49
1:D:145:LEU:HD11	1:D:179:LEU:HD13	1.95	0.49
1:L:106:ILE:H	1:L:111:ASN:HD21	1.61	0.49
1:L:186:ASP:CG	1:L:187:PRO:CD	2.86	0.49
1:M:89:LEU:HD21	1:M:101:MET:HG2	1.94	0.49
1:B:168:GLU:OE1	1:B:194:ILE:HG21	2.12	0.49
1:F:168:GLU:OE1	1:F:194:ILE:HG21	2.12	0.49
1:J:91:ASN:HB2	1:K:133:PRO:HB3	1.94	0.49
1:C:87:LYS:HA	1:C:100:THR:OG1	2.13	0.49
1:D:76:ILE:HG12	1:D:143:VAL:HG22	1.95	0.49
1:P:106:ILE:H	1:P:111:ASN:HD21	1.60	0.48
1:J:132:SER:O	1:J:135:GLU:HB2	2.13	0.48
1:I:186:ASP:HB3	1:I:189:ALA:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ALA:HA	1:B:182:VAL:O	2.13	0.48
1:R:145:LEU:HD12	1:R:154:TYR:CE1	2.49	0.48
1:C:186:ASP:HB3	1:C:189:ALA:CB	2.44	0.48
1:H:76:ILE:HG12	1:H:143:VAL:HG22	1.95	0.48
1:O:134:LEU:HD11	1:O:183:THR:HG21	1.96	0.48
1:O:187:PRO:HB3	1:P:131:PHE:CE1	2.49	0.48
1:C:146:THR:HB	1:C:151:VAL:HG22	1.96	0.48
1:H:179:LEU:HD23	1:H:197:ALA:HB3	1.96	0.48
1:L:107:MET:HE2	1:L:113:TYR:OH	2.13	0.48
1:D:102:LYS:HD2	1:D:170:ILE:HD12	1.96	0.48
1:H:105:GLN:HE22	1:H:114:ALA:N	2.03	0.48
1:M:81:ILE:HD11	1:M:134:LEU:HD23	1.95	0.48
1:N:168:GLU:OE2	1:N:196:HIS:HE1	1.97	0.48
1:Q:194:ILE:HG22	1:Q:196:HIS:CE1	2.49	0.48
1:I:119:HIS:CD2	1:I:121:PHE:CZ	3.02	0.48
1:Q:156:ILE:HG23	1:Q:195:VAL:HG13	1.96	0.47
1:R:146:THR:HG22	1:R:151:VAL:HG13	1.96	0.47
1:A:166:HIS:HB2	1:L:161:LYS:HB2	1.95	0.47
1:R:108:GLY:HA3	1:R:152:TYR:CD2	2.48	0.47
1:E:206:SER:O	1:E:206:SER:OG	2.30	0.47
1:P:86:PHE:HD1	1:P:93:GLU:HB3	1.75	0.47
1:B:67:ASN:O	1:B:69:PRO:HD3	2.14	0.47
1:D:94:LEU:HD13	1:D:118:HIS:CE1	2.48	0.47
1:G:105:GLN:HE22	1:G:114:ALA:H	1.62	0.47
1:K:94:LEU:CD2	1:K:116:ALA:O	2.62	0.47
1:B:145:LEU:HD12	1:B:154:TYR:CE1	2.49	0.47
1:J:157:THR:N	1:J:196:HIS:O	2.40	0.47
1:L:94:LEU:HD23	1:L:116:ALA:O	2.13	0.47
1:B:115:LEU:HB2	1:B:181:LEU:HD13	1.96	0.47
1:C:164:PRO:HD3	1:C:190:THR:OG1	2.14	0.47
1:E:206:SER:OG	1:E:209:ASP:C	2.57	0.47
1:L:106:ILE:H	1:L:111:ASN:ND2	2.11	0.47
1:H:78:ASP:HB2	1:H:141:MET:CE	2.44	0.47
1:I:137:ALA:C	1:I:138:LYS:HG2	2.40	0.47
1:J:153:THR:O	1:J:199:LEU:HD12	2.13	0.47
1:M:116:ALA:HA	1:M:182:VAL:O	2.14	0.47
1:M:154:TYR:HB3	1:M:197:ALA:HB1	1.95	0.47
1:H:119:HIS:HD2	1:H:121:PHE:CE2	2.32	0.47
1:L:86:PHE:HE1	1:L:97:GLY:HA3	1.78	0.47
1:L:185:THR:HG22	1:L:186:ASP:OD1	2.14	0.47
1:C:95:SER:O	1:C:119:HIS:ND1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:TYR:HD1	1:M:152:TYR:H	1.63	0.46
1:R:154:TYR:HB3	1:R:197:ALA:HB1	1.97	0.46
1:B:166:HIS:HB2	1:K:161:LYS:HB2	1.98	0.46
1:D:89:LEU:HD13	1:E:136:HIS:HB3	1.98	0.46
1:E:152:TYR:CD1	1:E:152:TYR:N	2.83	0.46
1:K:145:LEU:HD12	1:K:154:TYR:CE1	2.50	0.46
1:F:83:LEU:HD21	1:F:121:PHE:HZ	1.76	0.46
1:G:106:ILE:H	1:G:111:ASN:ND2	2.00	0.46
1:L:109:GLY:C	1:L:111:ASN:OD1	2.58	0.46
1:M:183:THR:CG2	1:M:193:ILE:O	2.58	0.46
1:R:108:GLY:HA3	1:R:152:TYR:CE2	2.50	0.46
1:B:102:LYS:HB2	1:B:105:GLN:HG3	1.98	0.46
1:H:119:HIS:CD2	1:H:121:PHE:CE2	3.03	0.46
1:M:183:THR:O	1:M:192:ARG:HG3	2.15	0.46
1:A:173:THR:HG21	1:A:176:LYS:HD2	1.97	0.46
1:E:207:THR:O	1:E:208:ALA:HB3	2.15	0.46
1:L:186:ASP:CG	1:L:187:PRO:HD2	2.40	0.46
1:K:154:TYR:HA	1:K:198:GLU:O	2.15	0.46
1:O:141:MET:HB2	1:O:156:ILE:HD12	1.96	0.46
1:A:98:ALA:HB1	1:A:115:LEU:HD13	1.98	0.46
1:G:74:ILE:HB	1:G:85:ILE:HD11	1.98	0.46
1:I:159:ILE:HD12	1:I:195:VAL:HG22	1.98	0.46
1:A:139:LYS:NZ	1:L:171:ASP:HB2	2.31	0.45
1:A:106:ILE:H	1:A:111:ASN:ND2	2.08	0.45
1:D:138:LYS:HB2	1:D:141:MET:HE3	1.98	0.45
1:G:182:VAL:HG22	1:G:194:ILE:HD12	1.98	0.45
1:J:105:GLN:HB3	1:J:113:TYR:CE1	2.51	0.45
1:O:165:GLU:H	1:O:165:GLU:HG3	1.62	0.45
1:P:107:MET:HG3	1:P:145:LEU:HD12	1.98	0.45
1:C:77:PRO:HG3	1:C:144:TYR:HE1	1.82	0.45
1:N:168:GLU:OE2	1:N:196:HIS:CE1	2.70	0.45
1:Q:186:ASP:OD1	1:Q:186:ASP:C	2.57	0.45
1:H:83:LEU:HA	1:H:84:PRO:HD2	1.73	0.45
1:O:179:LEU:HB3	1:O:197:ALA:HB3	1.99	0.45
1:E:186:ASP:HB2	1:E:189:ALA:CB	2.46	0.45
1:I:163:THR:HB	1:I:164:PRO:CD	2.47	0.45
1:J:67:ASN:HD22	1:J:69:PRO:HD3	1.81	0.45
1:D:152:TYR:CD1	1:D:152:TYR:N	2.84	0.45
1:L:147:ASP:N	1:L:150:LYS:O	2.49	0.45
1:A:105:GLN:HE22	1:A:114:ALA:H	1.61	0.45
1:A:139:LYS:HD2	1:A:157:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:TYR:HD2	1:C:202:THR:HB	1.82	0.45
1:G:119:HIS:HD2	1:G:121:PHE:CZ	2.35	0.45
1:E:105:GLN:HE22	1:E:114:ALA:N	2.10	0.45
1:H:106:ILE:N	1:H:106:ILE:HD12	2.32	0.45
1:H:186:ASP:O	1:H:189:ALA:HB3	2.17	0.45
1:M:94:LEU:HD13	1:M:118:HIS:CE1	2.52	0.45
1:E:190:THR:O	1:E:192:ARG:N	2.50	0.45
1:J:105:GLN:HE22	1:J:114:ALA:N	2.12	0.45
1:H:179:LEU:HB3	1:H:197:ALA:HB3	1.98	0.44
1:I:182:VAL:HG22	1:I:194:ILE:HD12	1.98	0.44
1:K:73:GLY:N	1:K:85:ILE:HD12	2.32	0.44
1:O:168:GLU:OE2	1:O:196:HIS:CE1	2.68	0.44
1:P:134:LEU:CD1	1:P:183:THR:HG21	2.47	0.44
1:K:183:THR:HG22	1:K:193:ILE:HB	1.98	0.44
1:Q:187:PRO:HD3	1:R:131:PHE:CZ	2.52	0.44
1:P:98:ALA:HB2	1:P:117:SER:HB2	1.98	0.44
1:J:116:ALA:HA	1:J:182:VAL:O	2.17	0.44
1:P:159:ILE:CD1	1:P:195:VAL:HG22	2.42	0.44
1:A:186:ASP:HB3	1:A:189:ALA:CB	2.39	0.44
1:K:111:ASN:HA	1:K:172:ASP:HB3	1.98	0.44
1:M:132:SER:O	1:M:135:GLU:HB2	2.18	0.44
1:B:167:VAL:O	1:B:167:VAL:HG23	2.18	0.44
1:G:119:HIS:CD2	1:G:121:PHE:CZ	3.05	0.44
1:G:121:PHE:CE2	1:G:133:PRO:HG3	2.52	0.44
1:K:95:SER:O	1:K:119:HIS:ND1	2.46	0.44
1:P:183:THR:HG23	1:P:193:ILE:O	2.17	0.44
1:L:183:THR:HB	1:L:193:ILE:O	2.17	0.44
1:Q:147:ASP:O	1:Q:148:LYS:C	2.58	0.44
1:C:186:ASP:HA	1:C:187:PRO:HD2	1.82	0.44
1:L:168:GLU:HA	1:L:168:GLU:OE2	2.18	0.44
1:B:90:GLY:O	1:B:94:LEU:HG	2.18	0.43
1:K:143:VAL:HG11	1:K:179:LEU:HD21	2.00	0.43
1:B:92:THR:O	1:B:93:GLU:C	2.61	0.43
1:C:109:GLY:O	1:C:177:SER:OG	2.20	0.43
1:E:183:THR:O	1:E:192:ARG:HG3	2.18	0.43
1:A:183:THR:HG22	1:A:184:CYS:N	2.34	0.43
1:P:102:LYS:HD3	1:P:170:ILE:HD12	2.00	0.43
1:I:134:LEU:HB3	1:I:193:ILE:HG21	1.99	0.43
1:K:83:LEU:HA	1:K:84:PRO:HD2	1.73	0.43
1:K:186:ASP:HB2	1:K:189:ALA:CB	2.47	0.43
1:A:102:LYS:NZ	1:A:112:ASN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:PHE:HD2	1:D:133:PRO:HG3	1.83	0.43
1:G:105:GLN:NE2	1:G:114:ALA:H	2.17	0.43
1:L:146:THR:HG22	1:L:151:VAL:HG13	2.00	0.43
1:D:160:SER:HA	1:I:166:HIS:CE1	2.53	0.43
1:J:134:LEU:HD12	1:J:183:THR:HG21	2.01	0.43
1:L:76:ILE:HB	1:L:81:ILE:HB	2.00	0.43
1:M:135:GLU:CG	3:M:403:HOH:O	2.66	0.43
1:Q:204:GLU:O	1:Q:205:PHE:CB	2.66	0.43
1:R:158:GLU:HG2	1:R:160:SER:OG	2.19	0.43
1:A:189:ALA:O	1:A:190:THR:HG22	2.18	0.43
1:B:113:TYR:CD2	1:B:145:LEU:HD13	2.54	0.43
1:K:134:LEU:HB3	1:K:193:ILE:HG21	2.01	0.43
1:L:77:PRO:HD3	1:L:142:LYS:O	2.18	0.43
1:P:168:GLU:OE1	1:P:168:GLU:HA	2.19	0.43
1:R:105:GLN:NE2	1:R:114:ALA:H	2.16	0.43
1:Q:204:GLU:O	1:Q:205:PHE:HB2	2.18	0.43
1:R:138:LYS:O	1:R:141:MET:HG3	2.19	0.43
1:L:98:ALA:HB3	1:L:115:LEU:CD2	2.48	0.43
1:L:137:ALA:O	1:L:159:ILE:HG13	2.19	0.43
1:P:70:VAL:HG22	1:P:86:PHE:HE2	1.83	0.43
1:A:102:LYS:HB2	1:A:105:GLN:NE2	2.33	0.42
1:B:107:MET:HG3	1:B:113:TYR:CE2	2.54	0.42
1:C:152:TYR:CD2	1:C:202:THR:HB	2.53	0.42
1:E:89:LEU:HD21	1:E:101:MET:HA	2.02	0.42
1:R:156:ILE:HD13	1:R:159:ILE:HD11	2.01	0.42
1:A:83:LEU:HA	1:A:84:PRO:HD2	1.89	0.42
1:E:119:HIS:NE2	1:E:121:PHE:CE2	2.87	0.42
1:O:144:TYR:CE2	1:O:153:THR:HG23	2.54	0.42
1:Q:70:VAL:HG22	1:Q:86:PHE:CE2	2.54	0.42
1:K:186:ASP:HB2	1:K:189:ALA:N	2.33	0.42
1:L:117:SER:OG	1:L:119:HIS:HB2	2.19	0.42
1:J:89:LEU:HD23	1:J:89:LEU:HA	1.85	0.42
1:R:138:LYS:N	1:R:141:MET:HE3	2.34	0.42
1:C:94:LEU:O	1:C:118:HIS:N	2.40	0.42
1:P:74:ILE:O	1:P:74:ILE:HG23	2.20	0.42
1:B:152:TYR:CD1	1:B:152:TYR:N	2.88	0.42
1:H:183:THR:O	1:H:192:ARG:HG2	2.19	0.42
1:A:145:LEU:HD12	1:A:154:TYR:CZ	2.54	0.42
1:C:108:GLY:HA2	1:C:154:TYR:OH	2.19	0.42
1:E:103:GLU:OE2	1:F:78:ASP:OD2	2.37	0.42
1:F:108:GLY:HA3	1:F:152:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:LYS:HD3	1:J:178:GLN:HE21	1.85	0.42
1:K:164:PRO:HD3	1:K:190:THR:HB	2.02	0.42
1:L:77:PRO:HD2	1:L:78:ASP:H	1.84	0.42
1:L:183:THR:O	1:L:192:ARG:HG2	2.20	0.42
1:M:133:PRO:C	1:M:135:GLU:N	2.75	0.42
1:A:152:TYR:N	1:A:152:TYR:HD2	2.15	0.42
1:A:153:THR:O	1:A:199:LEU:HD12	2.20	0.42
1:J:67:ASN:ND2	1:J:69:PRO:HD3	2.35	0.42
1:O:134:LEU:HD12	1:O:183:THR:HG21	2.02	0.42
1:R:86:PHE:O	1:R:99:GLY:HA2	2.20	0.42
1:E:173:THR:HA	1:E:174:PRO:HD2	1.77	0.41
1:P:135:GLU:OE2	1:P:135:GLU:HA	2.19	0.41
1:A:165:GLU:O	1:A:165:GLU:HG2	2.19	0.41
1:F:95:SER:O	1:F:119:HIS:ND1	2.53	0.41
1:A:177:SER:OG	1:A:199:LEU:CB	2.66	0.41
1:J:164:PRO:HA	1:J:192:ARG:HH21	1.86	0.41
1:O:133:PRO:C	1:O:135:GLU:H	2.29	0.41
1:A:160:SER:O	1:A:193:ILE:HA	2.21	0.41
1:A:163:THR:HB	1:A:164:PRO:HD2	2.03	0.41
1:D:144:TYR:HD2	1:D:153:THR:HG22	1.85	0.41
1:M:135:GLU:HG2	3:M:403:HOH:O	2.20	0.41
1:E:107:MET:HG3	1:E:145:LEU:HD13	2.03	0.41
1:F:145:LEU:HD13	1:F:154:TYR:CE1	2.56	0.41
1:J:147:ASP:HB3	1:J:149:SER:OG	2.20	0.41
1:M:89:LEU:HD13	1:N:136:HIS:HB3	2.02	0.41
1:R:111:ASN:HB2	1:R:172:ASP:OD1	2.20	0.41
1:K:78:ASP:OD1	1:K:78:ASP:N	2.53	0.41
1:K:102:LYS:HB2	1:K:105:GLN:NE2	2.35	0.41
1:L:186:ASP:CB	1:L:187:PRO:CD	2.99	0.41
1:O:86:PHE:O	1:O:99:GLY:HA2	2.21	0.41
1:Q:94:LEU:O	1:Q:118:HIS:HB2	2.21	0.41
1:M:162:VAL:HG11	1:M:166:HIS:CD2	2.56	0.41
1:N:92:THR:O	1:N:93:GLU:C	2.64	0.41
1:Q:186:ASP:HA	1:Q:187:PRO:HD2	1.86	0.41
1:H:105:GLN:NE2	1:H:114:ALA:H	2.06	0.41
1:O:106:ILE:H	1:O:111:ASN:ND2	2.14	0.41
1:R:107:MET:HE3	1:R:107:MET:HB2	1.87	0.41
1:J:81:ILE:HD11	1:J:133:PRO:HB2	2.03	0.40
1:O:105:GLN:HE22	1:O:114:ALA:H	1.61	0.40
1:P:115:LEU:O	1:P:181:LEU:HA	2.21	0.40
1:Q:205:PHE:HD1	1:Q:205:PHE:HA	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:ALA:HA	1:G:182:VAL:O	2.21	0.40
1:K:109:GLY:C	1:K:111:ASN:H	2.29	0.40
1:K:152:TYR:HD1	1:K:152:TYR:H	1.69	0.40
1:R:139:LYS:HG3	1:R:157:THR:O	2.20	0.40
1:B:137:ALA:HB3	1:B:159:ILE:CD1	2.51	0.40
1:E:179:LEU:HB3	1:E:197:ALA:HB3	2.03	0.40
1:L:133:PRO:C	1:L:135:GLU:H	2.30	0.40
1:R:77:PRO:C	1:R:79:VAL:N	2.79	0.40
1:B:121:PHE:CD1	1:B:121:PHE:C	2.96	0.40
1:C:102:LYS:HD2	1:C:170:ILE:HD12	2.04	0.40
1:F:145:LEU:HD12	1:F:145:LEU:N	2.36	0.40
1:H:78:ASP:HB3	1:H:141:MET:HE2	2.02	0.40
1:P:135:GLU:HB3	1:P:136:HIS:HD2	1.86	0.40
1:Q:154:TYR:CE2	1:Q:179:LEU:HB2	2.55	0.40
1:B:117:SER:O	1:B:183:THR:HA	2.22	0.40
1:C:168:GLU:OE2	1:C:196:HIS:HE1	2.04	0.40
1:E:183:THR:CG2	1:E:193:ILE:HB	2.52	0.40
1:H:81:ILE:HD11	1:H:133:PRO:HB2	2.04	0.40
1:L:107:MET:HE3	1:L:107:MET:HB2	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	125/160 (78%)	111 (89%)	12 (10%)	2 (2%)	7	30
1	B	116/160 (72%)	106 (91%)	9 (8%)	1 (1%)	14	44
1	C	121/160 (76%)	114 (94%)	6 (5%)	1 (1%)	16	47
1	D	121/160 (76%)	112 (93%)	9 (7%)	0	100	100
1	E	126/160 (79%)	109 (86%)	15 (12%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	128/160 (80%)	120 (94%)	8 (6%)	0	100	100
1	G	128/160 (80%)	116 (91%)	11 (9%)	1 (1%)	16	47
1	H	124/160 (78%)	108 (87%)	14 (11%)	2 (2%)	7	30
1	I	125/160 (78%)	111 (89%)	13 (10%)	1 (1%)	16	47
1	J	121/160 (76%)	112 (93%)	9 (7%)	0	100	100
1	K	123/160 (77%)	110 (89%)	12 (10%)	1 (1%)	16	47
1	L	121/160 (76%)	108 (89%)	9 (7%)	4 (3%)	3	17
1	M	122/160 (76%)	101 (83%)	20 (16%)	1 (1%)	16	47
1	N	133/160 (83%)	123 (92%)	10 (8%)	0	100	100
1	O	127/160 (79%)	120 (94%)	7 (6%)	0	100	100
1	P	128/160 (80%)	120 (94%)	8 (6%)	0	100	100
1	Q	129/160 (81%)	120 (93%)	9 (7%)	0	100	100
1	R	119/160 (74%)	102 (86%)	14 (12%)	3 (2%)	4	21
All	All	2237/2880 (78%)	2023 (90%)	195 (9%)	19 (1%)	16	47

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	L	186	ASP
1	L	187	PRO
1	A	148	LYS
1	E	91	ASN
1	H	134	LEU
1	R	78	ASP
1	R	163	THR
1	C	171	ASP
1	I	107	MET
1	K	176	LYS
1	L	77	PRO
1	M	134	LEU
1	R	107	MET
1	E	174	PRO
1	G	148	LYS
1	B	174	PRO
1	L	69	PRO
1	H	71	ILE

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	105/136 (77%)	94 (90%)	11 (10%)	6	26
1	B	101/136 (74%)	90 (89%)	11 (11%)	6	24
1	C	105/136 (77%)	93 (89%)	12 (11%)	5	23
1	D	107/136 (79%)	102 (95%)	5 (5%)	23	55
1	E	109/136 (80%)	92 (84%)	17 (16%)	2	12
1	F	106/136 (78%)	100 (94%)	6 (6%)	18	49
1	G	106/136 (78%)	98 (92%)	8 (8%)	12	39
1	H	106/136 (78%)	96 (91%)	10 (9%)	8	31
1	I	105/136 (77%)	93 (89%)	12 (11%)	5	23
1	J	107/136 (79%)	96 (90%)	11 (10%)	7	27
1	K	106/136 (78%)	90 (85%)	16 (15%)	3	13
1	L	104/136 (76%)	88 (85%)	16 (15%)	2	12
1	M	104/136 (76%)	88 (85%)	16 (15%)	2	12
1	N	111/136 (82%)	100 (90%)	11 (10%)	7	29
1	O	106/136 (78%)	97 (92%)	9 (8%)	10	35
1	P	109/136 (80%)	96 (88%)	13 (12%)	5	21
1	Q	110/136 (81%)	93 (84%)	17 (16%)	2	12
1	R	103/136 (76%)	86 (84%)	17 (16%)	2	11
All	All	1910/2448 (78%)	1692 (89%)	218 (11%)	5	23

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	VAL
1	A	146	THR
1	A	152	TYR
1	A	153	THR
1	A	155	THR
1	A	159	ILE

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Mol	Chain	Res	Type
1	A	167	VAL
1	A	180	THR
1	A	190	THR
1	A	191	GLU
1	A	198	GLU
1	B	68	LEU
1	B	83	LEU
1	B	92	THR
1	B	106	ILE
1	B	147	ASP
1	B	155	THR
1	B	159	ILE
1	B	165	GLU
1	B	173	THR
1	B	183	THR
1	B	195	VAL
1	C	68	LEU
1	C	92	THR
1	C	100	THR
1	C	103	GLU
1	C	115	LEU
1	C	139	LYS
1	C	146	THR
1	C	163	THR
1	C	183	THR
1	C	185	THR
1	C	190	THR
1	C	202	THR
1	D	71	ILE
1	D	92	THR
1	D	146	THR
1	D	155	THR
1	D	179	LEU
1	E	67	ASN
1	E	68	LEU
1	E	71	ILE
1	E	83	LEU
1	E	87	LYS
1	E	100	THR
1	E	146	THR
1	E	152	TYR
1	E	155	THR

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Mol	Chain	Res	Type
1	E	163	THR
1	E	167	VAL
1	E	183	THR
1	E	186	ASP
1	E	198	GLU
1	E	201	LYS
1	E	204	GLU
1	E	207	THR
1	F	71	ILE
1	F	91	ASN
1	F	146	THR
1	F	156	ILE
1	F	185	THR
1	F	194	ILE
1	G	70	VAL
1	G	95	SER
1	G	106	ILE
1	G	138	LYS
1	G	150	LYS
1	G	159	ILE
1	G	183	THR
1	G	192	ARG
1	H	71	ILE
1	H	78	ASP
1	H	79	VAL
1	H	100	THR
1	H	160	SER
1	H	163	THR
1	H	165	GLU
1	H	183	THR
1	H	185	THR
1	H	202	THR
1	I	81	ILE
1	I	100	THR
1	I	143	VAL
1	I	153	THR
1	I	157	THR
1	I	158	GLU
1	I	169	VAL
1	I	179	LEU
1	I	190	THR
1	I	193	ILE

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Mol	Chain	Res	Type
1	I	201	LYS
1	I	202	THR
1	J	92	THR
1	J	100	THR
1	J	102	LYS
1	J	103	GLU
1	J	121	PHE
1	J	147	ASP
1	J	153	THR
1	J	169	VAL
1	J	179	LEU
1	J	204	GLU
1	J	207	THR
1	K	71	ILE
1	K	78	ASP
1	K	79	VAL
1	K	100	THR
1	K	106	ILE
1	K	138	LYS
1	K	146	THR
1	K	152	TYR
1	K	172	ASP
1	K	176	LYS
1	K	179	LEU
1	K	183	THR
1	K	185	THR
1	K	192	ARG
1	K	198	GLU
1	K	201	LYS
1	L	71	ILE
1	L	95	SER
1	L	100	THR
1	L	115	LEU
1	L	143	VAL
1	L	146	THR
1	L	150	LYS
1	L	153	THR
1	L	159	ILE
1	L	160	SER
1	L	165	GLU
1	L	176	LYS
1	L	183	THR

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Mol	Chain	Res	Type
1	L	192	ARG
1	L	201	LYS
1	L	202	THR
1	M	71	ILE
1	M	79	VAL
1	M	89	LEU
1	M	95	SER
1	M	100	THR
1	M	106	ILE
1	M	139	LYS
1	M	146	THR
1	M	150	LYS
1	M	152	TYR
1	M	157	THR
1	M	163	THR
1	M	165	GLU
1	M	178	GLN
1	M	180	THR
1	M	193	ILE
1	N	76	ILE
1	N	78	ASP
1	N	93	GLU
1	N	138	LYS
1	N	143	VAL
1	N	167	VAL
1	N	176	LYS
1	N	179	LEU
1	N	183	THR
1	N	190	THR
1	N	192	ARG
1	O	68	LEU
1	O	138	LYS
1	O	146	THR
1	O	165	GLU
1	O	178	GLN
1	O	183	THR
1	O	185	THR
1	O	193	ILE
1	O	202	THR
1	P	66	HIS
1	P	71	ILE
1	P	82	ASN

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Mol	Chain	Res	Type
1	P	92	THR
1	P	135	GLU
1	P	138	LYS
1	P	145	LEU
1	P	146	THR
1	P	165	GLU
1	P	183	THR
1	P	192	ARG
1	P	201	LYS
1	P	202	THR
1	Q	71	ILE
1	Q	82	ASN
1	Q	104	ASN
1	Q	149	SER
1	Q	150	LYS
1	Q	151	VAL
1	Q	169	VAL
1	Q	179	LEU
1	Q	183	THR
1	Q	184	CYS
1	Q	186	ASP
1	Q	192	ARG
1	Q	193	ILE
1	Q	198	GLU
1	Q	202	THR
1	Q	204	GLU
1	Q	205	PHE
1	R	85	ILE
1	R	95	SER
1	R	138	LYS
1	R	149	SER
1	R	150	LYS
1	R	152	TYR
1	R	157	THR
1	R	162	VAL
1	R	163	THR
1	R	165	GLU
1	R	172	ASP
1	R	173	THR
1	R	177	SER
1	R	185	THR
1	R	194	ILE

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Mol	Chain	Res	Type
1	R	200	GLU
1	R	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	105	GLN
1	A	111	ASN
1	A	166	HIS
1	B	105	GLN
1	C	105	GLN
1	C	111	ASN
1	C	196	HIS
1	D	105	GLN
1	E	67	ASN
1	E	105	GLN
1	E	112	ASN
1	E	196	HIS
1	F	66	HIS
1	F	91	ASN
1	F	105	GLN
1	F	111	ASN
1	G	67	ASN
1	G	105	GLN
1	G	111	ASN
1	H	105	GLN
1	H	111	ASN
1	I	105	GLN
1	I	111	ASN
1	I	119	HIS
1	I	196	HIS
1	J	67	ASN
1	J	82	ASN
1	J	91	ASN
1	J	105	GLN
1	J	111	ASN
1	J	196	HIS
1	K	66	HIS
1	K	91	ASN
1	K	105	GLN
1	L	66	HIS

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Mol	Chain	Res	Type
1	L	105	GLN
1	M	105	GLN
1	M	111	ASN
1	M	166	HIS
1	N	91	ASN
1	N	105	GLN
1	N	111	ASN
1	O	105	GLN
1	O	111	ASN
1	P	82	ASN
1	P	91	ASN
1	P	105	GLN
1	Q	82	ASN
1	Q	105	GLN
1	R	105	GLN
1	R	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 73 ligands modelled in this entry, 73 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	129/160 (80%)	-0.04	2 (1%) 70 49	38, 56, 74, 83	0
1	B	124/160 (77%)	-0.10	3 (2%) 59 38	36, 52, 69, 83	0
1	C	129/160 (80%)	-0.25	1 (0%) 82 65	39, 50, 73, 80	0
1	D	129/160 (80%)	-0.15	3 (2%) 61 39	35, 50, 72, 85	0
1	E	134/160 (83%)	-0.15	1 (0%) 84 68	39, 55, 83, 87	0
1	F	132/160 (82%)	0.06	2 (1%) 72 52	38, 56, 73, 85	0
1	G	132/160 (82%)	-0.09	1 (0%) 82 65	42, 55, 72, 84	0
1	H	130/160 (81%)	-0.04	3 (2%) 61 39	41, 53, 73, 85	0
1	I	131/160 (81%)	-0.23	2 (1%) 72 52	39, 51, 77, 81	0
1	J	129/160 (80%)	-0.24	6 (4%) 36 19	37, 52, 74, 86	0
1	K	129/160 (80%)	0.04	3 (2%) 61 39	41, 57, 75, 86	0
1	L	127/160 (79%)	0.02	2 (1%) 70 49	44, 58, 75, 85	0
1	M	128/160 (80%)	-0.05	2 (1%) 70 49	46, 57, 78, 83	0
1	N	137/160 (85%)	-0.10	1 (0%) 84 68	37, 52, 73, 83	0
1	O	131/160 (81%)	-0.04	2 (1%) 72 52	32, 48, 68, 80	0
1	P	132/160 (82%)	-0.03	3 (2%) 61 39	27, 50, 70, 86	0
1	Q	133/160 (83%)	-0.04	1 (0%) 82 65	39, 54, 75, 85	0
1	R	125/160 (78%)	0.08	2 (1%) 70 49	45, 58, 75, 85	0
All	All	2341/2880 (81%)	-0.08	40 (1%) 69 48	27, 54, 75, 87	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	186	ASP	4.5
1	M	189	ALA	3.7
1	K	203	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	205	PHE	3.3
1	J	186	ASP	3.2
1	J	121	PHE	3.1
1	G	104	ASN	3.0
1	M	121	PHE	3.0
1	N	210	GLU	3.0
1	A	185	THR	3.0
1	O	190	THR	2.9
1	P	67	ASN	2.9
1	J	208	ALA	2.9
1	P	66	HIS	2.7
1	B	140	GLY	2.6
1	H	204	GLU	2.6
1	O	200	GLU	2.6
1	Q	206	SER	2.6
1	E	209	ASP	2.6
1	I	67	ASN	2.6
1	K	202	THR	2.5
1	J	201	LYS	2.5
1	B	121	PHE	2.5
1	B	188	GLU	2.4
1	D	205	PHE	2.3
1	D	130	LEU	2.3
1	A	155	THR	2.3
1	K	201	LYS	2.3
1	C	204	GLU	2.2
1	P	204	GLU	2.2
1	L	130	LEU	2.2
1	H	190	THR	2.2
1	I	190	THR	2.2
1	R	132	SER	2.1
1	F	171	ASP	2.1
1	J	203	GLY	2.1
1	H	149	SER	2.0
1	J	207	THR	2.0
1	L	188	GLU	2.0
1	D	203	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	ZN	B	305	1/1	0.93	0.12	47,47,47,47	0
2	ZN	I	301	1/1	0.93	0.05	82,82,82,82	0
2	ZN	B	304	1/1	0.94	0.09	97,97,97,97	0
2	ZN	M	304	1/1	0.94	0.07	88,88,88,88	0
2	ZN	B	306	1/1	0.95	0.07	77,77,77,77	0
2	ZN	C	305	1/1	0.95	0.09	88,88,88,88	0
2	ZN	H	304	1/1	0.96	0.05	71,71,71,71	0
2	ZN	N	304	1/1	0.96	0.08	77,77,77,77	0
2	ZN	Q	304	1/1	0.96	0.07	75,75,75,75	0
2	ZN	O	304	1/1	0.97	0.03	64,64,64,64	0
2	ZN	P	304	1/1	0.97	0.04	78,78,78,78	0
2	ZN	K	301	1/1	0.97	0.04	88,88,88,88	0
2	ZN	R	302	1/1	0.97	0.07	83,83,83,83	0
2	ZN	H	301	1/1	0.98	0.03	63,63,63,63	0
2	ZN	A	304	1/1	0.98	0.03	76,76,76,76	0
2	ZN	C	304	1/1	0.98	0.04	59,59,59,59	0
2	ZN	J	301	1/1	0.98	0.04	114,114,114,114	0
2	ZN	A	305	1/1	0.98	0.04	95,95,95,95	0
2	ZN	L	301	1/1	0.98	0.03	65,65,65,65	0
2	ZN	D	301	1/1	0.98	0.04	73,73,73,73	0
2	ZN	D	304	1/1	0.98	0.03	67,67,67,67	0
2	ZN	E	304	1/1	0.98	0.03	74,74,74,74	0
2	ZN	F	301	1/1	0.98	0.04	71,71,71,71	0
2	ZN	Q	301	1/1	0.98	0.02	76,76,76,76	0
2	ZN	G	302	1/1	0.98	0.07	74,74,74,74	0
2	ZN	G	306	1/1	0.98	0.04	71,71,71,71	0
2	ZN	J	302	1/1	0.99	0.04	53,53,53,53	0
2	ZN	B	302	1/1	0.99	0.02	36,36,36,36	0
2	ZN	K	302	1/1	0.99	0.04	53,53,53,53	0
2	ZN	K	303	1/1	0.99	0.02	59,59,59,59	0
2	ZN	G	303	1/1	0.99	0.02	65,65,65,65	0
2	ZN	L	302	1/1	0.99	0.04	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	G	304	1/1	0.99	0.03	48,48,48,48	0
2	ZN	M	306	1/1	0.99	0.04	66,66,66,66	0
2	ZN	N	301	1/1	0.99	0.02	65,65,65,65	0
2	ZN	C	301	1/1	0.99	0.02	61,61,61,61	0
2	ZN	O	301	1/1	0.99	0.02	39,39,39,39	0
2	ZN	E	301	1/1	0.99	0.02	70,70,70,70	0
2	ZN	P	301	1/1	0.99	0.03	65,65,65,65	0
2	ZN	P	302	1/1	0.99	0.05	33,33,33,33	0
2	ZN	E	303	1/1	0.99	0.02	46,46,46,46	0
2	ZN	A	301	1/1	0.99	0.02	48,48,48,48	0
2	ZN	Q	303	1/1	0.99	0.02	41,41,41,41	0
2	ZN	I	302	1/1	0.99	0.02	71,71,71,71	0
2	ZN	B	301	1/1	0.99	0.04	68,68,68,68	0
2	ZN	D	303	1/1	1.00	0.01	41,41,41,41	0
2	ZN	C	302	1/1	1.00	0.03	40,40,40,40	0
2	ZN	G	305	1/1	1.00	0.02	39,39,39,39	0
2	ZN	C	303	1/1	1.00	0.02	46,46,46,46	0
2	ZN	M	301	1/1	1.00	0.01	80,80,80,80	0
2	ZN	M	302	1/1	1.00	0.02	53,53,53,53	0
2	ZN	M	303	1/1	1.00	0.02	59,59,59,59	0
2	ZN	G	307	1/1	1.00	0.03	51,51,51,51	0
2	ZN	M	305	1/1	1.00	0.03	76,76,76,76	0
2	ZN	E	302	1/1	1.00	0.03	45,45,45,45	0
2	ZN	H	302	1/1	1.00	0.04	42,42,42,42	0
2	ZN	N	302	1/1	1.00	0.03	34,34,34,34	0
2	ZN	N	303	1/1	1.00	0.01	36,36,36,36	0
2	ZN	H	303	1/1	1.00	0.01	56,56,56,56	0
2	ZN	A	303	1/1	1.00	0.02	58,58,58,58	0
2	ZN	O	302	1/1	1.00	0.04	37,37,37,37	0
2	ZN	O	303	1/1	1.00	0.01	38,38,38,38	0
2	ZN	B	303	1/1	1.00	0.01	55,55,55,55	0
2	ZN	A	302	1/1	1.00	0.03	49,49,49,49	0
2	ZN	I	303	1/1	1.00	0.04	48,48,48,48	0
2	ZN	P	303	1/1	1.00	0.04	38,38,38,38	0
2	ZN	I	304	1/1	1.00	0.02	57,57,57,57	0
2	ZN	F	302	1/1	1.00	0.02	48,48,48,48	0
2	ZN	Q	302	1/1	1.00	0.03	53,53,53,53	0
2	ZN	G	301	1/1	1.00	0.01	45,45,45,45	0
2	ZN	J	303	1/1	1.00	0.01	40,40,40,40	0
2	ZN	R	301	1/1	1.00	0.01	69,69,69,69	0
2	ZN	D	302	1/1	1.00	0.05	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.