Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2024 – 11:44 PM EST

PDB ID	:	1NXB
Title	:	STRUCTURE AND FUNCTION OF SNAKE VENOM CURARIMIMETIC NEUROTOXINS
Authors	:	Tsernoglou, D.; Petsko, G.A.
Deposited on	:	1980-08-08
Resolution	:	1.38 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:

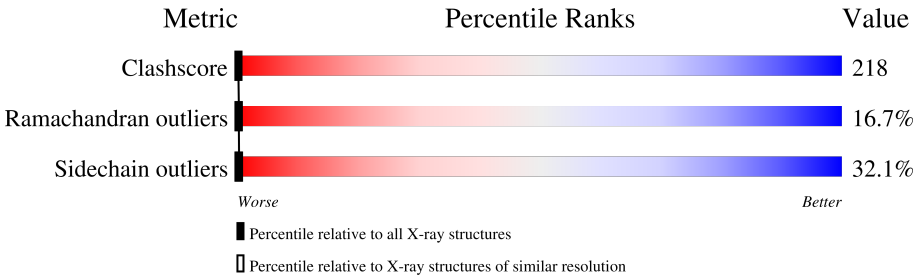
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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))
Clashscore	180529	4183 (1.40-1.36)
Ramachandran outliers	177936	4116 (1.40-1.36)
Sidechain outliers	177891	4115 (1.40-1.36)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	62	· 5% 48% 44%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	64	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 543 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.

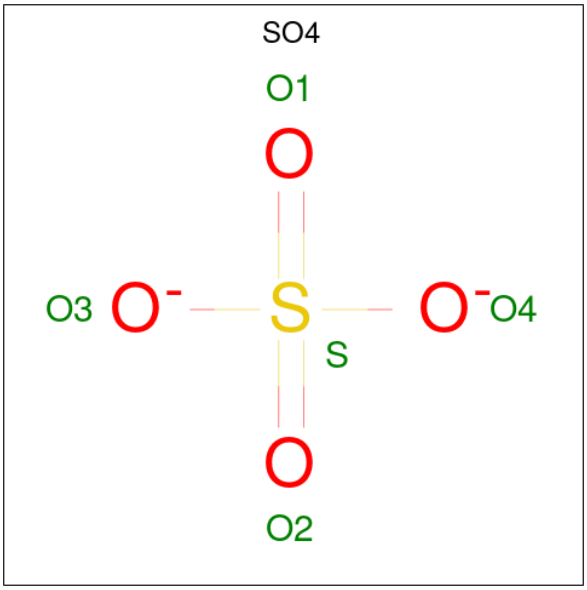
- Molecule 1 is a protein called NEUROTOXIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	62	472	283	87	94	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLN	HIS	conflict	UNP Q90VW1
A	7	HIS	GLN	conflict	UNP Q90VW1
A	26	HIS	ASN	conflict	UNP Q90VW1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	3	2	1	0	0
			Total	S			
2	A	1	1	1		0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	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. 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. 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.

Note EDS was not executed.

- Molecule 1: NEUROTOXIN B

Chain A:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.90Å 46.60Å 21.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.38	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.38)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	543	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	3.30	53/482 (11.0%)	6.38	225/647 (34.8%)

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	9	17

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	THR	C-N	-21.97	0.83	1.34
1	A	22	SER	C-N	18.91	1.77	1.34
1	A	17	CYS	CB-SG	-15.37	1.56	1.82
1	A	58	GLU	CD-OE2	-10.64	1.14	1.25
1	A	61	ASN	CG-ND2	-10.37	1.06	1.32
1	A	42	GLY	C-O	9.61	1.39	1.23
1	A	33	ARG	CZ-NH1	8.34	1.43	1.33
1	A	11	PRO	N-CA	-8.04	1.33	1.47
1	A	31	ASP	CB-CG	-7.83	1.35	1.51
1	A	62	ASN	C-OXT	7.70	1.38	1.23
1	A	1	ARG	CZ-NH2	7.64	1.43	1.33
1	A	23	SER	C-N	7.56	1.51	1.34
1	A	49	GLY	N-CA	7.47	1.57	1.46
1	A	38	GLU	CG-CD	7.22	1.62	1.51
1	A	32	PHE	CD2-CE2	7.14	1.53	1.39
1	A	33	ARG	NE-CZ	6.71	1.41	1.33
1	A	8	SER	CB-OG	6.62	1.50	1.42
1	A	12	GLN	CD-OE1	6.52	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	PRO	C-O	-6.42	1.10	1.23
1	A	56	GLU	CD-OE2	-6.39	1.18	1.25
1	A	29	TRP	CD1-NE1	6.31	1.48	1.38
1	A	62	ASN	CG-ND2	-6.29	1.17	1.32
1	A	39	ARG	C-O	-6.27	1.11	1.23
1	A	34	GLY	N-CA	6.27	1.55	1.46
1	A	24	CYS	CB-SG	-6.21	1.71	1.82
1	A	26	HIS	CE1-NE2	-6.17	1.18	1.32
1	A	25	TYR	CG-CD1	6.10	1.47	1.39
1	A	48	PRO	CA-C	-6.03	1.40	1.52
1	A	36	ILE	N-CA	6.01	1.58	1.46
1	A	28	GLN	N-CA	5.88	1.58	1.46
1	A	29	TRP	NE1-CE2	-5.87	1.29	1.37
1	A	21	GLU	CD-OE1	-5.80	1.19	1.25
1	A	43	CYS	CB-SG	5.77	1.92	1.82
1	A	27	LYS	CE-NZ	5.72	1.63	1.49
1	A	4	PHE	C-O	5.71	1.34	1.23
1	A	25	TYR	CG-CD2	-5.71	1.31	1.39
1	A	30	SER	C-N	-5.70	1.21	1.34
1	A	37	ILE	CA-CB	-5.62	1.42	1.54
1	A	40	GLY	C-O	5.61	1.32	1.23
1	A	23	SER	CB-OG	-5.60	1.34	1.42
1	A	60	CYS	CA-CB	-5.58	1.41	1.53
1	A	44	PRO	CA-C	-5.55	1.41	1.52
1	A	51	LYS	C-O	-5.51	1.12	1.23
1	A	59	VAL	C-O	5.49	1.33	1.23
1	A	27	LYS	N-CA	5.43	1.57	1.46
1	A	19	PRO	C-N	-5.40	1.23	1.33
1	A	51	LYS	CD-CE	5.34	1.64	1.51
1	A	43	CYS	C-O	5.30	1.33	1.23
1	A	26	HIS	N-CA	5.27	1.56	1.46
1	A	10	GLN	C-N	5.25	1.44	1.34
1	A	60	CYS	C-O	5.18	1.33	1.23
1	A	39	ARG	CD-NE	5.10	1.55	1.46
1	A	24	CYS	N-CA	-5.01	1.36	1.46

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	ASP	CB-CG-OD2	-35.20	86.62	118.30
1	A	25	TYR	CZ-CE2-CD2	30.59	147.33	119.80
1	A	31	ASP	CB-CG-OD1	30.50	145.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	TYR	CG-CD2-CE2	-25.68	100.76	121.30
1	A	32	PHE	CB-CG-CD1	-24.57	103.60	120.80
1	A	58	GLU	OE1-CD-OE2	-21.66	97.31	123.30
1	A	42	GLY	CA-C-O	21.48	159.27	120.60
1	A	37	ILE	CB-CG1-CD1	19.77	169.26	113.90
1	A	48	PRO	CA-N-CD	-19.50	84.21	111.50
1	A	39	ARG	CD-NE-CZ	-17.65	98.89	123.60
1	A	6	GLN	OE1-CD-NE2	17.41	161.94	121.90
1	A	4	PHE	CB-CG-CD1	-17.38	108.63	120.80
1	A	10	GLN	CG-CD-OE1	16.16	153.93	121.60
1	A	7	HIS	N-CA-CB	15.85	139.13	110.60
1	A	6	GLN	CG-CD-NE2	-15.33	79.90	116.70
1	A	42	GLY	N-CA-C	15.04	150.69	113.10
1	A	29	TRP	NE1-CE2-CZ2	-14.98	113.92	130.40
1	A	61	ASN	CB-CG-OD1	-14.95	91.69	121.60
1	A	50	ILE	CB-CA-C	-14.92	81.76	111.60
1	A	42	GLY	O-C-N	-14.43	99.61	122.70
1	A	40	GLY	O-C-N	-14.23	99.92	122.70
1	A	29	TRP	CD1-NE1-CE2	-14.12	96.29	109.00
1	A	55	CYS	O-C-N	-13.84	100.56	122.70
1	A	54	CYS	O-C-N	-13.78	100.65	122.70
1	A	56	GLU	N-CA-C	13.76	148.16	111.00
1	A	52	LEU	CA-CB-CG	13.63	146.66	115.30
1	A	44	PRO	CB-CA-C	13.42	145.55	112.00
1	A	56	GLU	CB-CA-C	-13.20	83.99	110.40
1	A	9	SER	N-CA-CB	-13.05	90.92	110.50
1	A	5	ASN	CB-CG-OD1	13.02	147.65	121.60
1	A	29	TRP	NE1-CE2-CD2	12.90	120.20	107.30
1	A	61	ASN	O-C-N	12.77	143.13	122.70
1	A	46	VAL	CG1-CB-CG2	12.71	131.24	110.90
1	A	53	SER	O-C-N	12.55	142.78	122.70
1	A	60	CYS	O-C-N	-12.48	102.73	122.70
1	A	25	TYR	OH-CZ-CE2	12.19	153.03	120.10
1	A	50	ILE	O-C-N	12.07	142.02	122.70
1	A	32	PHE	O-C-N	-11.99	103.52	122.70
1	A	39	ARG	O-C-N	-11.99	102.82	123.20
1	A	31	ASP	CA-CB-CG	11.98	139.76	113.40
1	A	26	HIS	CG-ND1-CE1	11.95	124.92	108.20
1	A	12	GLN	OE1-CD-NE2	11.90	149.27	121.90
1	A	47	LYS	CA-C-O	-11.85	95.22	120.10
1	A	23	SER	N-CA-CB	-11.71	92.94	110.50
1	A	32	PHE	CB-CA-C	11.52	133.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	THR	CA-CB-CG2	11.51	128.51	112.40
1	A	47	LYS	CA-C-N	11.44	149.14	117.10
1	A	45	THR	CA-CB-CG2	-11.36	96.50	112.40
1	A	43	CYS	N-CA-CB	-11.33	90.21	110.60
1	A	32	PHE	CB-CG-CD2	11.18	128.62	120.80
1	A	47	LYS	N-CA-CB	11.15	130.68	110.60
1	A	46	VAL	N-CA-CB	-11.12	87.03	111.50
1	A	58	GLU	CA-C-O	-10.90	97.21	120.10
1	A	11	PRO	O-C-N	10.87	140.09	122.70
1	A	58	GLU	CA-C-N	10.83	141.03	117.20
1	A	45	THR	CA-C-N	10.76	140.88	117.20
1	A	44	PRO	O-C-N	-10.75	105.50	122.70
1	A	6	GLN	C-N-CA	10.51	147.98	121.70
1	A	4	PHE	CZ-CE2-CD2	-10.37	107.65	120.10
1	A	25	TYR	CB-CG-CD1	-10.37	114.78	121.00
1	A	37	ILE	N-CA-CB	10.31	134.51	110.80
1	A	54	CYS	CA-C-N	10.25	139.75	117.20
1	A	28	GLN	OE1-CD-NE2	10.23	145.42	121.90
1	A	7	HIS	O-C-N	10.19	139.00	122.70
1	A	44	PRO	CA-N-CD	-10.17	97.27	111.50
1	A	40	GLY	C-N-CA	10.09	146.93	121.70
1	A	48	PRO	N-CA-CB	-10.02	91.28	103.30
1	A	62	ASN	N-CA-CB	10.01	128.61	110.60
1	A	32	PHE	CZ-CE2-CD2	-9.81	108.32	120.10
1	A	25	TYR	CE1-CZ-CE2	-9.81	104.10	119.80
1	A	43	CYS	C-N-CD	-9.67	99.33	120.60
1	A	24	CYS	CA-CB-SG	9.62	131.32	114.00
1	A	33	ARG	CG-CD-NE	-9.51	91.84	111.80
1	A	55	CYS	CA-C-O	9.46	139.97	120.10
1	A	60	CYS	C-N-CA	9.46	145.34	121.70
1	A	53	SER	N-CA-CB	-9.38	96.42	110.50
1	A	36	ILE	O-C-N	9.34	137.64	122.70
1	A	61	ASN	CA-CB-CG	9.32	133.91	113.40
1	A	56	GLU	N-CA-CB	9.24	127.24	110.60
1	A	27	LYS	O-C-N	9.23	137.47	122.70
1	A	32	PHE	CA-CB-CG	-9.22	91.78	113.90
1	A	37	ILE	CA-CB-CG2	-9.21	92.48	110.90
1	A	57	SER	C-N-CA	9.14	144.55	121.70
1	A	56	GLU	CG-CD-OE1	-9.13	100.03	118.30
1	A	32	PHE	CA-C-N	9.13	137.28	117.20
1	A	13	THR	CA-CB-CG2	-9.05	99.74	112.40
1	A	37	ILE	CA-CB-CG1	9.01	128.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	HIS	ND1-CG-CD2	-8.98	93.42	106.00
1	A	38	GLU	CA-CB-CG	8.97	133.14	113.40
1	A	39	ARG	CG-CD-NE	-8.90	93.11	111.80
1	A	62	ASN	CB-CA-C	-8.81	92.78	110.40
1	A	5	ASN	OD1-CG-ND2	-8.76	101.75	121.90
1	A	62	ASN	CA-CB-CG	-8.70	94.25	113.40
1	A	24	CYS	CA-C-O	-8.68	101.86	120.10
1	A	59	VAL	O-C-N	-8.63	108.89	122.70
1	A	31	ASP	O-C-N	8.53	136.35	122.70
1	A	25	TYR	N-CA-CB	8.52	125.93	110.60
1	A	45	THR	CA-C-O	-8.46	102.34	120.10
1	A	10	GLN	OE1-CD-NE2	-8.41	102.55	121.90
1	A	23	SER	N-CA-C	8.41	133.71	111.00
1	A	16	THR	O-C-N	8.40	136.15	122.70
1	A	60	CYS	N-CA-CB	8.39	125.70	110.60
1	A	25	TYR	CD1-CG-CD2	8.37	127.11	117.90
1	A	39	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	A	29	TRP	CB-CG-CD1	8.34	137.84	127.00
1	A	56	GLU	OE1-CD-OE2	8.29	133.25	123.30
1	A	13	THR	O-C-N	-8.26	109.49	122.70
1	A	32	PHE	CE1-CZ-CE2	8.20	134.77	120.00
1	A	8	SER	CA-C-N	-8.19	99.19	117.20
1	A	52	LEU	N-CA-CB	8.13	126.66	110.40
1	A	58	GLU	CG-CD-OE1	8.09	134.48	118.30
1	A	13	THR	N-CA-CB	-8.00	95.11	110.30
1	A	51	LYS	CD-CE-NZ	-7.92	93.48	111.70
1	A	14	THR	OG1-CB-CG2	7.90	128.16	110.00
1	A	1	ARG	CA-C-N	-7.78	100.09	117.20
1	A	45	THR	CB-CA-C	-7.76	90.65	111.60
1	A	13	THR	CB-CA-C	7.75	132.53	111.60
1	A	29	TRP	CG-CD1-NE1	7.72	117.82	110.10
1	A	53	SER	CA-C-N	-7.69	100.29	117.20
1	A	9	SER	O-C-N	-7.61	110.52	122.70
1	A	16	THR	CA-CB-OG1	-7.55	93.14	109.00
1	A	41	CYS	O-C-N	7.55	136.03	123.20
1	A	50	ILE	CA-C-N	-7.53	100.64	117.20
1	A	49	GLY	CA-C-O	7.49	134.08	120.60
1	A	42	GLY	CA-C-N	-7.46	100.78	117.20
1	A	47	LYS	CB-CG-CD	7.40	130.84	111.60
1	A	27	LYS	CD-CE-NZ	-7.39	94.70	111.70
1	A	55	CYS	N-CA-C	-7.37	91.10	111.00
1	A	46	VAL	CA-C-O	-7.35	104.67	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	PHE	CG-CD1-CE1	-7.33	112.74	120.80
1	A	59	VAL	C-N-CA	7.28	139.91	121.70
1	A	15	LYS	CB-CA-C	-7.26	95.88	110.40
1	A	32	PHE	CD1-CG-CD2	7.19	127.64	118.30
1	A	1	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	50	ILE	N-CA-CB	7.18	127.31	110.80
1	A	48	PRO	CB-CA-C	7.12	129.79	112.00
1	A	10	GLN	N-CA-C	7.11	130.20	111.00
1	A	57	SER	CA-C-N	7.10	132.82	117.20
1	A	51	LYS	N-CA-C	7.08	130.12	111.00
1	A	49	GLY	CA-C-N	-7.08	101.64	117.20
1	A	36	ILE	CB-CA-C	-7.07	97.45	111.60
1	A	2	ILE	O-C-N	7.06	134.00	122.70
1	A	4	PHE	CG-CD1-CE1	-7.03	113.07	120.80
1	A	50	ILE	N-CA-C	7.02	129.96	111.00
1	A	39	ARG	CA-C-O	6.93	134.66	120.10
1	A	55	CYS	CB-CA-C	6.89	124.19	110.40
1	A	39	ARG	N-CA-CB	6.79	122.82	110.60
1	A	39	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	33	ARG	N-CA-C	-6.74	92.81	111.00
1	A	27	LYS	C-N-CA	-6.70	104.94	121.70
1	A	50	ILE	CA-CB-CG2	6.70	124.30	110.90
1	A	38	GLU	O-C-N	6.60	133.26	122.70
1	A	28	GLN	CG-CD-OE1	-6.59	108.42	121.60
1	A	24	CYS	CA-C-N	6.57	131.65	117.20
1	A	52	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	A	35	THR	CA-CB-OG1	-6.45	95.46	109.00
1	A	25	TYR	CE1-CZ-OH	-6.44	102.70	120.10
1	A	12	GLN	CG-CD-NE2	-6.42	101.28	116.70
1	A	48	PRO	C-N-CA	-6.40	108.85	122.30
1	A	8	SER	CA-C-O	6.40	133.53	120.10
1	A	40	GLY	CA-C-N	6.39	131.26	117.20
1	A	52	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	A	35	THR	N-CA-C	-6.38	93.77	111.00
1	A	2	ILE	CA-C-O	-6.37	106.73	120.10
1	A	4	PHE	CE1-CZ-CE2	6.35	131.43	120.00
1	A	5	ASN	CA-CB-CG	-6.33	99.48	113.40
1	A	55	CYS	N-CA-CB	-6.32	99.23	110.60
1	A	21	GLU	OE1-CD-OE2	6.30	130.86	123.30
1	A	51	LYS	CA-C-O	-6.26	106.95	120.10
1	A	61	ASN	CB-CG-ND2	6.24	131.68	116.70
1	A	48	PRO	O-C-N	-6.23	112.60	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	PRO	CA-CB-CG	-6.21	92.19	104.00
1	A	57	SER	O-C-N	-6.21	112.77	122.70
1	A	4	PHE	CD1-CG-CD2	6.11	126.25	118.30
1	A	33	ARG	CA-C-O	-6.10	107.28	120.10
1	A	44	PRO	N-CA-CB	-6.08	95.91	102.60
1	A	12	GLN	CG-CD-OE1	-6.08	109.45	121.60
1	A	59	VAL	CA-C-N	6.03	130.47	117.20
1	A	54	CYS	C-N-CA	6.00	136.69	121.70
1	A	26	HIS	ND1-CE1-NE2	-5.95	96.81	109.90
1	A	4	PHE	CB-CG-CD2	5.90	124.93	120.80
1	A	46	VAL	CA-CB-CG2	5.89	119.74	110.90
1	A	17	CYS	CA-CB-SG	5.81	124.46	114.00
1	A	55	CYS	C-N-CA	5.79	136.17	121.70
1	A	50	ILE	CB-CG1-CD1	5.76	130.03	113.90
1	A	39	ARG	C-N-CA	5.75	134.38	122.30
1	A	3	CYS	CA-C-N	5.73	129.81	117.20
1	A	1	ARG	CA-C-O	5.72	132.12	120.10
1	A	15	LYS	N-CA-CB	-5.68	100.38	110.60
1	A	29	TRP	N-CA-CB	5.68	120.82	110.60
1	A	11	PRO	N-CA-CB	5.67	110.11	103.30
1	A	1	ARG	N-CA-C	5.66	126.28	111.00
1	A	34	GLY	O-C-N	5.64	131.73	122.70
1	A	39	ARG	CB-CA-C	-5.60	99.20	110.40
1	A	61	ASN	CA-C-O	-5.59	108.35	120.10
1	A	29	TRP	CB-CG-CD2	-5.58	119.35	126.60
1	A	33	ARG	CA-C-N	5.57	127.35	116.20
1	A	28	GLN	N-CA-C	-5.54	96.05	111.00
1	A	10	GLN	CG-CD-NE2	-5.51	103.49	116.70
1	A	2	ILE	CB-CG1-CD1	-5.50	98.49	113.90
1	A	6	GLN	CB-CA-C	-5.47	99.46	110.40
1	A	38	GLU	CA-C-N	-5.45	105.20	117.20
1	A	28	GLN	N-CA-CB	-5.44	100.81	110.60
1	A	51	LYS	CG-CD-CE	-5.43	95.60	111.90
1	A	4	PHE	O-C-N	5.40	131.34	122.70
1	A	21	GLU	CG-CD-OE2	-5.33	107.63	118.30
1	A	38	GLU	CG-CD-OE1	-5.31	107.67	118.30
1	A	39	ARG	CA-CB-CG	5.27	124.99	113.40
1	A	1	ARG	CB-CA-C	5.25	120.90	110.40
1	A	31	ASP	CA-C-O	-5.25	109.07	120.10
1	A	14	THR	C-N-CA	5.23	134.78	121.70
1	A	34	GLY	C-N-CA	-5.23	108.62	121.70
1	A	29	TRP	CD1-CG-CD2	-5.23	102.12	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	TRP	CE2-CD2-CG	-5.22	103.13	107.30
1	A	45	THR	OG1-CB-CG2	-5.21	98.02	110.00
1	A	32	PHE	C-N-CA	5.19	134.68	121.70
1	A	38	GLU	CB-CA-C	-5.18	100.03	110.40
1	A	6	GLN	CA-CB-CG	5.18	124.79	113.40
1	A	56	GLU	CB-CG-CD	-5.17	100.24	114.20
1	A	38	GLU	N-CA-C	-5.13	97.14	111.00
1	A	27	LYS	CB-CA-C	-5.12	100.16	110.40
1	A	25	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	A	62	ASN	CB-CG-ND2	5.03	128.78	116.70
1	A	28	GLN	O-C-N	5.02	130.74	122.70
1	A	50	ILE	CG1-CB-CG2	-5.01	100.38	111.40

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	ARG	CA
1	A	7	HIS	CA
1	A	14	THR	CB
1	A	32	PHE	CA
1	A	44	PRO	CA
1	A	51	LYS	CA
1	A	52	LEU	CA
1	A	56	GLU	CA
1	A	60	CYS	CA

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ARG	Sidechain
1	A	15	LYS	Peptide
1	A	3	CYS	Peptide
1	A	32	PHE	Peptide
1	A	33	ARG	Sidechain
1	A	39	ARG	Sidechain
1	A	42	GLY	Peptide
1	A	44	PRO	Mainchain
1	A	45	THR	Peptide
1	A	46	VAL	Peptide
1	A	47	LYS	Mainchain
1	A	49	GLY	Peptide
1	A	54	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	55	CYS	Peptide
1	A	57	SER	Mainchain
1	A	61	ASN	Peptide
1	A	9	SER	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	472	0	427	196	32
2	A	4	0	0	3	0
3	A	67	0	0	62	32
All	All	543	0	427	197	35

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 218.

All (197) 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:A:50:ILE:HD12	1:A:51:LYS:CA	1.36	1.50
1:A:26:HIS:CD2	1:A:37:ILE:HD13	1.45	1.50
1:A:26:HIS:CG	1:A:37:ILE:HD13	1.56	1.40
1:A:1:ARG:NH1	1:A:22:SER:O	1.56	1.39
1:A:16:THR:C	1:A:17:CYS:CA	1.89	1.38
1:A:22:SER:C	1:A:23:SER:N	1.77	1.38
1:A:50:ILE:CG1	1:A:51:LYS:N	1.77	1.33
1:A:16:THR:CA	1:A:17:CYS:N	1.91	1.31
1:A:50:ILE:CG1	1:A:51:LYS:H	1.27	1.30
1:A:52:LEU:HB2	3:A:100:HOH:O	1.16	1.28
1:A:14:THR:O	3:A:81:HOH:O	1.53	1.25
1:A:50:ILE:CD1	1:A:51:LYS:CA	2.14	1.25
1:A:59:VAL:CA	3:A:69:HOH:O	1.85	1.24
1:A:10:GLN:CD	3:A:76:HOH:O	1.75	1.24
1:A:4:PHE:CD1	3:A:130:HOH:O	1.72	1.23
1:A:35:THR:HB	3:A:110:HOH:O	1.35	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD12	1:A:51:LYS:C	1.59	1.22
1:A:6:GLN:CB	3:A:72:HOH:O	1.87	1.21
1:A:26:HIS:O	3:A:100:HOH:O	1.55	1.21
1:A:42:GLY:O	1:A:43:CYS:CB	1.73	1.21
1:A:53:SER:C	3:A:108:HOH:O	1.80	1.20
1:A:50:ILE:HD12	1:A:51:LYS:CB	1.71	1.20
1:A:10:GLN:NE2	3:A:76:HOH:O	1.74	1.17
1:A:15:LYS:NZ	2:A:64:SO4:S	2.16	1.17
1:A:27:LYS:NZ	1:A:38:GLU:OE1	1.77	1.16
1:A:1:ARG:NH2	1:A:58:GLU:OE1	1.80	1.14
1:A:50:ILE:HG13	1:A:51:LYS:N	1.42	1.14
1:A:52:LEU:CD2	3:A:100:HOH:O	1.81	1.14
1:A:10:GLN:HB2	1:A:11:PRO:CD	1.80	1.09
1:A:25:TYR:HB2	1:A:52:LEU:HD21	1.23	1.09
1:A:50:ILE:CD1	1:A:51:LYS:CB	2.30	1.09
1:A:50:ILE:HD11	1:A:51:LYS:HG2	1.34	1.09
1:A:22:SER:O	1:A:56:GLU:CG	2.01	1.08
1:A:8:SER:O	1:A:9:SER:C	1.93	1.07
1:A:29:TRP:CH2	3:A:101:HOH:O	2.07	1.07
1:A:52:LEU:HD23	3:A:100:HOH:O	1.45	1.07
1:A:14:THR:HG22	3:A:81:HOH:O	1.55	1.06
1:A:10:GLN:OE1	3:A:76:HOH:O	1.72	1.06
1:A:26:HIS:CG	1:A:37:ILE:CD1	2.38	1.05
1:A:26:HIS:CD2	1:A:37:ILE:CD1	2.39	1.05
1:A:27:LYS:NZ	1:A:38:GLU:CD	2.09	1.04
1:A:16:THR:O	1:A:17:CYS:N	1.93	1.02
1:A:27:LYS:HZ2	1:A:38:GLU:CD	1.62	1.01
1:A:46:VAL:HG12	1:A:47:LYS:H	1.18	1.01
1:A:29:TRP:HH2	3:A:101:HOH:O	1.42	1.00
1:A:41:CYS:SG	3:A:88:HOH:O	2.18	1.00
1:A:29:TRP:O	3:A:104:HOH:O	1.78	0.99
1:A:53:SER:O	3:A:108:HOH:O	1.80	0.97
1:A:13:THR:C	3:A:80:HOH:O	2.02	0.97
1:A:50:ILE:HD12	1:A:52:LEU:N	1.80	0.96
1:A:29:TRP:C	3:A:105:HOH:O	2.04	0.95
1:A:46:VAL:CG1	3:A:122:HOH:O	2.14	0.94
1:A:50:ILE:CD1	1:A:52:LEU:N	2.31	0.94
1:A:19:PRO:O	3:A:91:HOH:O	1.86	0.93
1:A:6:GLN:HB3	3:A:72:HOH:O	1.54	0.93
1:A:50:ILE:HD13	1:A:52:LEU:H	1.32	0.93
1:A:50:ILE:HD11	1:A:51:LYS:CG	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG13	3:A:123:HOH:O	1.47	0.92
1:A:29:TRP:CA	3:A:105:HOH:O	2.18	0.92
1:A:46:VAL:HG12	1:A:47:LYS:N	1.76	0.91
1:A:25:TYR:HB2	1:A:52:LEU:CD2	1.99	0.91
1:A:46:VAL:HG13	3:A:122:HOH:O	1.68	0.91
1:A:8:SER:O	1:A:9:SER:O	1.89	0.90
1:A:50:ILE:CD1	1:A:52:LEU:H	1.84	0.90
1:A:50:ILE:CD1	1:A:51:LYS:HG2	2.02	0.89
1:A:42:GLY:O	1:A:43:CYS:HB2	0.84	0.88
1:A:43:CYS:O	3:A:115:HOH:O	1.91	0.88
1:A:1:ARG:NH1	1:A:22:SER:C	2.27	0.88
1:A:16:THR:C	1:A:17:CYS:N	0.83	0.88
1:A:26:HIS:ND1	1:A:37:ILE:HD13	1.88	0.88
1:A:50:ILE:CD1	1:A:51:LYS:CG	2.52	0.87
1:A:46:VAL:HA	3:A:125:HOH:O	1.73	0.86
1:A:46:VAL:CG1	1:A:47:LYS:N	2.38	0.86
1:A:22:SER:O	1:A:56:GLU:HG2	1.77	0.84
1:A:26:HIS:NE2	1:A:37:ILE:HD13	1.93	0.84
1:A:10:GLN:HB2	1:A:11:PRO:HD3	1.60	0.81
1:A:50:ILE:CD1	1:A:51:LYS:N	2.33	0.81
1:A:16:THR:O	3:A:87:HOH:O	2.00	0.80
1:A:41:CYS:CB	3:A:88:HOH:O	2.29	0.80
1:A:46:VAL:CG1	1:A:50:ILE:CG2	2.60	0.79
1:A:19:PRO:HD2	3:A:90:HOH:O	1.81	0.79
1:A:56:GLU:OE1	1:A:56:GLU:CA	2.29	0.79
1:A:50:ILE:HD12	1:A:51:LYS:HB3	1.64	0.79
1:A:27:LYS:HZ3	1:A:38:GLU:CD	1.87	0.77
2:A:64:SO4:S	3:A:82:HOH:O	2.42	0.77
1:A:47:LYS:HD3	1:A:48:PRO:N	2.00	0.77
1:A:25:TYR:N	3:A:113:HOH:O	2.12	0.76
1:A:36:ILE:HG22	1:A:37:ILE:N	2.01	0.75
1:A:47:LYS:H	1:A:50:ILE:HG22	1.51	0.75
1:A:4:PHE:N	3:A:130:HOH:O	1.99	0.74
1:A:45:THR:O	3:A:125:HOH:O	2.06	0.73
1:A:6:GLN:CA	3:A:72:HOH:O	2.26	0.73
1:A:50:ILE:HG13	1:A:51:LYS:H	0.59	0.73
1:A:46:VAL:CG1	1:A:50:ILE:HG21	2.19	0.73
1:A:10:GLN:HB2	1:A:11:PRO:HD2	1.70	0.72
1:A:12:GLN:C	1:A:13:THR:HG22	2.07	0.72
1:A:46:VAL:O	3:A:124:HOH:O	2.07	0.72
1:A:14:THR:CG2	3:A:81:HOH:O	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ARG:CZ	1:A:58:GLU:OE1	2.37	0.72
1:A:50:ILE:CD1	1:A:51:LYS:HB3	2.18	0.72
1:A:31:ASP:OD1	1:A:33:ARG:HD3	1.90	0.71
1:A:46:VAL:HG22	1:A:52:LEU:CD1	2.20	0.71
1:A:26:HIS:CE1	1:A:37:ILE:HD13	2.25	0.70
1:A:22:SER:O	1:A:56:GLU:HG3	1.90	0.70
1:A:35:THR:HG23	3:A:104:HOH:O	1.89	0.70
1:A:1:ARG:O	1:A:17:CYS:HB2	1.91	0.69
1:A:46:VAL:CG1	1:A:50:ILE:HG22	2.21	0.69
1:A:46:VAL:CA	3:A:125:HOH:O	2.36	0.69
1:A:16:THR:HA	1:A:17:CYS:N	2.02	0.69
1:A:7:HIS:C	1:A:9:SER:N	2.44	0.68
1:A:25:TYR:HE1	1:A:27:LYS:HD2	1.57	0.68
1:A:47:LYS:N	1:A:50:ILE:HG22	2.08	0.68
1:A:4:PHE:CG	3:A:130:HOH:O	2.16	0.68
1:A:4:PHE:O	3:A:98:HOH:O	2.12	0.67
1:A:41:CYS:HB2	3:A:88:HOH:O	1.91	0.67
1:A:22:SER:OG	1:A:56:GLU:HG2	1.94	0.67
1:A:52:LEU:HD22	3:A:100:HOH:O	1.70	0.66
1:A:1:ARG:NE	1:A:58:GLU:OE1	2.29	0.66
1:A:22:SER:O	1:A:56:GLU:CB	2.44	0.65
1:A:46:VAL:HG22	1:A:52:LEU:HD12	1.78	0.65
1:A:26:HIS:O	1:A:52:LEU:HD23	1.98	0.63
1:A:47:LYS:HB3	3:A:124:HOH:O	1.99	0.63
1:A:56:GLU:OE1	1:A:56:GLU:N	2.32	0.63
1:A:29:TRP:HA	3:A:105:HOH:O	1.90	0.62
1:A:50:ILE:HD11	1:A:51:LYS:CB	2.19	0.62
1:A:16:THR:O	1:A:17:CYS:CA	2.40	0.61
1:A:22:SER:O	1:A:56:GLU:HB3	2.01	0.61
1:A:25:TYR:CB	1:A:52:LEU:HD21	2.15	0.60
1:A:38:GLU:OE2	3:A:101:HOH:O	2.15	0.60
1:A:26:HIS:ND1	1:A:37:ILE:CD1	2.58	0.60
1:A:6:GLN:HB2	3:A:72:HOH:O	1.75	0.59
1:A:46:VAL:HG11	3:A:122:HOH:O	1.93	0.59
1:A:50:ILE:CG1	1:A:51:LYS:CA	2.51	0.59
1:A:43:CYS:O	1:A:44:PRO:O	2.20	0.59
1:A:27:LYS:HD2	1:A:38:GLU:HB3	1.85	0.59
1:A:46:VAL:HG12	1:A:50:ILE:HG22	1.82	0.59
1:A:7:HIS:O	1:A:9:SER:N	2.37	0.58
1:A:50:ILE:HD13	1:A:52:LEU:N	2.04	0.58
1:A:22:SER:C	1:A:56:GLU:CG	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:H	1:A:39:ARG:HH22	1.53	0.56
1:A:25:TYR:O	3:A:97:HOH:O	2.17	0.56
1:A:50:ILE:HG13	1:A:51:LYS:CG	2.34	0.56
1:A:6:GLN:O	1:A:39:ARG:HD3	2.05	0.56
1:A:40:GLY:HA3	3:A:85:HOH:O	2.06	0.55
1:A:46:VAL:HG13	1:A:50:ILE:CG2	2.34	0.55
1:A:58:GLU:HA	2:A:63:SO4:O2	2.07	0.55
1:A:30:SER:CB	1:A:35:THR:HA	2.37	0.55
1:A:51:LYS:O	1:A:52:LEU:HB3	2.06	0.55
1:A:46:VAL:HG11	1:A:50:ILE:HG21	1.86	0.54
1:A:40:GLY:HA3	3:A:112:HOH:O	2.07	0.54
1:A:36:ILE:CG2	1:A:37:ILE:N	2.70	0.54
1:A:50:ILE:CG1	1:A:51:LYS:HG2	2.38	0.54
1:A:22:SER:C	1:A:56:GLU:HG2	2.29	0.53
1:A:26:HIS:CE1	1:A:37:ILE:CD1	2.91	0.52
1:A:25:TYR:CE1	1:A:27:LYS:HD2	2.42	0.52
1:A:26:HIS:O	1:A:52:LEU:HB2	2.10	0.52
1:A:47:LYS:HD3	1:A:48:PRO:CA	2.39	0.52
1:A:30:SER:HA	1:A:34:GLY:O	2.10	0.52
1:A:39:ARG:HB3	3:A:98:HOH:O	2.10	0.51
1:A:7:HIS:O	1:A:8:SER:C	2.49	0.51
1:A:1:ARG:NH1	1:A:56:GLU:HB3	2.26	0.50
1:A:46:VAL:CG1	1:A:47:LYS:H	1.99	0.50
1:A:46:VAL:CG2	1:A:52:LEU:HD12	2.42	0.50
1:A:50:ILE:CG1	1:A:51:LYS:CG	2.90	0.49
1:A:28:GLN:HA	1:A:36:ILE:O	2.13	0.49
1:A:1:ARG:HH11	1:A:22:SER:C	2.03	0.49
1:A:26:HIS:HA	1:A:37:ILE:HD12	1.93	0.49
1:A:40:GLY:N	3:A:98:HOH:O	2.45	0.48
1:A:16:THR:C	1:A:17:CYS:HA	2.19	0.48
1:A:26:HIS:C	1:A:52:LEU:HD23	2.34	0.48
1:A:37:ILE:HD11	1:A:39:ARG:HD2	1.94	0.48
1:A:59:VAL:C	3:A:69:HOH:O	2.33	0.48
1:A:7:HIS:CE1	3:A:74:HOH:O	2.66	0.47
1:A:40:GLY:CA	3:A:85:HOH:O	2.62	0.47
1:A:22:SER:C	1:A:23:SER:CA	2.76	0.47
1:A:46:VAL:HG22	1:A:52:LEU:HD11	1.96	0.46
1:A:10:GLN:HE21	1:A:10:GLN:HB3	1.16	0.46
1:A:6:GLN:HG2	1:A:13:THR:H	1.80	0.46
1:A:28:GLN:O	1:A:51:LYS:HA	2.16	0.46
1:A:2:ILE:HD13	1:A:2:ILE:HG21	1.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:SER:HB2	1:A:35:THR:HA	1.97	0.45
1:A:6:GLN:HB3	1:A:13:THR:HG23	1.98	0.45
1:A:46:VAL:HG12	1:A:50:ILE:CG2	2.42	0.44
1:A:22:SER:C	1:A:56:GLU:HG3	2.37	0.44
1:A:10:GLN:HG3	3:A:72:HOH:O	2.18	0.43
1:A:7:HIS:CE1	3:A:76:HOH:O	2.71	0.43
1:A:26:HIS:NE2	1:A:37:ILE:CD1	2.73	0.43
1:A:29:TRP:N	3:A:102:HOH:O	2.51	0.43
1:A:57:SER:O	1:A:60:CYS:SG	2.77	0.42
1:A:39:ARG:NH2	3:A:111:HOH:O	2.39	0.42
1:A:46:VAL:HG13	1:A:50:ILE:HG22	1.99	0.41
1:A:12:GLN:C	1:A:13:THR:CG2	2.56	0.41
1:A:27:LYS:CD	1:A:38:GLU:HB3	2.49	0.41
1:A:30:SER:CA	1:A:34:GLY:O	2.68	0.41
1:A:10:GLN:CB	1:A:11:PRO:HD3	2.42	0.41
1:A:11:PRO:O	1:A:13:THR:CG2	2.68	0.41
1:A:29:TRP:CG	1:A:30:SER:N	2.85	0.40

All (35) 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:A:1:ARG:NH1	3:A:95:HOH:O[1_556]	0.23	1.97
3:A:114:HOH:O	3:A:119:HOH:O[2_665]	0.27	1.93
3:A:89:HOH:O	3:A:110:HOH:O[4_556]	0.51	1.69
1:A:55:CYS:C	3:A:66:HOH:O[1_556]	0.61	1.59
1:A:55:CYS:C	3:A:128:HOH:O[1_556]	0.69	1.51
1:A:55:CYS:O	3:A:128:HOH:O[1_556]	0.92	1.28
1:A:56:GLU:N	3:A:66:HOH:O[1_556]	0.93	1.27
1:A:60:CYS:CB	3:A:74:HOH:O[1_556]	1.09	1.11
1:A:56:GLU:N	3:A:128:HOH:O[1_556]	1.10	1.10
1:A:1:ARG:CZ	3:A:95:HOH:O[1_556]	1.15	1.05
1:A:58:GLU:OE1	3:A:65:HOH:O[1_556]	1.37	0.83
1:A:55:CYS:O	3:A:66:HOH:O[1_556]	1.43	0.77
3:A:86:HOH:O	3:A:107:HOH:O[4_556]	1.43	0.77
1:A:58:GLU:CB	3:A:129:HOH:O[1_556]	1.44	0.76
1:A:58:GLU:CA	3:A:129:HOH:O[1_556]	1.52	0.68
1:A:58:GLU:OE2	3:A:65:HOH:O[1_556]	1.53	0.67
1:A:56:GLU:CG	3:A:94:HOH:O[1_556]	1.54	0.66
1:A:33:ARG:NH1	3:A:108:HOH:O[1_554]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:C	3:A:129:HOH:O[1_556]	1.65	0.55
1:A:33:ARG:NH1	1:A:53:SER:OG[1_554]	1.69	0.51
1:A:22:SER:O	3:A:95:HOH:O[1_556]	1.74	0.46
1:A:35:THR:O	3:A:89:HOH:O[4_456]	1.84	0.36
1:A:55:CYS:CA	3:A:66:HOH:O[1_556]	1.85	0.35
1:A:48:PRO:CD	3:A:92:HOH:O[2_665]	1.88	0.32
1:A:56:GLU:CD	3:A:94:HOH:O[1_556]	1.89	0.31
1:A:58:GLU:CD	3:A:65:HOH:O[1_556]	1.91	0.29
1:A:56:GLU:CA	3:A:66:HOH:O[1_556]	1.92	0.28
1:A:1:ARG:NE	3:A:65:HOH:O[1_556]	1.95	0.25
1:A:12:GLN:OE1	1:A:50:ILE:CD1[3_646]	1.95	0.25
1:A:35:THR:CB	3:A:89:HOH:O[4_456]	1.98	0.22
1:A:60:CYS:CA	3:A:74:HOH:O[1_556]	2.03	0.17
1:A:4:PHE:CE2	1:A:51:LYS:CE[3_646]	2.13	0.07
1:A:1:ARG:NE	3:A:95:HOH:O[1_556]	2.14	0.06
1:A:35:THR:C	3:A:89:HOH:O[4_456]	2.16	0.04
1:A:55:CYS:CA	3:A:128:HOH:O[1_556]	2.16	0.04

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	60/62 (97%)	42 (70%)	8 (13%)	10 (17%)	0 0

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	44	PRO
1	A	47	LYS
1	A	48	PRO
1	A	56	GLU
1	A	60	CYS

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Mol	Chain	Res	Type
1	A	8	SER
1	A	9	SER
1	A	50	ILE
1	A	59	VAL

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	56/57 (98%)	38 (68%)	18 (32%)	0 0

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	6	GLN
1	A	7	HIS
1	A	8	SER
1	A	9	SER
1	A	13	THR
1	A	21	GLU
1	A	27	LYS
1	A	28	GLN
1	A	37	ILE
1	A	44	PRO
1	A	46	VAL
1	A	47	LYS
1	A	48	PRO
1	A	51	LYS
1	A	52	LEU
1	A	56	GLU
1	A	60	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	10	GLN

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 2 ligands modelled in this entry, 1 is modelled with single atom - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	63	-	2,2,4	2.44	1 (50%)	1,1,6	1.27	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	63	SO4	O1-S	3.03	1.58	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	63	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	22:SER	C	23:SER	N	1.77
1	A	16:THR	C	17:CYS	N	0.83

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.