



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:36 am BST

PDB ID : 3SDP
Title : THE 2.1 ANGSTROMS RESOLUTION STRUCTURE OF IRON SUPER-
OXIDE DISMUTASE FROM PSEUDOMONAS OVALIS
Authors : Stoddard, B.L.; Ringe, D.; Petsko, G.A.
Deposited on : 1991-05-06
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

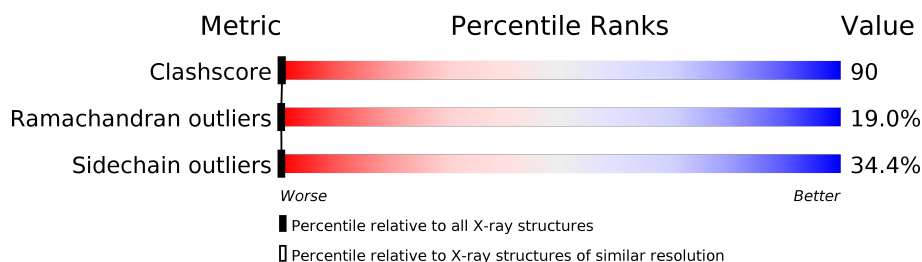
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	195	
1	B	195	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3090 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 IRON SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1454	937	239	275	3			
1	B	186	Total	C	N	O	S	0	0	0
			1454	937	239	275	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	GLY	CONFLICT	UNP P09223
B	85	ALA	GLY	CONFLICT	UNP P09223

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

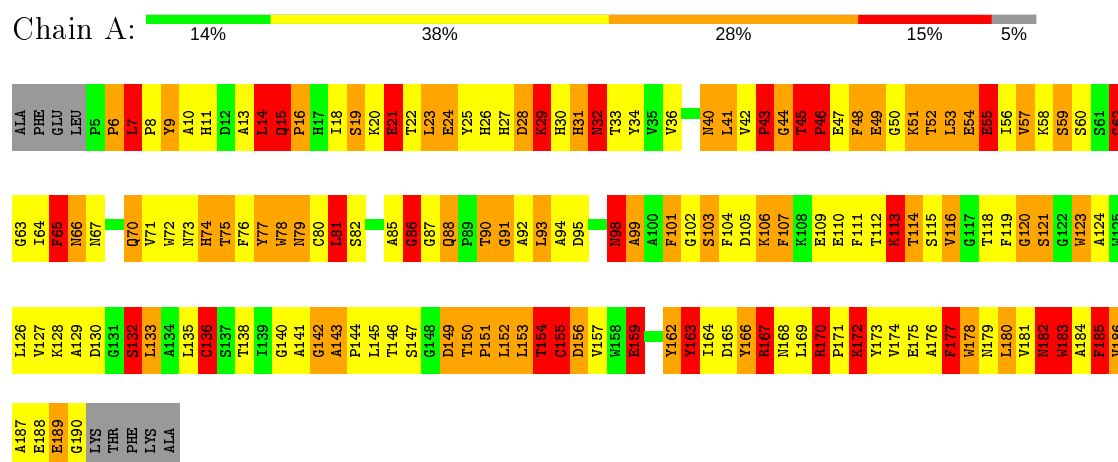
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	78	Total	O	0	0
			78	78		

3 Residue-property plots

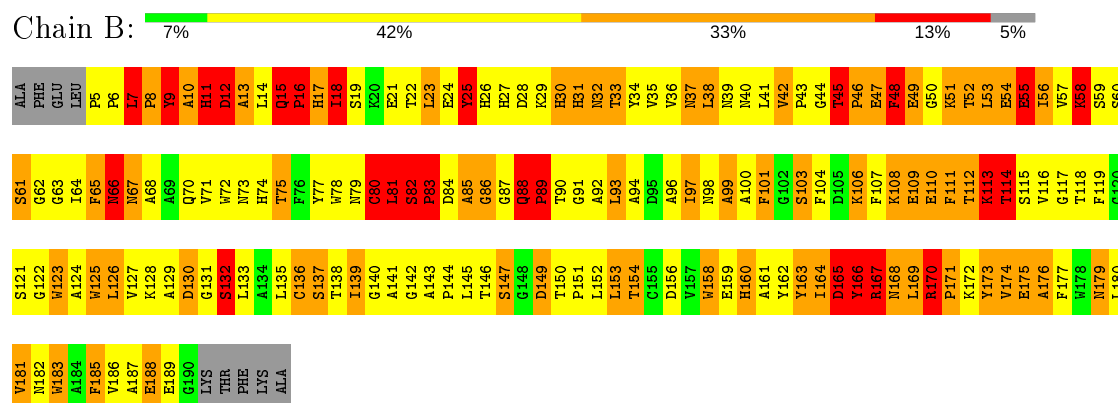
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: IRON SUPEROXIDE DISMUTASE



• Molecule 1: IRON SUPEROXIDE DISMUTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.90 Å 49.10 Å 61.70 Å 90.00° 106.80° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.232 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3090	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: FE

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	1.81	20/1504 (1.3%)	2.31	66/2058 (3.2%)
1	B	1.89	24/1504 (1.6%)	2.38	72/2058 (3.5%)
All	All	1.85	44/3008 (1.5%)	2.35	138/4116 (3.4%)

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	PRO	N-CD	20.58	1.76	1.47
1	A	45	THR	C-O	13.87	1.49	1.23
1	B	54	GLU	CD-OE2	8.97	1.35	1.25
1	A	189	GLU	CD-OE2	8.54	1.35	1.25
1	B	24	GLU	CD-OE2	7.68	1.34	1.25
1	A	55	GLU	CD-OE1	-7.60	1.17	1.25
1	B	109	GLU	CD-OE1	7.36	1.33	1.25
1	A	54	GLU	CD-OE2	7.09	1.33	1.25
1	B	159	GLU	CD-OE1	-6.97	1.18	1.25
1	B	47	GLU	CD-OE2	6.97	1.33	1.25
1	B	110	GLU	CD-OE1	-6.95	1.18	1.25
1	B	188	GLU	CD-OE2	6.79	1.33	1.25
1	A	121	SER	CB-OG	6.38	1.50	1.42
1	B	175	GLU	CD-OE2	6.27	1.32	1.25
1	B	59	SER	CB-OG	-6.27	1.34	1.42
1	A	62	GLY	N-CA	-6.22	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	GLY	C-O	6.11	1.33	1.23
1	A	21	GLU	CD-OE2	6.05	1.32	1.25
1	A	86	GLY	N-CA	-6.02	1.37	1.46
1	B	159	GLU	CD-OE2	6.01	1.32	1.25
1	A	110	GLU	CD-OE1	5.88	1.32	1.25
1	A	55	GLU	CD-OE2	5.84	1.32	1.25
1	A	189	GLU	CD-OE1	-5.76	1.19	1.25
1	A	49	GLU	CD-OE2	5.58	1.31	1.25
1	A	136	CYS	N-CA	5.53	1.57	1.46
1	A	48	PHE	CE2-CZ	5.53	1.47	1.37
1	A	62	GLY	CA-C	-5.49	1.43	1.51
1	A	136	CYS	CA-CB	-5.46	1.42	1.53
1	B	49	GLU	CD-OE1	-5.46	1.19	1.25
1	B	109	GLU	CD-OE2	-5.45	1.19	1.25
1	A	54	GLU	CD-OE1	-5.34	1.19	1.25
1	B	188	GLU	CD-OE1	-5.31	1.19	1.25
1	A	6	PRO	N-CD	5.29	1.55	1.47
1	B	86	GLY	CA-C	-5.27	1.43	1.51
1	B	111	PHE	CG-CD2	5.26	1.46	1.38
1	B	9	TYR	CE1-CZ	5.24	1.45	1.38
1	B	24	GLU	CD-OE1	-5.24	1.19	1.25
1	B	55	GLU	CD-OE2	-5.22	1.20	1.25
1	B	147	SER	CB-OG	-5.19	1.35	1.42
1	B	86	GLY	C-O	5.13	1.31	1.23
1	B	131	GLY	CA-C	5.13	1.60	1.51
1	B	86	GLY	N-CA	-5.08	1.38	1.46
1	A	65	PHE	CE1-CZ	5.08	1.47	1.37
1	A	6	PRO	N-CA	-5.03	1.38	1.47

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	PRO	CA-N-CD	-21.85	80.91	111.50
1	A	45	THR	CA-C-O	-19.61	78.92	120.10
1	A	155	CYS	CA-CB-SG	-18.93	79.92	114.00
1	A	167	ARG	NE-CZ-NH2	17.74	129.17	120.30
1	B	82	SER	O-C-N	17.23	153.84	121.10
1	B	86	GLY	N-CA-C	16.36	153.99	113.10
1	A	45	THR	CA-C-N	13.24	154.16	117.10
1	B	82	SER	C-N-CD	-12.90	92.22	120.60
1	A	159	GLU	OE1-CD-OE2	12.71	138.55	123.30
1	A	45	THR	O-C-N	-12.63	97.10	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	PRO	N-CA-CB	12.61	118.44	103.30
1	A	156	ASP	CB-CG-OD1	-12.34	107.19	118.30
1	A	136	CYS	CA-CB-SG	12.24	136.03	114.00
1	B	82	SER	C-N-CA	12.01	172.46	122.00
1	A	62	GLY	N-CA-C	11.78	142.56	113.10
1	B	87	GLY	C-N-CA	11.07	149.37	121.70
1	B	166	TYR	CA-CB-CG	10.19	132.77	113.40
1	A	81	LEU	CA-CB-CG	10.14	138.62	115.30
1	B	170	ARG	CD-NE-CZ	10.01	137.61	123.60
1	B	82	SER	CA-C-O	-9.84	99.44	120.10
1	B	108	LYS	CA-CB-CG	9.39	134.06	113.40
1	A	167	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	B	25	TYR	CA-CB-CG	9.22	130.93	113.40
1	B	123	TRP	CA-CB-CG	9.22	131.22	113.70
1	A	188	GLU	N-CA-C	8.99	135.27	111.00
1	A	95	ASP	CB-CG-OD1	8.64	126.07	118.30
1	A	178	TRP	CB-CA-C	8.53	127.46	110.40
1	B	109	GLU	CA-CB-CG	8.36	131.80	113.40
1	A	53	LEU	CA-CB-CG	8.15	134.04	115.30
1	A	156	ASP	CB-CG-OD2	8.02	125.51	118.30
1	B	67	ASN	CA-CB-CG	8.01	131.03	113.40
1	B	167	ARG	N-CA-CB	7.95	124.91	110.60
1	B	101	PHE	CB-CA-C	7.91	126.21	110.40
1	B	125	TRP	CD1-CG-CD2	-7.62	100.20	106.30
1	A	101	PHE	CB-CG-CD2	-7.56	115.51	120.80
1	B	88	GLN	N-CA-C	7.48	131.19	111.00
1	B	84	ASP	C-N-CA	7.44	140.30	121.70
1	A	150	THR	N-CA-C	7.41	131.00	111.00
1	B	89	PRO	CA-N-CD	-7.28	101.30	111.50
1	B	12	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	182	ASN	CB-CA-C	7.23	124.85	110.40
1	A	156	ASP	CA-CB-CG	-7.21	97.54	113.40
1	A	135	LEU	CA-CB-CG	7.16	131.76	115.30
1	B	183	TRP	CA-CB-CG	7.06	127.11	113.70
1	B	25	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	A	9	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	B	166	TYR	CA-C-N	7.01	132.62	117.20
1	B	46	PRO	C-N-CA	6.92	138.99	121.70
1	A	23	LEU	CB-CA-C	6.90	123.32	110.20
1	A	153	LEU	N-CA-CB	6.90	124.20	110.40
1	B	101	PHE	CB-CG-CD1	-6.88	115.98	120.80
1	B	47	GLU	C-N-CA	6.81	138.72	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	SER	CA-C-O	6.79	134.37	120.10
1	B	86	GLY	CA-C-N	6.75	129.71	116.20
1	A	46	PRO	N-CD-CG	6.65	113.18	103.20
1	B	48	PHE	CB-CG-CD2	-6.62	116.17	120.80
1	A	119	PHE	CB-CG-CD1	-6.55	116.21	120.80
1	B	32	ASN	N-CA-C	-6.52	93.40	111.00
1	B	81	LEU	N-CA-C	6.48	128.49	111.00
1	B	183	TRP	N-CA-CB	6.45	122.20	110.60
1	A	85	ALA	C-N-CA	6.44	135.83	122.30
1	B	17	HIS	C-N-CA	6.41	137.72	121.70
1	B	101	PHE	N-CA-C	-6.38	93.77	111.00
1	A	46	PRO	CA-N-CD	-6.31	102.67	111.50
1	B	67	ASN	CB-CA-C	6.29	122.97	110.40
1	B	7	LEU	CA-CB-CG	6.28	129.75	115.30
1	B	181	VAL	O-C-N	6.27	132.73	122.70
1	B	16	PRO	N-CA-C	6.22	128.26	112.10
1	B	32	ASN	N-CA-CB	6.18	121.73	110.60
1	B	84	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	129	ALA	N-CA-C	-6.14	94.41	111.00
1	B	85	ALA	CB-CA-C	-6.11	100.94	110.10
1	B	113	LYS	N-CA-CB	6.07	121.53	110.60
1	A	44	GLY	C-N-CA	6.04	136.79	121.70
1	B	159	GLU	CG-CD-OE1	6.01	130.33	118.30
1	A	21	GLU	CA-CB-CG	5.99	126.58	113.40
1	B	49	GLU	OE1-CD-OE2	5.98	130.47	123.30
1	B	131	GLY	N-CA-C	-5.97	98.17	113.10
1	A	172	LYS	CB-CG-CD	5.96	127.09	111.60
1	B	117	GLY	N-CA-C	5.94	127.94	113.10
1	B	47	GLU	N-CA-C	5.92	127.00	111.00
1	A	162	TYR	CB-CG-CD1	5.86	124.51	121.00
1	A	16	PRO	N-CA-C	5.85	127.31	112.10
1	B	85	ALA	N-CA-C	5.80	126.66	111.00
1	A	98	ASN	CB-CA-C	5.79	121.99	110.40
1	A	149	ASP	CB-CA-C	5.79	121.99	110.40
1	A	85	ALA	N-CA-C	5.74	126.50	111.00
1	B	31	HIS	N-CA-CB	-5.73	100.29	110.60
1	A	116	VAL	CA-CB-CG2	5.65	119.38	110.90
1	B	84	ASP	CA-CB-CG	5.63	125.78	113.40
1	A	29	LYS	N-CA-C	-5.62	95.83	111.00
1	A	178	TRP	CA-C-N	-5.59	104.90	117.20
1	A	136	CYS	CB-CA-C	5.58	121.56	110.40
1	B	17	HIS	CA-C-O	5.58	131.81	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	TYR	CA-CB-CG	5.54	123.92	113.40
1	A	15	GLN	CA-CB-CG	5.51	125.53	113.40
1	A	186	VAL	CA-CB-CG1	5.50	119.15	110.90
1	A	102	GLY	N-CA-C	-5.50	99.36	113.10
1	A	130	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	132	SER	N-CA-C	5.49	125.81	111.00
1	B	125	TRP	CG-CD2-CE3	-5.48	128.96	133.90
1	B	9	TYR	CD1-CE1-CZ	-5.48	114.86	119.80
1	B	165	ASP	C-N-CA	5.45	135.33	121.70
1	A	77	TYR	CA-CB-CG	5.44	123.74	113.40
1	A	178	TRP	N-CA-C	-5.44	96.32	111.00
1	B	38	LEU	N-CA-C	5.42	125.62	111.00
1	A	49	GLU	N-CA-C	-5.42	96.38	111.00
1	B	18	ILE	N-CA-C	-5.40	96.42	111.00
1	B	170	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	185	PHE	CB-CA-C	5.37	121.14	110.40
1	A	54	GLU	CA-C-O	5.37	131.37	120.10
1	A	163	TYR	CG-CD1-CE1	5.36	125.58	121.30
1	B	89	PRO	N-CA-CB	-5.35	96.72	102.60
1	B	158	TRP	N-CA-C	-5.32	96.64	111.00
1	B	15	GLN	CB-CA-C	5.32	121.03	110.40
1	A	24	GLU	N-CA-CB	5.26	120.06	110.60
1	A	111	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	B	49	GLU	CA-CB-CG	5.24	124.93	113.40
1	A	167	ARG	N-CA-CB	5.24	120.03	110.60
1	A	156	ASP	N-CA-CB	5.23	120.02	110.60
1	A	65	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	A	186	VAL	CB-CA-C	5.21	121.30	111.40
1	A	185	PHE	N-CA-CB	5.21	119.97	110.60
1	B	125	TRP	CG-CD1-NE1	5.18	115.28	110.10
1	B	114	THR	N-CA-C	-5.17	97.03	111.00
1	A	60	SER	N-CA-C	5.17	124.96	111.00
1	B	175	GLU	CG-CD-OE1	5.17	128.63	118.30
1	B	160	HIS	CG-ND1-CE1	-5.11	99.06	105.70
1	A	154	THR	CA-CB-OG1	-5.08	98.32	109.00
1	B	179	ASN	N-CA-CB	5.08	119.75	110.60
1	A	170	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	186	VAL	N-CA-C	-5.05	97.36	111.00
1	B	132	SER	N-CA-C	5.05	124.64	111.00
1	B	89	PRO	CB-CA-C	5.05	124.61	112.00
1	A	49	GLU	N-CA-CB	5.04	119.68	110.60
1	B	80	CYS	CB-CA-C	-5.04	100.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	TRP	CA-C-N	-5.03	106.14	117.20
1	A	74	HIS	CA-CB-CG	-5.03	105.06	113.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	THR	Mainchain,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	1454	0	1355	262	1
1	B	1454	0	1355	263	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	102	0	0	23	9
3	B	78	0	0	7	9
All	All	3090	0	2710	503	10

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 90.

All (503) 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:B:83:PRO:N	1:B:83:PRO:CD	1.76	1.44
1:A:133:LEU:HD11	3:A:658:HOH:O	1.25	1.32
1:A:92:ALA:HB2	3:A:646:HOH:O	1.40	1.19
1:A:156:ASP:OD1	1:A:157:VAL:N	1.79	1.15
1:A:33:THR:CG2	3:A:605:HOH:O	1.93	1.13
1:A:184:ALA:CB	3:A:683:HOH:O	1.97	1.12
1:B:16:PRO:HD2	1:B:83:PRO:HB3	1.31	1.12
1:A:46:PRO:HG3	1:A:65:PHE:HZ	1.09	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLY:HA3	1:A:66:ASN:HB2	1.14	1.10
1:B:5:PRO:N	1:B:6:PRO:HD3	1.64	1.09
1:B:82:SER:C	1:B:83:PRO:CD	2.20	1.09
1:A:7:LEU:N	1:A:8:PRO:HD3	1.57	1.08
1:A:15:GLN:HB3	1:A:16:PRO:HD3	1.12	1.07
1:A:46:PRO:HG3	1:A:65:PHE:CZ	1.92	1.04
1:A:92:ALA:CB	3:A:646:HOH:O	1.96	1.04
1:A:7:LEU:H	1:A:8:PRO:HD3	0.87	1.03
1:A:14:LEU:H	1:A:23:LEU:HD12	1.24	1.02
1:A:42:VAL:H	1:A:43:PRO:HD2	1.25	1.01
1:B:183:TRP:HE3	1:B:186:VAL:HG21	1.23	1.01
1:B:42:VAL:HB	1:B:43:PRO:HD3	1.42	1.01
1:B:170:ARG:O	1:B:172:LYS:N	1.92	1.01
1:A:143:ALA:HB1	3:A:632:HOH:O	1.58	1.00
1:A:184:ALA:HB1	3:A:683:HOH:O	1.58	0.97
1:A:114:THR:HG22	1:A:136:CYS:HB3	1.42	0.97
1:A:33:THR:HG21	3:A:605:HOH:O	1.55	0.97
1:A:7:LEU:H	1:A:8:PRO:CD	1.78	0.96
1:B:72:TRP:HZ3	1:B:143:ALA:HB1	1.27	0.95
1:B:183:TRP:CE3	1:B:186:VAL:HG21	2.00	0.95
1:A:14:LEU:HB3	1:A:18:ILE:O	1.66	0.95
1:B:93:LEU:HD12	1:B:187:ALA:HA	1.45	0.95
1:A:159:GLU:OE1	1:B:160:HIS:HB3	1.66	0.94
1:B:166:TYR:HA	1:B:169:LEU:HD21	1.47	0.94
1:A:118:THR:HG23	1:A:157:VAL:HG11	1.52	0.92
1:A:180:LEU:HD22	1:A:180:LEU:H	1.31	0.92
1:B:58:LYS:HD2	1:B:145:LEU:O	1.68	0.92
1:A:62:GLY:CA	1:A:66:ASN:HB2	2.00	0.91
1:A:172:LYS:O	1:A:176:ALA:HB3	1.69	0.91
1:A:15:GLN:CB	1:A:16:PRO:HD3	1.96	0.91
1:A:25:TYR:CD1	1:B:167:ARG:HG3	2.05	0.91
1:A:156:ASP:OD1	1:A:156:ASP:C	2.02	0.89
1:B:34:TYR:CZ	1:B:70:GLN:NE2	2.40	0.89
1:B:125:TRP:CE3	1:B:154:THR:HG23	2.08	0.89
1:A:56:ILE:O	1:A:57:VAL:HG23	1.73	0.88
1:A:115:SER:O	1:A:157:VAL:HG21	1.74	0.88
1:A:9:TYR:OH	1:A:23:LEU:HD13	1.74	0.88
1:B:38:LEU:O	1:B:43:PRO:HD2	1.72	0.88
1:B:116:VAL:HG22	1:B:173:TYR:CE2	2.08	0.88
1:B:182:ASN:O	1:B:186:VAL:HG13	1.74	0.88
1:A:7:LEU:N	1:A:8:PRO:CD	2.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:O	1:A:98:ASN:ND2	2.06	0.87
1:A:53:LEU:HD13	1:A:72:TRP:CZ3	2.09	0.87
1:B:37:ASN:HD22	1:B:37:ASN:H	1.21	0.87
1:A:70:GLN:HG3	1:B:119:PHE:HZ	1.39	0.86
1:A:42:VAL:N	1:A:43:PRO:HD2	1.90	0.86
1:B:41:LEU:HA	1:B:46:PRO:HD2	1.56	0.86
1:A:76:PHE:HD2	1:A:154:THR:HG1	1.25	0.85
1:A:178:TRP:CE3	1:A:180:LEU:HD21	2.11	0.85
1:B:71:VAL:O	1:B:75:THR:HG23	1.77	0.85
1:A:91:GLY:HA2	1:A:94:ALA:HB3	1.59	0.84
1:A:15:GLN:HB3	1:A:16:PRO:CD	2.03	0.84
1:B:166:TYR:HA	1:B:169:LEU:CD2	2.08	0.84
1:B:72:TRP:CZ3	1:B:143:ALA:HB1	2.13	0.84
1:A:123:TRP:NE1	1:A:155:CYS:O	2.12	0.83
1:B:111:PHE:O	1:B:112:THR:HG23	1.77	0.83
1:B:170:ARG:C	1:B:172:LYS:H	1.79	0.83
1:A:114:THR:CG2	1:A:136:CYS:HB3	2.08	0.83
1:A:42:VAL:HA	1:A:49:GLU:HG2	1.61	0.83
1:A:106:LYS:HD2	1:A:106:LYS:N	1.95	0.82
1:B:81:LEU:O	1:B:181:VAL:N	2.09	0.82
1:A:28:ASP:HA	1:A:31:HIS:HB2	1.61	0.82
1:A:76:PHE:CZ	1:A:152:LEU:HB2	2.14	0.81
1:B:57:VAL:O	1:B:58:LYS:HB2	1.80	0.81
1:A:171:PRO:O	1:A:175:GLU:HB3	1.80	0.80
1:A:151:PRO:HD2	1:A:152:LEU:HD23	1.61	0.80
1:A:93:LEU:HD23	1:A:187:ALA:HA	1.61	0.80
1:A:64:ILE:O	1:A:67:ASN:HB2	1.82	0.80
1:A:78:TRP:CD1	1:A:79:ASN:N	2.50	0.80
1:A:127:VAL:HA	1:A:151:PRO:HG2	1.63	0.80
1:B:62:GLY:O	1:B:64:ILE:N	2.14	0.80
1:A:159:GLU:CD	1:B:160:HIS:HB3	2.02	0.79
1:B:14:LEU:O	1:B:15:GLN:O	2.01	0.79
1:B:126:LEU:HB3	1:B:152:LEU:HB2	1.65	0.79
1:A:165:ASP:O	1:A:168:ASN:HB2	1.83	0.78
1:A:62:GLY:HA3	1:A:66:ASN:CB	2.07	0.78
1:B:5:PRO:N	1:B:6:PRO:CD	2.45	0.78
3:A:724:HOH:O	1:B:64:ILE:HD11	1.83	0.77
1:A:41:LEU:O	1:A:46:PRO:HD2	1.84	0.77
1:A:67:ASN:O	1:A:71:VAL:HG23	1.84	0.77
1:B:129:ALA:O	1:B:130:ASP:HB2	1.85	0.77
1:A:53:LEU:HD12	1:A:54:GLU:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:CD2	1:A:180:LEU:H	1.98	0.76
1:B:26:HIS:CE1	1:B:161:ALA:HA	2.20	0.76
1:B:73:ASN:OD1	1:B:125:TRP:HH2	1.69	0.76
1:B:16:PRO:CD	1:B:83:PRO:HB3	2.14	0.76
1:A:159:GLU:OE1	1:B:160:HIS:CB	2.33	0.75
1:A:112:THR:HA	1:A:173:TYR:HE1	1.51	0.75
1:A:88:GLN:O	1:A:88:GLN:HG2	1.85	0.75
1:B:123:TRP:HZ3	1:B:140:GLY:HA2	1.52	0.75
1:A:14:LEU:CB	1:A:18:ILE:O	2.33	0.75
1:A:168:ASN:O	1:A:171:PRO:HD2	1.85	0.75
1:B:166:TYR:O	1:B:169:LEU:HD11	1.87	0.74
1:B:5:PRO:HG3	1:B:38:LEU:HD11	1.70	0.74
1:A:13:ALA:HB3	1:A:20:LYS:HZ2	1.52	0.74
1:B:53:LEU:O	1:B:56:ILE:HG22	1.87	0.74
1:B:85:ALA:HB3	1:B:179:ASN:OD1	1.86	0.74
1:A:187:ALA:HB1	3:A:687:HOH:O	1.88	0.74
1:A:28:ASP:OD2	1:A:32:ASN:ND2	2.22	0.72
1:B:85:ALA:CA	1:B:181:VAL:HB	2.19	0.72
1:B:72:TRP:HZ3	1:B:143:ALA:CB	2.03	0.71
1:A:78:TRP:HD1	1:A:79:ASN:H	1.38	0.71
1:B:37:ASN:HD22	1:B:37:ASN:N	1.86	0.71
1:A:180:LEU:N	1:A:180:LEU:HD22	2.03	0.71
1:B:56:ILE:HG23	1:B:57:VAL:N	2.06	0.71
1:A:53:LEU:CD1	1:A:54:GLU:H	2.02	0.71
1:B:161:ALA:O	3:B:768:HOH:O	2.08	0.71
1:B:85:ALA:HA	1:B:181:VAL:HB	1.73	0.71
1:B:42:VAL:CB	1:B:43:PRO:HD3	2.16	0.71
1:B:37:ASN:O	1:B:42:VAL:HG23	1.90	0.71
1:A:75:THR:O	1:A:78:TRP:CD1	2.43	0.71
1:B:56:ILE:HG12	1:B:68:ALA:HB3	1.71	0.71
1:A:14:LEU:N	1:A:23:LEU:HD12	2.01	0.71
1:B:162:TYR:HB3	1:B:172:LYS:HD3	1.73	0.70
1:B:88:GLN:HB3	1:B:89:PRO:CD	2.21	0.70
1:B:61:SER:HB2	1:B:65:PHE:CB	2.21	0.70
1:B:182:ASN:HB3	1:B:185:PHE:HB3	1.73	0.70
1:A:14:LEU:O	1:A:15:GLN:HB2	1.90	0.70
1:B:174:VAL:HG12	1:B:175:GLU:H	1.57	0.70
1:A:15:GLN:OE1	1:A:16:PRO:HG3	1.92	0.70
1:A:86:GLY:O	1:A:88:GLN:N	2.25	0.70
1:A:114:THR:HG22	1:A:136:CYS:CB	2.19	0.69
1:B:57:VAL:HG23	1:B:58:LYS:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:CD2	1:A:187:ALA:HA	2.21	0.69
1:B:9:TYR:OH	1:B:23:LEU:HD12	1.92	0.69
1:A:80:CYS:HA	1:A:181:VAL:CG1	2.22	0.69
1:A:112:THR:HG23	1:A:113:LYS:H	1.58	0.69
1:B:56:ILE:CG2	1:B:57:VAL:N	2.56	0.69
1:A:29:LYS:O	1:A:33:THR:HB	1.93	0.69
1:B:36:VAL:HG12	1:B:67:ASN:HD21	1.57	0.68
1:A:32:ASN:N	1:A:32:ASN:HD22	1.92	0.68
1:B:11:HIS:CE1	1:B:83:PRO:HD3	2.29	0.68
1:B:37:ASN:H	1:B:37:ASN:ND2	1.92	0.68
1:A:115:SER:OG	1:A:124:ALA:CB	2.42	0.67
1:A:62:GLY:HA2	1:A:66:ASN:N	2.09	0.67
1:A:126:LEU:O	1:A:152:LEU:HA	1.93	0.67
1:A:171:PRO:HA	1:A:175:GLU:HB2	1.76	0.67
1:A:127:VAL:HA	1:A:151:PRO:CG	2.25	0.67
1:B:61:SER:HG	1:B:65:PHE:HD2	1.40	0.67
1:A:53:LEU:HD13	1:A:72:TRP:CH2	2.29	0.66
1:A:53:LEU:HD12	1:A:54:GLU:N	2.09	0.66
1:A:70:GLN:HG3	1:B:119:PHE:CZ	2.27	0.66
1:A:132:SER:O	1:A:133:LEU:HB2	1.93	0.66
1:B:143:ALA:O	1:B:146:THR:HG23	1.95	0.66
1:B:144:PRO:HG2	1:B:151:PRO:HD3	1.76	0.66
1:A:76:PHE:HD2	1:A:154:THR:OG1	1.79	0.66
1:B:61:SER:HB2	1:B:65:PHE:HB2	1.78	0.66
1:A:77:TYR:HB2	1:A:154:THR:HG21	1.78	0.65
1:A:79:ASN:O	1:A:181:VAL:HB	1.95	0.65
1:B:114:THR:HB	1:B:124:ALA:HB1	1.79	0.65
1:A:28:ASP:HB3	1:B:167:ARG:CZ	2.27	0.65
1:A:18:ILE:HG23	1:A:22:THR:HG21	1.79	0.65
1:A:115:SER:OG	1:A:124:ALA:HB3	1.97	0.65
1:B:51:LYS:HE3	1:B:56:ILE:CD1	2.27	0.65
1:A:30:HIS:O	1:A:34:TYR:HB2	1.97	0.65
1:A:46:PRO:HG2	1:A:48:PHE:HD2	1.62	0.65
1:B:34:TYR:OH	1:B:70:GLN:NE2	2.30	0.65
1:B:52:THR:C	1:B:54:GLU:H	2.00	0.65
1:A:40:ASN:ND2	1:A:40:ASN:O	2.30	0.65
1:A:154:THR:O	1:A:155:CYS:HB3	1.98	0.64
1:A:128:LYS:HG2	1:A:151:PRO:HG3	1.78	0.64
1:A:142:GLY:O	1:A:143:ALA:HB3	1.97	0.64
1:A:62:GLY:HA2	1:A:66:ASN:H	1.62	0.64
1:B:33:THR:O	1:B:34:TYR:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:HE1	1:A:59:SER:HB3	1.61	0.63
1:A:171:PRO:O	1:A:175:GLU:CB	2.46	0.63
1:A:53:LEU:HD13	1:A:72:TRP:HZ3	1.56	0.63
1:A:80:CYS:HA	1:A:181:VAL:HG12	1.80	0.63
1:B:66:ASN:ND2	1:B:141:ALA:HA	2.14	0.63
1:A:162:TYR:CE1	1:A:169:LEU:HD13	2.34	0.63
1:B:56:ILE:CG2	1:B:57:VAL:H	2.12	0.63
1:A:25:TYR:HD1	1:B:167:ARG:HG3	1.60	0.63
1:A:14:LEU:H	1:A:23:LEU:CD1	2.07	0.62
1:B:118:THR:OG1	1:B:138:THR:HG21	1.99	0.62
1:A:167:ARG:HB3	1:B:29:LYS:CE	2.29	0.62
1:B:174:VAL:HG12	1:B:175:GLU:N	2.15	0.62
1:B:34:TYR:CE1	1:B:70:GLN:NE2	2.68	0.62
1:A:109:GLU:C	1:A:112:THR:HG22	2.20	0.62
1:A:109:GLU:O	1:A:112:THR:HG22	2.00	0.62
1:A:63:GLY:HA2	3:A:625:HOH:O	2.00	0.62
1:A:25:TYR:CD1	1:B:167:ARG:CG	2.80	0.62
1:B:98:ASN:ND2	1:B:103:SER:HA	2.15	0.61
1:A:32:ASN:H	1:A:32:ASN:HD22	1.47	0.61
1:B:81:LEU:O	1:B:181:VAL:HG12	2.00	0.61
1:B:167:ARG:O	1:B:168:ASN:HB2	1.98	0.61
1:A:70:GLN:NE2	1:A:74:HIS:CE1	2.69	0.61
1:B:34:TYR:CD2	1:B:70:GLN:HB3	2.35	0.61
1:B:73:ASN:OD1	1:B:125:TRP:CH2	2.53	0.61
1:A:50:GLY:O	1:A:51:LYS:HB2	2.01	0.61
1:B:53:LEU:CD1	3:B:717:HOH:O	2.49	0.61
1:A:177:PHE:O	1:A:177:PHE:CG	2.54	0.60
1:A:45:THR:C	1:A:46:PRO:O	2.39	0.60
1:A:128:LYS:HE3	1:A:151:PRO:HB3	1.83	0.60
1:A:42:VAL:N	1:A:43:PRO:CD	2.62	0.60
1:A:14:LEU:HD23	1:A:16:PRO:HD2	1.82	0.60
1:B:140:GLY:CA	1:B:158:TRP:HZ3	2.14	0.60
1:B:10:ALA:O	1:B:11:HIS:HB3	2.00	0.60
1:B:129:ALA:HB2	1:B:149:ASP:OD2	2.01	0.60
1:A:116:VAL:HB	1:A:173:TYR:OH	2.01	0.60
1:A:19:SER:OG	1:A:164:ILE:CD1	2.49	0.60
1:A:128:LYS:N	1:A:151:PRO:HG3	2.16	0.60
1:A:128:LYS:NZ	1:A:190:GLY:O	2.25	0.60
1:B:7:LEU:O	1:B:8:PRO:O	2.19	0.60
1:B:140:GLY:HA2	1:B:158:TRP:HZ3	1.66	0.60
1:A:25:TYR:HD1	1:B:167:ARG:CG	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASN:HA	1:B:70:GLN:HG3	1.82	0.59
1:B:9:TYR:OH	1:B:23:LEU:CD1	2.50	0.59
1:B:30:HIS:O	1:B:34:TYR:HB2	2.02	0.59
1:B:121:SER:HB3	1:B:158:TRP:CD2	2.37	0.59
1:B:12:ASP:HB3	1:B:15:GLN:HB3	1.84	0.59
1:B:28:ASP:O	1:B:32:ASN:OD1	2.20	0.59
1:A:123:TRP:CD1	1:A:155:CYS:SG	2.96	0.59
1:A:118:THR:CG2	1:A:157:VAL:HG11	2.31	0.59
1:B:14:LEU:O	1:B:15:GLN:C	2.42	0.59
1:B:61:SER:HB2	1:B:65:PHE:HB3	1.84	0.58
1:B:128:LYS:NZ	1:B:189:GLU:OE1	2.35	0.58
1:A:70:GLN:HE22	1:A:123:TRP:HH2	1.50	0.58
1:A:167:ARG:HB3	1:B:29:LYS:HE2	1.84	0.58
1:B:141:ALA:O	3:B:763:HOH:O	2.17	0.58
1:B:98:ASN:O	1:B:99:ALA:HB2	2.03	0.58
1:B:172:LYS:O	1:B:176:ALA:HB3	2.03	0.58
1:B:72:TRP:CZ2	1:B:145:LEU:HD12	2.38	0.58
1:B:170:ARG:HB2	1:B:171:PRO:HD3	1.85	0.58
1:B:67:ASN:O	1:B:70:GLN:HB2	2.04	0.57
1:B:5:PRO:CG	1:B:38:LEU:HD11	2.33	0.57
1:B:10:ALA:O	1:B:11:HIS:CB	2.52	0.57
1:A:127:VAL:CA	1:A:151:PRO:HG2	2.33	0.57
1:A:164:ILE:O	1:A:165:ASP:HB2	2.03	0.57
1:A:178:TRP:HA	1:A:180:LEU:CD2	2.35	0.57
1:B:72:TRP:CH2	1:B:145:LEU:HD12	2.40	0.57
1:B:45:THR:HB	1:B:46:PRO:HD3	1.87	0.57
1:A:142:GLY:O	1:A:143:ALA:CB	2.53	0.57
1:B:140:GLY:C	1:B:142:GLY:H	2.08	0.57
1:B:78:TRP:HA	1:B:78:TRP:CE3	2.40	0.57
1:A:101:PHE:HB3	1:A:107:PHE:HA	1.87	0.56
1:B:112:THR:C	1:B:114:THR:H	2.06	0.56
1:A:62:GLY:CA	1:A:66:ASN:H	2.18	0.56
1:A:73:ASN:HB3	1:A:123:TRP:CZ2	2.41	0.56
1:A:144:PRO:O	1:A:147:SER:OG	2.22	0.56
1:B:53:LEU:HD12	3:B:717:HOH:O	2.05	0.56
1:B:170:ARG:NH1	1:B:170:ARG:HB2	2.21	0.56
1:B:22:THR:O	1:B:25:TYR:HD1	1.88	0.56
1:A:112:THR:HA	1:A:173:TYR:CE1	2.38	0.56
1:A:14:LEU:HD22	1:A:18:ILE:H	1.71	0.56
1:A:159:GLU:OE1	1:B:160:HIS:N	2.39	0.56
1:A:182:ASN:HB2	3:A:636:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TRP:CE3	1:B:154:THR:CG2	2.87	0.56
1:A:77:TYR:O	1:A:80:CYS:HB2	2.06	0.55
1:B:66:ASN:HD22	1:B:141:ALA:HA	1.72	0.55
1:B:82:SER:HA	1:B:85:ALA:HB2	1.86	0.55
1:A:92:ALA:HB3	3:A:646:HOH:O	1.84	0.55
1:A:30:HIS:HA	1:A:34:TYR:CD2	2.42	0.55
1:B:82:SER:C	1:B:83:PRO:HD3	2.22	0.55
1:B:39:ASN:H	1:B:39:ASN:ND2	2.05	0.55
1:B:112:THR:C	1:B:114:THR:N	2.60	0.55
1:B:183:TRP:HE3	1:B:186:VAL:CG2	2.09	0.54
1:A:168:ASN:C	1:A:171:PRO:HD2	2.27	0.54
1:B:34:TYR:C	1:B:36:VAL:H	2.10	0.54
1:A:19:SER:OG	1:A:164:ILE:HD12	2.08	0.54
1:A:54:GLU:HB2	1:A:72:TRP:CE3	2.42	0.54
1:B:34:TYR:C	1:B:36:VAL:N	2.61	0.54
1:B:41:LEU:HD23	1:B:65:PHE:CD1	2.43	0.54
1:B:160:HIS:C	1:B:160:HIS:CD2	2.81	0.54
1:B:98:ASN:O	1:B:99:ALA:CB	2.56	0.54
1:A:157:VAL:O	1:A:157:VAL:CG1	2.56	0.54
1:A:98:ASN:N	1:A:98:ASN:HD22	2.04	0.54
1:A:153:LEU:HD21	1:A:180:LEU:HD12	1.90	0.54
1:B:183:TRP:HA	1:B:186:VAL:HG22	1.89	0.54
1:A:70:GLN:NE2	1:A:74:HIS:HE1	2.04	0.54
1:B:7:LEU:N	1:B:8:PRO:HD3	2.23	0.54
1:A:185:PHE:HE1	1:A:189:GLU:H	1.55	0.54
1:A:141:ALA:HB2	1:B:119:PHE:CE2	2.44	0.53
1:A:46:PRO:CG	1:A:48:PHE:HD2	2.22	0.53
1:B:122:GLY:HA3	1:B:138:THR:HA	1.90	0.53
1:A:167:ARG:HD2	3:A:705:HOH:O	2.08	0.53
1:A:13:ALA:HB3	1:A:20:LYS:HG2	1.90	0.53
1:B:40:ASN:O	1:B:41:LEU:HD12	2.08	0.53
1:A:178:TRP:HA	1:A:180:LEU:HD21	1.91	0.53
1:B:181:VAL:HG22	1:B:182:ASN:H	1.73	0.53
1:B:88:GLN:HB3	1:B:89:PRO:HD2	1.91	0.53
1:B:88:GLN:HG2	1:B:94:ALA:HA	1.91	0.52
1:B:170:ARG:C	1:B:172:LYS:N	2.48	0.52
1:B:34:TYR:HE2	1:B:74:HIS:CE1	2.27	0.52
1:B:74:HIS:CE1	1:B:123:TRP:HZ2	2.28	0.52
1:B:85:ALA:HA	1:B:181:VAL:CB	2.38	0.52
1:B:61:SER:OG	1:B:65:PHE:HD2	1.93	0.52
1:A:105:ASP:HB3	1:A:106:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:H	1:A:66:ASN:HB2	1.74	0.52
1:A:76:PHE:CD2	1:A:154:THR:OG1	2.56	0.52
1:B:104:PHE:O	1:B:108:LYS:HG3	2.10	0.52
1:B:125:TRP:CE3	1:B:151:PRO:HB3	2.44	0.52
1:B:35:VAL:HA	1:B:37:ASN:ND2	2.25	0.52
1:B:82:SER:HB3	1:B:179:ASN:OD1	2.10	0.52
1:A:115:SER:HB2	1:A:173:TYR:CE1	2.45	0.52
1:B:166:TYR:O	1:B:169:LEU:CD1	2.56	0.52
1:B:18:ILE:CG2	1:B:23:LEU:HD21	2.39	0.52
1:B:145:LEU:CD2	1:B:150:THR:HG22	2.40	0.51
1:B:85:ALA:HB3	1:B:179:ASN:CG	2.30	0.51
1:A:76:PHE:O	1:A:79:ASN:ND2	2.44	0.51
1:A:112:THR:HG23	1:A:113:LYS:N	2.23	0.51
1:B:51:LYS:NZ	1:B:56:ILE:HD12	2.26	0.51
1:B:51:LYS:HE3	1:B:56:ILE:HD13	1.93	0.50
1:A:115:SER:O	1:A:118:THR:HG22	2.11	0.50
1:A:30:HIS:HA	1:A:34:TYR:HD2	1.76	0.50
1:A:172:LYS:HD2	1:A:172:LYS:O	2.10	0.50
1:B:104:PHE:HA	1:B:107:PHE:HB3	1.93	0.50
1:A:183:TRP:O	1:A:187:ALA:HB2	2.12	0.50
1:B:126:LEU:HD13	1:B:152:LEU:HD12	1.92	0.50
1:A:15:GLN:CB	1:A:16:PRO:CD	2.77	0.50
1:A:19:SER:OG	1:A:164:ILE:HD11	2.11	0.50
1:B:127:VAL:HG21	1:B:144:PRO:HG3	1.93	0.50
1:B:37:ASN:ND2	1:B:37:ASN:N	2.57	0.50
1:A:46:PRO:HB2	1:A:48:PHE:CD2	2.47	0.50
1:A:52:THR:O	1:A:55:GLU:HB2	2.12	0.50
1:B:103:SER:HB2	1:B:106:LYS:HB2	1.93	0.50
1:A:173:TYR:HA	1:A:177:PHE:HB3	1.94	0.49
1:A:167:ARG:HB3	1:B:29:LYS:HE3	1.93	0.49
1:A:25:TYR:CE1	1:B:167:ARG:HB2	2.47	0.49
1:B:12:ASP:O	1:B:13:ALA:HB2	2.11	0.49
1:A:23:LEU:O	1:A:27:HIS:HB3	2.12	0.49
1:B:37:ASN:HA	1:B:41:LEU:HD22	1.94	0.49
1:B:53:LEU:HD21	1:B:71:VAL:CG1	2.42	0.49
1:B:97:ILE:HA	1:B:101:PHE:CD2	2.47	0.49
1:B:22:THR:HA	1:B:25:TYR:CD1	2.48	0.49
1:A:101:PHE:O	1:A:103:SER:O	2.30	0.49
1:A:166:TYR:C	1:A:168:ASN:H	2.16	0.49
1:A:27:HIS:HD2	3:A:611:HOH:O	1.95	0.49
1:B:32:ASN:OD1	1:B:33:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ALA:HA	1:A:144:PRO:HD3	1.71	0.49
1:A:77:TYR:CE1	1:A:81:LEU:HD11	2.48	0.49
1:A:98:ASN:O	1:A:99:ALA:HB2	2.13	0.48
1:B:145:LEU:HD21	1:B:150:THR:HG22	1.93	0.48
1:A:51:LYS:HB3	1:A:55:GLU:HB3	1.96	0.48
1:B:36:VAL:CG1	1:B:67:ASN:HD21	2.24	0.48
1:B:118:THR:HB	1:B:138:THR:HB	1.94	0.48
1:B:150:THR:HA	1:B:151:PRO:HD2	1.60	0.48
1:B:41:LEU:O	1:B:46:PRO:O	2.32	0.48
1:A:159:GLU:OE1	1:B:160:HIS:CA	2.60	0.48
1:A:63:GLY:CA	3:A:625:HOH:O	2.60	0.48
1:A:151:PRO:CG	1:A:152:LEU:H	2.27	0.48
1:B:137:SER:O	1:B:137:SER:OG	2.24	0.48
1:B:82:SER:OG	1:B:179:ASN:O	2.30	0.48
1:A:36:VAL:CG1	1:A:64:ILE:HG23	2.44	0.48
1:A:62:GLY:C	1:A:66:ASN:H	2.17	0.48
1:B:41:LEU:CA	1:B:46:PRO:HD2	2.38	0.48
1:B:89:PRO:O	1:B:94:ALA:HB2	2.14	0.48
1:B:91:GLY:O	1:B:94:ALA:HB3	2.13	0.48
1:A:182:ASN:O	1:A:184:ALA:N	2.44	0.48
1:A:78:TRP:CD1	1:A:79:ASN:HB3	2.49	0.47
1:B:33:THR:O	1:B:35:VAL:N	2.46	0.47
1:B:174:VAL:CG1	1:B:175:GLU:N	2.77	0.47
1:B:114:THR:O	1:B:118:THR:HG23	2.14	0.47
1:B:15:GLN:OE1	1:B:18:ILE:HB	2.14	0.47
1:A:183:TRP:CE3	1:A:186:VAL:HG11	2.49	0.47
1:B:125:TRP:HA	1:B:153:LEU:O	2.15	0.47
1:B:22:THR:O	1:B:26:HIS:CB	2.63	0.47
1:A:44:GLY:O	1:A:45:THR:HG23	2.14	0.47
1:B:39:ASN:HD22	1:B:39:ASN:H	1.62	0.47
1:A:150:THR:O	1:A:150:THR:OG1	2.28	0.47
1:A:162:TYR:HB3	1:A:172:LYS:HG3	1.97	0.47
1:A:25:TYR:CE1	1:B:167:ARG:N	2.83	0.47
1:A:28:ASP:HB3	1:B:167:ARG:NH1	2.30	0.47
1:B:22:THR:O	1:B:26:HIS:HB2	2.15	0.47
1:A:93:LEU:HD23	3:A:687:HOH:O	2.14	0.47
1:A:127:VAL:HA	1:A:151:PRO:CD	2.44	0.47
1:B:34:TYR:O	1:B:36:VAL:N	2.38	0.47
1:B:57:VAL:C	1:B:58:LYS:HD3	2.36	0.46
1:B:34:TYR:CE2	1:B:70:GLN:HB3	2.50	0.46
1:A:163:TYR:O	1:A:163:TYR:CD1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:HB2	3:A:679:HOH:O	2.14	0.46
1:B:72:TRP:CH2	1:B:151:PRO:HG3	2.50	0.46
1:B:92:ALA:O	1:B:96:ALA:N	2.48	0.46
1:A:184:ALA:HB2	3:A:683:HOH:O	1.88	0.46
1:B:132:SER:O	1:B:133:LEU:HD23	2.16	0.46
1:B:123:TRP:CZ3	1:B:140:GLY:HA2	2.41	0.46
1:A:128:LYS:HG2	1:A:151:PRO:CG	2.45	0.46
1:A:149:ASP:N	1:A:149:ASP:OD1	2.48	0.46
1:A:98:ASN:HD22	1:A:98:ASN:H	1.63	0.46
1:B:22:THR:HA	1:B:25:TYR:CE1	2.50	0.46
1:B:36:VAL:C	1:B:38:LEU:H	2.18	0.46
1:B:53:LEU:HD21	1:B:71:VAL:HB	1.97	0.46
1:B:97:ILE:HA	1:B:101:PHE:HD2	1.80	0.46
1:B:118:THR:HG21	1:B:138:THR:OG1	2.15	0.46
1:B:52:THR:O	1:B:53:LEU:HB2	2.15	0.46
1:A:181:VAL:O	1:A:182:ASN:C	2.53	0.46
1:B:35:VAL:HA	1:B:37:ASN:HD21	1.79	0.46
1:B:52:THR:C	1:B:54:GLU:N	2.68	0.46
1:A:107:PHE:CE2	1:A:126:LEU:HD22	2.51	0.46
1:A:21:GLU:O	1:A:25:TYR:HD2	1.99	0.46
1:A:26:HIS:ND1	3:A:634:HOH:O	2.14	0.46
1:B:108:LYS:HB2	1:B:108:LYS:NZ	2.28	0.45
1:B:70:GLN:O	1:B:74:HIS:ND1	2.42	0.45
1:A:150:THR:N	1:A:151:PRO:HD3	2.30	0.45
1:A:169:LEU:O	1:A:172:LYS:HB3	2.16	0.45
1:B:72:TRP:CZ2	1:B:151:PRO:HG3	2.51	0.45
1:A:154:THR:O	1:A:155:CYS:CB	2.63	0.45
1:B:108:LYS:HB2	1:B:108:LYS:HZ3	1.80	0.45
1:B:51:LYS:CE	1:B:56:ILE:HD12	2.47	0.45
1:A:104:PHE:CD1	1:A:104:PHE:C	2.90	0.45
1:A:163:TYR:C	1:A:163:TYR:CD1	2.90	0.45
1:B:48:PHE:O	1:B:50:GLY:N	2.50	0.45
1:A:98:ASN:N	1:A:98:ASN:ND2	2.64	0.45
1:B:133:LEU:HD11	3:B:760:HOH:O	2.16	0.45
1:A:25:TYR:HE1	1:B:167:ARG:HB2	1.81	0.45
1:A:33:THR:HG23	3:A:605:HOH:O	1.84	0.45
1:A:52:THR:O	1:A:53:LEU:C	2.54	0.45
1:B:127:VAL:HG22	1:B:151:PRO:HA	1.98	0.45
1:B:51:LYS:HE3	1:B:56:ILE:HD12	1.98	0.45
1:B:5:PRO:HD2	3:B:717:HOH:O	2.17	0.44
1:B:12:ASP:OD2	1:B:81:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HG22	1:B:57:VAL:H	1.83	0.44
1:A:151:PRO:HD2	1:A:152:LEU:CD2	2.41	0.44
1:B:121:SER:HB3	1:B:158:TRP:CG	2.52	0.44
1:B:185:PHE:C	1:B:185:PHE:CD1	2.91	0.44
1:A:13:ALA:HB1	1:A:23:LEU:HB2	1.99	0.44
1:A:114:THR:HG22	1:A:136:CYS:CA	2.48	0.44
1:B:167:ARG:C	1:B:168:ASN:HD22	2.21	0.44
1:B:78:TRP:HA	1:B:78:TRP:HE3	1.82	0.44
1:A:63:GLY:N	1:A:66:ASN:HB2	2.33	0.44
1:B:77:TYR:O	1:B:80:CYS:HB2	2.18	0.44
1:A:112:THR:CG2	1:A:113:LYS:H	2.28	0.43
1:B:156:ASP:OD1	1:B:158:TRP:HB2	2.18	0.43
1:A:173:TYR:C	1:A:175:GLU:H	2.22	0.43
1:A:9:TYR:HB2	1:A:27:HIS:CE1	2.53	0.43
1:A:46:PRO:C	1:A:48:PHE:H	2.21	0.43
1:B:113:LYS:HE3	1:B:113:LYS:HB3	1.91	0.43
1:A:157:VAL:HG13	1:A:157:VAL:O	2.18	0.43
1:A:127:VAL:CA	1:A:151:PRO:CG	2.93	0.43
1:B:18:ILE:HG21	1:B:23:LEU:HD21	1.99	0.43
1:A:154:THR:HB	1:A:155:CYS:H	1.42	0.43
1:B:170:ARG:HG3	1:B:170:ARG:HH11	1.84	0.43
1:B:93:LEU:CD1	1:B:187:ALA:HA	2.33	0.43
1:B:52:THR:HB	1:B:54:GLU:CD	2.39	0.43
1:B:25:TYR:O	1:B:29:LYS:HG3	2.19	0.43
1:B:39:ASN:N	1:B:39:ASN:ND2	2.67	0.43
1:A:109:GLU:O	1:A:112:THR:CG2	2.64	0.42
1:A:10:ALA:HB3	1:A:11:HIS:CE1	2.54	0.42
1:A:62:GLY:CA	1:A:66:ASN:N	2.80	0.42
1:B:82:SER:CB	1:B:179:ASN:O	2.68	0.42
1:A:70:GLN:HE21	1:A:70:GLN:HA	1.84	0.42
1:B:30:HIS:NE2	1:B:75:THR:HG22	2.34	0.42
1:B:169:LEU:N	1:B:169:LEU:HD12	2.34	0.42
1:B:180:LEU:HD11	1:B:183:TRP:CE2	2.55	0.42
1:B:57:VAL:HG23	1:B:58:LYS:CD	2.45	0.42
1:B:125:TRP:CD2	1:B:154:THR:HG23	2.52	0.42
1:B:170:ARG:CG	1:B:170:ARG:HH11	2.32	0.42
1:B:17:HIS:O	1:B:18:ILE:HG13	2.18	0.42
1:B:152:LEU:HD22	1:B:188:GLU:HB2	2.02	0.42
1:B:83:PRO:HD2	1:B:83:PRO:C	2.37	0.42
1:A:163:TYR:O	1:A:166:TYR:CE1	2.72	0.42
1:B:16:PRO:HB2	1:B:17:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ALA:HB3	1:B:101:PHE:CD2	2.54	0.42
1:B:23:LEU:O	1:B:27:HIS:N	2.50	0.42
1:B:88:GLN:CB	1:B:89:PRO:CD	2.90	0.42
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.84	0.41
1:B:15:GLN:HG2	1:B:23:LEU:HD11	2.02	0.41
1:B:156:ASP:HB3	1:B:161:ALA:HB2	2.02	0.41
1:A:32:ASN:N	1:A:32:ASN:ND2	2.63	0.41
1:A:56:ILE:O	1:A:57:VAL:CG2	2.57	0.41
1:B:18:ILE:CG2	1:B:23:LEU:CD2	2.98	0.41
1:A:115:SER:O	1:A:157:VAL:CG2	2.55	0.41
1:B:163:TYR:C	1:B:165:ASP:H	2.22	0.41
1:B:51:LYS:HD3	1:B:55:GLU:O	2.20	0.41
1:A:106:LYS:H	1:A:106:LYS:HD2	1.79	0.41
1:B:51:LYS:CE	1:B:56:ILE:CD1	2.97	0.41
1:A:120:GLY:O	1:A:121:SER:HB2	2.20	0.41
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.83	0.41
1:A:58:LYS:NZ	3:A:618:HOH:O	2.51	0.41
1:B:160:HIS:CE1	3:B:767:HOH:O	2.73	0.41
1:A:162:TYR:HD2	1:A:164:ILE:O	2.04	0.41
1:A:88:GLN:O	1:A:88:GLN:CG	2.63	0.41
1:A:167:ARG:CD	3:A:705:HOH:O	2.67	0.41
1:A:184:ALA:O	1:A:187:ALA:HB3	2.19	0.41
1:B:167:ARG:O	1:B:168:ASN:CB	2.65	0.41
1:A:14:LEU:HB2	1:A:23:LEU:CD1	2.51	0.41
1:A:170:ARG:N	1:A:171:PRO:CD	2.84	0.41
1:B:37:ASN:O	1:B:41:LEU:HB3	2.21	0.41
1:A:25:TYR:CE1	1:B:167:ARG:CB	3.04	0.41
1:A:46:PRO:CG	1:A:65:PHE:CZ	2.84	0.41
1:A:164:ILE:O	1:A:165:ASP:CB	2.69	0.41
1:A:178:TRP:HE3	1:A:180:LEU:HD21	1.79	0.41
1:A:66:ASN:HD22	1:A:66:ASN:HA	1.81	0.41
1:A:21:GLU:OE1	1:B:166:TYR:CE2	2.74	0.41
1:A:162:TYR:HB2	1:A:164:ILE:O	2.20	0.41
1:A:14:LEU:HB3	1:A:15:GLN:H	1.41	0.40
1:A:70:GLN:HE22	1:A:74:HIS:CE1	2.39	0.40
1:A:15:GLN:OE1	1:A:16:PRO:CG	2.65	0.40
1:A:80:CYS:O	1:A:181:VAL:N	2.54	0.40
1:B:183:TRP:CA	1:B:186:VAL:HG22	2.50	0.40
1:B:34:TYR:CZ	1:B:70:GLN:CD	2.94	0.40
1:A:9:TYR:HH	1:A:23:LEU:HD13	1.79	0.40
1:B:143:ALA:C	1:B:145:LEU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:TYR:HA	1:B:177:PHE:HB3	2.04	0.40
1:A:174:VAL:HG22	1:A:174:VAL:O	2.22	0.40
1:B:170:ARG:N	1:B:171:PRO:HD2	2.37	0.40

All (10) 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)
3:A:651:HOH:O	3:B:706:HOH:O[2_756]	0.29	1.91
3:A:653:HOH:O	3:B:708:HOH:O[2_756]	0.54	1.66
3:A:603:HOH:O	3:B:737:HOH:O[2_846]	0.72	1.48
3:A:623:HOH:O	3:A:677:HOH:O[1_565]	0.92	1.28
3:A:635:HOH:O	3:B:776:HOH:O[1_556]	1.16	1.04
3:A:621:HOH:O	3:B:773:HOH:O[2_856]	1.20	1.00
3:A:668:HOH:O	3:B:709:HOH:O[2_756]	1.56	0.64
3:A:652:HOH:O	3:B:742:HOH:O[2_756]	1.66	0.54
1:A:45:THR:CG2	3:B:702:HOH:O[1_565]	2.06	0.14
3:A:688:HOH:O	3:B:713:HOH:O[2_756]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/195 (94%)	110 (60%)	42 (23%)	32 (17%)	0	0
1	B	184/195 (94%)	105 (57%)	41 (22%)	38 (21%)	0	0
All	All	368/390 (94%)	215 (58%)	83 (23%)	70 (19%)	0	0

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	LEU

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Mol	Chain	Res	Type
1	A	15	GLN
1	A	19	SER
1	A	31	HIS
1	A	43	PRO
1	A	45	THR
1	A	46	PRO
1	A	57	VAL
1	A	90	THR
1	A	99	ALA
1	A	151	PRO
1	A	155	CYS
1	A	166	TYR
1	A	183	TRP
1	B	8	PRO
1	B	10	ALA
1	B	13	ALA
1	B	16	PRO
1	B	18	ILE
1	B	47	GLU
1	B	48	PHE
1	B	49	GLU
1	B	56	ILE
1	B	61	SER
1	B	63	GLY
1	B	82	SER
1	B	83	PRO
1	B	88	GLN
1	B	89	PRO
1	B	99	ALA
1	B	130	ASP
1	B	163	TYR
1	B	164	ILE
1	B	166	TYR
1	B	171	PRO
1	A	62	GLY
1	A	87	GLY
1	A	120	GLY
1	A	138	THR
1	A	140	GLY
1	A	142	GLY
1	A	154	THR
1	B	9	TYR

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Mol	Chain	Res	Type
1	B	11	HIS
1	B	15	GLN
1	B	44	GLY
1	B	58	LYS
1	B	112	THR
1	B	115	SER
1	B	136	CYS
1	A	32	ASN
1	A	51	LYS
1	A	86	GLY
1	A	143	ALA
1	B	168	ASN
1	A	7	LEU
1	A	91	GLY
1	A	133	LEU
1	B	42	VAL
1	B	45	THR
1	B	81	LEU
1	B	176	ALA
1	A	113	LYS
1	A	152	LEU
1	A	177	PHE
1	B	66	ASN
1	A	182	ASN
1	B	86	GLY
1	B	174	VAL
1	B	139	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	151/158 (96%)	101 (67%)	50 (33%)	0	0
1	B	151/158 (96%)	97 (64%)	54 (36%)	0	0
All	All	302/316 (96%)	198 (66%)	104 (34%)	0	0

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	7	LEU
1	A	14	LEU
1	A	21	GLU
1	A	24	GLU
1	A	28	ASP
1	A	29	LYS
1	A	32	ASN
1	A	40	ASN
1	A	41	LEU
1	A	43	PRO
1	A	45	THR
1	A	47	GLU
1	A	52	THR
1	A	55	GLU
1	A	59	SER
1	A	65	PHE
1	A	66	ASN
1	A	70	GLN
1	A	75	THR
1	A	78	TRP
1	A	79	ASN
1	A	81	LEU
1	A	82	SER
1	A	88	GLN
1	A	90	THR
1	A	93	LEU
1	A	98	ASN
1	A	103	SER
1	A	106	LYS
1	A	107	PHE
1	A	113	LYS
1	A	114	THR
1	A	123	TRP
1	A	132	SER
1	A	136	CYS
1	A	145	LEU
1	A	146	THR
1	A	154	THR
1	A	155	CYS
1	A	159	GLU
1	A	163	TYR

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Mol	Chain	Res	Type
1	A	167	ARG
1	A	170	ARG
1	A	172	LYS
1	A	177	PHE
1	A	179	ASN
1	A	180	LEU
1	A	183	TRP
1	A	185	PHE
1	B	7	LEU
1	B	9	TYR
1	B	11	HIS
1	B	12	ASP
1	B	15	GLN
1	B	19	SER
1	B	21	GLU
1	B	23	LEU
1	B	25	TYR
1	B	30	HIS
1	B	31	HIS
1	B	33	THR
1	B	37	ASN
1	B	45	THR
1	B	51	LYS
1	B	52	THR
1	B	53	LEU
1	B	55	GLU
1	B	58	LYS
1	B	65	PHE
1	B	66	ASN
1	B	75	THR
1	B	79	ASN
1	B	80	CYS
1	B	81	LEU
1	B	82	SER
1	B	89	PRO
1	B	90	THR
1	B	93	LEU
1	B	97	ILE
1	B	103	SER
1	B	106	LYS
1	B	109	GLU
1	B	110	GLU

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Mol	Chain	Res	Type
1	B	113	LYS
1	B	114	THR
1	B	126	LEU
1	B	132	SER
1	B	135	LEU
1	B	136	CYS
1	B	137	SER
1	B	139	ILE
1	B	147	SER
1	B	149	ASP
1	B	153	LEU
1	B	154	THR
1	B	164	ILE
1	B	165	ASP
1	B	166	TYR
1	B	167	ARG
1	B	169	LEU
1	B	170	ARG
1	B	173	TYR
1	B	185	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	32	ASN
1	A	39	ASN
1	A	66	ASN
1	A	67	ASN
1	A	70	GLN
1	A	79	ASN
1	A	179	ASN
1	A	182	ASN
1	B	11	HIS
1	B	26	HIS
1	B	37	ASN
1	B	39	ASN
1	B	66	ASN
1	B	67	ASN
1	B	70	GLN
1	B	79	ASN
1	B	88	GLN

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Mol	Chain	Res	Type
1	B	98	ASN
1	B	168	ASN
1	B	182	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.