



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:22 AM UTC

PDB ID : 1ENQ / pdb_00001enq
Title : CO-CRYSTALS OF DEMETALLIZED CONCAVALIN A WITH ZINC
HAVING A ZINC ION BOUND IN THE S1 SITE
Authors : Bouckaert, J.; Loris, R.; Poortmans, F.; Wyns, L.
Deposited on : 1996-03-20
Resolution : 2.50 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

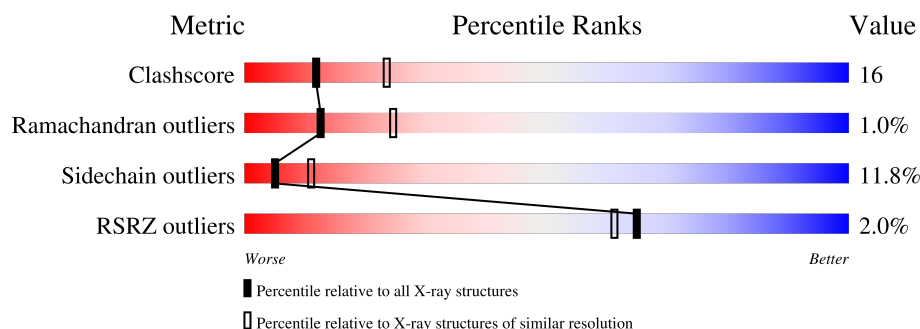
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	2% 55% 31% 9% • •
1	B	237	2% 58% 32% 7% • •
1	C	237	3% 54% 34% 8% • •
1	D	237	% 57% 31% 6% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7335 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 CONCAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	3	0	1
			1766	1117	294	353	2			
1	B	233	Total	C	N	O	S	12	0	1
			1780	1126	297	355	2			
1	C	231	Total	C	N	O	S	15	0	1
			1764	1116	294	352	2			
1	D	226	Total	C	N	O	S	16	0	2
			1726	1094	289	341	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	conflict	UNP P02866
A	155	GLU	ARG	conflict	UNP P02866
B	151	ASP	GLU	conflict	UNP P02866
B	155	GLU	ARG	conflict	UNP P02866
C	151	ASP	GLU	conflict	UNP P02866
C	155	GLU	ARG	conflict	UNP P02866
D	151	ASP	GLU	conflict	UNP P02866
D	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

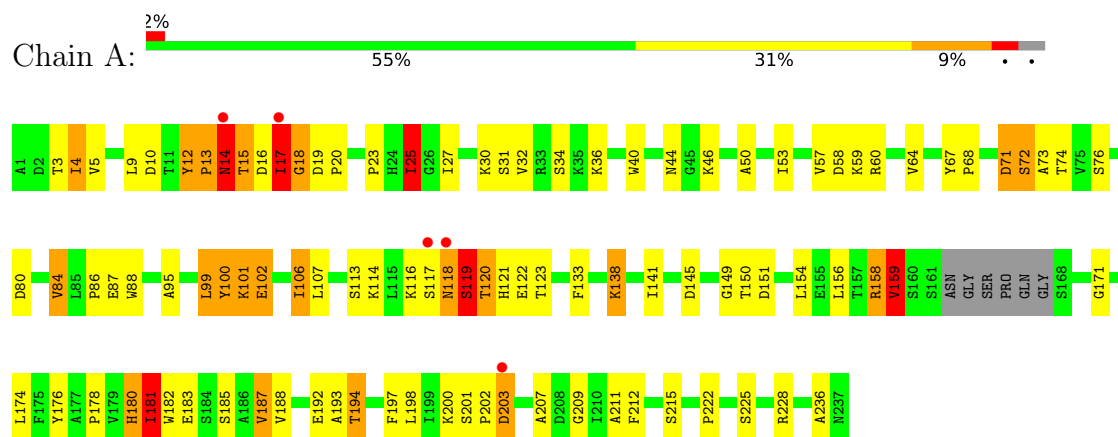
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	89	Total 89	O 89	0	0
3	C	54	Total 54	O 54	0	0
3	D	64	Total 64	O 64	0	0

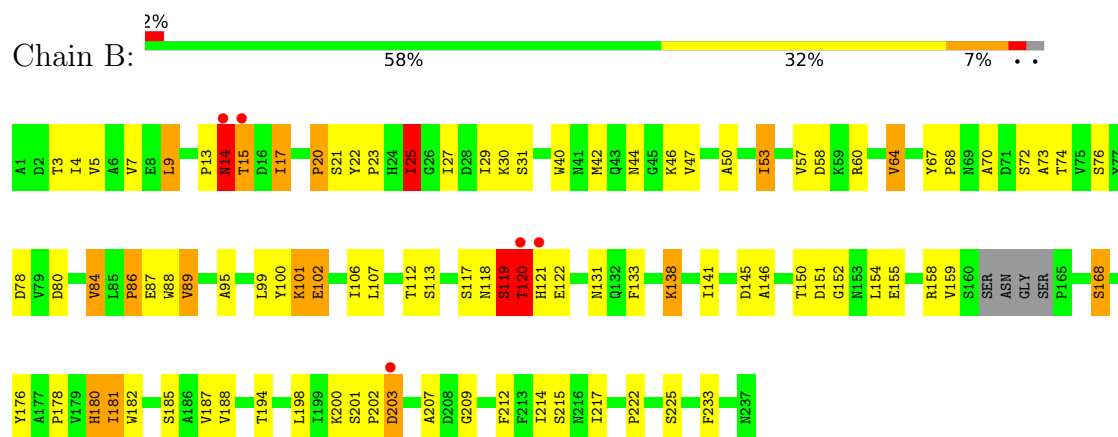
3 Residue-property plots [i](#)

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

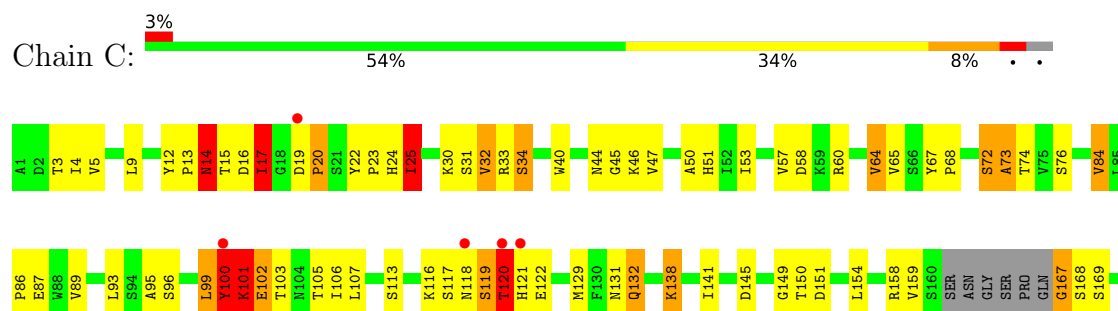
• Molecule 1: CONCANAVALIN A

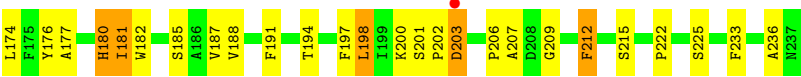


• Molecule 1: CONCANAVALIN A

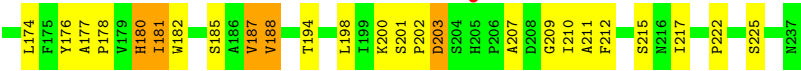
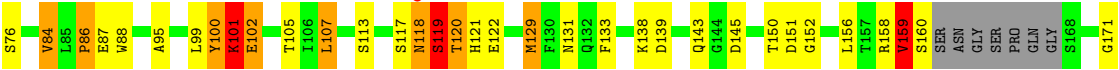


• Molecule 1: CONCANAVALIN A





● Molecule 1: CONCANAVALIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.23Å 113.03Å 122.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (10.00-2.50) 92.6 (10.00-2.50)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.198 , 0.284 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7335	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.73	24/1806 (1.3%)	1.55	31/2460 (1.3%)
1	B	1.60	19/1821 (1.0%)	1.55	28/2480 (1.1%)
1	C	1.54	14/1804 (0.8%)	1.58	36/2457 (1.5%)
1	D	1.48	12/1765 (0.7%)	1.48	28/2402 (1.2%)
All	All	1.59	69/7196 (1.0%)	1.54	123/9799 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	9

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	ILE	CA-CB	9.88	1.67	1.54
1	A	141	ILE	CA-CB	-8.96	1.43	1.54
1	C	14	ASN	N-CA	-8.64	1.35	1.46
1	A	5	VAL	CA-CB	-8.62	1.43	1.54
1	B	17	ILE	CA-CB	8.34	1.65	1.54
1	B	14	ASN	CA-CB	8.12	1.63	1.52
1	A	27	ILE	CA-CB	-7.75	1.44	1.54
1	A	71	ASP	CA-C	-7.38	1.43	1.52
1	A	14	ASN	N-CA	-7.29	1.36	1.46
1	C	17	ILE	CA-C	7.02	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	ILE	CA-C	6.92	1.61	1.52
1	C	25	ILE	CA-CB	6.80	1.63	1.54
1	A	211	ALA	CA-CB	-6.79	1.42	1.53
1	B	207	ALA	CA-CB	-6.77	1.44	1.53
1	B	13	PRO	C-N	6.77	1.43	1.33
1	D	27	ILE	CA-CB	-6.74	1.46	1.54
1	A	197	PHE	CA-C	-6.68	1.44	1.52
1	D	24	HIS	CD2-NE2	6.68	1.45	1.37
1	D	129	MET	SD-CE	6.63	1.96	1.79
1	A	27	ILE	C-O	-6.57	1.17	1.24
1	A	123	THR	CA-CB	-6.57	1.44	1.53
1	A	194	THR	C-O	-6.44	1.16	1.23
1	A	4	ILE	C-O	-6.38	1.17	1.24
1	B	80	ASP	C-O	-6.34	1.16	1.23
1	A	67	TYR	CA-C	-6.32	1.46	1.52
1	A	64	VAL	CA-CB	-6.30	1.46	1.54
1	D	57	VAL	C-O	-6.27	1.17	1.24
1	B	17	ILE	N-CA	6.25	1.54	1.46
1	C	168	SER	CA-C	6.25	1.61	1.52
1	C	84	VAL	CA-CB	-6.17	1.48	1.55
1	A	68	PRO	CA-C	-6.16	1.44	1.52
1	A	181	ILE	CA-C	-6.14	1.44	1.52
1	B	14	ASN	N-CA	6.08	1.54	1.46
1	B	27	ILE	C-O	-6.04	1.17	1.24
1	B	13	PRO	CA-C	6.01	1.60	1.53
1	C	191	PHE	CA-C	-6.00	1.45	1.52
1	B	42	MET	SD-CE	-5.87	1.64	1.79
1	C	13	PRO	C-N	-5.85	1.25	1.33
1	A	114	LYS	C-O	-5.83	1.16	1.23
1	D	67	TYR	CA-C	-5.72	1.46	1.52
1	A	133	PHE	CA-C	-5.69	1.45	1.52
1	D	143	GLN	CA-C	-5.68	1.45	1.52
1	D	7	VAL	CA-C	-5.60	1.45	1.52
1	D	22	TYR	CA-C	5.60	1.57	1.52
1	A	57	VAL	CA-CB	-5.57	1.47	1.54
1	B	112	THR	CA-CB	-5.54	1.44	1.53
1	C	17	ILE	N-CA	5.51	1.53	1.46
1	D	159	VAL	C-N	-5.43	1.25	1.33
1	A	159	VAL	CA-CB	5.42	1.59	1.53
1	B	70	ALA	CA-C	-5.41	1.46	1.53
1	A	194	THR	CA-CB	-5.33	1.43	1.53
1	A	27	ILE	CA-C	-5.33	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	ILE	CA-CB	-5.30	1.47	1.54
1	C	132	GLN	N-CA	-5.28	1.40	1.46
1	B	89	VAL	CA-CB	5.28	1.61	1.54
1	A	106	ILE	CA-CB	-5.26	1.48	1.54
1	D	180	HIS	CA-C	5.26	1.59	1.52
1	A	72	SER	C-O	-5.22	1.17	1.23
1	B	214	ILE	C-O	-5.22	1.18	1.24
1	A	183	GLU	CA-C	-5.22	1.46	1.52
1	C	129	MET	SD-CE	5.22	1.92	1.79
1	C	32	VAL	CA-CB	-5.22	1.48	1.54
1	D	159	VAL	CA-CB	5.15	1.68	1.54
1	D	84	VAL	CA-CB	-5.13	1.49	1.55
1	B	102	GLU	N-CA	-5.12	1.39	1.46
1	C	116	LYS	C-O	-5.12	1.17	1.24
1	B	25	ILE	CA-C	5.07	1.58	1.52
1	C	120	THR	CA-CB	5.07	1.62	1.53
1	B	57	VAL	CA-CB	-5.06	1.47	1.54

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	THR	N-CA-C	-14.09	80.23	107.57
1	C	15	THR	N-CA-C	-13.30	84.16	108.24
1	B	15	THR	N-CA-C	-12.09	84.11	107.57
1	B	13	PRO	CA-C-O	-10.65	113.43	121.31
1	B	5	VAL	N-CA-C	-8.87	95.69	108.11
1	C	3	THR	N-CA-C	-8.68	95.37	109.96
1	C	121	HIS	N-CA-C	8.68	126.16	113.40
1	D	176	TYR	N-CA-C	8.52	120.64	111.36
1	C	207	ALA	N-CA-C	-8.25	95.85	108.96
1	B	84	VAL	CB-CA-C	-7.99	103.85	111.44
1	B	3	THR	N-CA-C	-7.92	96.31	109.46
1	D	203	ASP	N-CA-C	-7.79	97.90	110.20
1	D	3	THR	N-CA-C	-7.62	96.81	109.46
1	D	5	VAL	N-CA-C	-7.47	97.65	108.11
1	D	84	VAL	CB-CA-C	-7.35	104.45	111.44
1	C	25	ILE	N-CA-C	-7.21	98.09	108.48
1	B	14	ASN	N-CA-CB	7.21	121.16	110.49
1	D	12	TYR	CA-C-N	7.12	128.75	119.84
1	D	12	TYR	C-N-CA	7.12	128.75	119.84
1	C	212	PHE	N-CA-C	-7.11	98.02	109.96
1	D	25	ILE	N-CA-C	-7.09	98.25	108.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	VAL	CB-CA-C	-7.06	99.62	110.50
1	A	64	VAL	CB-CA-C	-7.06	99.63	110.50
1	A	84	VAL	N-CA-C	7.03	117.60	111.56
1	B	138	LYS	N-CA-C	7.00	121.08	112.54
1	C	12	TYR	CA-C-N	7.00	128.59	119.84
1	C	12	TYR	C-N-CA	7.00	128.59	119.84
1	C	102	GLU	N-CA-C	-6.87	98.29	108.79
1	A	138	LYS	N-CA-C	6.80	120.83	112.54
1	B	212	PHE	N-CA-C	-6.76	98.67	109.76
1	D	57	VAL	N-CA-C	-6.75	104.27	110.82
1	A	25	ILE	N-CA-C	-6.75	98.74	108.53
1	A	9	LEU	N-CA-C	-6.71	93.67	107.70
1	A	12	TYR	CA-C-N	6.66	128.16	119.84
1	A	12	TYR	C-N-CA	6.66	128.16	119.84
1	A	176	TYR	N-CA-C	6.65	118.61	111.36
1	A	84	VAL	CB-CA-C	-6.64	105.13	111.44
1	D	207	ALA	N-CA-C	-6.60	98.51	109.46
1	C	5	VAL	N-CA-C	-6.59	99.00	108.48
1	A	102	GLU	N-CA-C	-6.57	98.30	108.42
1	A	207	ALA	N-CA-C	-6.50	98.67	109.46
1	C	67	TYR	N-CA-C	-6.36	99.22	109.58
1	A	3	THR	N-CA-C	-6.35	98.92	109.46
1	D	121	HIS	N-CA-C	6.32	122.69	113.40
1	B	25	ILE	N-CA-C	-6.32	99.37	108.53
1	B	176	TYR	N-CA-C	6.26	119.08	111.82
1	A	57	VAL	N-CA-C	-6.25	105.06	110.74
1	A	212	PHE	N-CA-C	-6.14	99.64	109.96
1	B	207	ALA	N-CA-C	-6.14	99.19	108.96
1	C	180	HIS	CA-C-O	-6.11	114.74	121.58
1	A	203	ASP	N-CA-C	-6.11	101.25	110.28
1	C	176	TYR	N-CA-C	6.02	118.81	111.82
1	A	121	HIS	CA-C-N	-5.98	113.20	122.05
1	A	121	HIS	C-N-CA	-5.98	113.20	122.05
1	B	233	PHE	CA-C-N	5.98	125.68	119.64
1	B	233	PHE	C-N-CA	5.98	125.68	119.64
1	D	7	VAL	N-CA-C	-5.96	97.22	107.24
1	D	101	LYS	N-CA-C	-5.94	99.05	108.73
1	D	131	ASN	N-CA-C	-5.92	105.37	113.30
1	A	67	TYR	N-CA-C	-5.85	100.05	109.58
1	C	167	GLY	CA-C-N	5.85	132.71	121.54
1	C	167	GLY	C-N-CA	5.85	132.71	121.54
1	B	64	VAL	CB-CA-C	-5.84	101.50	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	PRO	N-CA-C	-5.84	102.43	111.13
1	C	9	LEU	N-CA-C	-5.82	95.99	107.69
1	C	57	VAL	N-CA-C	-5.79	105.20	110.82
1	A	5	VAL	N-CA-C	-5.79	100.00	108.11
1	B	73	ALA	N-CA-C	-5.78	99.76	109.07
1	C	203	ASP	N-CA-C	-5.78	101.08	110.20
1	A	178	PRO	N-CA-C	-5.77	102.40	111.34
1	A	73	ALA	N-CA-C	-5.76	99.79	109.07
1	C	138	LYS	N-CA-C	5.75	119.56	112.54
1	D	9	LEU	N-CA-C	-5.75	96.14	107.69
1	C	24	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
1	B	131	ASN	N-CA-C	-5.72	105.02	113.61
1	D	67	TYR	N-CA-C	-5.72	100.26	109.58
1	B	9	LEU	N-CA-C	-5.71	96.22	107.69
1	D	73	ALA	N-CA-C	-5.69	99.91	109.07
1	D	212	PHE	N-CA-C	-5.69	100.40	109.96
1	B	67	TYR	N-CA-C	-5.64	99.28	109.09
1	C	101	LYS	N-CA-C	-5.62	100.08	109.24
1	B	57	VAL	N-CA-C	-5.60	105.39	110.82
1	B	180	HIS	CA-C-O	-5.59	115.31	121.58
1	A	119	SER	N-CA-C	-5.56	98.67	108.23
1	B	86	PRO	N-CA-C	-5.53	102.89	111.13
1	C	233	PHE	CA-C-N	5.53	125.23	119.64
1	C	233	PHE	C-N-CA	5.53	125.23	119.64
1	C	84	VAL	CB-CA-C	-5.50	105.31	111.80
1	C	13	PRO	CA-C-N	-5.48	112.67	122.32
1	C	13	PRO	C-N-CA	-5.48	112.67	122.32
1	B	102	GLU	N-CA-C	-5.47	100.42	108.79
1	C	73	ALA	N-CA-C	-5.46	100.28	109.07
1	A	18	GLY	CA-C-O	5.45	125.04	119.10
1	B	58	ASP	CB-CA-C	-5.45	100.20	110.67
1	C	64	VAL	CB-CA-C	-5.45	102.11	110.50
1	C	141	ILE	N-CA-C	-5.42	99.93	107.80
1	B	203	ASP	N-CA-C	-5.42	101.64	110.20
1	C	121	HIS	CB-CA-C	-5.40	101.17	111.06
1	D	178	PRO	N-CA-C	-5.40	102.62	111.21
1	C	34	SER	N-CA-C	5.40	118.30	110.42
1	C	119	SER	N-CA-C	-5.39	99.33	110.80
1	C	58	ASP	N-CA-C	5.38	118.07	111.82
1	D	119	SER	N-CA-C	-5.35	99.40	110.80
1	B	119	SER	N-CA-C	-5.29	99.13	108.23
1	A	58	ASP	CB-CA-C	-5.25	100.59	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	CA-C-N	5.24	129.03	122.43
1	A	158	ARG	C-N-CA	5.24	129.03	122.43
1	C	131	ASN	N-CA-C	-5.22	106.30	113.30
1	D	138	LYS	N-CA-C	5.22	119.27	113.01
1	A	149	GLY	N-CA-C	5.21	120.89	114.69
1	A	192	GLU	N-CA-CB	-5.21	101.77	110.99
1	D	102	GLU	N-CA-C	-5.20	100.84	108.79
1	A	180	HIS	CA-C-O	-5.14	115.82	121.58
1	B	178	PRO	N-CA-C	-5.13	103.39	111.34
1	D	105	THR	N-CA-C	5.13	117.09	108.73
1	D	217	ILE	N-CA-C	5.13	117.47	111.05
1	D	84	VAL	N-CA-C	5.12	115.96	111.56
1	B	7	VAL	N-CA-C	-5.12	100.28	107.75
1	A	100	TYR	N-CA-C	5.12	118.09	110.52
1	B	121	HIS	N-CA-C	5.09	120.89	113.40
1	D	100	TYR	N-CA-C	5.09	118.06	110.52
1	C	100	TYR	N-CA-C	5.02	117.95	110.52
1	C	149	GLY	N-CA-C	5.00	120.64	114.69

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TYR	Sidechain
1	A	13	PRO	Mainchain
1	B	100	TYR	Sidechain
1	B	14	ASN	Mainchain
1	B	168	SER	Mainchain
1	C	100	TYR	Sidechain
1	C	14	ASN	Mainchain
1	D	100	TYR	Sidechain
1	D	13	PRO	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	1766	0	1717	67	0
1	B	1780	0	1731	47	0
1	C	1764	0	1715	65	0
1	D	1726	0	1683	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	88	0	0	11	0
3	B	89	0	0	3	0
3	C	54	0	0	5	0
3	D	64	0	0	6	0
All	All	7335	0	6846	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (218) 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:C:20:PRO:HB3	1:C:22:TYR:CE1	2.05	0.92
1:C:145:ASP:HB3	1:C:158:ARG:HB2	1.57	0.86
1:D:145:ASP:HB3	1:D:158:ARG:HB2	1.63	0.81
1:C:132:GLN:HG3	3:C:275:HOH:O	1.80	0.80
3:A:283:HOH:O	1:C:120:THR:HG23	1.82	0.78
1:C:17:ILE:HD12	1:C:33:ARG:HE	1.47	0.76
1:B:78:ASP:HB3	3:B:313:HOH:O	1.87	0.74
1:A:12:TYR:C	1:A:14:ASN:H	1.95	0.74
1:B:145:ASP:HB3	1:B:158:ARG:HB2	1.70	0.74
1:D:60:ARG:HD2	1:D:76:SER:HB3	1.70	0.73
1:B:120:THR:HA	3:B:282:HOH:O	1.89	0.72
1:B:117:SER:HB2	1:B:122:GLU:HB2	1.74	0.70
1:C:117:SER:HB2	1:C:122:GLU:HB2	1.75	0.69
1:A:17:ILE:HD11	1:A:236:ALA:HB1	1.75	0.69
1:A:118:ASN:OD1	1:C:68:PRO:HA	1.92	0.68
1:A:17:ILE:CD1	1:A:236:ALA:HB1	2.22	0.68
1:A:71:ASP:HB2	3:A:324:HOH:O	1.93	0.68
1:A:145:ASP:HB3	1:A:158:ARG:HB2	1.76	0.67
1:A:87:GLU:HG3	1:A:182:TRP:O	1.94	0.67
1:B:60:ARG:HD2	1:B:76:SER:HB3	1.76	0.67
1:B:101:LYS:O	1:B:101:LYS:HG2	1.93	0.67
1:C:17:ILE:HD12	1:C:33:ARG:NE	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ILE:CD1	1:C:33:ARG:HE	2.10	0.65
1:C:222:PRO:HG2	1:C:225:SER:HB3	1.78	0.65
1:D:23:PRO:HB2	1:D:40:TRP:O	1.98	0.64
1:A:187:VAL:HG21	3:C:268:HOH:O	1.98	0.62
1:A:16:ASP:O	1:A:17:ILE:HG23	2.00	0.62
1:C:101:LYS:O	1:C:101:LYS:HG2	1.99	0.62
1:D:117:SER:HB2	1:D:122:GLU:HB2	1.81	0.62
1:A:101:LYS:O	1:A:101:LYS:HG2	2.00	0.62
1:A:119:SER:O	1:A:122:GLU:HG2	2.00	0.61
1:D:51:HIS:HB3	3:D:239:HOH:O	1.99	0.61
1:D:181:ILE:HD13	1:D:182:TRP:HD1	1.65	0.61
1:A:181:ILE:HD12	1:A:181:ILE:N	2.16	0.61
1:C:102:GLU:HA	1:C:200:LYS:O	2.00	0.61
1:D:30:LYS:HE2	1:D:84:VAL:HG13	1.83	0.61
1:D:181:ILE:HD13	1:D:182:TRP:CD1	2.35	0.61
1:A:117:SER:HB2	1:A:122:GLU:HB2	1.83	0.61
1:A:17:ILE:HG13	1:A:17:ILE:O	2.01	0.60
1:B:15:THR:HG23	1:B:21:SER:HB3	1.82	0.60
1:C:150:THR:O	1:C:151:ASP:HB2	2.02	0.60
1:A:17:ILE:CD1	1:A:236:ALA:O	2.50	0.60
1:A:17:ILE:HD11	1:A:236:ALA:O	2.02	0.60
1:A:30:LYS:HE2	1:A:84:VAL:HG13	1.84	0.59
1:B:44:ASN:HD21	1:B:201:SER:HB3	1.67	0.59
1:D:87:GLU:HG3	1:D:182:TRP:O	2.02	0.59
1:A:36:LYS:NZ	3:A:284:HOH:O	2.35	0.58
1:B:182:TRP:HB2	3:B:258:HOH:O	2.03	0.58
1:A:60:ARG:HD2	1:A:76:SER:HB3	1.85	0.58
1:B:87:GLU:HG3	1:B:182:TRP:O	2.05	0.56
1:B:181:ILE:HD13	1:B:182:TRP:HD1	1.70	0.56
1:C:86:PRO:O	1:C:181:ILE:HD11	2.06	0.56
1:D:101:LYS:O	1:D:101:LYS:HG2	2.05	0.56
1:A:181:ILE:HD12	1:A:181:ILE:H	1.71	0.56
1:B:181:ILE:HD13	1:B:182:TRP:CD1	2.41	0.56
1:D:222:PRO:HG2	1:D:225:SER:HB3	1.88	0.55
1:B:50:ALA:O	1:B:194:THR:HA	2.06	0.55
1:C:4:ILE:HD13	1:C:215:SER:HB3	1.86	0.55
1:B:23:PRO:HB2	1:B:40:TRP:O	2.07	0.55
1:A:13:PRO:O	1:A:15:THR:N	2.40	0.55
1:B:222:PRO:HG2	1:B:225:SER:HB3	1.87	0.55
1:C:145:ASP:CB	1:C:158:ARG:HB2	2.35	0.55
1:C:87:GLU:HG3	1:C:182:TRP:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ILE:HG13	1:C:33:ARG:HG2	1.89	0.54
1:A:181:ILE:HD13	1:A:182:TRP:CD1	2.42	0.54
1:B:101:LYS:O	1:B:202:PRO:HD2	2.07	0.54
1:A:106:ILE:HB	1:A:154:LEU:HB3	1.87	0.54
1:C:60:ARG:HD2	1:C:76:SER:HB3	1.89	0.54
1:A:25:ILE:CG2	1:A:40:TRP:HB2	2.38	0.54
1:B:106:ILE:HB	1:B:154:LEU:HB3	1.90	0.54
1:C:23:PRO:HB2	1:C:40:TRP:O	2.08	0.54
1:C:100:TYR:O	1:C:167:GLY:HA3	2.08	0.53
1:A:150:THR:O	1:A:151:ASP:HB2	2.08	0.53
1:B:95:ALA:HA	1:B:209:GLY:O	2.09	0.53
1:A:181:ILE:HD13	1:A:182:TRP:HD1	1.74	0.53
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.91	0.53
1:D:9:LEU:HB3	1:D:40:TRP:CZ3	2.44	0.53
1:C:89:VAL:HG22	1:C:181:ILE:HG13	1.91	0.53
1:C:174:LEU:HD12	1:C:174:LEU:N	2.23	0.53
1:A:4:ILE:HD13	1:A:215:SER:HB3	1.90	0.53
1:C:30:LYS:HE2	1:C:84:VAL:HG13	1.92	0.53
1:A:102:GLU:HA	1:A:200:LYS:O	2.08	0.52
1:C:181:ILE:HD13	1:C:182:TRP:CD1	2.43	0.52
1:B:20:PRO:HB3	1:B:22:TYR:CE1	2.44	0.52
1:B:68:PRO:HA	1:D:118:ASN:OD1	2.08	0.52
1:A:88:TRP:CG	1:B:138:LYS:HD2	2.44	0.52
1:C:32:VAL:HG22	1:C:32:VAL:O	2.10	0.52
1:A:95:ALA:HA	1:A:209:GLY:O	2.10	0.52
1:A:17:ILE:O	1:A:17:ILE:CG1	2.56	0.52
1:C:20:PRO:HB3	1:C:22:TYR:CZ	2.44	0.52
1:A:87:GLU:HG2	1:A:180:HIS:CD2	2.46	0.51
1:C:51:HIS:CD2	3:C:268:HOH:O	2.62	0.51
1:C:138:LYS:HD2	1:D:88:TRP:CG	2.46	0.51
1:B:47:VAL:O	1:B:68:PRO:HD3	2.11	0.51
1:D:50:ALA:O	1:D:194:THR:HA	2.09	0.51
1:D:25:ILE:CG2	1:D:40:TRP:HB2	2.40	0.51
1:C:103:THR:HG22	1:C:159:VAL:HG12	1.92	0.51
1:D:86:PRO:O	1:D:181:ILE:HD11	2.10	0.51
1:B:30:LYS:HE2	1:B:84:VAL:HG13	1.94	0.50
1:D:107:LEU:N	1:D:107:LEU:CD2	2.74	0.50
1:C:87:GLU:HG2	1:C:180:HIS:CD2	2.46	0.50
1:D:70:ALA:HB2	3:D:264:HOH:O	2.11	0.50
1:C:20:PRO:CB	1:C:22:TYR:CE1	2.90	0.50
1:D:87:GLU:HG2	1:D:180:HIS:CD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HD2	1:B:88:TRP:CG	2.47	0.49
1:C:93:LEU:HD23	1:C:212:PHE:HA	1.94	0.49
1:D:145:ASP:CB	1:D:158:ARG:HB2	2.38	0.49
1:B:4:ILE:HD13	1:B:215:SER:HB3	1.93	0.49
1:B:86:PRO:O	1:B:181:ILE:HD11	2.13	0.49
1:A:16:ASP:HB2	1:A:19:ASP:OD2	2.12	0.49
1:D:44:ASN:HD21	1:D:201:SER:HB3	1.77	0.49
1:B:119:SER:O	1:B:122:GLU:HG2	2.13	0.49
1:D:119:SER:O	1:D:122:GLU:HG2	2.13	0.49
1:D:159:VAL:HG22	1:D:160:SER:N	2.27	0.49
1:A:16:ASP:O	1:A:17:ILE:CG2	2.61	0.49
1:D:51:HIS:HD2	3:D:241:HOH:O	1.95	0.48
1:A:25:ILE:HG23	1:A:40:TRP:HB2	1.94	0.48
1:A:193:ALA:C	3:A:304:HOH:O	2.56	0.48
1:A:116:LYS:NZ	3:A:286:HOH:O	2.45	0.48
1:A:187:VAL:HG11	3:A:280:HOH:O	2.13	0.48
1:D:150:THR:O	1:D:151:ASP:HB2	2.13	0.48
1:A:59:LYS:HD3	1:A:80:ASP:HB2	1.96	0.48
1:A:101:LYS:O	1:A:202:PRO:HD2	2.14	0.47
1:A:228:ARG:HD3	3:A:298:HOH:O	2.14	0.47
1:A:16:ASP:C	1:A:17:ILE:HG23	2.39	0.47
1:C:181:ILE:HD13	1:C:182:TRP:HD1	1.79	0.47
1:D:101:LYS:O	1:D:202:PRO:HD2	2.14	0.47
1:C:22:TYR:CD1	1:C:22:TYR:C	2.92	0.47
1:B:87:GLU:HG2	1:B:180:HIS:CD2	2.49	0.47
1:B:122:GLU:OE1	1:B:122:GLU:HA	2.14	0.47
1:C:44:ASN:HD21	1:C:201:SER:HB3	1.78	0.47
1:D:32:VAL:O	1:D:32:VAL:HG22	2.15	0.47
1:A:23:PRO:HB2	1:A:40:TRP:O	2.14	0.47
1:A:222:PRO:HG2	1:A:225:SER:HB3	1.96	0.47
1:B:150:THR:O	1:B:151:ASP:HB2	2.13	0.47
1:C:50:ALA:O	1:C:194:THR:HA	2.15	0.47
1:D:133:PHE:O	1:D:152:GLY:HA2	2.14	0.47
1:C:4:ILE:HD13	1:C:215:SER:CB	2.44	0.47
1:D:95:ALA:HA	1:D:209:GLY:O	2.15	0.47
1:A:50:ALA:O	1:A:194:THR:HA	2.15	0.47
1:C:65:VAL:O	1:C:72:SER:HA	2.15	0.46
1:C:101:LYS:O	1:C:202:PRO:HD2	2.16	0.46
1:D:102:GLU:HA	1:D:200:LYS:O	2.15	0.46
1:C:96:SER:HA	1:C:169:SER:O	2.16	0.46
1:A:17:ILE:HD13	1:A:236:ALA:HB1	1.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HD3	1:B:202:PRO:HG3	1.98	0.46
1:C:17:ILE:CD1	1:C:236:ALA:O	2.63	0.46
1:A:60:ARG:NH2	3:C:290:HOH:O	2.49	0.46
1:A:101:LYS:HB3	1:A:101:LYS:HE3	1.64	0.45
1:C:25:ILE:CG2	1:C:40:TRP:HB2	2.47	0.45
1:D:181:ILE:HD12	1:D:181:ILE:N	2.30	0.45
1:B:101:LYS:HB3	1:B:101:LYS:HE3	1.63	0.45
1:A:32:VAL:HG22	1:A:32:VAL:O	2.16	0.45
1:C:181:ILE:HD12	1:C:181:ILE:N	2.31	0.45
1:D:51:HIS:CD2	3:D:241:HOH:O	2.70	0.45
1:D:159:VAL:CG2	1:D:160:SER:N	2.80	0.45
1:D:129:MET:CE	3:D:254:HOH:O	2.65	0.45
1:A:13:PRO:C	1:A:15:THR:N	2.74	0.44
1:A:86:PRO:O	1:A:181:ILE:HD11	2.18	0.44
1:A:44:ASN:HD21	1:A:201:SER:HB3	1.81	0.44
1:C:222:PRO:HG2	1:C:225:SER:CB	2.47	0.44
1:B:133:PHE:O	1:B:152:GLY:HA2	2.18	0.44
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.90	0.44
1:A:174:LEU:N	1:A:174:LEU:HD12	2.32	0.44
1:C:106:ILE:HB	1:C:154:LEU:HB3	2.00	0.43
1:D:47:VAL:O	1:D:68:PRO:HD3	2.18	0.43
1:B:25:ILE:CG2	1:B:40:TRP:HB2	2.48	0.43
1:C:73:ALA:HA	3:C:291:HOH:O	2.18	0.43
1:B:119:SER:HB2	1:B:122:GLU:HG2	1.99	0.43
1:B:181:ILE:N	1:B:181:ILE:HD12	2.33	0.43
1:C:95:ALA:HA	1:C:209:GLY:O	2.18	0.43
1:A:12:TYR:C	1:A:14:ASN:N	2.69	0.43
1:C:17:ILE:HG13	1:C:17:ILE:O	2.19	0.43
1:D:25:ILE:HG23	1:D:40:TRP:HB2	2.00	0.43
1:A:87:GLU:HG2	1:A:180:HIS:NE2	2.34	0.42
1:C:45:GLY:C	1:C:198:LEU:HD21	2.44	0.42
1:C:87:GLU:HG2	1:C:180:HIS:NE2	2.35	0.42
1:C:177:ALA:HB2	1:D:177:ALA:HB2	2.01	0.42
1:A:10:ASP:OD1	1:A:12:TYR:HB2	2.19	0.42
1:B:29:ILE:O	1:B:30:LYS:HB2	2.19	0.42
1:C:16:ASP:O	1:C:17:ILE:HG23	2.19	0.42
1:C:101:LYS:HB3	1:C:101:LYS:HE3	1.57	0.42
1:C:181:ILE:HD12	1:C:181:ILE:H	1.83	0.42
1:A:4:ILE:HD13	1:A:215:SER:CB	2.50	0.42
1:A:159:VAL:HG12	3:A:249:HOH:O	2.19	0.42
1:B:119:SER:O	1:B:120:THR:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:CB	1:B:158:ARG:HB2	2.45	0.42
1:A:17:ILE:HD12	1:A:236:ALA:O	2.20	0.42
1:B:9:LEU:HB3	1:B:40:TRP:CZ3	2.55	0.42
1:C:102:GLU:OE1	1:C:206:PRO:HB2	2.19	0.41
1:B:20:PRO:HB3	1:B:22:TYR:CZ	2.55	0.41
1:D:156:LEU:O	1:D:171:GLY:HA3	2.20	0.41
1:D:187:VAL:HG22	1:D:188:VAL:HG12	2.01	0.41
1:A:14:ASN:O	1:A:19:ASP:HB3	2.20	0.41
1:A:32:VAL:HG22	3:A:299:HOH:O	2.20	0.41
1:B:146:ALA:HA	1:B:155:GLU:O	2.20	0.41
1:C:89:VAL:CG2	1:C:181:ILE:HG13	2.50	0.41
1:A:118:ASN:HA	3:A:280:HOH:O	2.21	0.41
1:C:201:SER:HB3	1:C:206:PRO:HG3	2.02	0.41
1:B:102:GLU:HA	1:B:200:LYS:O	2.21	0.41
1:C:17:ILE:CD1	1:C:33:ARG:NE	2.77	0.41
1:B:22:TYR:CD1	1:B:22:TYR:C	2.98	0.41
1:D:139:ASP:OD1	1:D:139:ASP:N	2.50	0.41
1:B:89:VAL:HG22	1:B:181:ILE:HG13	2.01	0.41
1:B:4:ILE:HD13	1:B:215:SER:CB	2.51	0.41
1:B:53:ILE:HD12	1:B:53:ILE:HG21	1.85	0.41
1:C:16:ASP:C	1:C:17:ILE:HG23	2.46	0.41
1:C:17:ILE:C	1:C:19:ASP:H	2.28	0.41
1:C:20:PRO:C	1:C:22:TYR:H	2.28	0.41
1:A:18:GLY:N	3:A:294:HOH:O	2.49	0.40
1:D:174:LEU:N	1:D:174:LEU:HD12	2.36	0.40
1:A:145:ASP:CB	1:A:158:ARG:HB2	2.47	0.40
1:C:47:VAL:O	1:C:68:PRO:HD3	2.21	0.40
1:C:99:LEU:HD12	1:C:99:LEU:HA	1.85	0.40
1:C:105:THR:O	1:C:197:PHE:HA	2.21	0.40
1:D:210:ILE:HG22	1:D:211:ALA:N	2.37	0.40
1:A:156:LEU:O	1:A:171:GLY:HA3	2.22	0.40
1:D:40:TRP:CD1	3:D:277:HOH:O	2.73	0.40

There are no symmetry-related clashes.

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	227/237 (96%)	211 (93%)	14 (6%)	2 (1%)	14	27
1	B	229/237 (97%)	217 (95%)	9 (4%)	3 (1%)	9	18
1	C	227/237 (96%)	207 (91%)	18 (8%)	2 (1%)	14	27
1	D	220/237 (93%)	204 (93%)	14 (6%)	2 (1%)	14	27
All	All	903/948 (95%)	839 (93%)	55 (6%)	9 (1%)	12	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	B	17	ILE
1	B	120	THR
1	C	17	ILE
1	A	120	THR
1	C	120	THR
1	D	120	THR
1	D	159	VAL
1	B	168	SER

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	198/203 (98%)	174 (88%)	24 (12%)	5	10
1	B	199/203 (98%)	175 (88%)	24 (12%)	5	10
1	C	197/203 (97%)	173 (88%)	24 (12%)	5	10
1	D	193/203 (95%)	172 (89%)	21 (11%)	6	13
All	All	787/812 (97%)	694 (88%)	93 (12%)	5	11

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	17	ILE
1	A	20	PRO
1	A	25	ILE
1	A	31	SER
1	A	34	SER
1	A	46	LYS
1	A	53	ILE
1	A	72	SER
1	A	74	THR
1	A	99	LEU
1	A	101	LYS
1	A	107	LEU
1	A	113	SER
1	A	118	ASN
1	A	119	SER
1	A	120	THR
1	A	159	VAL
1	A	181	ILE
1	A	185	SER
1	A	187	VAL
1	A	188	VAL
1	A	198	LEU
1	A	203	ASP
1	B	14	ASN
1	B	20	PRO
1	B	25	ILE
1	B	31	SER
1	B	46	LYS
1	B	53	ILE
1	B	64	VAL
1	B	72	SER
1	B	74	THR
1	B	99	LEU
1	B	101	LYS
1	B	107	LEU
1	B	113	SER
1	B	118	ASN
1	B	119	SER
1	B	120	THR
1	B	159	VAL
1	B	181	ILE
1	B	185	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	187	VAL
1	B	188	VAL
1	B	198	LEU
1	B	203	ASP
1	B	217	ILE
1	C	14	ASN
1	C	17	ILE
1	C	20	PRO
1	C	25	ILE
1	C	31	SER
1	C	34	SER
1	C	46	LYS
1	C	53	ILE
1	C	64	VAL
1	C	72	SER
1	C	74	THR
1	C	99	LEU
1	C	101	LYS
1	C	107	LEU
1	C	113	SER
1	C	118	ASN
1	C	119	SER
1	C	120	THR
1	C	181	ILE
1	C	185	SER
1	C	187	VAL
1	C	188	VAL
1	C	198	LEU
1	C	203	ASP
1	D	25	ILE
1	D	31	SER
1	D	34	SER
1	D	46	LYS
1	D	53	ILE
1	D	72	SER
1	D	74	THR
1	D	99	LEU
1	D	101	LYS
1	D	107	LEU
1	D	113	SER
1	D	118	ASN
1	D	119	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	120	THR
1	D	159	VAL
1	D	181	ILE
1	D	185	SER
1	D	187	VAL
1	D	188	VAL
1	D	198	LEU
1	D	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	153	ASN
1	A	237	ASN
1	B	43	GLN
1	B	51	HIS
1	B	121	HIS
1	B	153	ASN
1	B	237	ASN
1	C	43	GLN
1	C	121	HIS
1	C	153	ASN
1	C	237	ASN
1	D	43	GLN
1	D	237	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 4 ligands modelled in this entry, 4 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/237 (97%)	-0.41	5 (2%) 62 58	15, 32, 89, 115	1 (0%)
1	B	233/237 (98%)	-0.44	5 (2%) 63 59	15, 32, 91, 117	3 (1%)
1	C	229/237 (96%)	-0.22	6 (2%) 57 52	18, 38, 93, 121	0
1	D	226/237 (95%)	-0.35	2 (0%) 81 78	17, 38, 80, 114	4 (1%)
All	All	919/948 (96%)	-0.36	18 (1%) 65 61	15, 35, 91, 121	8 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	THR	4.0
1	A	14	ASN	3.6
1	A	118	ASN	3.5
1	C	118	ASN	3.1
1	D	118	ASN	3.0
1	A	17	ILE	2.8
1	A	117	SER	2.8
1	B	14	ASN	2.7
1	C	120	THR	2.6
1	D	205	HIS	2.6
1	C	100	TYR	2.6
1	B	203	ASP	2.4
1	B	120	THR	2.3
1	B	121	HIS	2.3
1	C	19	ASP	2.3
1	C	203	ASP	2.1
1	C	121	HIS	2.1
1	A	203	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	238	1/1	0.94	0.05	38,38,38,38	0
2	ZN	C	238	1/1	0.98	0.03	52,52,52,52	0
2	ZN	D	238	1/1	0.98	0.04	51,51,51,51	0
2	ZN	B	238	1/1	0.99	0.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.