



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:27 PM UTC

PDB ID : 2ZQB / pdb_00002zqb
Title : Crystal structure of a psychrotrophic RNaseHI variant with sextuple thermostabilizing mutations
Authors : Angkawidjaja, C.; Kanaya, S.
Deposited on : 2008-08-07
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

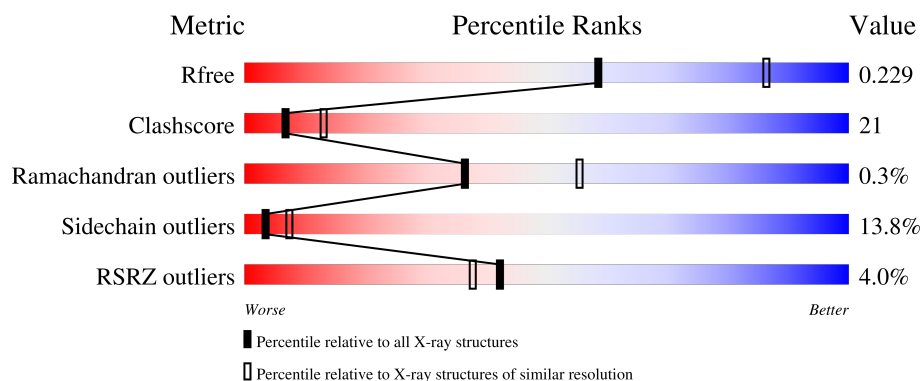
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	158	 3% 46% 35% 13% • 6%
1	B	158	 6% 51% 32% 9% • 7%
1	C	158	 4% 48% 34% 13% • •
1	D	158	 3% 50% 34% 11% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4941 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 Ribonuclease HI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1173	743	211	211	8			
1	B	147	Total	C	N	O	S	0	0	0
			1154	732	207	207	8			
1	C	151	Total	C	N	O	S	0	0	0
			1183	749	215	211	8			
1	D	152	Total	C	N	O	S	0	0	0
			1192	754	216	214	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LYS	ASN	engineered mutation	UNP Q8EE30
A	39	GLY	ASP	engineered mutation	UNP Q8EE30
A	76	VAL	MET	engineered mutation	UNP Q8EE30
A	90	ASN	LYS	engineered mutation	UNP Q8EE30
A	97	GLY	ARG	engineered mutation	UNP Q8EE30
A	136	HIS	ASP	engineered mutation	UNP Q8EE30
B	29	LYS	ASN	engineered mutation	UNP Q8EE30
B	39	GLY	ASP	engineered mutation	UNP Q8EE30
B	76	VAL	MET	engineered mutation	UNP Q8EE30
B	90	ASN	LYS	engineered mutation	UNP Q8EE30
B	97	GLY	ARG	engineered mutation	UNP Q8EE30
B	136	HIS	ASP	engineered mutation	UNP Q8EE30
C	29	LYS	ASN	engineered mutation	UNP Q8EE30
C	39	GLY	ASP	engineered mutation	UNP Q8EE30
C	76	VAL	MET	engineered mutation	UNP Q8EE30
C	90	ASN	LYS	engineered mutation	UNP Q8EE30
C	97	GLY	ARG	engineered mutation	UNP Q8EE30
C	136	HIS	ASP	engineered mutation	UNP Q8EE30
D	29	LYS	ASN	engineered mutation	UNP Q8EE30
D	39	GLY	ASP	engineered mutation	UNP Q8EE30
D	76	VAL	MET	engineered mutation	UNP Q8EE30

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Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ASN	LYS	engineered mutation	UNP Q8EE30
D	97	GLY	ARG	engineered mutation	UNP Q8EE30
D	136	HIS	ASP	engineered mutation	UNP Q8EE30

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

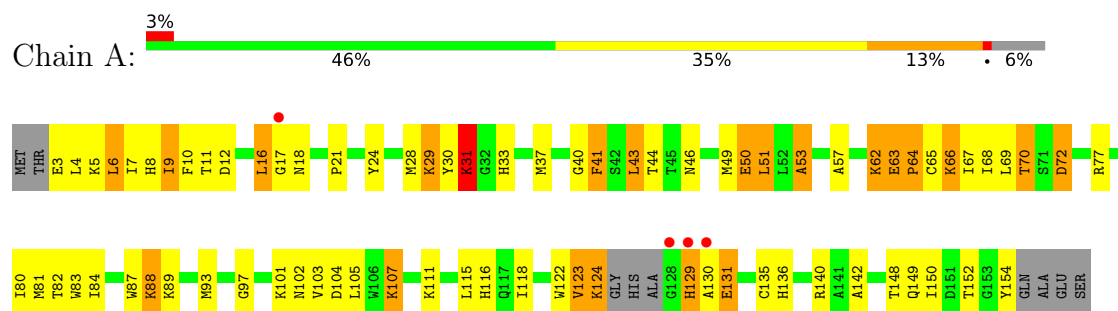
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		
3	B	49	Total	O	0	0
			49	49		
3	C	60	Total	O	0	0
			60	60		
3	D	56	Total	O	0	0
			56	56		

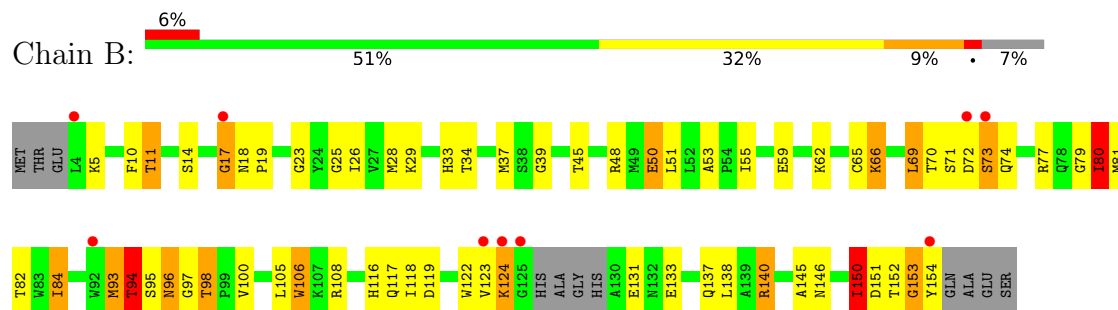
3 Residue-property plots [i](#)

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.

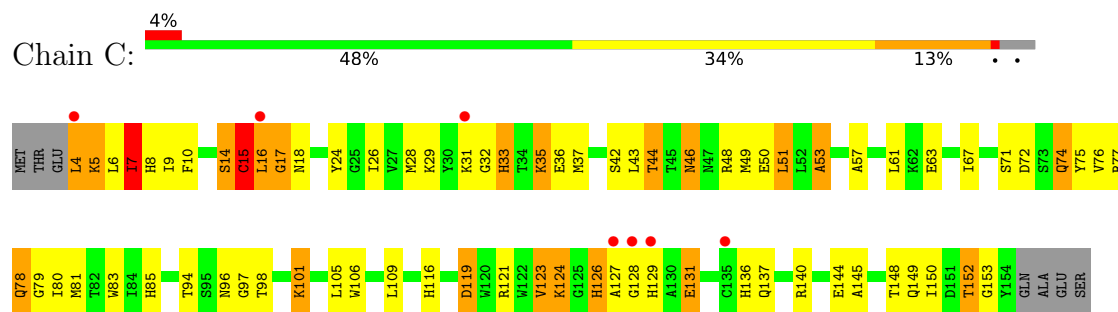
• Molecule 1: Ribonuclease HI



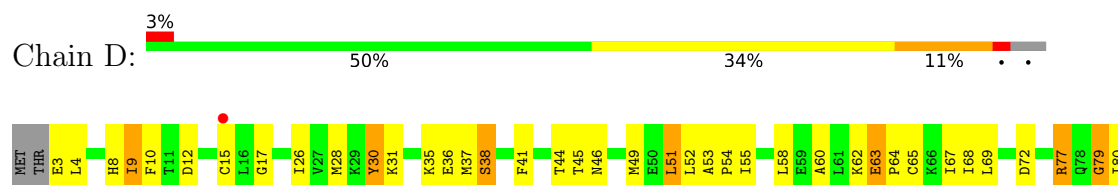
• Molecule 1: Ribonuclease HI

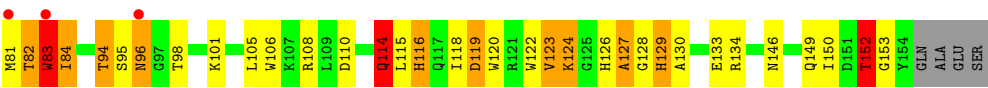


• Molecule 1: Ribonuclease HI



• Molecule 1: Ribonuclease HI





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.24Å 68.24Å 272.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 2.49 47.51 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.51-2.49) 99.8 (47.51-2.49)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.247 (Not available) , 0.229	Depositor DCC
R_{free} test set	1212 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4941	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.70	18/1201 (1.5%)	1.47	20/1623 (1.2%)
1	B	1.60	13/1181 (1.1%)	1.38	11/1596 (0.7%)
1	C	1.53	14/1213 (1.2%)	1.45	15/1641 (0.9%)
1	D	1.71	21/1222 (1.7%)	1.51	19/1653 (1.1%)
All	All	1.64	66/4817 (1.4%)	1.45	65/6513 (1.0%)

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	A	0	2
1	B	0	2
1	C	0	5
1	D	0	2
All	All	0	11

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	THR	C-O	-10.13	1.14	1.24
1	A	104	ASP	C-O	-7.54	1.15	1.24
1	A	7	ILE	C-O	-7.54	1.16	1.24
1	B	100	VAL	CA-C	7.03	1.61	1.52
1	A	8	HIS	C-O	-7.00	1.15	1.24
1	C	149	GLN	C-O	6.95	1.32	1.23
1	D	36	GLU	C-O	6.82	1.31	1.23
1	C	119	ASP	CA-C	6.70	1.61	1.52
1	A	30	TYR	C-N	6.69	1.43	1.33
1	C	98	THR	CA-CB	-6.68	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	THR	C-O	-6.60	1.15	1.23
1	D	130	ALA	C-O	-6.49	1.16	1.24
1	D	146	ASN	CA-CB	6.46	1.57	1.52
1	B	106	TRP	CA-C	6.37	1.61	1.52
1	A	29	LYS	C-O	-6.21	1.16	1.24
1	A	53	ALA	CA-C	6.11	1.59	1.52
1	A	57	ALA	C-O	6.05	1.31	1.24
1	D	10	PHE	C-N	-6.00	1.25	1.33
1	A	9	ILE	C-O	-5.99	1.17	1.24
1	A	41	PHE	C-O	-5.95	1.16	1.23
1	D	134	ARG	C-O	-5.95	1.17	1.24
1	A	107	LYS	C-O	-5.92	1.16	1.24
1	D	126	HIS	C-O	-5.92	1.16	1.24
1	D	77	ARG	C-O	-5.89	1.17	1.24
1	C	75	TYR	C-O	-5.88	1.17	1.24
1	D	150	ILE	CA-CB	5.87	1.61	1.54
1	B	80	ILE	CA-CB	5.87	1.61	1.54
1	D	129	HIS	C-O	-5.77	1.17	1.23
1	A	64	PRO	C-O	-5.76	1.17	1.23
1	D	133	GLU	CA-C	5.75	1.60	1.52
1	C	137	GLN	N-CA	5.75	1.53	1.46
1	D	38	SER	N-CA	-5.75	1.39	1.46
1	C	148	THR	N-CA	5.73	1.53	1.45
1	B	146	ASN	C-O	-5.71	1.21	1.23
1	C	43	LEU	C-O	-5.65	1.17	1.23
1	D	152	THR	C-O	-5.64	1.16	1.23
1	C	53	ALA	C-O	-5.62	1.19	1.24
1	B	69	LEU	C-O	-5.59	1.17	1.24
1	A	10	PHE	C-O	-5.59	1.17	1.24
1	A	30	TYR	C-O	-5.59	1.17	1.23
1	B	74	GLN	C-O	-5.58	1.17	1.24
1	B	70	THR	C-O	-5.56	1.17	1.24
1	B	11	THR	C-O	-5.52	1.17	1.23
1	B	26	ILE	CA-CB	-5.51	1.47	1.54
1	D	35	LYS	C-O	-5.48	1.16	1.23
1	B	108	ARG	C-O	-5.46	1.17	1.24
1	B	105	LEU	C-O	-5.45	1.17	1.24
1	D	146	ASN	N-CA	5.43	1.50	1.46
1	A	70	THR	C-O	5.42	1.30	1.24
1	B	50	GLU	C-O	-5.37	1.17	1.24
1	D	124	LYS	CA-C	5.37	1.59	1.52
1	D	12	ASP	C-O	-5.36	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	79	GLY	C-O	-5.29	1.16	1.23
1	D	119	ASP	C-O	-5.28	1.17	1.24
1	C	76	VAL	N-CA	-5.18	1.40	1.46
1	D	114	GLN	CA-C	-5.17	1.45	1.52
1	A	6	LEU	C-O	-5.16	1.17	1.24
1	B	116	HIS	C-O	-5.15	1.17	1.23
1	C	145	ALA	CA-CB	-5.15	1.46	1.53
1	C	149	GLN	CA-C	5.15	1.59	1.52
1	A	40	GLY	C-O	-5.12	1.16	1.23
1	D	41	PHE	C-O	-5.10	1.17	1.23
1	C	5	LYS	CA-C	5.07	1.59	1.52
1	D	108	ARG	C-O	-5.07	1.18	1.24
1	A	142	ALA	CA-CB	-5.05	1.45	1.53
1	C	137	GLN	CA-C	5.02	1.59	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	THR	N-CA-C	9.98	122.10	111.03
1	B	17	GLY	N-CA-C	-8.95	101.40	112.68
1	C	16	LEU	N-CA-C	8.43	122.66	111.28
1	B	153	GLY	N-CA-C	7.77	125.50	115.32
1	D	146	ASN	CA-C-N	-7.74	112.03	119.85
1	D	146	ASN	C-N-CA	-7.74	112.03	119.85
1	B	150	ILE	N-CA-C	7.59	119.50	108.58
1	A	62	LYS	N-CA-C	7.54	122.67	113.17
1	A	131	GLU	N-CA-C	-7.43	94.98	110.80
1	A	103	VAL	N-CA-C	7.25	118.88	110.62
1	A	123	VAL	N-CA-C	7.17	120.22	109.17
1	B	118	ILE	N-CA-C	7.09	118.10	107.75
1	A	84	ILE	N-CA-C	7.08	117.59	110.23
1	D	30	TYR	N-CA-C	7.00	120.96	107.44
1	D	30	TYR	CB-CA-C	-6.96	101.34	111.23
1	D	80	ILE	N-CA-C	6.96	123.81	109.34
1	C	15	CYS	N-CA-C	6.95	122.54	114.62
1	C	31	LYS	CB-CA-C	-6.72	108.81	116.54
1	A	62	LYS	CA-C-N	6.69	131.76	122.06
1	A	62	LYS	C-N-CA	6.69	131.76	122.06
1	A	50	GLU	N-CA-C	-6.68	104.08	111.36
1	A	150	ILE	N-CA-C	6.68	118.19	108.58
1	D	9	ILE	O-C-N	-6.59	116.13	122.98
1	D	9	ILE	CA-C-N	6.55	133.29	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	9	ILE	C-N-CA	6.55	133.29	121.89
1	B	18	ASN	N-CA-C	-6.51	95.42	109.81
1	A	129	HIS	N-CA-CB	-6.51	100.72	111.06
1	A	31	LYS	N-CA-CB	6.44	121.38	110.49
1	D	4	LEU	N-CA-C	6.43	119.00	108.52
1	D	68	ILE	N-CA-C	-6.37	98.56	107.80
1	C	7	ILE	N-CA-C	6.37	117.95	108.46
1	C	74	GLN	N-CA-C	-6.26	104.34	112.23
1	C	16	LEU	CB-CA-C	-6.25	102.98	112.11
1	D	35	LYS	N-CA-C	6.11	118.70	109.41
1	D	10	PHE	O-C-N	-6.09	115.95	123.44
1	C	129	HIS	N-CA-C	6.05	120.12	109.96
1	C	123	VAL	CB-CA-C	6.02	119.73	110.82
1	D	118	ILE	N-CA-C	5.98	116.62	107.77
1	A	72	ASP	CA-C-N	-5.94	114.86	122.77
1	A	72	ASP	C-N-CA	-5.94	114.86	122.77
1	A	6	LEU	N-CA-C	5.87	117.86	108.41
1	A	118	ILE	N-CA-C	5.82	116.69	108.36
1	A	152	THR	N-CA-CB	5.71	118.61	110.16
1	C	17	GLY	N-CA-C	-5.66	99.77	113.18
1	D	106	TRP	N-CA-C	5.58	118.09	111.33
1	D	49	MET	N-CA-C	-5.54	105.32	111.36
1	B	25	GLY	N-CA-C	-5.49	100.16	113.18
1	A	142	ALA	N-CA-C	-5.41	105.46	111.36
1	A	131	GLU	N-CA-CB	5.38	119.57	110.49
1	B	80	ILE	CA-CB-CG2	5.33	119.56	110.50
1	C	35	LYS	N-CA-C	5.31	118.21	109.72
1	D	63	GLU	CA-C-N	5.30	125.24	119.78
1	D	63	GLU	C-N-CA	5.30	125.24	119.78
1	B	98	THR	N-CA-C	5.27	116.06	109.57
1	B	116	HIS	N-CA-C	5.25	117.39	109.41
1	B	145	ALA	N-CA-C	-5.24	105.13	112.25
1	B	138	LEU	N-CA-C	5.19	116.63	111.07
1	C	32	GLY	N-CA-C	5.19	121.09	114.66
1	A	62	LYS	O-C-N	5.16	128.79	122.34
1	C	109	LEU	N-CA-C	-5.12	105.16	111.40
1	A	9	ILE	N-CA-C	5.04	115.22	108.17
1	D	116	HIS	CA-C-N	-5.03	116.08	122.77
1	D	116	HIS	C-N-CA	-5.03	116.08	122.77
1	C	15	CYS	CA-C-N	-5.01	115.41	122.63
1	C	15	CYS	C-N-CA	-5.01	115.41	122.63

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	LEU	Peptide
1	A	17	GLY	Peptide
1	B	124	LYS	Peptide
1	B	96	ASN	Peptide
1	C	126	HIS	Peptide
1	C	127	ALA	Peptide
1	C	128	GLY	Peptide
1	C	152	THR	Peptide
1	C	96	ASN	Peptide
1	D	127	ALA	Peptide
1	D	152	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1173	0	1165	57	0
1	B	1154	0	1152	36	0
1	C	1183	0	1175	55	0
1	D	1192	0	1181	61	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
3	A	59	0	0	5	0
3	B	49	0	0	1	0
3	C	60	0	0	8	0
3	D	56	0	0	6	0
All	All	4941	0	4673	201	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 21.

All (201) 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:D:84:ILE:HD12	1:D:84:ILE:O	1.39	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:HE3	1:A:124:LYS:CA	1.59	1.20
1:C:124:LYS:N	1:C:124:LYS:HD3	1.54	1.19
1:B:140:ARG:HH21	1:B:140:ARG:CG	1.60	1.15
1:C:124:LYS:HD3	1:C:124:LYS:H	0.96	1.10
1:D:84:ILE:HD12	1:D:84:ILE:C	1.75	1.09
1:A:16:LEU:O	1:A:16:LEU:HD12	1.52	1.08
1:D:79:GLY:O	1:D:84:ILE:HG23	1.59	1.02
1:A:16:LEU:HD21	1:A:140:ARG:HH21	1.20	1.00
1:B:140:ARG:HG3	1:B:140:ARG:NH2	1.48	0.99
1:A:124:LYS:HE3	1:A:124:LYS:HA	1.00	0.98
1:C:18:ASN:HD21	1:C:46:ASN:H	1.14	0.95
1:D:79:GLY:HA2	1:D:83:TRP:HB2	1.48	0.93
1:D:77:ARG:NH1	1:D:81:MET:HE1	1.81	0.93
1:C:124:LYS:N	1:C:124:LYS:CD	2.30	0.92
1:A:16:LEU:HD21	1:A:140:ARG:NH2	1.86	0.90
1:C:136:HIS:CE1	1:C:140:ARG:HD3	2.06	0.90
1:A:124:LYS:CA	1:A:124:LYS:CE	2.48	0.90
1:A:124:LYS:HA	1:A:124:LYS:CE	1.96	0.90
1:C:29:LYS:HE3	1:C:131:GLU:OE2	1.72	0.89
1:C:18:ASN:ND2	1:C:46:ASN:H	1.70	0.88
1:D:94:THR:HG23	1:D:98:THR:O	1.76	0.85
1:B:93:MET:HE2	1:B:97:GLY:O	1.78	0.84
1:D:51:LEU:HD22	1:D:55:ILE:HD11	1.58	0.83
1:A:16:LEU:O	1:A:16:LEU:CD1	2.30	0.80
1:D:3:GLU:O	1:D:3:GLU:HG3	1.84	0.77
1:C:36:GLU:HB2	1:D:38:SER:O	1.89	0.73
1:A:129:HIS:O	1:A:130:ALA:HB3	1.89	0.72
1:D:84:ILE:C	1:D:84:ILE:CD1	2.53	0.72
1:D:84:ILE:O	1:D:84:ILE:CD1	2.30	0.71
1:B:140:ARG:HH21	1:B:140:ARG:HG3	0.67	0.70
1:B:153:GLY:O	1:B:154:TYR:HB3	1.89	0.70
1:A:101:LYS:HE3	2:A:159:SO4:O3	1.92	0.70
1:A:123:VAL:HG11	1:A:129:HIS:HD2	1.58	0.69
1:A:43:LEU:HD13	1:A:154:TYR:HE2	1.58	0.68
1:A:33:HIS:ND1	3:A:190:HOH:O	2.26	0.68
1:A:12:ASP:HB2	1:A:135:CYS:HB3	1.76	0.68
1:D:53:ALA:HB3	1:D:54:PRO:CD	2.25	0.67
1:B:94:THR:HG23	1:B:98:THR:O	1.93	0.67
1:C:33:HIS:HB3	3:C:214:HOH:O	1.94	0.67
1:B:140:ARG:CG	1:B:140:ARG:NH2	2.30	0.66
1:C:24:TYR:HB2	1:C:53:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:TYR:CZ	1:D:31:LYS:HE2	2.31	0.66
1:A:65:CYS:H	1:A:116:HIS:HD2	1.44	0.66
1:D:26:ILE:HB	1:D:37:MET:HB2	1.78	0.66
1:C:136:HIS:O	1:C:140:ARG:HG2	1.96	0.65
1:A:18:ASN:ND2	1:A:46:ASN:H	1.95	0.65
1:C:33:HIS:N	1:C:33:HIS:ND1	2.44	0.65
1:B:79:GLY:HA3	1:B:106:TRP:CH2	2.32	0.64
1:C:78:GLN:HB3	1:C:83:TRP:CZ3	2.32	0.64
1:C:4:LEU:C	1:C:4:LEU:HD12	2.22	0.64
1:D:64:PRO:HA	1:D:116:HIS:CD2	2.33	0.63
1:D:96:ASN:N	1:D:96:ASN:OD1	2.30	0.63
1:D:120:TRP:CE3	1:D:122:TRP:CH2	2.87	0.63
1:D:96:ASN:O	1:D:98:THR:N	2.31	0.62
1:C:18:ASN:HD21	1:C:46:ASN:N	1.94	0.62
1:C:51:LEU:HD13	1:C:105:LEU:HB3	1.82	0.62
1:C:124:LYS:H	1:C:124:LYS:CD	1.82	0.62
1:A:9:ILE:HG12	1:A:28:MET:HG2	1.82	0.61
1:A:4:LEU:HB3	1:A:65:CYS:HA	1.81	0.61
1:D:77:ARG:NH1	1:D:81:MET:CE	2.60	0.61
1:A:12:ASP:OD2	1:A:136:HIS:HA	2.00	0.61
1:B:77:ARG:HG3	1:B:122:TRP:CE2	2.37	0.59
1:D:110:ASP:O	1:D:114:GLN:HG2	2.01	0.59
1:A:46:ASN:O	1:A:50:GLU:HG3	2.02	0.59
1:B:11:THR:HB	1:B:53:ALA:HB1	1.84	0.59
1:D:123:VAL:CG2	1:D:129:HIS:CE1	2.85	0.59
1:C:9:ILE:HG12	1:C:28:MET:HG2	1.85	0.59
1:B:55:ILE:O	1:B:59:GLU:HG3	2.02	0.58
1:C:51:LEU:HD13	1:C:105:LEU:CB	2.33	0.58
1:B:93:MET:C	1:B:94:THR:O	2.44	0.58
1:D:77:ARG:HH12	1:D:81:MET:HE1	1.67	0.57
1:D:96:ASN:C	1:D:98:THR:H	2.12	0.57
1:A:83:TRP:HB3	1:A:87:TRP:CZ2	2.40	0.57
1:A:88:LYS:NZ	3:A:205:HOH:O	2.28	0.56
1:C:10:PHE:CE1	1:C:131:GLU:HG3	2.40	0.56
1:D:53:ALA:HB3	1:D:54:PRO:HD3	1.87	0.56
1:A:67:ILE:HD12	1:A:116:HIS:HB3	1.87	0.56
1:A:6:LEU:CD2	1:C:144:GLU:HB3	2.35	0.55
1:C:4:LEU:C	1:C:4:LEU:CD1	2.80	0.55
1:B:29:LYS:HE3	1:B:131:GLU:HG2	1.89	0.55
1:B:93:MET:O	1:B:94:THR:O	2.25	0.55
1:A:6:LEU:HD23	1:C:144:GLU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ASP:HB2	3:D:230:HOH:O	2.06	0.55
1:C:35:LYS:HD2	3:D:257:HOH:O	2.05	0.54
1:C:18:ASN:ND2	1:C:46:ASN:N	2.49	0.54
1:C:26:ILE:HB	1:C:37:MET:HB2	1.88	0.54
1:A:69:LEU:HD23	1:A:70:THR:N	2.22	0.54
1:D:82:THR:OG1	1:D:83:TRP:N	2.41	0.54
1:A:62:LYS:C	1:A:63:GLU:HG3	2.33	0.53
1:D:15:CYS:O	1:D:17:GLY:O	2.26	0.53
1:A:43:LEU:HD13	1:A:154:TYR:CE2	2.39	0.53
1:B:72:ASP:CG	1:B:72:ASP:O	2.50	0.53
1:D:123:VAL:HG21	1:D:129:HIS:CE1	2.43	0.53
1:A:51:LEU:HD13	1:A:105:LEU:HB2	1.90	0.53
1:B:150:ILE:HG12	1:B:151:ASP:N	2.23	0.52
1:D:96:ASN:HB2	1:D:98:THR:HG23	1.91	0.52
1:A:129:HIS:O	1:A:130:ALA:CB	2.58	0.52
1:C:33:HIS:HB3	3:D:246:HOH:O	2.09	0.52
1:D:152:THR:O	1:D:153:GLY:O	2.28	0.52
1:D:69:LEU:C	1:D:69:LEU:HD23	2.35	0.52
1:D:51:LEU:HD22	1:D:55:ILE:CD1	2.33	0.52
1:A:29:LYS:NZ	1:A:131:GLU:OE2	2.43	0.51
1:A:51:LEU:HD13	1:A:105:LEU:CB	2.40	0.51
1:C:101:LYS:HE3	2:C:159:SO4:O3	2.10	0.51
1:D:94:THR:HG21	1:D:98:THR:OG1	2.09	0.51
1:C:33:HIS:HA	1:D:149:GLN:OE1	2.11	0.51
1:A:44:THR:OG1	1:A:49:MET:HE3	2.10	0.51
1:C:74:GLN:HE22	1:C:77:ARG:HH11	1.57	0.51
1:A:149:GLN:NE2	1:B:34:THR:H	2.10	0.50
1:D:51:LEU:HD13	1:D:105:LEU:HB2	1.92	0.50
1:D:65:CYS:N	1:D:116:HIS:HD2	2.08	0.50
1:C:48:ARG:NH2	1:C:153:GLY:HA2	2.27	0.50
1:A:3:GLU:N	3:A:210:HOH:O	2.44	0.50
1:B:50:GLU:CD	1:B:73:SER:HB2	2.37	0.50
1:C:16:LEU:N	3:C:181:HOH:O	2.44	0.50
1:D:129:HIS:HB3	3:D:219:HOH:O	2.11	0.50
1:D:94:THR:CG2	1:D:98:THR:O	2.56	0.49
1:B:45:THR:OG1	1:B:48:ARG:HG3	2.12	0.49
1:D:54:PRO:O	1:D:58:LEU:HG	2.13	0.49
1:A:101:LYS:O	1:A:102:ASN:HB2	2.12	0.49
1:D:53:ALA:CB	1:D:54:PRO:CD	2.90	0.49
1:B:11:THR:HB	1:B:53:ALA:CB	2.42	0.48
1:D:72:ASP:OD2	1:D:72:ASP:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASP:OD2	1:C:121:ARG:NH2	2.32	0.47
1:A:24:TYR:HB2	1:A:53:ALA:HB2	1.96	0.47
1:C:26:ILE:HD13	1:C:57:ALA:HB2	1.96	0.47
1:B:72:ASP:O	1:B:72:ASP:OD2	2.33	0.47
1:D:52:LEU:HA	1:D:55:ILE:HD12	1.97	0.47
1:B:23:GLY:HA2	1:B:39:GLY:O	2.15	0.47
1:A:49:MET:HA	1:A:49:MET:HE2	1.97	0.46
1:D:58:LEU:HD22	1:D:67:ILE:HD13	1.96	0.46
1:A:80:ILE:HG22	1:A:81:MET:CE	2.46	0.46
1:D:51:LEU:HD13	1:D:105:LEU:CB	2.45	0.46
1:D:94:THR:CG2	1:D:98:THR:OG1	2.63	0.46
1:A:21:PRO:HD2	3:A:166:HOH:O	2.16	0.46
1:D:96:ASN:C	1:D:98:THR:N	2.69	0.46
1:A:72:ASP:HB3	3:A:184:HOH:O	2.15	0.46
1:B:72:ASP:HB3	1:B:123:VAL:O	2.15	0.46
1:C:8:HIS:CE1	3:C:199:HOH:O	2.68	0.46
1:C:74:GLN:HE22	1:C:77:ARG:HD3	1.80	0.46
1:B:66:LYS:HB2	1:B:66:LYS:HE2	1.42	0.46
1:C:44:THR:HG21	1:C:49:MET:HE3	1.98	0.46
1:A:83:TRP:HB3	1:A:87:TRP:CE2	2.51	0.46
1:C:85:HIS:HE1	3:C:191:HOH:O	1.99	0.46
1:D:94:THR:OG1	1:D:95:SER:N	2.47	0.46
1:A:123:VAL:HG12	3:D:256:HOH:O	2.15	0.45
1:D:30:TYR:OH	1:D:31:LYS:HE2	2.16	0.45
1:B:72:ASP:CB	1:B:123:VAL:O	2.65	0.45
1:C:94:THR:O	1:C:97:GLY:HA2	2.17	0.45
1:A:93:MET:HE3	1:A:97:GLY:HA2	1.97	0.45
1:C:5:LYS:HD2	1:C:63:GLU:OE2	2.17	0.45
1:D:9:ILE:HG12	1:D:28:MET:HG2	1.98	0.45
1:C:15:CYS:O	1:C:16:LEU:HB2	2.16	0.45
1:C:131:GLU:H	1:C:131:GLU:HG2	1.43	0.45
1:B:77:ARG:HA	1:B:122:TRP:CZ2	2.53	0.44
1:D:44:THR:OG1	1:D:45:THR:N	2.50	0.44
1:B:23:GLY:CA	1:B:39:GLY:O	2.65	0.44
1:B:82:THR:CG2	3:B:186:HOH:O	2.64	0.44
1:C:67:ILE:HD12	1:C:116:HIS:HB3	1.98	0.44
1:A:69:LEU:HD23	1:A:69:LEU:C	2.43	0.44
1:A:31:LYS:HB3	1:C:16:LEU:HB3	1.99	0.44
1:B:79:GLY:HA3	1:B:106:TRP:CZ3	2.52	0.43
1:C:46:ASN:O	1:C:50:GLU:HG3	2.17	0.43
1:D:94:THR:OG1	1:D:96:ASN:O	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:HIS:HB3	3:C:168:HOH:O	2.19	0.43
1:D:8:HIS:ND1	3:D:210:HOH:O	2.29	0.43
1:A:12:ASP:HB2	1:A:135:CYS:CB	2.47	0.43
1:D:123:VAL:HG22	1:D:129:HIS:NE2	2.34	0.43
1:B:69:LEU:C	1:B:69:LEU:HD23	2.44	0.43
1:C:6:LEU:HD12	1:C:7:ILE:N	2.33	0.43
1:B:28:MET:HE3	1:B:37:MET:SD	2.58	0.43
1:A:148:THR:O	1:A:149:GLN:C	2.60	0.43
1:B:17:GLY:C	1:B:19:PRO:O	2.62	0.43
1:A:122:TRP:O	1:D:128:GLY:HA3	2.19	0.42
1:D:37:MET:HE1	1:D:60:ALA:CB	2.49	0.42
1:A:72:ASP:O	1:A:72:ASP:CG	2.63	0.42
1:A:65:CYS:N	1:A:116:HIS:HD2	2.14	0.42
1:D:37:MET:HE1	1:D:60:ALA:HB2	1.99	0.42
1:A:77:ARG:HA	1:A:122:TRP:CH2	2.55	0.42
1:B:10:PHE:CD2	1:B:10:PHE:N	2.87	0.42
1:A:41:PHE:CD2	1:A:41:PHE:N	2.88	0.42
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.83	0.42
1:A:149:GLN:NE2	1:B:33:HIS:HA	2.34	0.42
1:C:79:GLY:HA3	1:C:106:TRP:CH2	2.54	0.42
1:B:73:SER:O	1:B:73:SER:OG	2.37	0.42
1:C:17:GLY:N	3:C:181:HOH:O	2.52	0.41
1:D:127:ALA:HA	1:D:128:GLY:HA2	1.93	0.41
1:A:64:PRO:HB3	1:A:115:LEU:O	2.21	0.41
1:D:69:LEU:C	1:D:69:LEU:CD2	2.93	0.41
1:D:114:GLN:HG2	1:D:114:GLN:H	1.45	0.41
1:A:6:LEU:HD13	1:A:66:LYS:HG2	2.03	0.41
1:B:80:ILE:HA	1:B:84:ILE:HD12	2.02	0.41
1:C:85:HIS:CE1	3:C:191:HOH:O	2.74	0.41
1:C:140:ARG:HG2	1:C:140:ARG:H	1.69	0.41
1:D:120:TRP:HB3	1:D:122:TRP:CZ2	2.56	0.41
1:A:68:ILE:CD1	3:C:172:HOH:O	2.69	0.40
1:C:14:SER:OG	1:C:140:ARG:HD2	2.21	0.40
1:C:140:ARG:O	1:C:144:GLU:HG3	2.20	0.40
1:C:6:LEU:C	1:C:7:ILE:HG12	2.47	0.40
1:D:152:THR:O	1:D:153:GLY:C	2.64	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	145/158 (92%)	136 (94%)	9 (6%)	0	100	100
1	B	143/158 (90%)	133 (93%)	9 (6%)	1 (1%)	18	34
1	C	149/158 (94%)	139 (93%)	10 (7%)	0	100	100
1	D	150/158 (95%)	140 (93%)	9 (6%)	1 (1%)	18	34
All	All	587/632 (93%)	548 (93%)	37 (6%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	THR
1	D	83	TRP

5.3.2 Protein sidechains [i](#)

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	123/129 (95%)	110 (89%)	13 (11%)	6	14
1	B	121/129 (94%)	98 (81%)	23 (19%)	1	3
1	C	123/129 (95%)	105 (85%)	18 (15%)	3	6
1	D	124/129 (96%)	110 (89%)	14 (11%)	5	12
All	All	491/516 (95%)	423 (86%)	68 (14%)	3	7

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	31	LYS
1	A	37	MET
1	A	43	LEU
1	A	51	LEU
1	A	63	GLU
1	A	66	LYS
1	A	82	THR
1	A	88	LYS
1	A	89	LYS
1	A	107	LYS
1	A	111	LYS
1	A	124	LYS
1	B	5	LYS
1	B	14	SER
1	B	51	LEU
1	B	62	LYS
1	B	65	CYS
1	B	66	LYS
1	B	71	SER
1	B	73	SER
1	B	80	ILE
1	B	81	MET
1	B	84	ILE
1	B	93	MET
1	B	94	THR
1	B	95	SER
1	B	96	ASN
1	B	117	GLN
1	B	119	ASP
1	B	124	LYS
1	B	133	GLU
1	B	137	GLN
1	B	140	ARG
1	B	150	ILE
1	B	152	THR
1	C	4	LEU
1	C	7	ILE
1	C	14	SER
1	C	15	CYS
1	C	33	HIS
1	C	42	SER
1	C	46	ASN

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Mol	Chain	Res	Type
1	C	51	LEU
1	C	71	SER
1	C	72	ASP
1	C	78	GLN
1	C	80	ILE
1	C	81	MET
1	C	101	LYS
1	C	123	VAL
1	C	124	LYS
1	C	131	GLU
1	C	150	ILE
1	D	46	ASN
1	D	51	LEU
1	D	62	LYS
1	D	63	GLU
1	D	82	THR
1	D	83	TRP
1	D	84	ILE
1	D	94	THR
1	D	96	ASN
1	D	101	LYS
1	D	114	GLN
1	D	115	LEU
1	D	123	VAL
1	D	124	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	47	ASN
1	A	116	HIS
1	A	129	HIS
1	A	149	GLN
1	B	47	ASN
1	B	90	ASN
1	B	117	GLN
1	B	132	ASN
1	B	146	ASN
1	C	18	ASN
1	C	74	GLN
1	C	117	GLN

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Mol	Chain	Res	Type
1	C	126	HIS
1	C	132	ASN
1	C	136	HIS
1	C	146	ASN
1	D	47	ASN
1	D	74	GLN
1	D	90	ASN
1	D	114	GLN
1	D	116	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	SO4	A	159	-	4,4,4	0.46	0	6,6,6	0.18	0
2	SO4	B	159	-	4,4,4	0.17	0	6,6,6	0.82	0
2	SO4	C	159	-	4,4,4	0.32	0	6,6,6	0.84	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	159	SO4	1	0
2	C	159	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	149/158 (94%)	-0.03	4 (2%)	56	51	10, 24, 42, 51	0
1	B	147/158 (93%)	0.27	9 (6%)	27	23	12, 29, 48, 66	0
1	C	151/158 (95%)	0.14	7 (4%)	37	33	9, 28, 47, 58	0
1	D	152/158 (96%)	0.04	4 (2%)	57	52	11, 24, 50, 55	0
All	All	599/632 (94%)	0.10	24 (4%)	42	38	9, 26, 47, 66	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	GLY	4.6
1	D	15	CYS	4.6
1	B	154	TYR	4.0
1	A	128	GLY	3.9
1	B	73	SER	3.8
1	B	72	ASP	3.6
1	D	81	MET	3.5
1	C	129	HIS	3.4
1	D	83	TRP	3.4
1	C	31	LYS	3.4
1	A	129	HIS	3.2
1	C	127	ALA	3.1
1	A	17	GLY	2.9
1	B	124	LYS	2.8
1	C	4	LEU	2.8
1	C	135	CYS	2.4
1	C	16	LEU	2.4
1	C	128	GLY	2.3
1	B	4	LEU	2.3
1	A	130	ALA	2.2
1	B	17	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	123	VAL	2.2
1	D	96	ASN	2.2
1	B	92	TRP	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
2	SO4	C	159	5/5	0.92	0.12	49,50,54,55	0
2	SO4	B	159	5/5	0.94	0.11	43,43,46,48	0
2	SO4	A	159	5/5	0.97	0.10	39,40,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.