



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:53 PM UTC

PDB ID : 1CIC / pdb_00001cic
Title : IDIOTOPE-ANTI-IDIOTOPE FAB-FAB COMPLEX; D1.3-E225
Authors : Bentley, G.A.
Deposited on : 1999-03-31
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

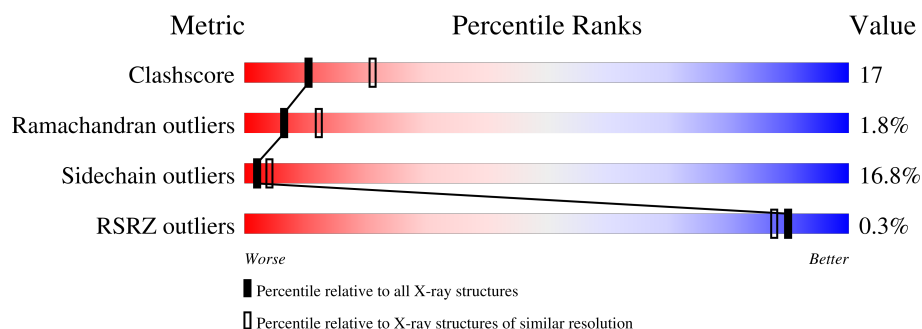
1 Overall quality at a glance

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	214	43% 38% 16% .
2	B	217	50% 32% 16% .
3	C	214	43% 39% 15% .
4	D	218	51% 35% 11% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6733 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 PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1668	1038	283	338	9			

- Molecule 2 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1629	1030	262	329	8			

- Molecule 3 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1665	1037	281	340	7			

- Molecule 4 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1643	1030	279	326	8			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	33	Total	O	0	0
			33	33		
5	C	34	Total	O	0	0
			34	34		
5	D	36	Total	O	0	0
			36	36		

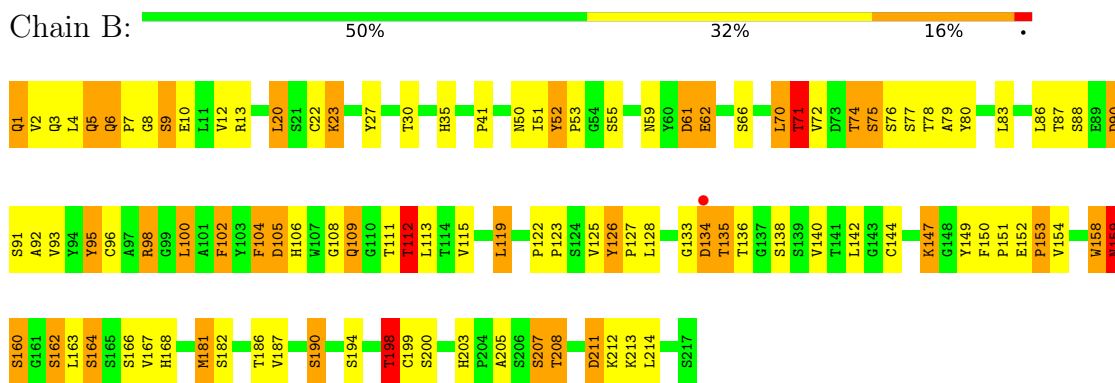
3 Residue-property plots

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 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.

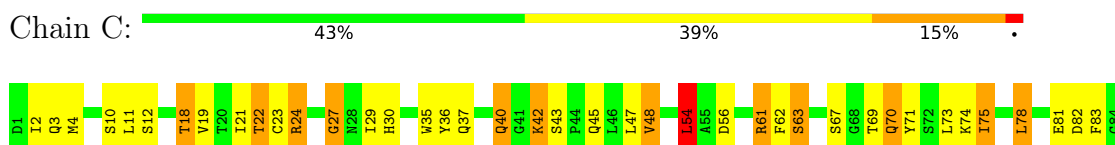
• Molecule 1: PROTEIN (IG HEAVY CHAIN V REGIONS)

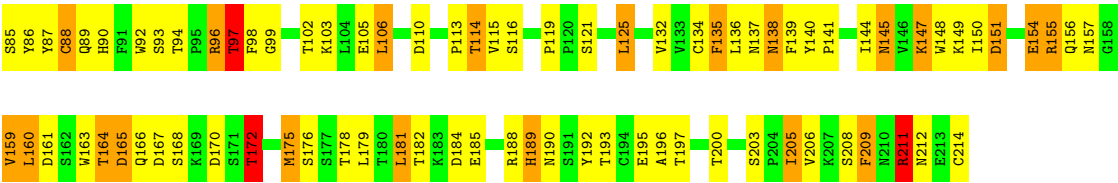


• Molecule 2: PROTEIN (IG HEAVY CHAIN V REGIONS)

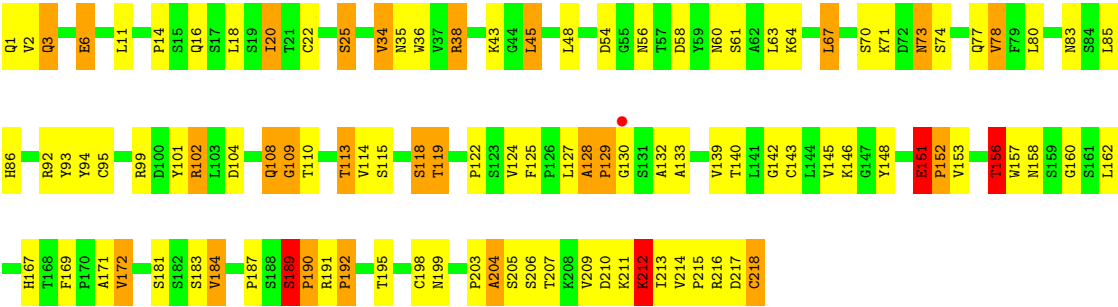


• Molecule 3: PROTEIN (IG HEAVY CHAIN V REGIONS)





• Molecule 4: PROTEIN (IG HEAVY CHAIN V REGIONS)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.11Å 77.65Å 96.75Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50 7.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.50) 77.2 (7.00-2.53)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	203.33 (at 2.51Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.179 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6733	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 ⓘ

5.1 Standard geometry ⓘ

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	1.18	1/1707 (0.1%)	2.13	62/2315 (2.7%)
2	B	1.30	2/1676 (0.1%)	2.17	73/2294 (3.2%)
3	C	1.28	3/1705 (0.2%)	2.17	82/2315 (3.5%)
4	D	1.31	2/1684 (0.1%)	2.16	73/2300 (3.2%)
All	All	1.27	8/6772 (0.1%)	2.16	290/9224 (3.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	189	SER	N-CA	5.73	1.51	1.46
2	B	35	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	140	TYR	CA-CB	5.64	1.62	1.53
3	C	172	THR	CA-CB	5.55	1.62	1.53
4	D	109	GLY	N-CA	5.43	1.50	1.45
3	C	21	ILE	C-N	-5.15	1.26	1.33
3	C	47	LEU	CA-C	5.14	1.56	1.52
2	B	102	PHE	C-N	-5.12	1.27	1.33

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	56	ASP	CA-CB-CG	12.74	125.34	112.60
4	D	6	GLU	CA-CB-CG	11.34	136.79	114.10
2	B	106	HIS	CA-CB-CG	-10.85	102.95	113.80
4	D	133	ALA	N-CA-C	10.60	123.89	111.71
1	A	128	GLY	N-CA-C	10.23	129.86	114.61
2	B	59	ASN	CA-CB-CG	10.15	122.75	112.60
1	A	61	ARG	CA-CB-CG	10.01	134.12	114.10
4	D	45	LEU	N-CA-CB	-9.71	95.70	109.97
2	B	6	GLN	OE1-CD-NE2	9.52	132.12	122.60
2	B	71	THR	N-CA-CB	-9.18	96.33	111.66
1	A	138	ASN	N-CA-C	8.99	123.53	111.30
1	A	61	ARG	N-CA-C	-8.87	101.53	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	172	THR	N-CA-CB	-8.79	96.39	110.46
3	C	145	ASN	CA-CB-CG	8.71	121.31	112.60
1	A	138	ASN	N-CA-CB	-8.57	99.36	111.62
2	B	152	GLU	CA-CB-CG	8.46	131.01	114.10
1	A	82	ASP	N-CA-C	-8.40	102.59	113.17
4	D	130	GLY	N-CA-C	-8.25	100.72	111.37
1	A	198	HIS	CA-CB-CG	8.21	122.01	113.80
2	B	199	CYS	CA-C-O	-8.03	111.88	120.80
3	C	114	THR	CA-C-O	-8.00	111.90	120.46
4	D	171	ALA	CA-C-O	-7.99	112.86	121.56
4	D	58	ASP	CA-CB-CG	7.96	120.56	112.60
1	A	1	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	37	GLN	OE1-CD-NE2	7.89	130.49	122.60
2	B	111	THR	CA-C-O	-7.87	111.88	120.30
2	B	102	PHE	N-CA-C	7.82	123.89	113.72
3	C	87	TYR	O-C-N	7.80	132.31	123.27
1	A	77	ASN	N-CA-CB	-7.79	99.86	111.71
2	B	79	ALA	CA-C-O	-7.75	112.40	121.16
3	C	164	THR	CA-CB-CG2	7.70	123.59	110.50
2	B	100	LEU	N-CA-C	-7.68	99.75	110.35
4	D	172	VAL	CA-C-O	-7.67	111.70	120.67
3	C	96	ARG	N-CA-C	-7.66	100.21	110.55
1	A	29	VAL	N-CA-CB	-7.62	98.65	111.23
3	C	164	THR	CA-CB-OG1	-7.62	98.17	109.60
4	D	217	ASP	CA-CB-CG	7.59	120.19	112.60
4	D	16	GLN	CA-C-N	7.56	135.49	122.64
4	D	16	GLN	C-N-CA	7.56	135.49	122.64
3	C	29	ILE	CA-C-O	7.55	126.84	119.97
2	B	108	GLY	N-CA-C	-7.47	101.09	112.89
3	C	61	ARG	CD-NE-CZ	-7.44	113.98	124.40
1	A	205	ILE	N-CA-CB	7.43	118.62	110.53
4	D	213	ILE	N-CA-CB	7.40	119.97	111.39
1	A	3	VAL	O-C-N	7.38	130.92	123.18
3	C	61	ARG	NE-CZ-NH2	7.37	125.83	119.20
3	C	99	GLY	N-CA-C	-7.35	101.02	112.85
3	C	22	THR	N-CA-CB	-7.29	98.61	111.08
1	A	61	ARG	N-CA-CB	7.27	121.54	110.28
4	D	67	LEU	N-CA-CB	-7.11	99.05	110.63
1	A	30	ARG	CA-C-O	-7.10	110.35	120.51
2	B	87	THR	N-CA-C	-7.05	99.02	109.81
4	D	210	ASP	CA-C-O	-7.04	112.75	120.36
4	D	2	VAL	N-CA-C	-7.04	99.60	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	LYS	N-CA-C	-6.99	101.26	109.93
3	C	165	ASP	N-CA-C	-6.98	100.71	110.35
1	A	202	THR	N-CA-C	-6.97	104.59	113.23
2	B	111	THR	O-C-N	6.96	131.34	123.27
4	D	92	ARG	CA-C-O	-6.96	112.85	120.43
2	B	7	PRO	CA-C-N	6.92	127.62	119.94
2	B	7	PRO	C-N-CA	6.92	127.62	119.94
2	B	100	LEU	CA-C-O	-6.92	114.06	121.88
4	D	6	GLU	CB-CG-CD	6.89	124.32	112.60
2	B	198	THR	CA-C-O	-6.89	112.67	120.32
2	B	75	SER	CA-C-O	-6.85	112.53	120.20
2	B	74	THR	CA-CB-CG2	6.83	122.10	110.50
2	B	158	TRP	CA-C-O	6.82	127.82	120.32
3	C	147	LYS	N-CA-CB	6.81	121.75	110.52
1	A	3	VAL	CA-C-O	-6.79	113.28	120.48
2	B	104	PHE	CA-C-O	-6.78	113.05	120.30
2	B	20	LEU	N-CA-CB	-6.76	100.03	109.97
4	D	83	ASN	CB-CG-ND2	6.76	126.54	116.40
2	B	78	THR	CA-CB-OG1	-6.74	99.48	109.60
3	C	30	HIS	CA-C-O	-6.70	114.19	122.03
3	C	24	ARG	CA-CB-CG	6.67	127.44	114.10
3	C	132	VAL	CA-C-O	-6.62	113.37	120.59
3	C	209	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	101	GLY	N-CA-C	-6.57	103.37	112.18
2	B	164	SER	N-CA-C	-6.57	103.22	113.02
1	A	29	VAL	CA-C-N	6.56	134.07	121.54
1	A	29	VAL	C-N-CA	6.56	134.07	121.54
3	C	97	THR	CA-CB-CG2	6.55	121.63	110.50
1	A	96	PHE	CA-CB-CG	6.54	120.33	113.80
3	C	54	LEU	N-CA-CB	-6.52	100.39	109.97
3	C	114	THR	CB-CA-C	6.51	121.41	110.79
1	A	108	ARG	CA-CB-CG	6.51	127.12	114.10
2	B	153	PRO	CA-C-N	6.51	133.04	122.69
2	B	153	PRO	C-N-CA	6.51	133.04	122.69
3	C	212	ASN	CA-CB-CG	6.50	119.11	112.60
3	C	81	GLU	CB-CA-C	-6.50	96.60	110.32
4	D	70	SER	CA-C-O	-6.50	114.49	121.38
1	A	52	SER	O-C-N	6.45	127.85	121.85
4	D	14	PRO	CA-C-N	6.45	137.58	125.66
4	D	14	PRO	C-N-CA	6.45	137.58	125.66
3	C	114	THR	N-CA-C	-6.44	96.59	107.99
4	D	95	CYS	N-CA-C	-6.44	98.90	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	TRP	CA-C-O	6.42	128.30	120.92
3	C	151	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	108	ARG	CD-NE-CZ	-6.41	115.42	124.40
3	C	105	GLU	CB-CG-CD	6.39	123.47	112.60
4	D	145	VAL	CB-CA-C	6.36	117.66	111.23
3	C	139	PHE	CA-CB-CG	6.36	120.16	113.80
2	B	152	GLU	CA-C-O	-6.35	114.10	120.64
4	D	167	HIS	CA-C-O	-6.35	113.50	120.30
2	B	3	GLN	CA-CB-CG	6.35	126.80	114.10
4	D	192	PRO	N-CD-CG	-6.34	96.20	103.80
1	A	114	THR	N-CA-C	-6.33	97.37	108.20
3	C	98	PHE	CA-C-O	-6.31	114.02	120.71
3	C	157	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	51	ALA	CA-C-O	-6.28	111.53	120.51
4	D	61	SER	CA-C-O	-6.27	113.86	120.63
2	B	159	ASN	OD1-CG-ND2	6.26	128.86	122.60
1	A	102	THR	O-C-N	6.25	131.28	123.28
3	C	114	THR	CA-CB-OG1	-6.24	100.24	109.60
3	C	61	ARG	NE-CZ-NH1	-6.20	115.30	121.50
2	B	51	ILE	CB-CG1-CD1	6.18	126.78	113.80
4	D	156	THR	CA-CB-OG1	-6.18	100.34	109.60
4	D	94	TYR	O-C-N	6.16	130.81	123.24
1	A	73	LEU	N-CA-C	-6.14	99.19	109.07
2	B	98	ARG	NE-CZ-NH2	-6.13	113.68	119.20
4	D	60	ASN	CA-CB-CG	6.13	118.73	112.60
4	D	189	SER	CA-C-N	6.12	127.49	119.84
4	D	189	SER	C-N-CA	6.12	127.49	119.84
3	C	73	LEU	CA-C-O	-6.11	113.54	120.32
2	B	186	THR	CA-C-O	-6.11	113.83	120.36
1	A	99	GLY	CA-C-N	6.10	129.28	120.38
1	A	99	GLY	C-N-CA	6.10	129.28	120.38
4	D	212	LYS	CA-CB-CG	6.10	126.29	114.10
4	D	118	SER	N-CA-C	6.09	118.96	109.52
3	C	27	GLY	CA-C-O	-6.08	114.74	121.37
4	D	3	GLN	CA-CB-CG	6.06	126.22	114.10
1	A	202	THR	CA-C-O	6.06	126.36	119.27
3	C	71	TYR	CA-C-O	-6.05	114.57	121.40
4	D	35	ASN	CA-CB-CG	6.02	118.62	112.60
3	C	182	THR	N-CA-C	-5.97	100.83	110.32
2	B	126	TYR	O-C-N	5.96	126.69	121.39
3	C	138	ASN	N-CA-C	5.95	119.84	111.52
1	A	67	SER	CA-C-O	-5.93	111.99	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	56	ASN	OD1-CG-ND2	-5.93	116.67	122.60
2	B	112	THR	CB-CA-C	5.91	119.76	110.19
4	D	151	GLU	CG-CD-OE1	5.91	131.99	118.40
2	B	8	GLY	N-CA-C	5.91	119.35	112.50
4	D	125	PHE	CA-CB-CG	5.90	119.70	113.80
3	C	88	CYS	N-CA-C	-5.88	101.03	110.14
4	D	171	ALA	O-C-N	5.87	129.79	122.86
2	B	199	CYS	N-CA-C	-5.84	100.18	109.76
3	C	97	THR	CA-CB-OG1	-5.84	100.84	109.60
2	B	111	THR	N-CA-C	-5.84	98.90	108.41
3	C	47	LEU	CA-C-N	5.83	131.11	123.06
3	C	47	LEU	C-N-CA	5.83	131.11	123.06
1	A	42	GLN	CA-CB-CG	5.83	125.75	114.10
1	A	32	ALA	CA-C-O	-5.81	115.38	122.64
3	C	97	THR	N-CA-CB	-5.80	100.64	111.13
2	B	5	GLN	CB-CG-CD	5.80	122.45	112.60
2	B	5	GLN	CA-CB-CG	5.77	125.64	114.10
2	B	74	THR	CA-CB-OG1	-5.77	100.95	109.60
2	B	159	ASN	CA-CB-CG	-5.77	106.83	112.60
3	C	42	LYS	N-CA-C	-5.76	100.75	109.85
4	D	184	VAL	N-CA-C	-5.75	99.94	108.45
1	A	42	GLN	CB-CA-C	5.74	121.30	110.62
1	A	99	GLY	N-CA-C	-5.72	102.31	112.54
3	C	166	GLN	OE1-CD-NE2	5.71	128.31	122.60
2	B	90	ASP	CA-CB-CG	5.71	118.31	112.60
4	D	108	GLN	CB-CG-CD	5.71	122.30	112.60
4	D	169	PHE	CA-C-N	5.69	125.69	119.89
4	D	169	PHE	C-N-CA	5.69	125.69	119.89
3	C	160	LEU	O-C-N	5.69	129.96	123.31
4	D	67	LEU	CA-C-O	-5.68	114.58	121.28
2	B	61	ASP	N-CA-C	-5.67	100.58	109.25
1	A	37	GLN	CA-C-O	-5.67	114.70	120.71
2	B	105	ASP	CA-C-N	5.66	130.77	122.39
2	B	105	ASP	C-N-CA	5.66	130.77	122.39
2	B	71	THR	OG1-CB-CG2	5.65	120.60	109.30
4	D	128	ALA	CB-CA-C	5.64	117.32	108.63
3	C	135	PHE	CA-CB-CG	5.64	119.44	113.80
4	D	61	SER	O-C-N	5.63	128.09	122.12
3	C	185	GLU	CB-CG-CD	5.63	122.17	112.60
4	D	14	PRO	CB-CA-C	5.62	118.42	111.23
2	B	96	CYS	N-CA-C	-5.58	101.07	109.95
4	D	101	TYR	N-CA-C	5.58	119.27	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	VAL	N-CA-C	-5.58	101.48	108.84
3	C	172	THR	CA-CB-OG1	-5.57	101.24	109.60
1	A	85	ASP	CB-CA-C	5.54	119.34	109.38
1	A	207	LYS	N-CA-C	-5.53	99.89	108.90
3	C	137	ASN	N-CA-C	5.52	118.81	109.76
3	C	94	THR	CB-CA-C	5.51	117.15	108.88
4	D	56	ASN	CB-CG-ND2	5.50	124.65	116.40
4	D	34	VAL	O-C-N	5.50	129.13	123.20
3	C	137	ASN	OD1-CG-ND2	-5.49	117.11	122.60
3	C	114	THR	CA-CB-CG2	5.49	119.83	110.50
3	C	96	ARG	CA-C-N	5.49	131.59	121.94
3	C	96	ARG	C-N-CA	5.49	131.59	121.94
2	B	53	PRO	CA-C-N	5.48	126.07	119.98
2	B	53	PRO	C-N-CA	5.48	126.07	119.98
3	C	54	LEU	CB-CA-C	5.48	119.02	109.65
4	D	78	VAL	CA-C-O	-5.48	114.64	120.39
4	D	43	LYS	N-CA-CB	5.47	119.13	110.87
3	C	70	GLN	CA-C-O	-5.47	114.31	120.32
3	C	140	TYR	CA-C-O	-5.46	114.76	119.72
3	C	63	SER	CB-CA-C	-5.45	102.28	110.24
2	B	71	THR	CB-CA-C	5.44	122.14	110.45
1	A	90	HIS	CA-C-O	-5.43	114.46	120.38
4	D	92	ARG	N-CA-C	-5.43	100.39	109.24
4	D	20	ILE	CA-C-O	-5.43	114.69	120.39
1	A	12	SER	CA-C-O	-5.42	114.41	120.54
2	B	144	CYS	O-C-N	5.42	129.97	123.36
2	B	211	ASP	CA-C-O	-5.42	114.51	120.36
4	D	56	ASN	CA-CB-CG	5.41	118.01	112.60
4	D	101	TYR	N-CA-CB	-5.41	103.96	112.13
3	C	62	PHE	CA-C-O	-5.41	114.89	121.05
1	A	75	ILE	O-C-N	5.40	129.42	123.10
4	D	67	LEU	N-CA-C	5.39	118.85	110.17
3	C	89	GLN	CG-CD-NE2	-5.39	108.31	116.40
4	D	108	GLN	CA-CB-CG	5.39	124.87	114.10
2	B	168	HIS	N-CA-CB	5.37	119.28	110.90
3	C	24	ARG	CA-C-O	-5.37	115.02	120.71
3	C	73	LEU	O-C-N	5.36	129.59	123.31
3	C	164	THR	CB-CA-C	5.34	118.61	109.80
4	D	38	ARG	N-CA-CB	-5.34	101.66	111.37
1	A	213	GLU	CA-CB-CG	5.33	124.77	114.10
2	B	208	THR	N-CA-C	5.33	118.05	110.10
3	C	48	VAL	CA-C-O	-5.33	114.43	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	94	THR	N-CA-C	-5.32	102.11	110.14
1	A	23	CYS	CA-C-O	-5.28	113.78	120.28
1	A	165	ASP	N-CA-C	-5.28	101.93	110.32
4	D	73	ASN	CA-C-O	-5.27	114.96	120.55
4	D	181	SER	CA-C-O	-5.26	115.09	120.99
1	A	24	LYS	CB-CA-C	5.26	119.22	109.70
1	A	204	PRO	CA-C-O	-5.26	115.60	121.23
4	D	25	SER	N-CA-CB	-5.23	101.67	111.13
4	D	104	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	167	VAL	CA-C-O	-5.22	114.26	121.51
2	B	78	THR	CA-C-O	-5.22	115.07	120.70
1	A	90	HIS	N-CA-CB	-5.21	102.39	110.57
3	C	63	SER	O-C-N	5.19	130.45	123.34
3	C	181	LEU	CA-CB-CG	5.19	134.46	116.30
3	C	22	THR	OG1-CB-CG2	5.18	119.67	109.30
3	C	141	PRO	CA-C-N	5.18	127.74	120.28
3	C	141	PRO	C-N-CA	5.18	127.74	120.28
2	B	133	GLY	CA-C-N	5.18	131.43	121.54
2	B	133	GLY	C-N-CA	5.18	131.43	121.54
4	D	119	THR	CA-CB-OG1	-5.17	101.84	109.60
1	A	101	GLY	O-C-N	5.17	127.28	122.47
1	A	98	PHE	CA-CB-CG	5.16	118.96	113.80
2	B	52	TYR	CB-CA-C	5.16	115.27	110.17
3	C	21	ILE	N-CA-C	-5.15	101.06	108.53
3	C	61	ARG	CA-C-N	-5.14	114.06	121.42
3	C	61	ARG	C-N-CA	-5.14	114.06	121.42
4	D	133	ALA	CA-C-O	-5.14	114.29	120.10
4	D	132	ALA	CA-C-N	5.13	127.67	120.28
4	D	132	ALA	C-N-CA	5.13	127.67	120.28
1	A	83	LEU	N-CA-C	-5.13	101.77	109.15
1	A	164	THR	CA-CB-OG1	-5.13	101.91	109.60
4	D	85	LEU	CA-C-N	5.13	131.43	122.82
4	D	85	LEU	C-N-CA	5.13	131.43	122.82
3	C	37	GLN	OE1-CD-NE2	-5.12	117.48	122.60
2	B	50	ASN	CA-C-O	-5.12	115.12	121.11
4	D	34	VAL	CA-C-O	-5.12	114.93	120.36
3	C	18	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	163	TRP	CA-C-N	5.11	129.88	121.39
1	A	163	TRP	C-N-CA	5.11	129.88	121.39
3	C	189	HIS	CA-C-O	-5.11	115.94	121.36
2	B	122	PRO	CB-CA-C	5.11	117.15	110.92
2	B	190	SER	N-CA-C	-5.10	107.01	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	TYR	CA-CB-CG	5.09	123.06	113.90
3	C	138	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	93	SER	CB-CA-C	5.08	120.06	110.62
4	D	140	THR	CA-CB-OG1	-5.07	101.99	109.60
4	D	77	GLN	CG-CD-NE2	-5.07	108.79	116.40
2	B	79	ALA	N-CA-C	-5.07	101.90	109.95
1	A	155	ARG	N-CA-CB	5.06	118.72	110.37
4	D	115	SER	N-CA-C	5.05	116.52	108.79
2	B	30	THR	CA-C-O	-5.05	110.83	118.91
3	C	167	ASP	CA-C-N	5.05	127.36	120.54
3	C	167	ASP	C-N-CA	5.05	127.36	120.54
1	A	13	THR	CA-C-O	-5.05	115.88	121.33
1	A	83	LEU	CB-CA-C	5.04	118.34	110.67
2	B	70	LEU	CA-C-O	5.04	126.72	120.92
2	B	93	VAL	N-CA-C	-5.04	101.15	108.36
4	D	77	GLN	O-C-N	5.04	129.41	123.27
2	B	22	CYS	N-CA-CB	-5.03	102.59	110.79
3	C	75	ILE	N-CA-CB	5.03	118.01	111.67
2	B	30	THR	CA-CB-OG1	-5.03	102.06	109.60
2	B	111	THR	CA-C-N	-5.03	116.08	122.77
2	B	111	THR	C-N-CA	-5.03	116.08	122.77
3	C	164	THR	N-CA-CB	-5.02	102.72	110.56
2	B	98	ARG	N-CA-CB	5.02	118.39	110.56
3	C	147	LYS	O-C-N	5.01	129.05	123.19
1	A	77	ASN	CA-CB-CG	5.01	117.61	112.60
2	B	88	SER	O-C-N	5.00	127.85	122.15

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	1668	0	1589	73	0
2	B	1629	0	1562	46	0
3	C	1665	0	1582	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1643	0	1612	44	0
5	A	25	0	0	0	0
5	B	33	0	0	1	0
5	C	34	0	0	0	0
5	D	36	0	0	0	0
All	All	6733	0	6345	215	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 17.

All (215) 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)
3:C:4:MET:HG2	3:C:97:THR:HG22	1.24	1.15
4:D:195:THR:HG23	4:D:212:LYS:HE3	1.21	1.09
4:D:187:PRO:O	4:D:190:PRO:HD2	1.57	1.05
1:A:193:THR:HG22	1:A:208:SER:HB3	1.47	0.96
2:B:119:LEU:HD12	2:B:119:LEU:H	1.33	0.94
3:C:4:MET:HG2	3:C:97:THR:CG2	2.02	0.89
3:C:4:MET:CG	3:C:97:THR:HG22	2.03	0.89
3:C:161:ASP:HB3	3:C:175:MET:HE2	1.54	0.88
1:A:190:ASN:HA	1:A:211:ARG:HB2	1.54	0.87
3:C:145:ASN:HB2	3:C:197:THR:HB	1.62	0.81
3:C:189:HIS:O	3:C:211:ARG:HD3	1.81	0.80
1:A:193:THR:HG22	1:A:208:SER:CB	2.13	0.78
4:D:195:THR:HG23	4:D:212:LYS:CE	2.10	0.78
4:D:67:LEU:HD11	4:D:80:LEU:HD11	1.66	0.78
1:A:207:LYS:NZ	1:A:207:LYS:HA	1.99	0.76
2:B:119:LEU:HD12	2:B:119:LEU:N	1.99	0.76
4:D:195:THR:CG2	4:D:212:LYS:HE3	2.10	0.76
2:B:160:SER:HB2	2:B:162:SER:OG	1.86	0.75
2:B:10:GLU:HB2	2:B:113:LEU:HD12	1.69	0.74
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.67	0.74
4:D:187:PRO:HG2	4:D:190:PRO:HG2	1.69	0.73
3:C:150:ILE:HD11	3:C:179:LEU:HD21	1.73	0.71
1:A:9:LYS:HD2	1:A:9:LYS:N	2.06	0.69
3:C:138:ASN:HA	3:C:172:THR:HG23	1.75	0.68
2:B:147:LYS:HB2	2:B:147:LYS:HZ1	1.59	0.68
1:A:136:LEU:HD13	1:A:175:MET:HE2	1.74	0.68
2:B:123:PRO:HB3	2:B:149:TYR:HB3	1.76	0.67
2:B:159:ASN:HD22	2:B:163:LEU:HD23	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.28	0.66
3:C:113:PRO:HG3	3:C:144:ILE:HD11	1.77	0.66
2:B:147:LYS:HB2	2:B:147:LYS:NZ	2.10	0.66
3:C:170:ASP:OD1	3:C:172:THR:HB	1.96	0.66
4:D:86:HIS:O	4:D:114:VAL:HG11	1.97	0.65
3:C:205:ILE:HD12	3:C:205:ILE:H	1.62	0.65
1:A:91:CYS:HB3	2:B:102:PHE:HB3	1.80	0.64
1:A:59:PRO:HG2	1:A:62:PHE:CD2	2.32	0.64
3:C:190:ASN:ND2	3:C:211:ARG:HB2	2.12	0.64
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.79	0.64
2:B:86:LEU:HA	2:B:90:ASP:OD2	1.99	0.63
1:A:189:HIS:O	1:A:211:ARG:HD3	1.98	0.62
3:C:40:GLN:HE21	3:C:165:ASP:HB3	1.66	0.61
2:B:119:LEU:H	2:B:119:LEU:CD1	2.07	0.60
2:B:147:LYS:NZ	2:B:147:LYS:CB	2.64	0.60
2:B:198:THR:HG23	2:B:213:LYS:HG2	1.83	0.60
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.84	0.59
1:A:146:VAL:HG21	1:A:175:MET:HE1	1.85	0.59
2:B:159:ASN:HD22	2:B:163:LEU:CD2	2.16	0.59
1:A:198:HIS:HD2	1:A:200:THR:OG1	1.85	0.59
1:A:44:PRO:O	1:A:45:LYS:HD2	2.04	0.58
3:C:163:TRP:CZ2	3:C:175:MET:HE3	2.39	0.58
1:A:207:LYS:HA	1:A:207:LYS:HZ3	1.68	0.58
3:C:190:ASN:HA	3:C:211:ARG:HG3	1.86	0.57
4:D:187:PRO:HG2	4:D:190:PRO:CG	2.34	0.57
2:B:71:THR:HG22	2:B:80:TYR:HB2	1.85	0.57
1:A:159:VAL:HA	1:A:178:THR:O	2.04	0.57
2:B:181:MET:HG2	2:B:182:SER:N	2.18	0.57
2:B:91:SER:O	2:B:92:ALA:HB2	2.05	0.57
3:C:205:ILE:HD12	3:C:205:ILE:N	2.21	0.56
3:C:24:ARG:HG3	3:C:24:ARG:HH11	1.70	0.55
1:A:17:ASP:O	1:A:78:VAL:HG23	2.07	0.55
1:A:181:LEU:HD22	1:A:185:GLU:CD	2.32	0.55
2:B:198:THR:HG23	2:B:212:LYS:C	2.32	0.55
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.37	0.55
1:A:125:LEU:HD22	1:A:183:LYS:HG3	1.88	0.54
1:A:207:LYS:HA	1:A:207:LYS:HZ2	1.71	0.54
3:C:85:SER:HA	3:C:102:THR:O	2.08	0.54
3:C:151:ASP:OD2	3:C:189:HIS:HB3	2.07	0.54
3:C:78:LEU:HD13	3:C:106:LEU:HD12	1.90	0.54
1:A:39:LYS:HD2	1:A:42:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LYS:HB2	3:C:193:THR:HB	1.91	0.53
1:A:205:ILE:HD12	1:A:205:ILE:H	1.72	0.53
1:A:148:TRP:O	1:A:155:ARG:N	2.41	0.53
3:C:149:LYS:O	3:C:193:THR:N	2.42	0.52
2:B:1:GLN:OE1	2:B:1:GLN:N	2.43	0.52
3:C:90:HIS:HD2	3:C:92:TRP:H	1.57	0.52
4:D:195:THR:HA	4:D:212:LYS:NZ	2.25	0.52
1:A:28:ASP:OD1	1:A:30:ARG:HD2	2.09	0.51
4:D:195:THR:HA	4:D:212:LYS:HZ2	1.74	0.51
2:B:23:LYS:HD3	2:B:23:LYS:C	2.35	0.51
3:C:148:TRP:O	3:C:154:GLU:HA	2.11	0.51
4:D:189:SER:CB	4:D:190:PRO:HD3	2.41	0.51
2:B:142:LEU:HB3	2:B:214:LEU:HD22	1.93	0.51
2:B:6:GLN:O	2:B:109:GLN:NE2	2.43	0.51
1:A:121:SER:HB2	1:A:123:GLU:OE1	2.10	0.50
3:C:195:GLU:HG2	3:C:206:VAL:HG23	1.92	0.50
2:B:198:THR:HA	2:B:212:LYS:O	2.12	0.50
3:C:184:ASP:HB2	3:C:188:ARG:HH21	1.76	0.50
1:A:181:LEU:HD22	1:A:185:GLU:OE2	2.12	0.50
2:B:160:SER:C	2:B:162:SER:H	2.20	0.50
3:C:61:ARG:NH1	3:C:82:ASP:OD2	2.45	0.50
3:C:119:PRO:HB3	3:C:209:PHE:CE2	2.47	0.49
4:D:18:LEU:HD21	4:D:20:ILE:HD11	1.94	0.49
4:D:122:PRO:HD2	4:D:207:THR:HG21	1.94	0.49
1:A:4:MET:HE3	1:A:23:CYS:SG	2.52	0.49
1:A:59:PRO:HG2	1:A:62:PHE:CE2	2.47	0.49
4:D:187:PRO:HG2	4:D:190:PRO:CD	2.43	0.49
1:A:125:LEU:O	1:A:183:LYS:HD3	2.12	0.49
3:C:155:ARG:HE	3:C:179:LEU:HD11	1.77	0.49
4:D:1:GLN:HA	4:D:1:GLN:OE1	2.08	0.49
1:A:116:SER:O	1:A:134:CYS:HA	2.12	0.49
1:A:30:ARG:HH22	4:D:54:ASP:CG	2.21	0.48
1:A:131:SER:OG	1:A:180:THR:HG23	2.13	0.48
2:B:158:TRP:HB2	2:B:163:LEU:O	2.13	0.48
3:C:36:TYR:O	3:C:86:TYR:HA	2.13	0.48
4:D:11:LEU:HA	4:D:113:THR:O	2.14	0.48
2:B:2:VAL:HG13	2:B:27:TYR:CD1	2.48	0.48
3:C:116:SER:O	3:C:134:CYS:HA	2.14	0.48
3:C:145:ASN:N	3:C:197:THR:O	2.45	0.48
3:C:93:SER:O	3:C:96:ARG:HD2	2.13	0.48
3:C:160:LEU:HD22	4:D:172:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ASN:CG	3:C:211:ARG:HB2	2.38	0.48
2:B:134:ASP:O	2:B:135:THR:OG1	2.26	0.48
2:B:198:THR:CG2	2:B:213:LYS:HG2	2.44	0.48
2:B:83:LEU:HB3	2:B:86:LEU:HD21	1.96	0.47
1:A:110:ASP:OD2	1:A:199:LYS:HE2	2.13	0.47
2:B:76:SER:O	2:B:77:SER:HB2	2.12	0.47
4:D:119:THR:HG21	4:D:204:ALA:O	2.14	0.47
1:A:89:GLN:HE21	1:A:96:PHE:HB3	1.78	0.47
2:B:159:ASN:HB3	2:B:163:LEU:HG	1.96	0.47
4:D:124:VAL:HB	4:D:209:VAL:HG11	1.97	0.47
1:A:150:ILE:HG23	1:A:192:TYR:CE1	2.50	0.47
2:B:163:LEU:CD1	2:B:187:VAL:HG11	2.45	0.47
1:A:37:GLN:O	1:A:44:PRO:HA	2.15	0.47
1:A:112:ALA:HB2	1:A:200:THR:HB	1.97	0.47
4:D:127:LEU:HB2	4:D:142:GLY:C	2.40	0.46
4:D:203:PRO:O	4:D:205:SER:N	2.47	0.46
4:D:151:GLU:OE1	4:D:152:PRO:HA	2.15	0.46
1:A:139:PHE:CZ	1:A:144:ILE:HG21	2.51	0.46
1:A:15:VAL:HA	1:A:78:VAL:O	2.16	0.46
3:C:136:LEU:HD23	3:C:196:ALA:HB2	1.98	0.46
1:A:198:HIS:CD2	1:A:200:THR:OG1	2.67	0.46
4:D:203:PRO:C	4:D:205:SER:H	2.24	0.46
1:A:164:THR:HB	1:A:174:SER:O	2.16	0.45
1:A:122:SER:O	1:A:126:THR:HG23	2.16	0.45
2:B:86:LEU:HB3	2:B:115:VAL:HG21	1.98	0.45
3:C:214:CYS:SG	4:D:216:ARG:CZ	3.05	0.45
2:B:150:PHE:CG	2:B:151:PRO:HA	2.51	0.45
3:C:113:PRO:HG3	3:C:144:ILE:CD1	2.44	0.45
3:C:193:THR:HG23	3:C:206:VAL:HG23	1.98	0.45
4:D:205:SER:O	4:D:206:SER:HB2	2.16	0.45
1:A:112:ALA:HB2	1:A:200:THR:CB	2.47	0.45
1:A:169:LYS:HA	1:A:169:LYS:HD3	1.83	0.45
4:D:162:LEU:HG	4:D:184:VAL:HG21	1.98	0.44
1:A:205:ILE:HD12	1:A:205:ILE:N	2.32	0.44
3:C:24:ARG:HG3	3:C:24:ARG:NH1	2.30	0.44
1:A:13:THR:OG1	1:A:17:ASP:HB2	2.17	0.44
3:C:192:TYR:HB2	3:C:209:PHE:CE1	2.52	0.44
3:C:48:VAL:HG22	3:C:54:LEU:HD12	2.00	0.44
4:D:122:PRO:HB3	4:D:148:TYR:HB3	2.00	0.44
2:B:203:HIS:CE1	2:B:205:ALA:HB3	2.53	0.43
2:B:98:ARG:HD2	2:B:105:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:LYS:NZ	4:D:73:ASN:HD21	2.15	0.43
3:C:135:PHE:CE2	4:D:183:SER:HB3	2.54	0.43
3:C:145:ASN:O	3:C:196:ALA:HA	2.18	0.43
4:D:34:VAL:HG21	4:D:78:VAL:HG21	1.99	0.43
4:D:93:TYR:O	4:D:109:GLY:HA2	2.18	0.43
1:A:54:ARG:NH2	1:A:60:ASP:HB3	2.33	0.43
3:C:121:SER:O	3:C:125:LEU:HD22	2.18	0.43
3:C:196:ALA:HB3	3:C:205:ILE:HB	1.99	0.43
1:A:151:ASP:C	1:A:153:SER:H	2.26	0.43
4:D:156:THR:HG23	4:D:160:GLY:N	2.34	0.43
4:D:214:VAL:HA	4:D:215:PRO:HD3	1.84	0.43
4:D:128:ALA:HA	4:D:129:PRO:HD3	1.79	0.42
1:A:43:SER:HA	1:A:44:PRO:HD3	1.92	0.42
1:A:43:SER:HB3	2:B:95:TYR:CE2	2.54	0.42
2:B:1:GLN:OE1	2:B:1:GLN:CA	2.68	0.42
2:B:150:PHE:CE1	2:B:151:PRO:HB3	2.55	0.42
2:B:159:ASN:HB3	2:B:163:LEU:HB2	2.02	0.42
4:D:189:SER:N	4:D:190:PRO:CD	2.81	0.42
1:A:61:ARG:CZ	1:A:79:GLN:HG3	2.49	0.42
4:D:22:CYS:HB2	4:D:36:TRP:CH2	2.55	0.42
1:A:168:SER:HB2	1:A:169:LYS:NZ	2.35	0.42
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.55	0.42
3:C:150:ILE:HD13	3:C:192:TYR:HE1	1.83	0.42
4:D:187:PRO:C	4:D:190:PRO:HD2	2.37	0.42
1:A:107:LYS:HE2	1:A:107:LYS:HB2	1.60	0.42
1:A:80:SER:O	1:A:83:LEU:HB2	2.20	0.42
4:D:71:LYS:CE	4:D:73:ASN:HD21	2.33	0.42
1:A:161:ASP:HA	1:A:176:SER:O	2.20	0.42
1:A:59:PRO:HG2	1:A:62:PHE:HD2	1.78	0.42
3:C:159:VAL:HA	3:C:178:THR:O	2.20	0.42
4:D:99:ARG:O	4:D:102:ARG:HG2	2.19	0.42
1:A:61:ARG:HH11	1:A:82:ASP:CG	2.28	0.41
1:A:24:LYS:HA	1:A:69:THR:O	2.20	0.41
2:B:52:TYR:HD2	2:B:55:SER:OG	2.03	0.41
3:C:19:VAL:O	3:C:74:LYS:HA	2.20	0.41
3:C:110:ASP:HB3	3:C:200:THR:CG2	2.49	0.41
1:A:19:VAL:HG12	1:A:75:ILE:HB	2.03	0.41
3:C:115:VAL:HA	3:C:135:PHE:O	2.20	0.41
1:A:115:VAL:HA	1:A:135:PHE:O	2.20	0.41
1:A:89:GLN:HG2	1:A:90:HIS:N	2.36	0.41
1:A:121:SER:OG	2:B:126:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:SER:HA	2:B:112:THR:O	2.20	0.41
3:C:18:THR:HA	3:C:75:ILE:O	2.20	0.41
1:A:113:PRO:HG3	1:A:144:ILE:HD11	2.03	0.41
1:A:115:VAL:HG12	1:A:207:LYS:HG3	2.03	0.41
1:A:141:PRO:O	1:A:198:HIS:HE1	2.04	0.41
2:B:61:ASP:O	2:B:62:GLU:C	2.62	0.41
3:C:27:GLY:C	3:C:69:THR:HG22	2.45	0.41
4:D:127:LEU:HB2	4:D:142:GLY:CA	2.51	0.41
3:C:135:PHE:HD1	3:C:176:SER:HG	1.63	0.41
3:C:136:LEU:CD2	3:C:196:ALA:HB2	2.51	0.41
4:D:157:TRP:O	4:D:158:ASN:C	2.64	0.41
1:A:108:ARG:HG3	1:A:171:SER:HB2	2.03	0.41
3:C:83:PHE:CE1	3:C:168:SER:HA	2.56	0.41
1:A:193:THR:HG22	1:A:208:SER:OG	2.20	0.40
3:C:214:CYS:HG	4:D:218:CYS:CB	2.25	0.40
3:C:175:MET:HG2	3:C:176:SER:N	2.36	0.40
3:C:61:ARG:HH11	3:C:61:ARG:HD2	1.34	0.40
1:A:147:LYS:HG2	1:A:195:GLU:HB3	2.02	0.40
2:B:9:SER:HB3	5:B:229:HOH:O	2.21	0.40
1:A:9:LYS:N	1:A:9:LYS:CD	2.81	0.40
1:A:136:LEU:HD13	1:A:175:MET:CE	2.46	0.40
2:B:127:PRO:C	2:B:128:LEU:HD23	2.46	0.40
4:D:192:PRO:HB3	4:D:215:PRO:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	192 (91%)	15 (7%)	5 (2%)	4	8
2	B	215/217 (99%)	199 (93%)	11 (5%)	5 (2%)	5	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	212/214 (99%)	199 (94%)	11 (5%)	2 (1%)	14	27
4	D	216/218 (99%)	204 (94%)	9 (4%)	3 (1%)	9	17
All	All	855/863 (99%)	794 (93%)	46 (5%)	15 (2%)	6	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
2	B	134	ASP
2	B	159	ASN
3	C	211	ARG
4	D	129	PRO
1	A	30	ARG
1	A	199	LYS
4	D	204	ALA
2	B	135	THR
3	C	40	GLN
2	B	207	SER
1	A	81	GLU
4	D	190	PRO
1	A	60	ASP
2	B	41	PRO

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	191/191 (100%)	164 (86%)	27 (14%)	3	7
2	B	186/186 (100%)	147 (79%)	39 (21%)	1	2
3	C	189/189 (100%)	156 (82%)	33 (18%)	2	3
4	D	190/190 (100%)	162 (85%)	28 (15%)	3	6
All	All	756/756 (100%)	629 (83%)	127 (17%)	2	4

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	15	VAL
1	A	18	ARG
1	A	29	VAL
1	A	43	SER
1	A	45	LYS
1	A	56	THR
1	A	80	SER
1	A	81	GLU
1	A	91	CYS
1	A	100	SER
1	A	105	GLU
1	A	107	LYS
1	A	121	SER
1	A	147	LYS
1	A	164	THR
1	A	169	LYS
1	A	171	SER
1	A	180	THR
1	A	187	GLU
1	A	191	SER
1	A	201	SER
1	A	202	THR
1	A	205	ILE
1	A	207	LYS
1	A	208	SER
1	A	211	ARG
2	B	1	GLN
2	B	4	LEU
2	B	5	GLN
2	B	9	SER
2	B	12	VAL
2	B	13	ARG
2	B	20	LEU
2	B	23	LYS
2	B	62	GLU
2	B	66	SER
2	B	70	LEU
2	B	71	THR
2	B	72	VAL
2	B	74	THR
2	B	75	SER
2	B	100	LEU

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Mol	Chain	Res	Type
2	B	104	PHE
2	B	109	GLN
2	B	112	THR
2	B	119	LEU
2	B	125	VAL
2	B	136	THR
2	B	138	SER
2	B	140	VAL
2	B	147	LYS
2	B	153	PRO
2	B	154	VAL
2	B	160	SER
2	B	162	SER
2	B	164	SER
2	B	166	SER
2	B	181	MET
2	B	190	SER
2	B	194	SER
2	B	198	THR
2	B	200	SER
2	B	207	SER
2	B	208	THR
2	B	211	ASP
3	C	2	ILE
3	C	3	GLN
3	C	10	SER
3	C	11	LEU
3	C	12	SER
3	C	22	THR
3	C	23	CYS
3	C	42	LYS
3	C	43	SER
3	C	45	GLN
3	C	54	LEU
3	C	63	SER
3	C	67	SER
3	C	70	GLN
3	C	78	LEU
3	C	97	THR
3	C	103	LYS
3	C	106	LEU
3	C	114	THR

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Mol	Chain	Res	Type
3	C	125	LEU
3	C	147	LYS
3	C	154	GLU
3	C	155	ARG
3	C	156	GLN
3	C	159	VAL
3	C	164	THR
3	C	172	THR
3	C	175	MET
3	C	181	LEU
3	C	203	SER
3	C	205	ILE
3	C	208	SER
3	C	211	ARG
4	D	3	GLN
4	D	6	GLU
4	D	25	SER
4	D	38	ARG
4	D	45	LEU
4	D	48	LEU
4	D	63	LEU
4	D	64	LYS
4	D	74	SER
4	D	102	ARG
4	D	108	GLN
4	D	110	THR
4	D	113	THR
4	D	118	SER
4	D	139	VAL
4	D	143	CYS
4	D	146	LYS
4	D	151	GLU
4	D	152	PRO
4	D	153	VAL
4	D	156	THR
4	D	189	SER
4	D	191	ARG
4	D	198	CYS
4	D	199	ASN
4	D	211	LYS
4	D	212	LYS
4	D	218	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	89	GLN
1	A	90	HIS
1	A	198	HIS
1	A	212	ASN
2	B	50	ASN
2	B	59	ASN
2	B	159	ASN
2	B	168	HIS
3	C	31	ASN
3	C	40	GLN
3	C	45	GLN
3	C	90	HIS
3	C	137	ASN
3	C	190	ASN
3	C	210	ASN
4	D	73	ASN
4	D	83	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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	214/214 (100%)	-0.58	1 (0%) 87 85	11, 42, 83, 112	0
2	B	217/217 (100%)	-0.72	1 (0%) 87 85	10, 31, 64, 80	0
3	C	214/214 (100%)	-0.68	0 100 100	9, 30, 83, 112	0
4	D	218/218 (100%)	-0.82	1 (0%) 87 85	7, 27, 63, 99	0
All	All	863/863 (100%)	-0.70	3 (0%) 90 87	7, 33, 77, 112	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	134	ASP	3.5
4	D	130	GLY	3.2
1	A	156	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.