



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:32 AM UTC

PDB ID : 3SDP / pdb_00003sdp
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

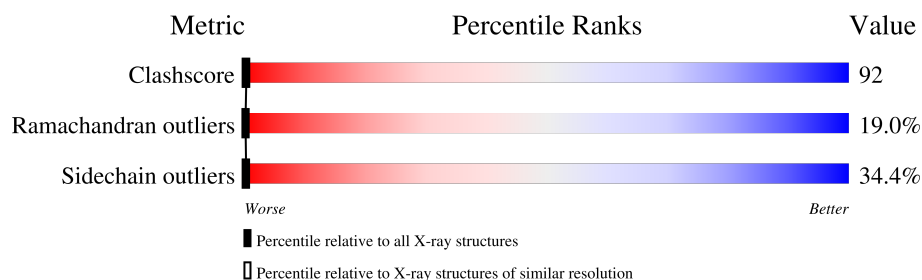
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 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 $\leq 5\%$.

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 (CCD ID: FE) (formula: Fe).

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

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	81.90Å 49.10Å 61.70Å 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	2.32	62/1504 (4.1%)	2.90	152/2058 (7.4%)
1	B	2.28	48/1504 (3.2%)	3.36	169/2058 (8.2%)
All	All	2.30	110/3008 (3.7%)	3.14	321/4116 (7.8%)

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	0	2

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	PRO	N-CD	20.66	1.76	1.47
1	A	45	THR	C-O	19.89	1.49	1.24
1	A	45	THR	CA-C	-9.44	1.41	1.52
1	A	136	CYS	N-CA	9.35	1.57	1.46
1	A	12	ASP	N-CA	8.79	1.56	1.45
1	A	124	ALA	N-CA	8.31	1.56	1.46
1	A	107	PHE	CA-C	8.29	1.63	1.53
1	B	32	ASN	CA-C	8.13	1.60	1.52
1	B	64	ILE	CA-CB	-7.69	1.43	1.54
1	A	136	CYS	CA-CB	-7.62	1.42	1.53
1	A	154	THR	N-CA	-7.59	1.36	1.46
1	B	17	HIS	CG-CD2	7.19	1.43	1.35
1	B	67	ASN	CA-CB	-7.11	1.44	1.54
1	B	76	PHE	N-CA	7.07	1.54	1.46
1	B	117	GLY	C-O	7.04	1.33	1.23
1	A	188	GLU	CA-C	-6.94	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	160	HIS	ND1-CE1	6.77	1.39	1.32
1	A	6	PRO	N-CA	-6.74	1.38	1.47
1	B	166	TYR	C-O	6.73	1.32	1.24
1	A	129	ALA	C-N	-6.64	1.24	1.33
1	A	16	PRO	CA-CB	6.56	1.63	1.53
1	A	11	HIS	CA-C	6.43	1.61	1.52
1	A	30	HIS	ND1-CE1	-6.42	1.26	1.32
1	B	65	PHE	CA-C	6.37	1.61	1.52
1	B	25	TYR	C-O	-6.33	1.16	1.24
1	B	146	THR	N-CA	6.33	1.54	1.46
1	B	107	PHE	C-O	-6.27	1.16	1.24
1	B	94	ALA	N-CA	6.25	1.53	1.46
1	A	62	GLY	CA-C	-6.25	1.43	1.51
1	B	105	ASP	N-CA	6.25	1.54	1.46
1	A	130	ASP	CA-CB	-6.23	1.44	1.53
1	A	143	ALA	C-N	6.17	1.40	1.34
1	A	69	ALA	C-O	6.15	1.31	1.24
1	A	27	HIS	CA-C	-6.13	1.44	1.52
1	B	167	ARG	CA-CB	-6.09	1.45	1.52
1	A	16	PRO	C-O	6.09	1.31	1.24
1	A	18	ILE	C-N	-6.08	1.25	1.33
1	B	9	TYR	N-CA	-6.08	1.38	1.46
1	A	105	ASP	C-O	-6.07	1.17	1.24
1	A	138	THR	C-O	6.04	1.31	1.24
1	B	86	GLY	CA-C	-6.00	1.43	1.51
1	A	117	GLY	C-O	5.99	1.30	1.24
1	A	62	GLY	N-CA	-5.96	1.36	1.45
1	B	177	PHE	CA-C	-5.96	1.44	1.52
1	B	71	VAL	CA-C	5.96	1.59	1.52
1	B	17	HIS	CA-C	-5.95	1.46	1.53
1	A	125	TRP	CA-C	5.95	1.59	1.52
1	A	170	ARG	N-CA	5.91	1.51	1.46
1	B	86	GLY	C-O	5.88	1.31	1.23
1	A	27	HIS	CE1-NE2	5.85	1.38	1.32
1	B	88	GLN	CA-CB	5.85	1.62	1.53
1	B	183	TRP	CA-CB	-5.84	1.43	1.53
1	A	56	ILE	N-CA	5.80	1.54	1.46
1	B	131	GLY	CA-C	5.80	1.60	1.51
1	A	185	PHE	N-CA	5.79	1.52	1.46
1	B	93	LEU	N-CA	5.77	1.53	1.46
1	B	89	PRO	C-O	5.77	1.31	1.24
1	B	62	GLY	C-O	-5.76	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	GLY	N-CA	-5.76	1.37	1.45
1	A	59	SER	CA-C	5.75	1.60	1.53
1	B	17	HIS	CE1-NE2	5.74	1.38	1.32
1	B	80	CYS	C-N	-5.72	1.25	1.33
1	A	12	ASP	C-O	5.70	1.31	1.23
1	A	135	LEU	N-CA	5.67	1.52	1.46
1	B	73	ASN	C-O	5.66	1.30	1.24
1	B	117	GLY	CA-C	-5.64	1.44	1.51
1	A	140	GLY	C-O	5.64	1.31	1.23
1	A	152	LEU	N-CA	-5.61	1.39	1.46
1	B	55	GLU	C-N	-5.61	1.26	1.33
1	A	155	CYS	N-CA	-5.61	1.39	1.46
1	A	49	GLU	CA-C	5.59	1.59	1.52
1	A	73	ASN	C-O	5.57	1.31	1.24
1	A	34	TYR	CA-CB	5.56	1.59	1.53
1	A	53	LEU	CA-CB	-5.56	1.44	1.53
1	A	169	LEU	CA-C	-5.54	1.45	1.52
1	A	35	VAL	C-N	-5.53	1.27	1.33
1	A	121	SER	CA-C	-5.48	1.45	1.52
1	B	16	PRO	CA-C	-5.48	1.44	1.52
1	A	188	GLU	CA-CB	5.47	1.60	1.53
1	B	83	PRO	N-CA	-5.44	1.40	1.47
1	A	73	ASN	C-N	-5.42	1.25	1.33
1	B	181	VAL	CA-C	5.41	1.59	1.52
1	B	6	PRO	C-O	5.40	1.30	1.24
1	A	127	VAL	CA-C	5.38	1.59	1.52
1	A	104	PHE	C-O	5.38	1.31	1.24
1	B	74	HIS	CE1-NE2	5.37	1.38	1.32
1	A	6	PRO	N-CD	5.37	1.55	1.47
1	A	153	LEU	CA-C	5.35	1.58	1.52
1	B	54	GLU	CD-OE2	5.35	1.35	1.25
1	B	154	THR	C-O	-5.33	1.16	1.23
1	A	129	ALA	C-O	5.32	1.30	1.24
1	B	85	ALA	N-CA	-5.31	1.38	1.45
1	A	87	GLY	N-CA	5.30	1.53	1.45
1	B	131	GLY	N-CA	5.30	1.53	1.45
1	B	7	LEU	CA-C	5.29	1.59	1.52
1	A	65	PHE	N-CA	5.27	1.52	1.46
1	B	82	SER	C-O	-5.26	1.17	1.24
1	B	177	PHE	C-O	5.25	1.30	1.24
1	A	49	GLU	CA-CB	-5.21	1.46	1.53
1	A	164	ILE	CA-C	5.21	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	HIS	CE1-NE2	5.21	1.37	1.32
1	B	17	HIS	ND1-CE1	-5.17	1.27	1.32
1	A	163	TYR	N-CA	5.16	1.52	1.46
1	A	129	ALA	CA-C	5.16	1.59	1.52
1	A	31	HIS	CE1-NE2	5.12	1.37	1.32
1	A	42	VAL	CA-C	-5.12	1.47	1.52
1	A	189	GLU	CD-OE2	5.11	1.35	1.25
1	A	101	PHE	N-CA	5.08	1.53	1.46
1	B	26	HIS	ND1-CE1	-5.03	1.27	1.32
1	B	98	ASN	CA-C	5.02	1.59	1.53

All (321) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	SER	CA-C-N	42.09	172.46	119.84
1	B	82	SER	C-N-CA	42.09	172.46	119.84
1	A	45	THR	CA-C-O	-30.11	78.92	120.16
1	B	82	SER	O-C-N	28.28	153.84	121.32
1	B	83	PRO	CA-N-CD	-22.21	80.91	112.00
1	A	45	THR	O-C-N	-21.06	97.10	121.32
1	B	67	ASN	CA-CB-CG	18.43	131.03	112.60
1	B	86	GLY	N-CA-C	17.22	153.99	113.18
1	A	188	GLU	N-CA-C	16.55	135.27	108.96
1	B	82	SER	CA-C-O	-15.12	99.44	120.16
1	A	156	ASP	CA-CB-CG	-15.06	97.54	112.60
1	A	155	CYS	CA-CB-SG	-14.99	79.92	114.40
1	B	83	PRO	N-CA-CB	14.46	118.44	103.25
1	A	29	LYS	N-CA-C	-14.25	95.83	111.36
1	B	32	ASN	N-CA-C	-13.97	93.40	112.12
1	B	101	PHE	N-CA-C	-13.55	93.77	111.24
1	A	67	ASN	N-CA-C	-13.32	97.53	114.04
1	B	84	ASP	CA-CB-CG	13.18	125.78	112.60
1	B	67	ASN	N-CA-C	-12.67	97.97	114.31
1	A	62	GLY	N-CA-C	12.40	142.56	113.18
1	B	85	ALA	N-CA-C	12.38	126.66	110.43
1	B	183	TRP	N-CA-C	-12.27	97.94	113.16
1	B	150	THR	CA-C-N	12.13	132.93	119.83
1	B	150	THR	C-N-CA	12.13	132.93	119.83
1	B	60	SER	CA-C-O	11.75	134.37	121.56
1	B	84	ASP	CA-C-N	11.50	140.30	120.87
1	B	84	ASP	C-N-CA	11.50	140.30	120.87
1	B	87	GLY	CA-C-N	11.30	149.37	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	GLY	C-N-CA	11.30	149.37	121.80
1	A	163	TYR	N-CA-C	-11.24	98.18	112.90
1	A	167	ARG	NE-CZ-NH2	11.08	129.17	119.20
1	B	101	PHE	CA-CB-CG	-11.06	102.74	113.80
1	B	113	LYS	N-CA-C	-10.87	100.05	113.20
1	B	166	TYR	CA-CB-CG	10.48	132.77	113.90
1	A	60	SER	N-CA-C	10.44	124.96	110.24
1	A	178	TRP	CB-CA-C	10.29	127.46	111.72
1	A	132	SER	N-CA-C	10.07	125.81	109.59
1	B	108	LYS	CA-CB-CG	9.98	134.06	114.10
1	B	105	ASP	N-CA-C	-9.89	100.58	111.36
1	A	55	GLU	N-CA-C	-9.84	101.27	113.28
1	B	167	ARG	N-CA-CB	9.77	124.91	110.35
1	B	88	GLN	N-CA-C	9.67	131.19	109.81
1	A	150	THR	N-CA-C	9.59	131.00	109.81
1	B	132	SER	N-CA-C	9.56	124.64	110.48
1	B	38	LEU	N-CA-C	9.54	125.62	112.93
1	B	25	TYR	CA-CB-CG	9.46	130.93	113.90
1	B	170	ARG	CD-NE-CZ	9.44	137.61	124.40
1	A	136	CYS	CA-CB-SG	9.40	136.03	114.40
1	A	143	ALA	CA-C-N	9.30	128.94	119.82
1	A	143	ALA	C-N-CA	9.30	128.94	119.82
1	B	101	PHE	CB-CA-C	9.30	126.21	110.86
1	B	123	TRP	CA-CB-CG	9.28	131.22	113.60
1	B	88	GLN	CA-C-N	9.27	131.42	119.84
1	B	88	GLN	C-N-CA	9.27	131.42	119.84
1	B	158	TRP	N-CA-C	-9.22	96.64	110.28
1	B	46	PRO	CA-C-N	9.13	138.99	121.54
1	B	46	PRO	C-N-CA	9.13	138.99	121.54
1	A	178	TRP	N-CA-C	-9.01	96.32	109.11
1	B	47	GLU	CA-C-N	9.00	138.72	121.54
1	B	47	GLU	C-N-CA	9.00	138.72	121.54
1	B	39	ASN	CA-CB-CG	-8.90	103.70	112.60
1	B	109	GLU	CA-CB-CG	8.85	131.80	114.10
1	B	60	SER	N-CA-C	8.84	122.96	110.50
1	B	32	ASN	CA-CB-CG	8.83	121.43	112.60
1	B	17	HIS	CA-C-N	8.75	137.72	121.97
1	B	17	HIS	C-N-CA	8.75	137.72	121.97
1	A	74	HIS	CA-CB-CG	-8.74	105.06	113.80
1	A	130	ASP	CA-CB-CG	8.73	121.33	112.60
1	A	22	THR	N-CA-C	-8.70	101.35	112.93
1	A	177	PHE	CA-CB-CG	8.67	122.47	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	LEU	N-CA-C	8.65	122.62	108.52
1	B	54	GLU	N-CA-C	-8.61	101.83	111.82
1	A	52	THR	N-CA-C	8.59	122.03	110.35
1	A	153	LEU	N-CA-CB	8.55	124.20	110.77
1	B	37	ASN	CA-CB-CG	8.53	121.13	112.60
1	A	123	TRP	N-CA-C	8.47	120.97	108.60
1	B	179	ASN	N-CA-CB	8.39	119.75	110.35
1	B	64	ILE	N-CA-C	-8.39	101.85	111.00
1	B	67	ASN	CB-CA-C	8.31	122.97	109.02
1	B	81	LEU	N-CA-C	8.30	128.49	110.80
1	A	45	THR	CA-C-N	-8.18	109.62	119.84
1	A	45	THR	C-N-CA	-8.18	109.62	119.84
1	A	76	PHE	CA-CB-CG	-8.15	105.65	113.80
1	B	181	VAL	O-C-N	8.13	132.73	122.57
1	B	160	HIS	ND1-CG-CD2	8.08	114.18	106.10
1	B	160	HIS	ND1-CE1-NE2	8.03	116.43	108.40
1	A	79	ASN	CA-CB-CG	8.01	120.61	112.60
1	B	82	SER	C-N-CD	-8.00	92.22	125.00
1	A	42	VAL	CA-C-N	7.99	129.82	119.84
1	A	42	VAL	C-N-CA	7.99	129.82	119.84
1	B	89	PRO	CB-CA-C	7.91	124.61	111.56
1	A	54	GLU	CA-C-O	7.89	131.37	121.58
1	A	185	PHE	CA-CB-CG	-7.83	105.97	113.80
1	A	130	ASP	N-CA-C	-7.77	100.94	110.88
1	B	31	HIS	N-CA-CB	-7.76	100.29	111.54
1	B	151	PRO	N-CA-C	7.72	122.93	111.03
1	A	129	ALA	N-CA-C	-7.70	94.41	110.80
1	B	183	TRP	N-CA-CB	7.69	122.20	110.44
1	B	16	PRO	N-CA-C	7.67	128.26	112.47
1	A	188	GLU	CA-C-O	7.66	129.01	120.43
1	B	89	PRO	CA-N-CD	-7.64	101.30	112.00
1	B	27	HIS	N-CA-C	-7.61	103.46	112.89
1	B	47	GLU	N-CA-C	7.60	127.00	110.80
1	B	31	HIS	N-CA-C	7.55	121.98	111.56
1	A	154	THR	CA-CB-OG1	-7.52	98.32	109.60
1	B	94	ALA	N-CA-C	-7.47	102.82	110.97
1	A	49	GLU	N-CA-C	-7.47	96.38	108.41
1	A	30	HIS	ND1-CE1-NE2	7.39	115.79	108.40
1	A	85	ALA	N-CA-C	7.37	126.50	110.80
1	A	85	ALA	CA-C-N	7.36	135.83	121.41
1	A	85	ALA	C-N-CA	7.36	135.83	121.41
1	B	12	ASP	CA-CB-CG	7.31	119.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ALA	N-CA-C	-7.30	102.97	112.68
1	B	166	TYR	CA-C-O	-7.30	110.07	120.51
1	A	64	ILE	N-CA-C	-7.29	103.06	111.00
1	A	149	ASP	CA-C-O	-7.26	113.15	121.72
1	A	182	ASN	CB-CA-C	7.25	124.85	110.42
1	A	105	ASP	N-CA-C	-7.23	103.40	111.28
1	B	165	ASP	CA-C-N	7.22	135.33	121.54
1	B	165	ASP	C-N-CA	7.22	135.33	121.54
1	A	16	PRO	N-CA-C	7.21	127.31	112.47
1	A	30	HIS	CA-CB-CG	7.18	120.98	113.80
1	A	71	VAL	N-CA-C	-7.14	103.57	110.42
1	B	183	TRP	CA-CB-CG	7.11	127.11	113.60
1	B	105	ASP	CA-C-N	7.07	129.63	120.44
1	B	105	ASP	C-N-CA	7.07	129.63	120.44
1	A	111	PHE	N-CA-C	-7.01	104.19	112.89
1	A	39	ASN	CA-CB-CG	6.99	119.59	112.60
1	B	161	ALA	N-CA-C	-6.98	104.03	112.54
1	A	107	PHE	N-CA-C	-6.96	102.02	112.04
1	B	76	PHE	O-C-N	6.96	130.18	122.11
1	A	149	ASP	CB-CA-C	6.95	121.99	109.83
1	B	17	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	172	LYS	CB-CG-CD	6.86	127.09	111.30
1	B	113	LYS	N-CA-CB	6.86	121.53	110.42
1	B	29	LYS	N-CA-C	-6.85	103.87	111.82
1	A	136	CYS	CB-CA-C	6.84	121.56	109.72
1	B	160	HIS	CB-CG-ND1	-6.84	112.44	122.70
1	A	24	GLU	N-CA-CB	6.80	120.06	110.07
1	B	31	HIS	CA-CB-CG	6.74	120.54	113.80
1	A	46	PRO	CA-N-CD	-6.67	102.67	112.00
1	B	177	PHE	CA-CB-CG	6.66	120.46	113.80
1	B	179	ASN	N-CA-C	-6.66	100.32	109.71
1	A	46	PRO	N-CD-CG	6.65	113.18	103.20
1	A	151	PRO	CA-C-N	6.59	134.13	121.54
1	A	151	PRO	C-N-CA	6.59	134.13	121.54
1	B	158	TRP	CA-C-O	-6.59	113.78	121.16
1	B	21	GLU	N-CA-C	-6.52	103.79	111.03
1	A	159	GLU	OE1-CD-OE2	6.52	138.55	122.90
1	A	72	TRP	N-CA-C	6.47	118.87	111.11
1	B	114	THR	N-CA-C	-6.47	97.03	110.80
1	A	40	ASN	CA-CB-CG	6.41	119.01	112.60
1	B	54	GLU	CA-C-O	6.40	127.33	119.97
1	B	146	THR	N-CA-C	-6.39	104.18	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	LEU	CA-CB-CG	6.38	138.62	116.30
1	A	159	GLU	CB-CG-CD	-6.37	101.78	112.60
1	A	129	ALA	CA-C-O	-6.36	111.41	120.51
1	B	131	GLY	N-CA-C	-6.33	98.17	113.18
1	A	185	PHE	CB-CA-C	6.29	121.14	111.02
1	A	175	GLU	CA-C-O	6.28	123.35	119.77
1	A	50	GLY	N-CA-C	-6.26	101.44	112.77
1	A	21	GLU	CA-CB-CG	6.24	126.58	114.10
1	A	66	ASN	CA-CB-CG	6.24	118.84	112.60
1	A	29	LYS	CA-C-O	6.23	127.03	120.42
1	B	117	GLY	N-CA-C	6.23	127.94	113.18
1	A	23	LEU	CB-CA-C	6.22	123.32	110.31
1	A	111	PHE	CA-CB-CG	6.22	120.02	113.80
1	B	89	PRO	N-CA-CB	-6.22	96.72	103.25
1	B	18	ILE	N-CA-C	-6.21	96.42	109.34
1	A	98	ASN	CB-CA-C	6.20	121.99	112.00
1	B	137	SER	N-CA-C	6.17	119.93	111.54
1	A	44	GLY	CA-C-N	6.15	136.79	121.80
1	A	44	GLY	C-N-CA	6.15	136.79	121.80
1	A	67	ASN	O-C-N	6.13	129.60	122.25
1	A	186	VAL	CB-CA-C	6.11	121.30	111.29
1	B	86	GLY	O-C-N	-6.09	114.79	122.70
1	B	66	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	169	LEU	N-CA-CB	-6.08	100.89	109.94
1	A	70	GLN	CB-CG-CD	6.06	122.91	112.60
1	B	5	PRO	CA-C-N	6.04	127.39	119.84
1	B	5	PRO	C-N-CA	6.04	127.39	119.84
1	B	166	TYR	N-CA-C	6.04	123.66	110.80
1	A	75	THR	N-CA-C	-6.03	105.01	112.90
1	B	160	HIS	CG-ND1-CE1	-6.03	99.06	109.30
1	B	35	VAL	CA-C-N	6.00	132.77	121.97
1	B	35	VAL	C-N-CA	6.00	132.77	121.97
1	B	74	HIS	CA-CB-CG	6.00	119.80	113.80
1	B	23	LEU	N-CA-C	5.99	117.61	111.14
1	B	127	VAL	CB-CA-C	5.98	119.67	110.82
1	B	169	LEU	CA-C-O	-5.97	113.48	120.53
1	B	130	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	187	ALA	N-CA-C	-5.97	98.08	110.80
1	B	160	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
1	B	48	PHE	CA-C-N	5.96	132.92	121.54
1	B	48	PHE	C-N-CA	5.96	132.92	121.54
1	A	49	GLU	N-CA-CB	5.95	119.68	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ALA	CA-C-N	5.95	132.90	121.54
1	A	13	ALA	C-N-CA	5.95	132.90	121.54
1	A	109	GLU	CA-C-O	5.93	126.70	119.11
1	B	95	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	119	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	170	ARG	O-C-N	5.87	125.02	120.38
1	B	29	LYS	CA-C-N	5.87	130.62	120.58
1	B	29	LYS	C-N-CA	5.87	130.62	120.58
1	B	17	HIS	CA-C-O	5.86	131.81	122.20
1	A	178	TRP	CA-C-O	5.84	129.98	121.86
1	A	102	GLY	N-CA-C	-5.83	99.36	113.18
1	A	167	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	B	183	TRP	CA-C-O	5.82	126.33	119.28
1	B	14	LEU	N-CA-C	-5.81	106.24	113.38
1	B	169	LEU	N-CA-C	5.79	119.56	111.56
1	A	186	VAL	N-CA-C	-5.76	97.36	109.34
1	A	184	ALA	O-C-N	5.75	129.16	122.09
1	B	126	LEU	N-CA-C	-5.73	99.39	108.73
1	B	32	ASN	N-CA-CB	5.72	121.73	110.63
1	A	15	GLN	CA-CB-CG	5.72	125.53	114.10
1	B	67	ASN	CA-C-O	5.71	125.11	118.77
1	B	157	VAL	CB-CA-C	5.71	120.18	112.36
1	A	75	THR	CA-CB-OG1	-5.71	101.04	109.60
1	A	92	ALA	N-CA-C	-5.68	98.71	110.80
1	A	163	TYR	CA-C-O	5.68	126.24	119.60
1	A	89	PRO	N-CA-C	-5.67	101.30	110.55
1	B	55	GLU	CA-C-O	5.67	127.17	120.70
1	A	29	LYS	CA-C-N	5.67	128.13	120.65
1	A	29	LYS	C-N-CA	5.67	128.13	120.65
1	A	185	PHE	N-CA-CB	5.66	119.97	110.92
1	A	113	LYS	CA-C-N	5.65	128.12	120.38
1	A	113	LYS	C-N-CA	5.65	128.12	120.38
1	A	105	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	167	ARG	N-CA-CB	5.64	120.03	110.49
1	B	69	ALA	N-CA-C	-5.64	105.12	112.23
1	B	24	GLU	N-CA-CB	5.64	116.83	110.35
1	B	162	TYR	N-CA-CB	-5.62	102.67	111.56
1	A	46	PRO	N-CA-CB	5.59	109.12	103.25
1	A	133	LEU	CA-C-N	5.58	131.00	121.29
1	A	133	LEU	C-N-CA	5.58	131.00	121.29
1	B	160	HIS	CB-CA-C	-5.58	100.78	110.09
1	A	9	TYR	CA-CB-CG	5.57	123.92	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	VAL	O-C-N	5.56	128.74	122.18
1	A	153	LEU	N-CA-C	-5.56	99.23	108.34
1	B	66	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	66	ASN	N-CA-C	-5.52	102.14	110.70
1	B	15	GLN	CB-CA-C	5.51	121.03	110.17
1	B	80	CYS	CB-CA-C	-5.50	100.31	109.55
1	A	156	ASP	N-CA-CB	5.48	120.02	110.81
1	B	55	GLU	CA-C-N	5.48	131.84	121.97
1	B	55	GLU	C-N-CA	5.48	131.84	121.97
1	B	135	LEU	CA-C-N	5.48	132.01	121.54
1	B	135	LEU	C-N-CA	5.48	132.01	121.54
1	A	61	SER	CA-C-N	5.48	132.14	121.41
1	A	61	SER	C-N-CA	5.48	132.14	121.41
1	A	77	TYR	CA-CB-CG	5.47	123.74	113.90
1	B	181	VAL	N-CA-C	-5.46	97.97	109.34
1	B	182	ASN	N-CA-C	-5.46	103.87	111.52
1	A	5	PRO	CA-C-N	5.45	126.65	119.84
1	A	5	PRO	C-N-CA	5.45	126.65	119.84
1	A	12	ASP	N-CA-C	-5.44	101.71	110.14
1	A	157	VAL	O-C-N	5.44	127.11	122.16
1	B	130	ASP	N-CA-C	-5.44	99.22	110.80
1	B	68	ALA	N-CA-C	-5.43	105.92	112.54
1	A	158	TRP	N-CA-C	-5.42	102.85	110.50
1	B	49	GLU	CA-CB-CG	5.42	124.93	114.10
1	A	139	ILE	CA-C-N	5.41	132.02	121.41
1	A	139	ILE	C-N-CA	5.41	132.02	121.41
1	B	177	PHE	O-C-N	-5.40	115.25	122.49
1	A	65	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	184	ALA	N-CA-C	-5.38	105.83	112.72
1	A	162	TYR	N-CA-C	5.37	116.20	107.23
1	A	185	PHE	CA-C-O	5.37	126.28	119.95
1	B	80	CYS	CA-C-N	5.36	131.77	121.54
1	B	80	CYS	C-N-CA	5.36	131.77	121.54
1	A	55	GLU	CA-C-N	5.34	128.47	122.59
1	A	55	GLU	C-N-CA	5.34	128.47	122.59
1	B	65	PHE	N-CA-C	-5.34	99.42	110.80
1	A	124	ALA	N-CA-C	-5.34	99.71	108.41
1	A	176	ALA	CA-C-O	-5.34	114.77	121.02
1	B	174	VAL	CB-CA-C	5.34	120.05	111.29
1	B	182	ASN	CB-CA-C	5.34	119.01	111.86
1	A	152	LEU	CA-C-O	5.30	128.09	120.51
1	A	12	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	VAL	CA-CB-CG2	5.28	119.38	110.40
1	A	68	ALA	O-C-N	5.28	127.50	122.07
1	B	59	SER	N-CA-C	5.28	119.71	113.12
1	A	43	PRO	CA-N-CD	-5.27	104.62	112.00
1	B	105	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	18	ILE	CA-C-N	5.27	131.61	121.54
1	A	18	ILE	C-N-CA	5.27	131.61	121.54
1	B	151	PRO	CB-CA-C	-5.27	105.00	111.64
1	B	40	ASN	N-CA-C	-5.26	99.59	110.80
1	A	89	PRO	CB-CA-C	5.24	117.24	111.11
1	B	84	ASP	CA-C-O	5.24	124.47	119.08
1	A	78	TRP	CA-C-O	5.22	126.27	120.63
1	A	147	SER	N-CA-C	-5.22	106.06	112.90
1	A	160	HIS	ND1-CG-CD2	5.22	111.32	106.10
1	A	140	GLY	N-CA-C	5.21	125.54	113.18
1	B	48	PHE	N-CA-C	5.20	121.86	110.80
1	B	159	GLU	CG-CD-OE1	5.18	130.33	118.40
1	B	136	CYS	CA-C-N	5.17	129.47	122.07
1	B	136	CYS	C-N-CA	5.17	129.47	122.07
1	B	46	PRO	N-CA-CB	5.17	105.81	102.92
1	B	81	LEU	N-CA-CB	-5.17	101.76	110.49
1	A	154	THR	N-CA-C	5.16	121.79	110.80
1	B	10	ALA	O-C-N	5.16	129.45	122.59
1	A	186	VAL	CA-CB-CG1	5.15	119.15	110.40
1	A	102	GLY	CA-C-N	5.14	129.84	122.23
1	A	102	GLY	C-N-CA	5.14	129.84	122.23
1	B	81	LEU	CA-C-O	5.13	127.85	120.51
1	B	185	PHE	N-CA-C	-5.12	107.20	113.50
1	A	45	THR	CA-CB-OG1	-5.11	101.93	109.60
1	B	125	TRP	N-CA-C	5.10	116.82	109.07
1	A	143	ALA	N-CA-C	5.09	121.06	109.81
1	B	31	HIS	ND1-CG-CD2	5.08	111.18	106.10
1	B	116	VAL	CA-C-N	5.08	131.36	121.41
1	B	116	VAL	C-N-CA	5.08	131.36	121.41
1	A	49	GLU	CA-C-O	-5.07	115.16	120.58
1	A	53	LEU	CA-CB-CG	5.07	134.04	116.30
1	A	167	ARG	CA-CB-CG	5.06	124.23	114.10
1	B	27	HIS	ND1-CG-CD2	5.04	111.14	106.10
1	B	76	PHE	N-CA-C	-5.04	104.73	111.24
1	B	154	THR	O-C-N	5.04	130.15	122.94
1	A	44	GLY	CA-C-O	5.03	129.32	120.57

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	THR	Peptide,Mainchain

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	1356	270	1
1	B	1454	0	1356	270	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	2712	518	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 92.

All (518) 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:B:82:SER:C	1:B:83:PRO:CD	2.20	1.13
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:A:46:PRO:HG3	1:A:65:PHE:HZ	1.09	1.12
1:B:16:PRO:HD2	1:B:83:PRO:HB3	1.31	1.12
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:156:ASP:OD1	1:A:156:ASP:C	2.02	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:H	1:A:180:LEU:HD22	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: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:9:TYR:OH	1:A:23:LEU:HD13	1.74	0.88
1:A:115:SER:O	1:A:157:VAL:HG21	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:170:ARG:C	1:B:172:LYS:H	1.79	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
1:A:94:ALA:O	1:A:98:ASN:ND2	2.06	0.87
1:A:76:PHE:HD2	1:A:154:THR:HG1	1.23	0.87
1:A:53:LEU:HD13	1:A:72:TRP:CZ3	2.09	0.87
1:B:37:ASN:H	1:B:37:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HA	1:B:46:PRO:HD2	1.56	0.86
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:159:GLU:CD	1:B:160:HIS:HB3	2.02	0.84
1:A:15:GLN:HB3	1:A:16:PRO:CD	2.03	0.84
1:B:72:TRP:CZ3	1:B:143:ALA:HB1	2.13	0.84
1:B:166:TYR:HA	1:B:169:LEU:CD2	2.08	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:A:42:VAL:HA	1:A:49:GLU:HG2	1.61	0.83
1:A:114:THR:CG2	1:A:136:CYS:HB3	2.08	0.83
1:A:183:TRP:CD1	1:A:183:TRP:H	1.96	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:64:ILE:O	1:A:67:ASN:HB2	1.82	0.80
1:A:93:LEU:HD23	1:A:187:ALA:HA	1.61	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: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
1:A:180:LEU:H	1:A:180:LEU:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD22	1:A:180:LEU:N	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:85:ALA:HA	1:B:181:VAL:HB	1.73	0.71
1:B:161:ALA:O	3:B:768:HOH:O	2.08	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
1:A:93:LEU:CD2	1:A:187:ALA:HA	2.21	0.69
1:B:52:THR:C	1:B:54:GLU:H	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:GLY:HA2	1:A:66:ASN:N	2.09	0.67
1:A:115:SER:OG	1:A:124:ALA:CB	2.42	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:109:GLU:C	1:A:112:THR:HG22	2.20	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:45:THR:C	1:A:46:PRO:O	2.39	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:A:40:ASN:O	1:A:40:ASN:ND2	2.30	0.65
1:A:154:THR:O	1:A:155:CYS:HB3	1.98	0.64
1:A:62:GLY:HA2	1:A:66:ASN:H	1.62	0.64
1:A:128:LYS:HG2	1:A:151:PRO:HG3	1.78	0.64
1:A:78:TRP:CD1	1:A:79:ASN:H	2.12	0.64
1:A:48:PHE:HE1	1:A:59:SER:HB3	1.61	0.63
1:A:142:GLY:O	1:A:143:ALA:HB3	1.97	0.63
1:A:53:LEU:HD13	1:A:72:TRP:HZ3	1.56	0.63
1:A:171:PRO:O	1:A:175:GLU:CB	2.46	0.63
1:B:14:LEU:O	1:B:15:GLN:C	2.42	0.63
1:A:80:CYS:HA	1:A:181:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:167:ARG:HB3	1:B:29:LYS:CE	2.29	0.62
1:B:118:THR:OG1	1:B:138:THR:HG21	1.99	0.62
1:B:34:TYR:CE1	1:B:70:GLN:NE2	2.68	0.62
1:B:174:VAL:HG12	1:B:175:GLU:N	2.15	0.62
1:A:63:GLY:HA2	3:A:625:HOH:O	2.00	0.62
1:A:109:GLU:O	1:A:112:THR:HG22	2.00	0.62
1:A:25:TYR:CD1	1:B:167:ARG:CG	2.80	0.62
1:B:33:THR:O	1:B:34:TYR:HB2	1.97	0.62
1:B:98:ASN:ND2	1:B:103:SER:HA	2.15	0.61
1:B:140:GLY:C	1:B:142:GLY:H	2.08	0.61
1:A:32:ASN:HD22	1:A:32:ASN:H	1.47	0.61
1:B:81:LEU:O	1:B:181:VAL:HG12	2.00	0.61
1:B:82:SER:C	1:B:83:PRO:HD3	2.22	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:B:53:LEU:CD1	3:B:717:HOH:O	2.49	0.61
1:B:112:THR:C	1:B:114:THR:H	2.06	0.61
1:A:177:PHE:CG	1:A:177:PHE:O	2.54	0.60
1:A:42:VAL:N	1:A:43:PRO:CD	2.62	0.60
1:A:128:LYS:HE3	1:A:151:PRO:HB3	1.83	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
1:B:67:ASN:HA	1:B:70:GLN:HG3	1.82	0.59
1:B:112:THR:C	1:B:114:THR:N	2.60	0.59
1:B:9:TYR:OH	1:B:23:LEU:CD1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASN:C	1:A:171:PRO:HD2	2.27	0.59
1:B:30:HIS:O	1:B:34:TYR:HB2	2.02	0.59
1:B:34:TYR:C	1:B:36:VAL:H	2.10	0.59
1:A:50:GLY:O	1:A:51:LYS:HB2	2.01	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:B:121:SER:HB3	1:B:158:TRP:CD2	2.37	0.59
1:A:118:THR:CG2	1:A:157:VAL:HG11	2.31	0.59
1:A:123:TRP:CD1	1:A:155:CYS:SG	2.96	0.59
1:B:160:HIS:C	1:B:160:HIS:CD2	2.81	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:98:ASN:O	1:B:99:ALA:HB2	2.03	0.58
1:B:141:ALA:O	3:B:763:HOH:O	2.17	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:34:TYR:C	1:B:36:VAL:N	2.61	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:78:TRP:HA	1:B:78:TRP:CE3	2.40	0.57
1:A:62:GLY:CA	1:A:66:ASN:H	2.18	0.56
1:A:101:PHE:HB3	1:A:107:PHE:HA	1.87	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:22:THR:O	1:B:25:TYR:HD1	1.88	0.56
1:B:170:ARG:HB2	1:B:170:ARG:NH1	2.21	0.56
1:A:112:THR:HA	1:A:173:TYR:CE1	2.38	0.56
1:B:85:ALA:HB3	1:B:179:ASN:CG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:HB2	3:A:636:HOH:O	2.06	0.56
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:39:ASN:ND2	1:B:39:ASN:H	2.05	0.55
1:B:183:TRP:HE3	1:B:186:VAL:CG2	2.09	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:41:LEU:HD23	1:B:65:PHE:CD1	2.43	0.54
1:B:98:ASN:O	1:B:99:ALA:CB	2.56	0.54
1:A:98:ASN:N	1:A:98:ASN:HD22	2.04	0.54
1:A:157:VAL:O	1:A:157:VAL:CG1	2.56	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:B:170:ARG:C	1:B:172:LYS:N	2.48	0.54
1:A:141:ALA:HB2	1:B:119:PHE:CE2	2.44	0.53
1:A:166:TYR:C	1:A:168:ASN:H	2.16	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:13:ALA:HB3	1:A:20:LYS:HG2	1.90	0.53
1:A:167:ARG:HD2	3:A:705:HOH:O	2.08	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:88:GLN:HB3	1:B:89:PRO:HD2	1.91	0.53
1:B:181:VAL:HG22	1:B:182:ASN:H	1.73	0.53
1:A:62:GLY:C	1:A:66:ASN:H	2.17	0.53
1:B:88:GLN:HG2	1:B:94:ALA:HA	1.91	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: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:A:105:ASP:HB3	1:A:106:LYS:HD2	1.91	0.52
1:B:35:VAL:HA	1:B:37:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:SER:HB3	1:B:179:ASN:OD1	2.10	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:A:115:SER:HB2	1:A:173:TYR:CE1	2.45	0.52
1:B:18:ILE:CG2	1:B:23:LEU:HD21	2.39	0.52
1:B:166:TYR:O	1:B:169:LEU:CD1	2.56	0.52
1:B:145:LEU:CD2	1:B:150:THR:HG22	2.40	0.51
1:B:57:VAL:C	1:B:58:LYS:HD3	2.36	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:36:VAL:C	1:B:38:LEU:H	2.18	0.51
1:A:181:VAL:O	1:A:182:ASN:C	2.53	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:B:52:THR:C	1:B:54:GLU:N	2.68	0.50
1:A:30:HIS:HA	1:A:34:TYR:HD2	1.76	0.50
1:A:115:SER:O	1:A:118:THR:HG22	2.11	0.50
1:A:172:LYS:O	1:A:172:LYS:HD2	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:37:ASN:N	1:B:37:ASN:ND2	2.57	0.50
1:B:127:VAL:HG21	1:B:144:PRO:HG3	1.93	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:A:104:PHE:CD1	1:A:104:PHE:C	2.90	0.50
1:B:103:SER:HB2	1:B:106:LYS:HB2	1.93	0.50
1:A:163:TYR:CD1	1:A:163:TYR:C	2.90	0.49
1:A:173:TYR:HA	1:A:177:PHE:HB3	1.94	0.49
1:A:25:TYR:CE1	1:B:167:ARG:HB2	2.47	0.49
1:A:52:THR:O	1:A:53:LEU:C	2.54	0.49
1:A:167:ARG:HB3	1:B:29:LYS:HE3	1.93	0.49
1:B:12:ASP:O	1:B:13:ALA:HB2	2.11	0.49
1:B:32:ASN:OD1	1:B:33:THR:OG1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PRO:HD2	1:B:83:PRO:C	2.37	0.49
1:A:101:PHE:O	1:A:103:SER:O	2.30	0.49
1:B:185:PHE:CD1	1:B:185:PHE:C	2.91	0.49
1:A:27:HIS:HD2	3:A:611:HOH:O	1.95	0.49
1:A:77:TYR:CE1	1:A:81:LEU:HD11	2.48	0.49
1:A:143:ALA:HA	1:A:144:PRO:HD3	1.71	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:167:ARG:C	1:B:168:ASN:HD22	2.21	0.48
1:B:118:THR:HB	1:B:138:THR:HB	1.94	0.48
1:B:41:LEU:O	1:B:46:PRO:O	2.32	0.48
1:B:150:THR:HA	1:B:151:PRO:HD2	1.60	0.48
1:A:159:GLU:OE1	1:B:160:HIS:CA	2.60	0.48
1:A:46:PRO:C	1:A:48:PHE:H	2.21	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:52:THR:HB	1:B:54:GLU:CD	2.39	0.48
1:B:82:SER:OG	1:B:179:ASN:O	2.30	0.48
1:B:137:SER:O	1:B:137:SER:OG	2.24	0.48
1:A:36:VAL:CG1	1:A:64:ILE:HG23	2.44	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:173:TYR:C	1:A:175:GLU:H	2.22	0.47
1:A:183:TRP:CE3	1:A:186:VAL:HG11	2.49	0.47
1:B:22:THR:O	1:B:26:HIS:CB	2.63	0.47
1:B:125:TRP:HA	1:B:153:LEU:O	2.15	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:A:44:GLY:O	1:A:45:THR:HG23	2.14	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:B:22:THR:O	1:B:26:HIS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:H	1:B:39:ASN:HD22	1.62	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:34:TYR:CE2	1:B:70:GLN:HB3	2.50	0.46
1:A:163:TYR:CD1	1:A:163:TYR:O	2.68	0.46
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:123:TRP:CZ3	1:B:140:GLY:HA2	2.41	0.46
1:B:132:SER:O	1:B:133:LEU:HD23	2.16	0.46
1:A:98:ASN:HD22	1:A:98:ASN:H	1.63	0.46
1:A:128:LYS:HG2	1:A:151:PRO:CG	2.45	0.46
1:A:149:ASP:OD1	1:A:149:ASP:N	2.48	0.46
1:B:22:THR:HA	1:B:25:TYR:CE1	2.50	0.46
1:B:53:LEU:HD21	1:B:71:VAL:HB	1.97	0.46
1:B:163:TYR:C	1:B:165:ASP:H	2.22	0.46
1:B:52:THR:O	1:B:53:LEU:HB2	2.15	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:62:GLY:C	1:B:64:ILE:H	2.19	0.46
1:B:35:VAL:HA	1:B:37:ASN:HD21	1.79	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:A:107:PHE:CE2	1:A:126:LEU:HD22	2.51	0.46
1:B:108:LYS:NZ	1:B:108:LYS:HB2	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:51:LYS:CE	1:B:56:ILE:HD12	2.47	0.45
1:B:34:TYR:CZ	1:B:70:GLN:CD	2.94	0.45
1:B:48:PHE:O	1:B:50:GLY:N	2.50	0.45
1:A:25:TYR:HE1	1:B:167:ARG:HB2	1.81	0.45
1:A:98:ASN:ND2	1:A:98:ASN:N	2.64	0.45
1:B:133:LEU:HD11	3:B:760:HOH:O	2.16	0.45
1:B:143:ALA:C	1:B:145:LEU:H	2.24	0.45
1:A:33:THR:HG23	3:A:605:HOH:O	1.84	0.45
1:B:127:VAL:HG22	1:B:151:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PRO:C	1:A:152:LEU:HG	2.42	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:85:ALA:HB1	1:B:180:LEU:C	2.42	0.44
1:B:12:ASP:OD2	1:B:81:LEU:HD23	2.18	0.44
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: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: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:A:127:VAL:C	1:A:151:PRO:CG	2.91	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:B:140:GLY:C	1:B:142:GLY:N	2.73	0.43
1:A:9:TYR:HB2	1:A:27:HIS:CE1	2.53	0.43
1:A:65:PHE:C	1:A:67:ASN:H	2.26	0.43
1:B:113:LYS:HE3	1:B:113:LYS:HB3	1.91	0.43
1:A:33:THR:C	1:A:35:VAL:H	2.26	0.43
1:A:157:VAL:O	1:A:157:VAL:HG13	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:93:LEU:CD1	1:B:187:ALA:HA	2.33	0.43
1:B:170:ARG:HG3	1:B:170:ARG:HH11	1.84	0.43
1:B:36:VAL:C	1:B:38:LEU:N	2.77	0.43
1:B:25:TYR:O	1:B:29:LYS:HG3	2.19	0.43
1:B:39:ASN:ND2	1:B:39:ASN:N	2.67	0.43
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:A:109:GLU:O	1:A:112:THR:CG2	2.64	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:A:72:TRP:CD1	1:A:72:TRP:C	2.97	0.42
1:B:30:HIS:NE2	1:B:75:THR:HG22	2.34	0.42
1:B:57:VAL:HG23	1:B:58:LYS:CD	2.45	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:17:HIS:O	1:B:18:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TRP:CD2	1:B:154:THR:HG23	2.52	0.42
1:B:170:ARG:HH11	1:B:170:ARG:CG	2.32	0.42
1:B:152:LEU:HD22	1:B:188:GLU:HB2	2.02	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
1:B:23:LEU:O	1:B:27:HIS:N	2.50	0.42
1:B:100:ALA:HB3	1:B:101:PHE:CD2	2.54	0.42
1:A:13:ALA:HB3	1:A:20:LYS:NZ	2.35	0.42
1:B:88:GLN:CB	1:B:89:PRO:CD	2.90	0.42
1:B:163:TYR:C	1:B:163:TYR:CD1	2.98	0.42
1:B:174:VAL:C	1:B:176:ALA:H	2.28	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: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:A:166:TYR:C	1:A:168:ASN:N	2.78	0.41
1:B:51:LYS:HD3	1:B:55:GLU:O	2.20	0.41
1:A:106:LYS:HD2	1:A:106:LYS:H	1.79	0.41
1:B:51:LYS:CE	1:B:56:ILE:CD1	2.97	0.41
1:A:31:HIS:C	1:A:33:THR:H	2.28	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:A:120:GLY:O	1:A:121:SER:HB2	2.20	0.41
1:B:160:HIS:CE1	3:B:767:HOH:O	2.73	0.41
1:A:88:GLN:O	1:A:88:GLN:CG	2.63	0.41
1:A:162:TYR:HD2	1:A:164:ILE:O	2.04	0.41
1:B:33:THR:C	1:B:35:VAL:N	2.78	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:A:14:LEU:HB2	1:A:23:LEU:CD1	2.51	0.41
1:A:127:VAL:C	1:A:151:PRO:HG3	2.44	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:21:GLU:OE1	1:B:166:TYR:CE2	2.74	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:66:ASN:HD22	1:A:66:ASN:HA	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:O	1:B:168:ASN:CB	2.65	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:106:LYS:C	1:B:106:LYS:HD3	2.47	0.40
1:B:173:TYR:HA	1:B:177:PHE:HB3	2.04	0.40
1:A:174:VAL:O	1:A:174:VAL:HG22	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Res	Type
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
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%)	102 (68%)	49 (32%)	0	0
1	B	151/158 (96%)	96 (64%)	55 (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	54	GLU
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	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	113	LYS
1	A	114	THR
1	A	132	SER
1	A	145	LEU
1	A	146	THR

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Mol	Chain	Res	Type
1	A	149	ASP
1	A	154	THR
1	A	157	VAL
1	A	159	GLU
1	A	163	TYR
1	A	167	ARG
1	A	169	LEU
1	A	170	ARG
1	A	172	LYS
1	A	179	ASN
1	A	180	LEU
1	A	183	TRP
1	A	185	PHE
1	A	186	VAL
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	36	VAL
1	B	37	ASN
1	B	41	LEU
1	B	45	THR
1	B	51	LYS
1	B	52	THR
1	B	53	LEU
1	B	55	GLU
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

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Mol	Chain	Res	Type
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
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	170	ARG
1	B	173	TYR
1	B	174	VAL
1	B	185	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	32	ASN
1	A	66	ASN
1	A	70	GLN
1	A	79	ASN
1	A	179	ASN
1	B	11	HIS
1	B	26	HIS
1	B	37	ASN
1	B	39	ASN
1	B	40	ASN

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Mol	Chain	Res	Type
1	B	66	ASN
1	B	67	ASN
1	B	70	GLN
1	B	79	ASN
1	B	88	GLN
1	B	98	ASN
1	B	168	ASN
1	B	182	ASN

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](#)

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 [i](#)

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.