



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:30 PM UTC

PDB ID : 2CNA / pdb_00002cna
Title : THE COVALENT AND THREE-DIMENSIONAL STRUCTURE OF
CONCANAVALIN A, IV.ATOMIC COORDINATES,HYDROGEN BOND-
ING,AND QUATERNARY STRUCTURE
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Deposited on : 1975-04-01
Resolution : 2.00 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

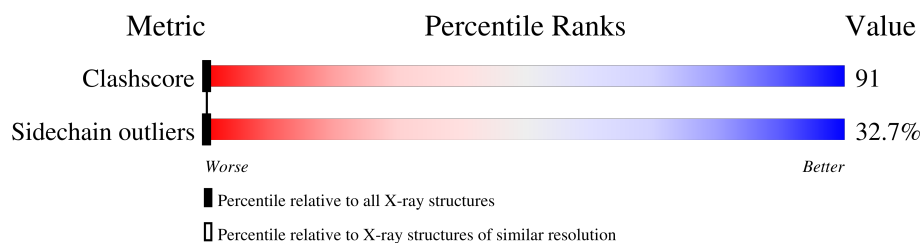
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1813 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 CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1807	1139	300	366	2			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

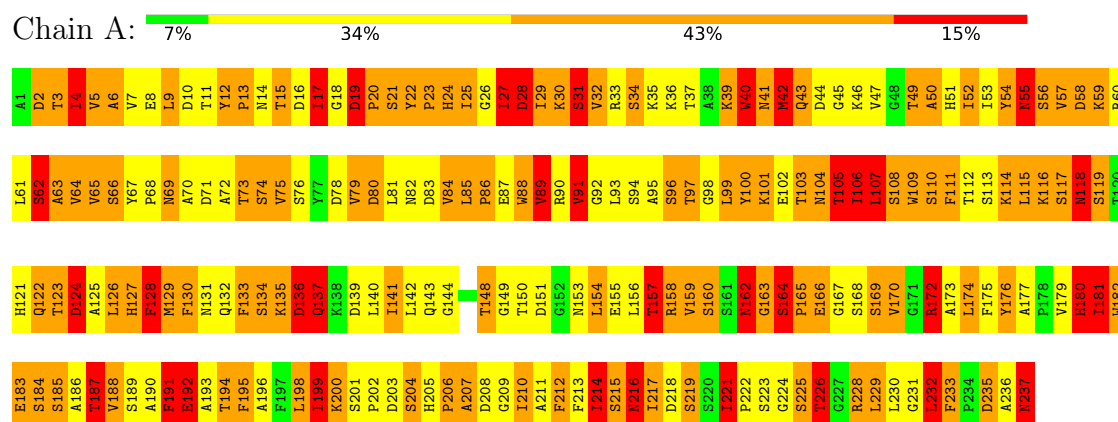
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: CONCAVALIN A



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	89.91Å 87.23Å 63.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1813	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: CA, MN

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	1.29	27/1849 (1.5%)	2.73	229/2519 (9.1%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	TRP	NE1-CE2	-8.67	1.27	1.37
1	A	182	TRP	NE1-CE2	-8.62	1.27	1.37
1	A	40	TRP	NE1-CE2	-8.61	1.27	1.37
1	A	109	TRP	NE1-CE2	-8.59	1.27	1.37
1	A	118	ASN	CG-OD1	8.37	1.39	1.23
1	A	162	ASN	CG-OD1	8.35	1.39	1.23
1	A	41	ASN	CG-OD1	8.34	1.39	1.23
1	A	216	ASN	CG-OD1	8.34	1.39	1.23
1	A	153	ASN	CG-OD1	8.32	1.39	1.23
1	A	131	ASN	CG-OD1	8.32	1.39	1.23
1	A	69	ASN	CG-OD1	8.31	1.39	1.23
1	A	55	ASN	CG-OD1	8.31	1.39	1.23
1	A	14	ASN	CG-OD1	8.28	1.39	1.23
1	A	237	ASN	CG-OD1	8.27	1.39	1.23
1	A	104	ASN	CG-OD1	8.26	1.39	1.23
1	A	131	ASN	CG-ND2	-5.25	1.22	1.33
1	A	118	ASN	CG-ND2	-5.25	1.22	1.33
1	A	14	ASN	CG-ND2	-5.24	1.22	1.33
1	A	82	ASN	CG-ND2	-5.24	1.22	1.33
1	A	162	ASN	CG-ND2	-5.24	1.22	1.33
1	A	237	ASN	CG-ND2	-5.24	1.22	1.33
1	A	153	ASN	CG-ND2	-5.24	1.22	1.33
1	A	104	ASN	CG-ND2	-5.23	1.22	1.33
1	A	69	ASN	CG-ND2	-5.23	1.22	1.33
1	A	41	ASN	CG-ND2	-5.21	1.22	1.33
1	A	55	ASN	CG-ND2	-5.17	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	ASN	CG-ND2	-5.14	1.22	1.33

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	N-CA-CB	18.74	142.16	110.49
1	A	56	SER	N-CA-CB	-18.35	83.40	110.01
1	A	158	ARG	CB-CA-C	-16.66	77.27	110.42
1	A	125	ALA	N-CA-C	14.82	131.63	108.07
1	A	225	SER	N-CA-C	-14.33	95.82	113.01
1	A	135	LYS	N-CA-C	-14.19	95.29	112.89
1	A	99	LEU	N-CA-CB	-14.10	89.96	110.40
1	A	99	LEU	N-CA-C	-14.04	95.86	113.55
1	A	187	THR	N-CA-CB	-13.32	93.40	110.98
1	A	95	ALA	CB-CA-C	-12.54	87.30	110.62
1	A	84	VAL	N-CA-C	12.42	123.47	111.67
1	A	122	GLN	CB-CA-C	-12.37	94.16	111.73
1	A	126	LEU	N-CA-C	12.06	129.57	109.06
1	A	99	LEU	CB-CA-C	-11.61	91.34	109.34
1	A	96	SER	N-CA-C	11.31	126.76	109.23
1	A	72	ALA	N-CA-C	10.88	126.38	110.28
1	A	213	PHE	N-CA-C	10.69	126.83	109.40
1	A	49	THR	CB-CA-C	-10.64	95.45	110.34
1	A	221	ILE	CB-CA-C	-10.61	99.43	110.89
1	A	47	VAL	N-CA-CB	10.52	122.00	110.53
1	A	41	ASN	N-CA-CB	-10.30	95.75	110.58
1	A	105	THR	N-CA-CB	-10.11	94.41	110.69
1	A	57	VAL	N-CA-CB	10.07	127.85	111.23
1	A	121	HIS	CB-CA-C	-9.98	92.05	110.62
1	A	180	HIS	N-CA-CB	9.96	127.29	110.46
1	A	4	ILE	N-CA-C	9.93	122.62	108.42
1	A	181	ILE	CB-CA-C	9.84	127.42	111.29
1	A	223	SER	CB-CA-C	9.80	124.96	110.26
1	A	124	ASP	N-CA-C	9.79	125.94	110.17
1	A	182	TRP	CB-CA-C	-9.76	88.59	110.07
1	A	128	PHE	CB-CA-C	9.64	124.99	110.14
1	A	183	GLU	N-CA-C	9.48	123.09	108.96
1	A	182	TRP	N-CA-CB	-9.29	95.53	111.69
1	A	125	ALA	CB-CA-C	-9.24	94.14	110.03
1	A	188	VAL	N-CA-CB	-9.19	96.06	111.23
1	A	190	ALA	N-CA-C	9.08	123.24	108.99
1	A	114	LYS	N-CA-C	9.06	123.56	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	SER	N-CA-C	-9.02	102.28	113.28
1	A	101	LYS	N-CA-CB	-8.97	96.00	110.63
1	A	53	ILE	CB-CA-C	-8.95	96.95	110.55
1	A	86	PRO	CB-CA-C	8.82	122.54	110.98
1	A	7	VAL	N-CA-C	-8.80	93.29	107.28
1	A	84	VAL	CB-CA-C	-8.78	101.44	111.80
1	A	226	THR	N-CA-CB	8.75	122.19	110.29
1	A	122	GLN	N-CA-CB	8.61	125.13	112.13
1	A	202	PRO	N-CA-C	-8.60	102.31	113.57
1	A	53	ILE	N-CA-C	8.53	123.02	108.95
1	A	6	ALA	CB-CA-C	-8.51	91.60	109.38
1	A	116	LYS	N-CA-CB	-8.49	96.03	109.87
1	A	31	SER	N-CA-C	8.43	120.37	108.74
1	A	40	TRP	N-CA-CB	-8.35	97.25	110.69
1	A	56	SER	N-CA-C	8.32	119.97	111.07
1	A	137	GLN	N-CA-CB	8.24	124.42	110.49
1	A	169	SER	N-CA-C	8.23	122.90	110.14
1	A	78	ASP	N-CA-CB	8.15	123.86	110.17
1	A	63	ALA	N-CA-C	8.03	122.19	109.50
1	A	8	GLU	N-CA-C	7.94	122.58	109.95
1	A	213	PHE	N-CA-CB	-7.92	97.06	110.83
1	A	187	THR	CB-CA-C	7.83	122.12	109.27
1	A	195	PHE	N-CA-CB	7.81	123.69	110.49
1	A	216	ASN	CB-CA-C	7.80	123.47	109.83
1	A	172	ARG	CB-CA-C	-7.78	95.92	111.17
1	A	115	LEU	N-CA-CB	-7.77	99.02	110.84
1	A	78	ASP	CB-CA-C	-7.77	97.24	110.22
1	A	5	VAL	N-CA-C	-7.74	97.27	108.11
1	A	154	LEU	N-CA-CB	7.67	122.92	110.42
1	A	130	PHE	N-CA-C	7.66	121.70	108.76
1	A	186	ALA	CB-CA-C	-7.63	97.28	109.80
1	A	129	MET	N-CA-C	7.63	121.36	109.07
1	A	117	SER	N-CA-C	7.60	121.87	109.94
1	A	194	THR	N-CA-CB	-7.59	98.48	111.69
1	A	20	PRO	CB-CA-C	7.56	124.04	111.56
1	A	54	TYR	N-CA-CB	-7.55	95.79	111.87
1	A	58	ASP	N-CA-C	7.54	121.73	112.23
1	A	205	HIS	CB-CA-C	7.47	124.88	110.17
1	A	126	LEU	N-CA-CB	-7.45	97.79	111.13
1	A	19	ASP	N-CA-CB	7.41	120.05	110.04
1	A	105	THR	CB-CA-C	7.41	122.72	109.38
1	A	184	SER	N-CA-CB	7.38	122.97	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASN	N-CA-C	7.34	121.30	108.52
1	A	29	ILE	CB-CA-C	-7.33	101.47	110.99
1	A	53	ILE	N-CA-CB	-7.28	100.22	112.44
1	A	154	LEU	N-CA-C	-7.27	96.88	108.73
1	A	232	LEU	N-CA-C	-7.24	104.31	113.43
1	A	12	TYR	N-CA-CB	7.23	123.23	110.37
1	A	39	LYS	N-CA-C	7.19	120.50	108.20
1	A	121	HIS	N-CA-CB	7.19	122.71	111.56
1	A	219	SER	N-CA-C	7.18	121.27	110.64
1	A	217	ILE	N-CA-CB	-7.13	96.66	110.78
1	A	115	LEU	N-CA-C	7.09	120.64	108.02
1	A	24	HIS	N-CA-CB	-7.09	99.82	111.66
1	A	131	ASN	N-CA-CB	-7.08	99.96	111.01
1	A	31	SER	N-CA-CB	-7.07	99.40	111.21
1	A	25	ILE	CB-CA-C	-6.93	100.14	110.82
1	A	228	ARG	N-CA-CB	-6.91	98.80	110.41
1	A	27	ILE	N-CA-CB	-6.83	102.79	110.99
1	A	116	LYS	N-CA-C	6.83	119.69	109.25
1	A	118	ASN	CB-CA-C	-6.72	97.40	110.11
1	A	206	PRO	N-CA-C	6.72	121.78	111.15
1	A	207	ALA	N-CA-C	6.68	125.04	110.80
1	A	125	ALA	N-CA-CB	-6.64	100.47	111.69
1	A	62	SER	N-CA-C	6.63	120.20	109.40
1	A	12	TYR	CB-CA-C	-6.62	97.13	110.17
1	A	43	GLN	CB-CA-C	6.61	121.82	111.77
1	A	180	HIS	CB-CA-C	-6.52	100.00	111.22
1	A	144	GLY	N-CA-C	6.52	128.63	113.18
1	A	22	TYR	N-CA-CB	-6.51	98.78	110.37
1	A	21	SER	N-CA-C	6.49	120.90	112.92
1	A	157	THR	N-CA-C	6.47	120.45	110.42
1	A	82	ASN	N-CA-C	-6.45	103.37	111.11
1	A	233	PHE	N-CA-C	6.43	119.70	109.40
1	A	235	ASP	N-CA-CB	-6.38	100.85	110.35
1	A	214	ILE	CB-CA-C	-6.38	101.33	110.83
1	A	106	ILE	N-CA-CB	-6.35	102.61	111.25
1	A	215	SER	N-CA-CB	-6.33	101.52	110.51
1	A	59	LYS	N-CA-CB	-6.30	102.37	111.70
1	A	100	TYR	CB-CA-C	6.25	119.85	109.53
1	A	136	ASP	CB-CA-C	6.24	122.83	110.42
1	A	119	SER	N-CA-CB	-6.24	99.95	110.49
1	A	163	GLY	N-CA-C	-6.24	98.40	113.18
1	A	141	ILE	N-CA-CB	6.23	119.49	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	HIS	N-CA-C	6.22	118.53	109.07
1	A	157	THR	CB-CA-C	-6.21	99.56	109.80
1	A	81	LEU	CB-CA-C	6.17	122.05	110.63
1	A	124	ASP	CB-CA-C	6.17	119.93	109.50
1	A	43	GLN	N-CA-CB	-6.16	99.42	110.82
1	A	107	LEU	CB-CA-C	6.15	122.54	111.03
1	A	176	TYR	CB-CA-C	6.15	120.44	110.96
1	A	113	SER	N-CA-C	6.09	117.99	107.93
1	A	108	SER	N-CA-CB	-6.08	100.68	111.08
1	A	141	ILE	CB-CA-C	-6.08	103.63	111.53
1	A	158	ARG	N-CA-C	6.01	123.61	110.80
1	A	151	ASP	N-CA-C	-5.98	103.31	111.56
1	A	54	TYR	N-CA-C	5.92	117.27	107.73
1	A	54	TYR	CB-CA-C	-5.91	99.46	110.56
1	A	170	VAL	N-CA-C	5.90	121.61	109.34
1	A	49	THR	N-CA-C	5.85	117.58	107.93
1	A	193	ALA	N-CA-CB	5.84	121.71	111.13
1	A	37	THR	N-CA-CB	5.82	121.68	111.55
1	A	91	VAL	N-CA-CB	-5.77	104.14	111.64
1	A	82	ASN	N-CA-CB	5.74	118.49	109.94
1	A	111	PHE	N-CA-C	5.72	117.71	108.34
1	A	52	ILE	N-CA-C	5.71	121.22	109.34
1	A	72	ALA	CB-CA-C	-5.71	99.89	109.65
1	A	131	ASN	CB-CG-ND2	5.68	124.92	116.40
1	A	118	ASN	CB-CG-ND2	5.68	124.92	116.40
1	A	55	ASN	CB-CG-ND2	5.67	124.91	116.40
1	A	41	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	123	THR	N-CA-CB	-5.66	100.92	110.49
1	A	162	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	10	ASP	N-CA-C	5.66	117.87	108.20
1	A	69	ASN	CB-CG-ND2	5.65	124.87	116.40
1	A	153	ASN	CB-CG-ND2	5.65	124.87	116.40
1	A	104	ASN	CB-CG-ND2	5.64	124.87	116.40
1	A	82	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	216	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	64	VAL	N-CA-CB	-5.64	105.01	112.34
1	A	198	LEU	N-CA-CB	5.64	120.06	110.87
1	A	14	ASN	CB-CG-ND2	5.63	124.85	116.40
1	A	162	ASN	N-CA-CB	-5.63	102.38	110.65
1	A	212	PHE	CB-CA-C	-5.61	101.80	110.78
1	A	237	ASN	CB-CG-ND2	5.61	124.82	116.40
1	A	81	LEU	N-CA-C	-5.60	105.27	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ALA	CB-CA-C	-5.60	97.68	109.38
1	A	117	SER	N-CA-CB	-5.59	99.95	110.07
1	A	194	THR	N-CA-C	-5.59	100.80	109.24
1	A	42	MET	N-CA-C	5.57	118.15	110.35
1	A	62	SER	CB-CA-C	-5.56	98.75	109.37
1	A	135	LYS	N-CA-CB	5.56	119.46	110.40
1	A	5	VAL	N-CA-CB	5.54	119.06	111.41
1	A	89	VAL	N-CA-CB	-5.54	102.09	111.23
1	A	81	LEU	N-CA-CB	-5.53	101.70	110.22
1	A	123	THR	CB-CA-C	5.52	121.41	110.42
1	A	2	ASP	N-CA-CB	5.50	119.79	110.49
1	A	192	GLU	N-CA-CB	5.49	120.04	110.81
1	A	134	SER	N-CA-C	5.49	117.86	109.95
1	A	159	VAL	N-CA-C	5.46	117.66	109.20
1	A	13	PRO	N-CA-C	5.45	123.69	112.47
1	A	79	VAL	N-CA-CB	-5.45	100.84	112.00
1	A	86	PRO	N-CA-C	-5.44	102.74	111.38
1	A	121	HIS	N-CA-C	5.42	117.08	108.79
1	A	159	VAL	N-CA-CB	-5.42	102.47	112.43
1	A	23	PRO	CB-CA-C	5.41	118.44	111.46
1	A	193	ALA	CB-CA-C	-5.39	99.00	109.68
1	A	9	LEU	N-CA-CB	5.35	119.20	110.37
1	A	71	ASP	N-CA-C	5.33	118.37	110.48
1	A	7	VAL	N-CA-CB	5.33	118.61	111.90
1	A	104	ASN	N-CA-CB	5.33	119.79	111.64
1	A	225	SER	CB-CA-C	5.32	121.02	110.17
1	A	148	THR	N-CA-CB	5.31	120.06	110.83
1	A	106	ILE	CB-CA-C	5.30	118.73	110.83
1	A	74	SER	N-CA-CB	-5.30	102.33	111.55
1	A	191	PHE	CB-CA-C	5.29	119.83	109.35
1	A	42	MET	CB-CA-C	5.29	117.97	109.61
1	A	95	ALA	N-CA-C	-5.29	100.70	108.79
1	A	42	MET	N-CA-CB	-5.27	100.87	109.56
1	A	74	SER	CB-CA-C	5.24	120.53	109.79
1	A	103	THR	CB-CA-C	5.23	118.34	109.50
1	A	127	HIS	N-CA-C	5.23	117.98	109.24
1	A	66	SER	N-CA-C	5.23	118.52	110.42
1	A	183	GLU	N-CA-CB	-5.23	103.30	111.56
1	A	200	LYS	N-CA-C	5.21	116.88	108.34
1	A	53	ILE	CA-CB-CG2	-5.18	101.69	110.50
1	A	27	ILE	N-CA-C	5.17	115.76	108.36
1	A	228	ARG	N-CA-C	-5.17	106.92	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ILE	CA-CB-CG2	-5.16	101.74	110.50
1	A	25	ILE	CA-CB-CG2	-5.14	101.76	110.50
1	A	141	ILE	CA-CB-CG2	-5.14	101.76	110.50
1	A	164	SER	N-CA-CB	-5.14	101.22	110.37
1	A	4	ILE	CA-CB-CG2	-5.13	101.77	110.50
1	A	198	LEU	CB-CA-C	-5.13	103.26	111.17
1	A	27	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	A	165	PRO	CB-CA-C	5.13	118.10	111.64
1	A	106	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	A	210	ILE	CA-CB-CG2	-5.12	101.79	110.50
1	A	199	ILE	CA-CB-CG2	-5.12	101.80	110.50
1	A	214	ILE	CA-CB-CG2	-5.12	101.81	110.50
1	A	181	ILE	CA-CB-CG2	-5.11	101.81	110.50
1	A	133	PHE	N-CA-CB	-5.11	102.29	110.46
1	A	52	ILE	CA-CB-CG2	-5.11	101.82	110.50
1	A	217	ILE	CA-CB-CG2	-5.11	101.82	110.50
1	A	28	ASP	N-CA-CB	5.08	118.53	110.55
1	A	17	ILE	CA-CB-CG2	-5.08	101.87	110.50
1	A	7	VAL	CB-CA-C	5.07	117.59	110.99
1	A	110	SER	N-CA-C	5.07	117.33	108.76
1	A	29	ILE	CA-CB-CG2	-5.07	101.88	110.50
1	A	177	ALA	CB-CA-C	5.07	117.58	109.62
1	A	201	SER	N-CA-C	5.06	119.67	108.73
1	A	50	ALA	N-CA-CB	-5.06	102.38	110.63

There are no chirality outliers.

There are no planarity outliers.

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	1807	0	1746	325	4
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	0	1	0
All	All	1813	0	1746	325	4

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 91.

All (325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HB	1:A:42:MET:CE	1.61	1.31
1:A:174:LEU:HD23	1:A:174:LEU:N	1.44	1.25
1:A:85:LEU:HD11	1:A:214:ILE:HG21	1.20	1.19
1:A:116:LYS:HD3	1:A:188:VAL:HG12	1.27	1.16
1:A:110:SER:OG	1:A:194:THR:HG22	1.42	1.16
1:A:11:THR:HB	1:A:42:MET:HE1	1.11	1.08
1:A:19:ASP:HB3	1:A:24:HIS:CE1	1.89	1.06
1:A:97:THR:HG22	1:A:169:SER:H	1.17	1.06
1:A:116:LYS:HB2	1:A:188:VAL:O	1.54	1.05
1:A:216:ASN:N	1:A:216:ASN:OD1	1.87	1.05
1:A:54:TYR:CD2	1:A:55:ASN:N	2.25	1.05
1:A:11:THR:CG2	1:A:42:MET:HE2	1.88	1.03
1:A:174:LEU:N	1:A:174:LEU:CD2	2.14	1.02
1:A:210:ILE:HG23	1:A:211:ALA:H	1.25	1.02
1:A:11:THR:CB	1:A:42:MET:CE	2.37	1.01
1:A:11:THR:HG22	1:A:42:MET:HE2	1.39	1.01
1:A:36:LYS:HD3	1:A:75:VAL:HG23	1.43	1.00
1:A:90:ARG:HD2	1:A:217:ILE:HA	1.44	0.99
1:A:88:TRP:CE2	1:A:180:HIS:NE2	2.31	0.99
1:A:191:PHE:HE1	1:A:214:ILE:HD11	1.27	0.98
1:A:143:GLN:OE1	1:A:172:ARG:HD2	1.64	0.98
1:A:56:SER:O	1:A:59:LYS:HG3	1.63	0.97
1:A:143:GLN:OE1	1:A:172:ARG:CD	2.14	0.96
1:A:173:ALA:C	1:A:174:LEU:HD23	1.89	0.96
1:A:137:GLN:HG3	1:A:140:LEU:HD12	1.48	0.95
1:A:142:LEU:HD23	1:A:173:ALA:HB2	1.46	0.94
1:A:210:ILE:CG2	1:A:211:ALA:N	2.30	0.94
1:A:133:PHE:CD2	1:A:154:LEU:HB2	2.03	0.92
1:A:4:ILE:HG12	1:A:5:VAL:N	1.84	0.92
1:A:19:ASP:HB3	1:A:24:HIS:NE2	1.85	0.92
1:A:174:LEU:HD23	1:A:174:LEU:H	1.29	0.91
1:A:128:PHE:CD1	1:A:175:PHE:CG	2.57	0.91
1:A:12:TYR:CE2	1:A:100:TYR:CE1	2.59	0.91
1:A:133:PHE:CE2	1:A:154:LEU:HB2	2.06	0.90
1:A:105:THR:HB	1:A:155:GLU:OE1	1.72	0.89
1:A:85:LEU:HD11	1:A:214:ILE:CG2	2.02	0.89
1:A:229:LEU:O	1:A:231:GLY:N	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HB2	1:A:166:GLU:HG2	1.56	0.88
1:A:128:PHE:CE1	1:A:175:PHE:HB2	2.08	0.88
1:A:110:SER:OG	1:A:194:THR:CG2	2.22	0.88
1:A:173:ALA:C	1:A:174:LEU:CD2	2.46	0.86
1:A:103:THR:HG22	1:A:105:THR:HG22	1.56	0.86
1:A:19:ASP:CB	1:A:24:HIS:CE1	2.59	0.85
1:A:134:SER:OG	1:A:137:GLN:N	2.10	0.85
1:A:54:TYR:CD2	1:A:54:TYR:C	2.55	0.84
1:A:88:TRP:CD2	1:A:180:HIS:CD2	2.66	0.84
1:A:116:LYS:HD3	1:A:188:VAL:CG1	2.07	0.84
1:A:117:SER:HB2	1:A:123:THR:HG21	1.58	0.84
1:A:225:SER:HB3	1:A:231:GLY:HA2	1.58	0.83
1:A:51:HIS:C	1:A:52:ILE:HG13	2.03	0.83
1:A:93:LEU:HB3	1:A:156:LEU:HD11	1.59	0.82
1:A:162:ASN:H	1:A:162:ASN:ND2	1.77	0.82
1:A:143:GLN:N	1:A:172:ARG:O	2.12	0.81
1:A:88:TRP:CE2	1:A:180:HIS:CD2	2.69	0.81
1:A:210:ILE:HG23	1:A:211:ALA:N	1.93	0.80
1:A:25:ILE:HG21	1:A:65:VAL:HG21	1.62	0.80
1:A:88:TRP:NE1	1:A:180:HIS:NE2	2.30	0.80
1:A:133:PHE:HD2	1:A:154:LEU:N	1.79	0.79
1:A:11:THR:CB	1:A:42:MET:HE2	2.08	0.79
1:A:85:LEU:CD1	1:A:214:ILE:HG21	2.09	0.79
1:A:133:PHE:CE2	1:A:154:LEU:CB	2.65	0.79
1:A:128:PHE:CD1	1:A:175:PHE:CD1	2.71	0.78
1:A:85:LEU:HD13	1:A:89:VAL:HG21	1.66	0.78
1:A:12:TYR:HB2	1:A:207:ALA:O	1.84	0.78
1:A:117:SER:CB	1:A:123:THR:HG21	2.14	0.78
1:A:89:VAL:HG22	1:A:215:SER:O	1.83	0.77
1:A:191:PHE:HD2	1:A:191:PHE:O	1.67	0.77
1:A:133:PHE:CD2	1:A:154:LEU:N	2.53	0.76
1:A:143:GLN:OE1	1:A:172:ARG:HD3	1.86	0.76
1:A:191:PHE:CE1	1:A:214:ILE:HD11	2.16	0.76
1:A:210:ILE:HG22	1:A:211:ALA:N	2.01	0.76
1:A:65:VAL:O	1:A:73:THR:HG23	1.87	0.75
1:A:191:PHE:C	1:A:191:PHE:CD2	2.63	0.75
1:A:56:SER:O	1:A:59:LYS:CG	2.33	0.75
1:A:11:THR:CG2	1:A:42:MET:CE	2.64	0.75
1:A:97:THR:CG2	1:A:167:GLY:HA2	2.16	0.75
1:A:105:THR:HG23	1:A:198:LEU:O	1.86	0.74
1:A:102:GLU:HG2	1:A:199:ILE:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:CD2	1:A:154:LEU:CB	2.69	0.74
1:A:222:PRO:HG2	1:A:225:SER:OG	1.87	0.74
1:A:179:VAL:HG12	1:A:181:ILE:HD13	1.68	0.74
1:A:128:PHE:CE1	1:A:175:PHE:CB	2.71	0.74
1:A:162:ASN:ND2	1:A:162:ASN:N	2.34	0.74
1:A:187:THR:HG23	1:A:188:VAL:HG23	1.70	0.74
1:A:191:PHE:HD2	1:A:191:PHE:C	1.94	0.74
1:A:128:PHE:CE1	1:A:175:PHE:CG	2.77	0.73
1:A:162:ASN:N	1:A:162:ASN:HD22	1.87	0.72
1:A:55:ASN:O	1:A:59:LYS:N	2.21	0.72
1:A:141:ILE:O	1:A:173:ALA:HA	1.89	0.72
1:A:44:ASP:OD2	1:A:44:ASP:C	2.32	0.72
1:A:11:THR:O	1:A:13:PRO:HD3	1.90	0.71
1:A:36:LYS:HD2	1:A:76:SER:O	1.88	0.71
1:A:122:GLN:O	1:A:122:GLN:HG2	1.90	0.71
1:A:124:ASP:OD2	1:A:124:ASP:N	2.23	0.71
1:A:89:VAL:HG21	1:A:214:ILE:CG2	2.19	0.71
1:A:222:PRO:CD	1:A:225:SER:OG	2.39	0.71
1:A:97:THR:HG22	1:A:169:SER:N	2.01	0.70
1:A:105:THR:CG2	1:A:198:LEU:O	2.40	0.70
1:A:142:LEU:HD23	1:A:173:ALA:CB	2.20	0.70
1:A:157:THR:HG23	1:A:158:ARG:N	2.06	0.70
1:A:128:PHE:HD1	1:A:175:PHE:CD1	2.09	0.70
1:A:36:LYS:HD3	1:A:75:VAL:CG2	2.21	0.69
1:A:89:VAL:HG12	1:A:179:VAL:HB	1.73	0.69
1:A:179:VAL:HG12	1:A:181:ILE:CD1	2.22	0.69
1:A:187:THR:CG2	1:A:188:VAL:HG23	2.23	0.69
1:A:105:THR:HG23	1:A:198:LEU:HB3	1.75	0.68
1:A:107:LEU:HD23	1:A:107:LEU:N	2.09	0.68
1:A:11:THR:CB	1:A:42:MET:HE1	2.05	0.68
1:A:187:THR:C	1:A:188:VAL:HG23	2.18	0.68
1:A:222:PRO:HD2	1:A:225:SER:OG	1.93	0.68
1:A:89:VAL:CG2	1:A:215:SER:O	2.42	0.67
1:A:33:ARG:HE	1:A:237:ASN:HB2	1.60	0.67
1:A:116:LYS:CD	1:A:188:VAL:HG12	2.16	0.67
1:A:54:TYR:CD2	1:A:55:ASN:CA	2.78	0.67
1:A:210:ILE:CG2	1:A:211:ALA:H	1.92	0.67
1:A:55:ASN:HB2	1:A:189:SER:O	1.96	0.66
1:A:106:ILE:C	1:A:107:LEU:HD23	2.20	0.66
1:A:224:GLY:C	1:A:226:THR:N	2.48	0.66
1:A:224:GLY:C	1:A:226:THR:H	2.02	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HG21	1:A:167:GLY:HA2	1.78	0.66
1:A:222:PRO:HG2	1:A:225:SER:HG	1.60	0.65
1:A:236:ALA:C	1:A:237:ASN:CG	2.63	0.65
1:A:173:ALA:CA	1:A:174:LEU:HD23	2.26	0.65
1:A:25:ILE:HD12	1:A:75:VAL:HG12	1.79	0.65
1:A:106:ILE:CD1	1:A:156:LEU:HG	2.27	0.65
1:A:56:SER:O	1:A:57:VAL:C	2.39	0.64
1:A:56:SER:HA	1:A:59:LYS:HG2	1.80	0.64
1:A:103:THR:HG22	1:A:105:THR:CG2	2.25	0.64
1:A:148:THR:HG22	1:A:154:LEU:CD1	2.28	0.64
1:A:221:ILE:HG22	1:A:225:SER:CB	2.29	0.63
1:A:222:PRO:CG	1:A:225:SER:OG	2.46	0.63
1:A:93:LEU:N	1:A:173:ALA:O	2.31	0.63
1:A:173:ALA:C	1:A:174:LEU:HD22	2.24	0.63
1:A:26:GLY:C	1:A:27:ILE:HD13	2.24	0.62
1:A:25:ILE:HD13	1:A:65:VAL:HG23	1.79	0.62
1:A:123:THR:C	1:A:124:ASP:OD2	2.43	0.62
1:A:96:SER:HB2	1:A:230:LEU:HA	1.82	0.61
1:A:51:HIS:C	1:A:52:ILE:CG1	2.74	0.61
1:A:85:LEU:HD22	1:A:86:PRO:HD2	1.82	0.61
1:A:215:SER:OG	1:A:219:SER:HB2	2.01	0.60
1:A:54:TYR:CG	1:A:55:ASN:N	2.68	0.60
1:A:28:ASP:HB3	1:A:31:SER:O	2.02	0.60
1:A:198:LEU:C	1:A:198:LEU:HD23	2.26	0.60
1:A:17:ILE:O	1:A:33:ARG:NH1	2.35	0.60
1:A:182:TRP:CG	1:A:183:GLU:N	2.70	0.60
1:A:92:GLY:HA2	1:A:174:LEU:HA	1.83	0.60
1:A:183:GLU:HG2	1:A:184:SER:H	1.67	0.60
1:A:9:LEU:O	1:A:209:GLY:HA3	2.02	0.59
1:A:85:LEU:CD1	1:A:89:VAL:HG21	2.31	0.59
1:A:97:THR:HG23	1:A:167:GLY:HA2	1.84	0.59
1:A:134:SER:HG	1:A:137:GLN:H	1.50	0.59
1:A:148:THR:HG22	1:A:154:LEU:HD13	1.84	0.59
1:A:100:TYR:CB	1:A:207:ALA:HA	2.32	0.59
1:A:44:ASP:OD2	1:A:45:GLY:N	2.36	0.58
1:A:12:TYR:CE2	1:A:100:TYR:CD1	2.91	0.58
1:A:133:PHE:CD2	1:A:154:LEU:CA	2.85	0.58
1:A:93:LEU:O	1:A:172:ARG:HB3	2.03	0.58
1:A:221:ILE:CG2	1:A:225:SER:CB	2.82	0.58
1:A:158:ARG:O	1:A:166:GLU:HB3	2.04	0.58
1:A:157:THR:CG2	1:A:158:ARG:N	2.63	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:HG22	1:A:18:GLY:N	2.19	0.58
1:A:55:ASN:ND2	1:A:58:ASP:H	2.02	0.57
1:A:85:LEU:HD13	1:A:89:VAL:CG2	2.34	0.57
1:A:89:VAL:CG1	1:A:179:VAL:HB	2.35	0.57
1:A:118:ASN:ND2	1:A:185:SER:O	2.38	0.57
1:A:128:PHE:CD1	1:A:175:PHE:CD2	2.92	0.57
1:A:137:GLN:HA	1:A:137:GLN:OE1	1.95	0.57
1:A:54:TYR:C	1:A:54:TYR:HD2	2.08	0.57
1:A:33:ARG:HE	1:A:237:ASN:CB	2.18	0.56
1:A:173:ALA:HA	1:A:174:LEU:HD23	1.86	0.56
1:A:27:ILE:HD13	1:A:27:ILE:N	2.21	0.56
1:A:141:ILE:O	1:A:174:LEU:HD23	2.06	0.56
1:A:102:GLU:CB	1:A:207:ALA:HB3	2.35	0.56
1:A:112:THR:HB	1:A:192:GLU:HG2	1.86	0.56
1:A:19:ASP:O	1:A:20:PRO:O	2.23	0.55
1:A:187:THR:C	1:A:188:VAL:CG2	2.78	0.55
1:A:211:ALA:HB2	1:A:230:LEU:HD23	1.87	0.55
1:A:4:ILE:HD11	1:A:6:ALA:HB2	1.87	0.55
1:A:12:TYR:CD2	1:A:100:TYR:CD1	2.94	0.55
1:A:12:TYR:CD1	1:A:12:TYR:C	2.84	0.55
1:A:98:GLY:HA2	1:A:168:SER:HA	1.88	0.55
1:A:229:LEU:C	1:A:231:GLY:H	2.15	0.55
1:A:11:THR:O	1:A:13:PRO:CD	2.54	0.55
1:A:12:TYR:HE2	1:A:100:TYR:CE1	2.21	0.55
1:A:68:PRO:C	1:A:70:ALA:H	2.15	0.54
1:A:229:LEU:C	1:A:231:GLY:N	2.66	0.54
1:A:211:ALA:HB1	1:A:232:LEU:HD21	1.90	0.53
1:A:149:GLY:O	1:A:150:THR:C	2.51	0.53
1:A:212:PHE:CD1	1:A:212:PHE:C	2.85	0.53
1:A:27:ILE:CG2	1:A:61:LEU:HD23	2.38	0.53
1:A:27:ILE:HG23	1:A:61:LEU:HD23	1.91	0.53
1:A:80:ASP:O	1:A:84:VAL:HG23	2.09	0.53
1:A:28:ASP:OD2	1:A:28:ASP:N	2.42	0.52
1:A:12:TYR:CE2	1:A:100:TYR:HE1	2.21	0.52
1:A:162:ASN:H	1:A:162:ASN:HD22	1.47	0.52
1:A:102:GLU:HB3	1:A:207:ALA:HB3	1.91	0.52
1:A:54:TYR:HD2	1:A:55:ASN:N	2.02	0.52
1:A:49:THR:HA	1:A:196:ALA:HA	1.92	0.52
1:A:133:PHE:CE2	1:A:154:LEU:HB3	2.44	0.52
1:A:29:ILE:O	1:A:30:LYS:HB2	2.11	0.52
1:A:141:ILE:HD11	1:A:176:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:O	1:A:137:GLN:C	2.53	0.51
1:A:225:SER:CB	1:A:231:GLY:HA2	2.33	0.51
1:A:211:ALA:HB1	1:A:232:LEU:CD2	2.41	0.50
1:A:117:SER:HB3	1:A:123:THR:HG21	1.93	0.50
1:A:86:PRO:HG3	1:A:216:ASN:HB3	1.94	0.50
1:A:27:ILE:O	1:A:35:LYS:N	2.40	0.50
1:A:51:HIS:O	1:A:52:ILE:CG1	2.59	0.50
1:A:67:TYR:CB	1:A:70:ALA:HB3	2.42	0.50
1:A:215:SER:OG	1:A:219:SER:CB	2.60	0.50
1:A:97:THR:CG2	1:A:167:GLY:CA	2.88	0.50
1:A:55:ASN:HD21	1:A:58:ASP:H	1.59	0.49
1:A:88:TRP:CZ2	1:A:180:HIS:NE2	2.80	0.49
1:A:128:PHE:HB2	1:A:175:PHE:CZ	2.47	0.49
1:A:228:ARG:C	1:A:230:LEU:H	2.20	0.49
1:A:26:GLY:HA3	1:A:36:LYS:O	2.12	0.49
1:A:89:VAL:HG21	1:A:214:ILE:HG22	1.95	0.49
1:A:221:ILE:HG22	1:A:225:SER:HB2	1.92	0.49
1:A:128:PHE:HE1	1:A:175:PHE:HB2	1.75	0.49
1:A:133:PHE:CG	1:A:154:LEU:HB2	2.48	0.48
1:A:106:ILE:HD12	1:A:156:LEU:HG	1.96	0.48
1:A:183:GLU:CG	1:A:184:SER:N	2.76	0.48
1:A:19:ASP:C	1:A:20:PRO:O	2.56	0.48
1:A:51:HIS:O	1:A:52:ILE:HG13	2.13	0.48
1:A:80:ASP:HB3	1:A:83:ASP:OD2	2.13	0.48
1:A:204:SER:C	1:A:206:PRO:HD3	2.38	0.48
1:A:3:THR:H	1:A:216:ASN:HD21	1.61	0.48
1:A:28:ASP:HB2	1:A:233:PHE:CZ	2.48	0.48
1:A:63:ALA:O	1:A:74:SER:HB2	2.14	0.48
1:A:91:VAL:HG21	1:A:111:PHE:CZ	2.49	0.48
1:A:36:LYS:HB3	1:A:75:VAL:CG2	2.44	0.48
1:A:32:VAL:O	1:A:34:SER:N	2.45	0.47
1:A:106:ILE:HD11	1:A:156:LEU:CD1	2.44	0.47
1:A:54:TYR:CD2	1:A:55:ASN:HA	2.49	0.47
1:A:100:TYR:HB3	1:A:207:ALA:HA	1.96	0.47
1:A:225:SER:HB3	1:A:231:GLY:CA	2.38	0.47
1:A:68:PRO:O	1:A:69:ASN:HB2	2.14	0.47
1:A:208:ASP:HB3	4:A:243:HOH:O	2.13	0.47
1:A:87:GLU:HG3	1:A:182:TRP:HE3	1.80	0.47
1:A:97:THR:HG21	1:A:167:GLY:CA	2.45	0.46
1:A:104:ASN:OD1	1:A:199:ILE:HD13	2.15	0.46
1:A:128:PHE:CB	1:A:175:PHE:CZ	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD11	1:A:176:TYR:CD1	2.51	0.46
1:A:22:TYR:HB2	1:A:23:PRO:HD2	1.96	0.46
1:A:229:LEU:O	1:A:230:LEU:C	2.57	0.46
1:A:91:VAL:HG21	1:A:111:PHE:CE1	2.50	0.46
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.74	0.46
1:A:41:ASN:O	1:A:43:GLN:HG3	2.15	0.46
1:A:97:THR:CG2	1:A:168:SER:N	2.78	0.46
1:A:173:ALA:CA	1:A:174:LEU:CD2	2.91	0.46
1:A:160:SER:HB2	1:A:164:SER:OG	2.17	0.45
1:A:108:SER:HA	1:A:130:PHE:O	2.16	0.45
1:A:221:ILE:CG2	1:A:225:SER:HB2	2.46	0.45
1:A:50:ALA:O	1:A:194:THR:HA	2.17	0.45
1:A:102:GLU:CG	1:A:199:ILE:HG23	2.43	0.45
1:A:92:GLY:CA	1:A:173:ALA:O	2.64	0.45
1:A:181:ILE:HD13	1:A:181:ILE:N	2.32	0.45
1:A:97:THR:HG22	1:A:168:SER:N	2.31	0.45
1:A:12:TYR:CD1	1:A:12:TYR:O	2.70	0.45
1:A:115:LEU:O	1:A:123:THR:HB	2.17	0.45
1:A:88:TRP:CZ2	1:A:180:HIS:CE1	3.05	0.45
1:A:97:THR:CG2	1:A:167:GLY:C	2.90	0.44
1:A:111:PHE:CB	1:A:128:PHE:CE2	3.00	0.44
1:A:50:ALA:N	1:A:195:PHE:O	2.43	0.44
1:A:133:PHE:CZ	1:A:154:LEU:HB2	2.51	0.44
1:A:183:GLU:HG2	1:A:184:SER:N	2.32	0.44
1:A:216:ASN:C	1:A:218:ASP:N	2.70	0.44
1:A:11:THR:OG1	1:A:102:GLU:OE2	2.24	0.44
1:A:12:TYR:O	1:A:12:TYR:HD1	2.01	0.44
1:A:217:ILE:H	1:A:217:ILE:HG23	1.39	0.44
1:A:51:HIS:CD2	1:A:194:THR:OG1	2.71	0.44
1:A:102:GLU:HB2	1:A:207:ALA:CB	2.47	0.44
1:A:103:THR:O	1:A:199:ILE:HA	2.17	0.44
1:A:93:LEU:O	1:A:172:ARG:CB	2.66	0.44
1:A:67:TYR:HB3	1:A:70:ALA:HB3	1.99	0.43
1:A:89:VAL:CG2	1:A:214:ILE:CG2	2.94	0.43
1:A:103:THR:OG1	1:A:165:PRO:HB3	2.17	0.43
1:A:212:PHE:CD1	1:A:212:PHE:O	2.71	0.43
1:A:136:ASP:O	1:A:137:GLN:O	2.36	0.43
1:A:148:THR:HG22	1:A:154:LEU:HD12	1.99	0.43
1:A:228:ARG:HG3	1:A:229:LEU:N	2.33	0.43
1:A:102:GLU:CB	1:A:207:ALA:CB	2.97	0.43
1:A:221:ILE:HG22	1:A:225:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:CD2	1:A:180:HIS:HD2	2.30	0.43
1:A:103:THR:HB	1:A:200:LYS:HB2	1.99	0.43
1:A:163:GLY:O	1:A:164:SER:C	2.62	0.43
1:A:22:TYR:CD1	1:A:39:LYS:NZ	2.78	0.43
1:A:60:ARG:HE	1:A:76:SER:HB3	1.82	0.43
1:A:63:ALA:C	1:A:64:VAL:CG2	2.91	0.43
1:A:111:PHE:HB2	1:A:128:PHE:CE2	2.53	0.43
1:A:92:GLY:HA2	1:A:173:ALA:O	2.19	0.42
1:A:198:LEU:C	1:A:198:LEU:CD2	2.91	0.42
1:A:4:ILE:HG12	1:A:5:VAL:C	2.44	0.42
1:A:26:GLY:HA2	1:A:75:VAL:HG11	2.02	0.42
1:A:102:GLU:HB2	1:A:207:ALA:HB3	2.01	0.42
1:A:109:TRP:O	1:A:130:PHE:N	2.48	0.42
1:A:166:GLU:HG3	1:A:167:GLY:N	2.33	0.42
1:A:102:GLU:HB2	1:A:207:ALA:H	1.84	0.42
1:A:170:VAL:O	1:A:170:VAL:HG13	2.20	0.42
1:A:118:ASN:O	1:A:119:SER:C	2.63	0.42
1:A:137:GLN:NE2	1:A:139:ASP:OD1	2.52	0.42
1:A:164:SER:HA	1:A:165:PRO:HD2	1.91	0.42
1:A:43:GLN:OE1	1:A:70:ALA:HB2	2.19	0.42
1:A:182:TRP:CE3	1:A:183:GLU:HA	2.55	0.42
1:A:128:PHE:HB2	1:A:175:PHE:CE2	2.55	0.42
1:A:142:LEU:HD11	1:A:148:THR:HG23	2.02	0.42
1:A:31:SER:OG	1:A:33:ARG:N	2.53	0.42
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.93	0.41
1:A:96:SER:CB	1:A:230:LEU:HA	2.49	0.41
1:A:222:PRO:CG	1:A:225:SER:HG	2.27	0.41
1:A:80:ASP:CB	1:A:83:ASP:OD2	2.68	0.41
1:A:158:ARG:HB2	1:A:166:GLU:CG	2.37	0.41
1:A:40:TRP:HE1	1:A:67:TYR:HE1	1.67	0.41
1:A:160:SER:CB	1:A:164:SER:OG	2.69	0.41
1:A:127:HIS:NE2	1:A:129:MET:HG3	2.36	0.41
1:A:101:LYS:NZ	1:A:203:ASP:OD1	2.54	0.41
1:A:204:SER:O	1:A:206:PRO:CD	2.69	0.41
1:A:36:LYS:CD	1:A:75:VAL:HG23	2.31	0.41
1:A:102:GLU:HG2	1:A:199:ILE:CG2	2.46	0.41
1:A:156:LEU:HD22	1:A:172:ARG:HA	2.03	0.41
1:A:33:ARG:O	1:A:34:SER:C	2.64	0.41
1:A:102:GLU:CG	1:A:199:ILE:CG2	2.99	0.41
1:A:93:LEU:O	1:A:172:ARG:CA	2.69	0.40
1:A:228:ARG:HG3	1:A:229:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HB2	1:A:217:ILE:HA	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:NE2	1:A:122:GLN:NE2[4_565]	1.49	0.71
1:A:57:VAL:CG1	1:A:62:SER:OG[3_655]	1.92	0.28
1:A:15:THR:OG1	1:A:184:SER:OG[8_555]	1.96	0.24
1:A:122:GLN:CD	1:A:122:GLN:NE2[4_565]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/202 (100%)	136 (67%)	66 (33%)	0 0

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	THR
1	A	4	ILE
1	A	15	THR
1	A	16	ASP
1	A	17	ILE
1	A	19	ASP

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Mol	Chain	Res	Type
1	A	21	SER
1	A	27	ILE
1	A	28	ASP
1	A	30	LYS
1	A	31	SER
1	A	32	VAL
1	A	34	SER
1	A	40	TRP
1	A	42	MET
1	A	46	LYS
1	A	55	ASN
1	A	62	SER
1	A	65	VAL
1	A	66	SER
1	A	73	THR
1	A	75	VAL
1	A	79	VAL
1	A	80	ASP
1	A	85	LEU
1	A	89	VAL
1	A	91	VAL
1	A	94	SER
1	A	97	THR
1	A	99	LEU
1	A	105	THR
1	A	106	ILE
1	A	107	LEU
1	A	114	LYS
1	A	118	ASN
1	A	124	ASP
1	A	126	LEU
1	A	128	PHE
1	A	132	GLN
1	A	135	LYS
1	A	136	ASP
1	A	137	GLN
1	A	157	THR
1	A	159	VAL
1	A	160	SER
1	A	162	ASN
1	A	164	SER
1	A	166	GLU

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Mol	Chain	Res	Type
1	A	172	ARG
1	A	174	LEU
1	A	180	HIS
1	A	181	ILE
1	A	185	SER
1	A	187	THR
1	A	191	PHE
1	A	192	GLU
1	A	199	ILE
1	A	214	ILE
1	A	216	ASN
1	A	221	ILE
1	A	226	THR
1	A	229	LEU
1	A	232	LEU
1	A	235	ASP
1	A	237	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	55	ASN
1	A	82	ASN
1	A	118	ASN
1	A	131	ASN
1	A	132	GLN
1	A	162	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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.