



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 PM UTC

PDB ID : 1DCL / pdb_00001dcl
Title : MCG, A LAMBDA V TYPE LIGHT-CHAIN DIMER (BENCE-JONES PROTEIN), CRYSTALLIZED FROM AMMONIUM SULFATE
Authors : Schiffer, M.; Xu, Z.B.
Deposited on : 1995-10-16
Resolution : 2.30 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

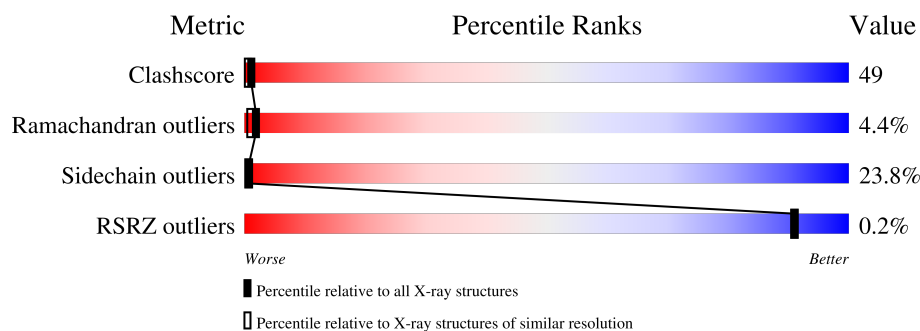
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

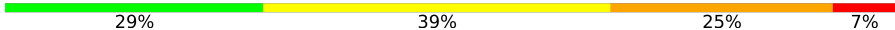
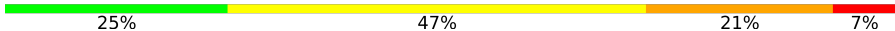
The reported resolution of this entry is 2.30 Å.

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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	216	
1	B	216	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3621 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 MCG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1604	1000	267	332	5			
1	B	216	Total	C	N	O	S	0	0	0
			1604	1000	267	332	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	PHE	conflict	UNP P01709
A	23	THR	SER	conflict	UNP P01709
A	28	ASN	ASP	conflict	UNP P01709
A	29	VAL	ILE	conflict	UNP P01709
A	31	GLY	ASN	conflict	UNP P01709
A	39	GLN	ARG	conflict	UNP P01709
A	42	ALA	PRO	conflict	UNP P01709
A	48	VAL	LEU	conflict	UNP P01709
A	49	ILE	MET	conflict	UNP P01709
A	54	ASN	THR	conflict	UNP P01709
A	62	ASP	ASN	conflict	UNP P01709
A	94	GLU	ALA	conflict	UNP P01709
A	97	ASP	ASN	conflict	UNP P01709
A	98	ASN	SER	conflict	UNP P01709
A	99	PHE	LEU	conflict	UNP P01709
A	100	VAL	ILE	conflict	UNP P01709
A	103	THR	GLY	conflict	UNP P01709
A	106	LYS	ARG	conflict	UNP P01709
A	107	VAL	LEU	conflict	UNP P01709
A	116	ASN	ALA	conflict	UNP P01709
A	118	THR	SER	conflict	UNP P01709
A	156	GLY	SER	conflict	UNP P01709
A	167	LYS	THR	conflict	UNP P01709
B	20	ILE	PHE	conflict	UNP P01709
B	23	THR	SER	conflict	UNP P01709

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Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASN	ASP	conflict	UNP P01709
B	29	VAL	ILE	conflict	UNP P01709
B	31	GLY	ASN	conflict	UNP P01709
B	39	GLN	ARG	conflict	UNP P01709
B	42	ALA	PRO	conflict	UNP P01709
B	48	VAL	LEU	conflict	UNP P01709
B	49	ILE	MET	conflict	UNP P01709
B	54	ASN	THR	conflict	UNP P01709
B	62	ASP	ASN	conflict	UNP P01709
B	94	GLU	ALA	conflict	UNP P01709
B	97	ASP	ASN	conflict	UNP P01709
B	98	ASN	SER	conflict	UNP P01709
B	99	PHE	LEU	conflict	UNP P01709
B	100	VAL	ILE	conflict	UNP P01709
B	103	THR	GLY	conflict	UNP P01709
B	106	LYS	ARG	conflict	UNP P01709
B	107	VAL	LEU	conflict	UNP P01709
B	116	ASN	ALA	conflict	UNP P01709
B	118	THR	SER	conflict	UNP P01709
B	156	GLY	SER	conflict	UNP P01709
B	167	LYS	THR	conflict	UNP P01709

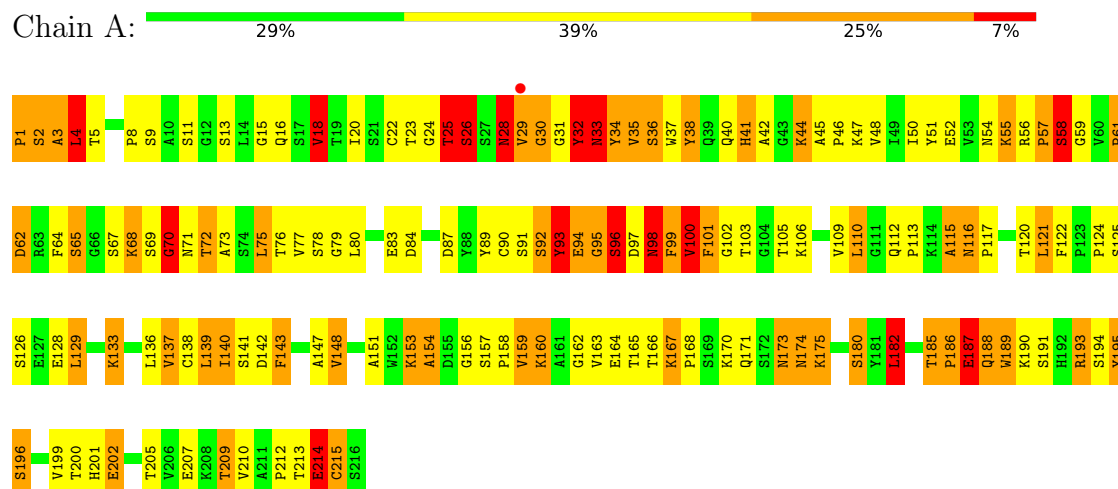
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	195	Total O 195 195	0	0
2	B	218	Total O 218 218	0	0

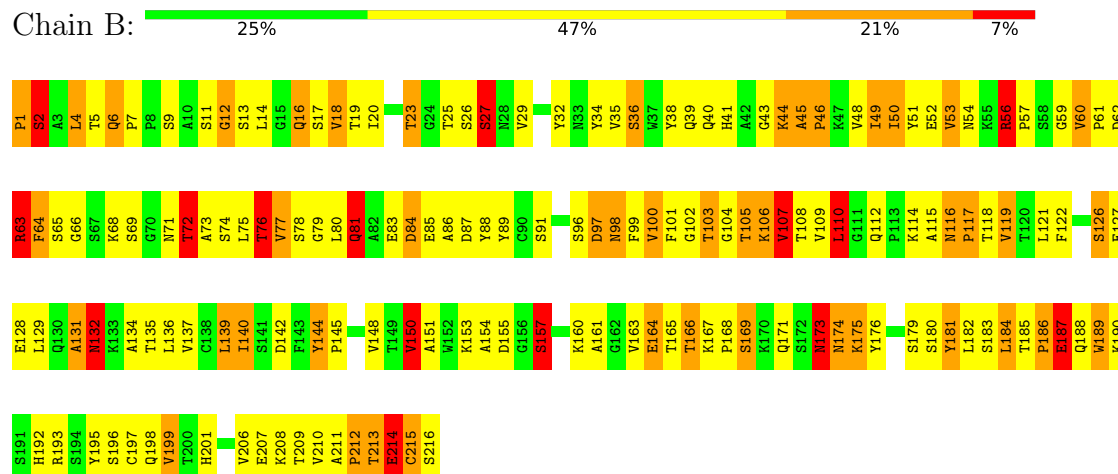
3 Residue-property plots

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: MCG



• Molecule 1: MCG



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.30Å 72.30Å 185.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30 62.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 49.7 (62.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.140 , (Not available) 0.149 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 14.8	EDS
L-test for twinning ¹	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3621	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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	1.34	2/1643 (0.1%)	2.56	125/2241 (5.6%)
1	B	1.36	7/1643 (0.4%)	2.53	120/2241 (5.4%)
All	All	1.35	9/3286 (0.3%)	2.54	245/4482 (5.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	GLY	N-CA	7.78	1.52	1.44
1	A	57	PRO	C-O	6.24	1.32	1.24
1	A	5	THR	CA-CB	6.14	1.61	1.53
1	B	103	THR	C-O	5.89	1.31	1.24
1	B	5	THR	CA-CB	5.68	1.60	1.53
1	B	169	SER	N-CA	5.33	1.52	1.46
1	B	12	GLY	N-CA	5.10	1.50	1.44
1	B	183	SER	N-CA	5.03	1.51	1.45
1	B	39	GLN	CD-NE2	-5.02	1.22	1.33

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PRO	CA-C-N	14.16	148.58	121.54
1	B	1	PRO	C-N-CA	14.16	148.58	121.54
1	B	174	ASN	CA-CB-CG	-13.03	99.57	112.60
1	A	159	VAL	CB-CA-C	12.10	125.24	111.08
1	A	92	SER	CA-C-N	11.18	142.89	121.54
1	A	92	SER	C-N-CA	11.18	142.89	121.54
1	A	54	ASN	CA-CB-CG	-10.81	101.79	112.60
1	B	187	GLU	CB-CG-CD	10.45	130.37	112.60
1	B	103	THR	CA-C-N	-9.98	112.02	122.30
1	B	103	THR	C-N-CA	-9.98	112.02	122.30
1	B	174	ASN	OD1-CG-ND2	9.69	132.29	122.60
1	A	59	GLY	N-CA-C	-9.66	101.32	114.95
1	A	41	HIS	CA-CB-CG	-9.40	104.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ASP	CA-CB-CG	-9.21	103.39	112.60
1	B	76	THR	N-CA-CB	9.09	124.84	110.57
1	A	62	ASP	CA-CB-CG	9.06	121.66	112.60
1	B	122	PHE	O-C-N	9.00	131.40	121.23
1	A	182	LEU	CA-C-O	-8.63	111.56	120.71
1	B	71	ASN	CA-CB-CG	-8.62	103.98	112.60
1	A	209	THR	CA-CB-OG1	-8.45	96.93	109.60
1	A	143	PHE	CA-CB-CG	8.32	122.12	113.80
1	B	139	LEU	CA-C-O	-8.31	111.12	120.43
1	B	63	ARG	CD-NE-CZ	-8.20	112.92	124.40
1	A	61	PRO	CA-C-N	8.17	134.57	120.68
1	A	61	PRO	C-N-CA	8.17	134.57	120.68
1	A	159	VAL	CA-C-O	8.07	130.26	120.74
1	B	116	ASN	CA-CB-CG	8.06	120.66	112.60
1	A	30	GLY	N-CA-C	-8.00	103.18	115.66
1	A	180	SER	N-CA-CB	7.95	125.84	111.37
1	A	138	CYS	CA-C-O	-7.80	109.67	120.52
1	A	52	GLU	CA-C-O	7.79	131.80	122.14
1	A	87	ASP	CA-C-O	-7.78	112.53	121.72
1	B	97	ASP	CA-C-N	7.78	134.30	121.39
1	B	97	ASP	C-N-CA	7.78	134.30	121.39
1	B	99	PHE	CA-C-O	7.67	129.48	120.66
1	B	56	ARG	CA-C-O	7.63	125.92	119.66
1	B	142	ASP	CA-CB-CG	-7.57	105.03	112.60
1	A	116	ASN	N-CA-CB	7.53	121.11	110.11
1	B	87	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	175	LYS	CA-C-O	-7.50	112.67	121.44
1	B	187	GLU	CA-CB-CG	7.42	128.95	114.10
1	A	28	ASN	CA-CB-CG	7.42	120.02	112.60
1	A	116	ASN	O-C-N	7.39	129.66	121.53
1	B	107	VAL	O-C-N	7.36	131.71	123.10
1	A	32	TYR	CA-C-N	7.29	135.47	121.54
1	A	32	TYR	C-N-CA	7.29	135.47	121.54
1	A	142	ASP	CA-CB-CG	-7.29	105.31	112.60
1	A	25	THR	CB-CA-C	7.26	120.59	109.34
1	A	180	SER	O-C-N	7.25	132.15	123.24
1	A	106	LYS	CA-C-O	-7.24	112.44	120.70
1	A	101	PHE	CA-CB-CG	7.24	121.04	113.80
1	B	12	GLY	CA-C-O	-7.24	114.58	121.38
1	A	195	TYR	CA-C-N	7.21	133.75	122.94
1	A	195	TYR	C-N-CA	7.21	133.75	122.94
1	B	150	VAL	CA-C-O	7.16	130.77	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	LYS	CA-C-O	-7.14	112.70	120.92
1	B	27	SER	N-CA-CB	-7.12	100.07	110.47
1	B	91	SER	O-C-N	7.11	131.44	123.48
1	A	28	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	B	127	GLU	CB-CG-CD	7.02	124.54	112.60
1	A	125	SER	CA-C-N	6.96	130.47	120.79
1	A	125	SER	C-N-CA	6.96	130.47	120.79
1	A	92	SER	CA-C-O	6.92	129.55	120.21
1	B	107	VAL	N-CA-CB	6.88	120.13	111.46
1	A	151	ALA	CA-C-O	-6.87	113.07	121.11
1	B	135	THR	CA-C-O	-6.85	112.96	120.36
1	A	75	LEU	CA-C-O	-6.80	113.26	120.80
1	B	144	TYR	CA-CB-CG	-6.80	101.67	113.90
1	A	79	GLY	CA-C-N	6.76	130.44	120.90
1	A	79	GLY	C-N-CA	6.76	130.44	120.90
1	A	196	SER	N-CA-C	6.76	120.42	109.40
1	B	131	ALA	CA-C-O	6.75	127.25	119.35
1	A	202	GLU	CB-CG-CD	6.74	124.05	112.60
1	B	169	SER	CB-CA-C	6.73	123.00	109.68
1	A	57	PRO	N-CA-C	6.72	122.26	113.86
1	A	34	TYR	N-CA-CB	6.70	118.05	110.35
1	A	52	GLU	CA-C-N	6.68	133.99	121.97
1	A	52	GLU	C-N-CA	6.68	133.99	121.97
1	A	98	ASN	CB-CA-C	6.66	120.68	110.62
1	B	175	LYS	N-CA-C	-6.62	99.25	109.52
1	A	5	THR	CA-C-O	-6.61	113.03	120.43
1	A	105	THR	O-C-N	6.55	131.75	123.23
1	B	117	PRO	O-C-N	6.55	130.99	123.00
1	A	94	GLU	CA-C-O	6.54	126.80	119.41
1	A	182	LEU	N-CA-C	-6.53	99.07	109.59
1	A	87	ASP	O-C-N	6.51	130.23	122.94
1	B	189	TRP	CA-C-N	6.46	131.63	120.58
1	B	189	TRP	C-N-CA	6.46	131.63	120.58
1	B	139	LEU	O-C-N	6.46	130.56	123.13
1	A	105	THR	CA-C-O	-6.44	113.75	120.70
1	A	106	LYS	O-C-N	6.42	131.36	123.01
1	B	105	THR	N-CA-CB	6.42	121.23	110.77
1	B	206	VAL	N-CA-CB	6.40	119.95	111.25
1	B	144	TYR	CA-C-O	-6.38	112.71	119.22
1	A	121	LEU	CA-C-O	6.37	127.37	120.43
1	A	67	SER	CA-C-O	-6.36	114.62	121.36
1	A	185	THR	O-C-N	6.36	129.90	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ASN	N-CA-CB	6.35	121.22	110.49
1	B	69	SER	CA-C-O	-6.33	115.18	119.68
1	A	115	ALA	CA-C-O	-6.32	113.51	120.33
1	B	39	GLN	CA-C-N	-6.31	111.73	122.33
1	B	39	GLN	C-N-CA	-6.31	111.73	122.33
1	A	168	PRO	CA-C-N	6.27	131.38	122.72
1	A	168	PRO	C-N-CA	6.27	131.38	122.72
1	B	4	LEU	CA-C-N	6.27	131.11	122.77
1	B	4	LEU	C-N-CA	6.27	131.11	122.77
1	A	65	SER	CA-C-N	6.24	126.48	122.18
1	A	65	SER	C-N-CA	6.24	126.48	122.18
1	B	193	ARG	CD-NE-CZ	-6.24	115.67	124.40
1	A	26	SER	CA-C-N	6.23	131.28	122.05
1	A	26	SER	C-N-CA	6.23	131.28	122.05
1	B	105	THR	O-C-N	6.23	131.25	123.28
1	A	90	CYS	N-CA-C	-6.21	100.05	109.85
1	B	164	GLU	CB-CG-CD	6.13	123.02	112.60
1	A	194	SER	CA-C-O	6.12	128.16	121.06
1	A	154	ALA	O-C-N	6.12	131.20	123.12
1	B	112	GLN	N-CA-C	-6.12	102.34	109.93
1	A	33	ASN	N-CA-C	6.05	123.68	110.80
1	A	175	LYS	CA-C-O	-6.04	114.03	121.88
1	B	128	GLU	N-CA-C	-6.02	105.42	112.89
1	B	107	VAL	CA-C-N	6.00	130.99	122.72
1	B	107	VAL	C-N-CA	6.00	130.99	122.72
1	A	94	GLU	N-CA-C	-5.98	106.11	113.41
1	B	132	ASN	OD1-CG-ND2	5.97	128.57	122.60
1	A	41	HIS	N-CA-C	-5.96	102.64	110.33
1	B	136	LEU	CA-C-O	-5.96	114.19	120.80
1	B	103	THR	O-C-N	-5.94	114.69	122.59
1	A	90	CYS	CA-C-O	-5.93	114.52	121.46
1	B	150	VAL	O-C-N	-5.93	116.81	123.03
1	B	197	CYS	CA-C-O	-5.92	113.81	120.32
1	B	169	SER	N-CA-CB	-5.92	100.41	111.13
1	B	50	ILE	O-C-N	5.91	129.43	123.10
1	B	72	THR	CA-C-O	5.89	127.06	120.70
1	B	157	SER	CB-CA-C	5.89	116.87	108.68
1	B	39	GLN	OE1-CD-NE2	5.89	128.49	122.60
1	B	182	LEU	CA-C-O	-5.88	113.98	120.33
1	A	48	VAL	CA-C-O	-5.85	113.87	120.95
1	B	77	VAL	N-CA-CB	-5.83	105.58	112.40
1	B	129	LEU	CB-CA-C	5.79	122.09	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	THR	OG1-CB-CG2	5.78	120.86	109.30
1	A	5	THR	O-C-N	5.77	129.77	123.13
1	A	186	PRO	N-CA-C	-5.76	100.60	112.47
1	A	38	TYR	O-C-N	-5.74	115.72	123.19
1	A	200	THR	CA-C-O	5.74	127.17	120.80
1	B	98	ASN	CA-C-N	5.73	132.01	122.73
1	B	98	ASN	C-N-CA	5.73	132.01	122.73
1	B	9	SER	N-CA-C	5.72	117.76	109.07
1	A	58	SER	CA-C-N	5.71	131.37	122.30
1	A	58	SER	C-N-CA	5.71	131.37	122.30
1	B	212	PRO	CA-C-N	5.70	130.83	122.39
1	B	212	PRO	C-N-CA	5.70	130.83	122.39
1	A	96	SER	CA-CB-OG	5.69	122.48	111.10
1	B	110	LEU	CA-CB-CG	5.69	136.21	116.30
1	A	100	VAL	CB-CA-C	5.69	120.15	111.68
1	A	42	ALA	N-CA-CB	-5.68	100.28	109.60
1	A	148	VAL	O-C-N	5.67	129.43	123.02
1	A	129	LEU	N-CA-CB	-5.65	101.59	110.30
1	A	76	THR	CA-C-O	-5.65	114.05	120.32
1	B	192	HIS	CA-CB-CG	-5.64	108.16	113.80
1	A	193	ARG	CD-NE-CZ	-5.64	116.51	124.40
1	B	180	SER	CA-C-O	-5.63	114.74	120.71
1	B	121	LEU	CB-CA-C	5.63	118.81	109.53
1	A	158	PRO	CA-C-O	-5.62	114.63	121.03
1	B	2	SER	N-CA-CB	5.59	119.94	110.49
1	B	115	ALA	CA-C-O	-5.58	113.39	120.20
1	B	76	THR	O-C-N	5.57	129.86	123.29
1	A	11	SER	O-C-N	5.56	129.50	123.10
1	B	173	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	102	GLY	CA-C-O	-5.53	115.73	122.75
1	B	122	PHE	CA-C-O	-5.53	115.28	119.59
1	B	165	THR	N-CA-CB	5.52	119.23	110.57
1	B	174	ASN	CA-C-O	-5.52	115.87	122.27
1	A	34	TYR	CA-CB-CG	-5.51	103.99	113.90
1	A	126	SER	CA-C-O	-5.50	115.02	121.07
1	B	164	GLU	CA-C-O	-5.49	114.43	120.30
1	B	199	VAL	CA-C-O	5.49	125.81	120.27
1	B	65	SER	O-C-N	5.49	129.74	123.48
1	B	189	TRP	CA-C-O	5.49	126.56	120.63
1	B	116	ASN	CB-CA-C	5.48	119.36	109.45
1	A	159	VAL	CA-CB-CG1	5.47	119.69	110.40
1	A	54	ASN	N-CA-CB	-5.46	103.15	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	SER	O-C-N	5.46	129.85	122.59
1	B	115	ALA	O-C-N	5.46	130.27	123.28
1	A	162	GLY	O-C-N	5.45	128.82	122.45
1	B	101	PHE	O-C-N	5.44	130.26	123.19
1	B	63	ARG	N-CA-C	-5.43	106.43	113.16
1	B	34	TYR	O-C-N	5.42	129.33	122.28
1	A	90	CYS	O-C-N	5.42	130.37	123.11
1	B	157	SER	N-CA-C	-5.39	102.87	110.31
1	A	58	SER	CA-C-O	5.38	128.20	120.51
1	B	66	GLY	CA-C-O	5.38	127.30	121.76
1	A	18	VAL	CB-CA-C	5.37	118.39	110.77
1	B	46	PRO	N-CA-C	-5.36	102.72	111.68
1	A	71	ASN	N-CA-C	-5.35	106.76	113.72
1	B	127	GLU	CG-CD-OE1	5.35	130.71	118.40
1	B	62	ASP	CA-CB-CG	-5.34	107.26	112.60
1	B	100	VAL	CA-C-N	-5.33	114.44	122.81
1	B	100	VAL	C-N-CA	-5.33	114.44	122.81
1	A	76	THR	O-C-N	5.33	129.55	123.31
1	A	189	TRP	CA-C-N	5.33	127.95	120.28
1	A	189	TRP	C-N-CA	5.33	127.95	120.28
1	B	186	PRO	CA-C-N	5.33	129.74	120.68
1	B	186	PRO	C-N-CA	5.33	129.74	120.68
1	B	187	GLU	CG-CD-OE1	5.33	130.65	118.40
1	B	81	GLN	N-CA-CB	5.32	118.63	110.70
1	A	125	SER	O-C-N	5.32	128.85	122.79
1	B	142	ASP	CA-C-O	5.32	128.01	121.84
1	A	187	GLU	CA-C-N	5.31	127.35	120.44
1	A	187	GLU	C-N-CA	5.31	127.35	120.44
1	A	20	ILE	CA-C-O	-5.30	114.66	121.40
1	B	151	ALA	O-C-N	5.29	129.41	123.27
1	A	115	ALA	O-C-N	5.27	130.08	123.12
1	A	4	LEU	CB-CA-C	5.27	119.22	110.74
1	B	45	ALA	N-CA-C	-5.26	102.38	110.01
1	A	18	VAL	CA-C-O	5.25	125.84	120.39
1	B	65	SER	CA-C-O	-5.23	114.26	120.43
1	B	64	PHE	N-CA-C	-5.22	100.67	109.07
1	B	29	VAL	O-C-N	5.21	127.16	121.94
1	B	84	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	139	LEU	O-C-N	5.20	129.15	123.22
1	A	126	SER	N-CA-C	-5.20	104.67	111.02
1	B	25	THR	N-CA-CB	5.18	119.25	110.49
1	A	25	THR	CA-CB-CG2	5.17	119.30	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	CA-C-O	5.17	125.72	119.31
1	A	174	ASN	N-CA-CB	-5.17	104.73	113.15
1	A	201	HIS	CA-C-O	-5.16	115.21	120.63
1	A	106	LYS	CB-CA-C	-5.16	102.35	111.22
1	A	70	GLY	O-C-N	5.14	129.38	122.70
1	A	188	GLN	CB-CA-C	-5.13	102.83	110.88
1	A	124	PRO	CA-C-O	-5.11	115.76	121.23
1	A	70	GLY	N-CA-C	-5.11	101.07	113.18
1	B	126	SER	O-C-N	5.11	127.61	122.09
1	A	205	THR	O-C-N	-5.10	116.38	123.12
1	B	23	THR	N-CA-C	5.09	117.27	109.07
1	B	27	SER	CA-C-O	5.08	125.15	119.41
1	B	72	THR	CA-CB-OG1	-5.08	101.98	109.60
1	B	181	TYR	CA-C-O	-5.08	115.17	121.11
1	A	116	ASN	N-CA-C	-5.08	103.07	110.08
1	B	6	GLN	OE1-CD-NE2	5.05	127.65	122.60
1	A	105	THR	N-CA-CB	5.03	119.58	110.83
1	A	77	VAL	CA-C-O	-5.03	114.78	120.66
1	B	36	SER	O-C-N	5.01	129.41	123.24
1	B	150	VAL	CB-CA-C	5.01	118.54	110.82
1	B	129	LEU	N-CA-C	-5.01	106.67	112.89
1	A	38	TYR	CA-C-O	5.01	126.77	121.11

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	1604	0	1542	176	0
1	B	1604	0	1542	145	1
2	A	195	0	0	24	4
2	B	218	0	0	15	2
All	All	3621	0	3084	308	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 49.

All (308) 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:31:GLY:O	1:A:32:TYR:HB2	1.42	1.14
1:A:93:TYR:CE1	1:A:96:SER:HB3	1.84	1.12
1:B:23:THR:HG23	1:B:72:THR:HG22	1.36	1.07
1:A:213:THR:O	1:A:214:GLU:HB2	1.55	1.06
1:B:160:LYS:H	1:B:160:LYS:HD3	1.11	1.05
1:A:25:THR:HG22	2:A:730:HOH:O	1.59	1.00
1:B:19:THR:HG23	1:B:76:THR:HG23	1.46	0.97
1:A:93:TYR:HE1	1:A:96:SER:HB3	1.25	0.94
1:A:29:VAL:HG13	1:A:30:GLY:H	1.31	0.94
1:B:64:PHE:CD1	1:B:77:VAL:HG22	2.04	0.92
1:A:24:GLY:CA	1:A:29:VAL:HG23	2.00	0.90
1:B:160:LYS:HD3	1:B:160:LYS:N	1.79	0.89
1:B:166:THR:HG22	1:B:179:SER:H	1.37	0.89
1:A:160:LYS:HD3	1:A:160:LYS:H	1.35	0.89
1:A:24:GLY:HA3	1:A:29:VAL:HG23	1.55	0.89
1:A:95:GLY:O	1:A:96:SER:CB	2.21	0.88
1:A:128:GLU:HG2	1:A:133:LYS:HB2	1.55	0.87
1:A:32:TYR:CD1	1:A:33:ASN:ND2	2.44	0.86
1:A:34:TYR:CD1	1:A:34:TYR:C	2.51	0.85
1:B:38:TYR:CE2	1:B:48:VAL:HG22	2.10	0.85
1:A:171:GLN:HE21	1:A:173:ASN:HD21	1.23	0.84
1:A:214:GLU:O	1:A:215:CYS:SG	2.36	0.84
1:B:160:LYS:H	1:B:160:LYS:CD	1.91	0.84
1:A:159:VAL:HG11	1:A:182:LEU:HD11	1.59	0.84
1:B:52:GLU:C	1:B:53:VAL:HG23	2.01	0.83
1:B:36:SER:HB3	1:B:51:TYR:HA	1.60	0.83
1:A:213:THR:O	1:A:214:GLU:CB	2.27	0.81
1:A:32:TYR:HD1	1:A:33:ASN:HD22	1.24	0.81
1:B:171:GLN:HE21	1:B:173:ASN:HD21	1.29	0.81
1:A:95:GLY:O	1:A:96:SER:HB3	1.79	0.80
1:A:34:TYR:C	1:A:34:TYR:HD1	1.89	0.80
1:B:64:PHE:CE1	1:B:77:VAL:HG22	2.17	0.79
1:A:112:GLN:HB2	1:A:113:PRO:CD	2.13	0.77
1:A:31:GLY:O	1:A:32:TYR:CB	2.25	0.77
1:B:186:PRO:O	1:B:190:LYS:HG2	1.85	0.77
1:A:69:SER:HB3	1:A:72:THR:HG23	1.66	0.76
1:A:122:PHE:O	1:A:136:LEU:HD23	1.86	0.75
1:B:175:LYS:HE2	2:B:575:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:HG3	2:B:589:HOH:O	1.83	0.75
1:A:4:LEU:HD23	1:A:22:CYS:SG	2.27	0.74
1:A:26:SER:HB3	2:A:674:HOH:O	1.87	0.74
1:A:214:GLU:HB3	2:A:932:HOH:O	1.87	0.73
1:A:214:GLU:CB	2:A:932:HOH:O	2.37	0.72
1:B:171:GLN:NE2	1:B:173:ASN:HD21	1.87	0.71
1:A:2:SER:O	1:A:3:ALA:O	2.08	0.71
1:A:4:LEU:HD11	1:A:29:VAL:HG22	1.73	0.71
1:B:185:THR:OG1	1:B:188:GLN:HG3	1.91	0.70
1:B:81:GLN:O	1:B:109:VAL:HG21	1.91	0.70
1:B:51:TYR:O	1:B:52:GLU:HB2	1.90	0.70
1:A:57:PRO:O	1:A:58:SER:HB2	1.92	0.70
1:B:154:ALA:HB2	1:B:195:TYR:CE1	2.27	0.69
1:A:26:SER:HB2	1:A:29:VAL:O	1.93	0.69
1:B:213:THR:HG23	2:B:895:HOH:O	1.93	0.69
1:B:52:GLU:O	1:B:53:VAL:HG23	1.93	0.69
1:A:24:GLY:HA2	1:A:29:VAL:HG23	1.74	0.68
1:A:29:VAL:HG22	1:A:30:GLY:N	2.08	0.68
1:B:52:GLU:C	1:B:53:VAL:CG2	2.67	0.68
1:A:121:LEU:O	2:A:610:HOH:O	2.11	0.68
1:A:173:ASN:ND2	1:A:175:LYS:H	1.92	0.68
1:A:30:GLY:CA	2:A:593:HOH:O	2.41	0.68
1:A:45:ALA:HB2	1:B:89:TYR:CD2	2.29	0.68
1:A:30:GLY:HA3	2:A:593:HOH:O	1.95	0.67
1:A:89:TYR:CE2	1:B:45:ALA:HA	2.29	0.67
1:A:69:SER:CB	1:A:72:THR:HG23	2.24	0.67
1:A:15:GLY:O	2:A:712:HOH:O	2.13	0.67
1:B:131:ALA:O	1:B:132:ASN:CB	2.41	0.67
1:A:65:SER:HA	2:A:783:HOH:O	1.95	0.66
1:B:57:PRO:HD2	1:B:60:VAL:HG21	1.76	0.66
1:A:93:TYR:CE1	1:A:98:ASN:O	2.49	0.66
1:A:34:TYR:CD1	1:A:34:TYR:O	2.48	0.66
1:A:98:ASN:ND2	1:A:100:VAL:CG1	2.59	0.65
1:B:160:LYS:N	1:B:160:LYS:CD	2.52	0.65
1:A:29:VAL:HG13	1:A:30:GLY:N	2.09	0.65
1:B:131:ALA:O	1:B:132:ASN:HB3	1.95	0.65
1:A:24:GLY:HA3	1:A:29:VAL:CG2	2.26	0.65
1:A:99:PHE:N	1:A:99:PHE:CD1	2.64	0.64
1:A:120:THR:HG22	1:A:122:PHE:CE1	2.32	0.64
1:A:115:ALA:O	1:A:143:PHE:HA	1.98	0.64
1:A:25:THR:CG2	2:A:730:HOH:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:O	1:A:96:SER:HB2	1.95	0.64
1:A:32:TYR:CE1	1:A:33:ASN:ND2	2.66	0.63
1:A:68:LYS:HE2	1:A:70:GLY:O	1.98	0.63
1:B:1:PRO:HG2	1:B:2:SER:H	1.64	0.62
1:B:134:ALA:O	1:B:184:LEU:HD23	1.99	0.62
1:A:196:SER:OG	1:A:209:THR:HG22	1.99	0.62
1:B:59:GLY:O	1:B:60:VAL:C	2.42	0.62
1:B:189:TRP:O	1:B:212:PRO:HG3	1.99	0.62
1:A:171:GLN:NE2	1:A:173:ASN:HD21	1.95	0.62
1:A:173:ASN:HD22	1:A:174:ASN:N	1.97	0.62
1:B:13:SER:H	1:B:16:GLN:HB3	1.64	0.62
1:A:173:ASN:HD22	1:A:173:ASN:C	2.06	0.62
1:B:174:ASN:OD1	1:B:174:ASN:N	2.28	0.61
1:A:97:ASP:O	1:B:57:PRO:HB2	2.00	0.61
1:A:136:LEU:HD21	1:A:210:VAL:HG21	1.83	0.61
1:A:9:SER:HB2	1:A:147:ALA:HB3	1.82	0.60
1:B:36:SER:HB2	1:B:50:ILE:O	2.01	0.60
1:A:1:PRO:HB3	1:A:100:VAL:CG1	2.30	0.60
1:A:171:GLN:HE21	1:A:173:ASN:ND2	1.96	0.60
1:A:140:ILE:HD13	1:A:199:VAL:HG21	1.82	0.60
1:B:119:VAL:HG22	1:B:208:LYS:HG3	1.83	0.60
1:A:4:LEU:HD11	1:A:29:VAL:CG2	2.30	0.60
1:A:153:LYS:CG	1:A:196:SER:HB2	2.32	0.60
1:B:49:ILE:HG22	1:B:60:VAL:HG13	1.84	0.60
1:B:4:LEU:N	1:B:4:LEU:HD23	2.16	0.60
1:B:18:VAL:O	1:B:76:THR:HG23	2.01	0.59
1:B:98:ASN:HA	2:B:604:HOH:O	2.02	0.59
1:B:1:PRO:CG	1:B:2:SER:H	2.15	0.59
1:A:154:ALA:HB2	1:A:159:VAL:HG21	1.84	0.59
1:B:106:LYS:HD2	2:B:912:HOH:O	2.02	0.59
1:A:167:LYS:HE2	1:B:43:GLY:HA3	1.85	0.59
1:A:98:ASN:ND2	1:A:100:VAL:HG12	2.18	0.59
1:A:112:GLN:HB2	1:A:113:PRO:HD3	1.85	0.59
1:A:93:TYR:CE1	1:A:95:GLY:O	2.56	0.59
1:A:213:THR:HG22	2:A:809:HOH:O	2.02	0.58
1:B:4:LEU:HB2	1:B:102:GLY:HA2	1.84	0.58
1:B:166:THR:HG22	1:B:179:SER:N	2.12	0.58
1:A:154:ALA:HB2	1:A:159:VAL:CG2	2.34	0.58
1:B:171:GLN:HE21	1:B:173:ASN:ND2	2.01	0.58
1:A:93:TYR:CE1	1:A:96:SER:CB	2.74	0.58
1:B:189:TRP:CZ2	1:B:212:PRO:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PHE:HD1	1:B:77:VAL:HG22	1.68	0.57
1:A:166:THR:CG2	1:A:167:LYS:H	2.17	0.57
1:B:40:GLN:NE2	1:B:44:LYS:O	2.36	0.57
1:A:38:TYR:HE1	1:A:91:SER:HB3	1.70	0.57
1:A:45:ALA:HB2	1:B:89:TYR:CE2	2.39	0.57
1:A:69:SER:N	1:A:72:THR:O	2.27	0.56
1:B:38:TYR:O	1:B:88:TYR:HA	2.05	0.56
1:A:4:LEU:HD13	1:A:100:VAL:CG2	2.36	0.56
1:B:211:ALA:C	1:B:213:THR:H	2.14	0.55
1:A:153:LYS:HG2	1:A:196:SER:HB2	1.89	0.55
1:A:4:LEU:CD1	1:A:29:VAL:HG22	2.37	0.55
1:B:13:SER:O	1:B:14:LEU:C	2.48	0.55
1:B:63:ARG:O	1:B:77:VAL:HA	2.07	0.55
1:A:99:PHE:HZ	1:B:51:TYR:CG	2.25	0.54
1:A:154:ALA:HB2	1:A:195:TYR:CE1	2.43	0.54
1:B:2:SER:O	1:B:100:VAL:HG23	2.06	0.54
1:B:4:LEU:HB2	1:B:102:GLY:CA	2.37	0.54
1:A:29:VAL:CG1	1:A:30:GLY:H	2.00	0.54
1:B:40:GLN:HB2	1:B:46:PRO:HA	1.90	0.54
1:B:12:GLY:HA3	1:B:80:LEU:CD1	2.37	0.54
1:B:36:SER:CB	1:B:50:ILE:O	2.56	0.53
1:B:213:THR:HG22	1:B:213:THR:O	2.08	0.53
1:A:35:VAL:HA	1:A:91:SER:O	2.08	0.53
1:A:22:CYS:HB3	1:A:73:ALA:HB3	1.90	0.53
1:A:93:TYR:CZ	1:A:98:ASN:O	2.62	0.53
1:A:4:LEU:CD1	1:A:29:VAL:CG2	2.87	0.53
1:A:24:GLY:HA3	1:A:29:VAL:CB	2.40	0.52
1:B:85:GLU:HA	1:B:107:VAL:O	2.09	0.52
1:B:57:PRO:HD2	1:B:60:VAL:CG2	2.40	0.52
1:B:57:PRO:HG2	1:B:60:VAL:CG2	2.39	0.52
1:A:31:GLY:HA3	2:A:918:HOH:O	2.09	0.52
1:B:157:SER:CB	2:B:735:HOH:O	2.57	0.52
1:A:98:ASN:HD21	1:A:100:VAL:CG1	2.22	0.52
1:B:48:VAL:N	2:B:719:HOH:O	2.11	0.52
1:A:166:THR:CG2	1:A:167:LYS:N	2.73	0.52
1:A:140:ILE:HD13	1:A:199:VAL:CG2	2.39	0.52
1:A:40:GLN:C	1:A:41:HIS:O	2.53	0.51
1:A:164:GLU:O	1:A:180:SER:CB	2.58	0.51
1:A:185:THR:C	1:A:187:GLU:N	2.64	0.51
1:A:32:TYR:HD2	2:A:685:HOH:O	1.91	0.51
1:A:173:ASN:ND2	1:A:173:ASN:C	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:CG1	1:A:80:LEU:HD22	2.40	0.51
1:A:32:TYR:CD2	2:A:685:HOH:O	2.53	0.51
1:B:14:LEU:HD22	2:B:585:HOH:O	2.11	0.51
1:A:45:ALA:CB	1:B:89:TYR:CD2	2.94	0.51
1:A:68:LYS:HA	1:A:73:ALA:HA	1.92	0.51
1:B:63:ARG:NH1	1:B:84:ASP:OD2	2.44	0.50
1:A:185:THR:O	1:A:186:PRO:C	2.53	0.50
1:B:114:LYS:HG2	1:B:145:PRO:HD3	1.94	0.50
1:A:24:GLY:HA3	1:A:29:VAL:HA	1.93	0.50
1:A:38:TYR:HA	1:A:47:LYS:O	2.11	0.50
1:A:214:GLU:HB2	2:A:932:HOH:O	2.05	0.50
1:B:53:VAL:CG1	1:B:68:LYS:HB2	2.42	0.50
1:B:63:ARG:HH12	1:B:84:ASP:CG	2.20	0.50
1:A:28:ASN:O	1:A:29:VAL:HB	2.10	0.50
1:A:164:GLU:O	1:A:180:SER:HA	2.12	0.50
1:A:4:LEU:HD13	1:A:100:VAL:HG23	1.93	0.50
1:A:214:GLU:O	1:A:215:CYS:CB	2.60	0.50
1:B:41:HIS:CD2	1:B:86:ALA:HB2	2.47	0.50
1:A:214:GLU:C	1:A:215:CYS:SG	2.95	0.49
1:A:34:TYR:CD2	1:A:94:GLU:HG2	2.47	0.49
1:B:214:GLU:CG	1:B:215:CYS:H	2.25	0.49
1:A:121:LEU:HD11	1:A:136:LEU:HD22	1.93	0.49
1:A:160:LYS:HD3	1:A:160:LYS:N	2.17	0.49
1:A:185:THR:OG1	1:A:188:GLN:N	2.30	0.49
1:A:22:CYS:O	1:A:72:THR:HA	2.12	0.49
1:A:56:ARG:NE	1:A:64:PHE:O	2.44	0.49
1:A:193:ARG:HD3	1:A:193:ARG:C	2.38	0.49
1:B:116:ASN:HB3	1:B:117:PRO:HD2	1.95	0.49
1:B:49:ILE:O	1:B:57:PRO:HD2	2.13	0.49
1:B:196:SER:CB	1:B:208:LYS:O	2.60	0.49
1:A:4:LEU:HG	1:A:29:VAL:CG2	2.43	0.49
1:B:160:LYS:HD3	1:B:161:ALA:N	2.28	0.49
1:A:30:GLY:C	2:A:593:HOH:O	2.56	0.48
1:A:99:PHE:HB3	2:A:885:HOH:O	2.12	0.48
1:A:98:ASN:C	1:A:98:ASN:HD22	2.21	0.48
1:A:128:GLU:HG2	1:A:133:LYS:CB	2.36	0.48
1:A:97:ASP:O	1:B:57:PRO:CB	2.62	0.48
1:A:166:THR:HG22	1:A:167:LYS:N	2.29	0.48
1:B:148:VAL:HG12	1:B:201:HIS:HB2	1.96	0.48
1:A:98:ASN:ND2	1:A:98:ASN:C	2.71	0.47
1:B:7:PRO:O	1:B:105:THR:OG1	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:SER:H	1:B:16:GLN:CB	2.27	0.47
1:B:96:SER:O	1:B:97:ASP:HB2	2.14	0.47
1:B:176:TYR:CD1	1:B:176:TYR:N	2.83	0.47
1:B:27:SER:O	1:B:32:TYR:HE1	1.98	0.47
1:B:35:VAL:HG11	1:B:73:ALA:HB1	1.96	0.47
1:B:56:ARG:HG2	1:B:60:VAL:HB	1.95	0.47
1:B:60:VAL:HA	1:B:61:PRO:HD3	1.73	0.47
1:A:40:GLN:O	1:A:41:HIS:C	2.55	0.47
1:A:153:LYS:HG3	1:A:196:SER:HB2	1.96	0.47
1:B:19:THR:HG23	1:B:76:THR:CG2	2.32	0.47
1:B:57:PRO:HG2	1:B:60:VAL:HG23	1.95	0.47
1:B:154:ALA:O	1:B:155:ASP:HB2	2.13	0.47
1:A:45:ALA:HB1	1:A:46:PRO:HD2	1.96	0.47
1:A:139:LEU:HD22	1:B:137:VAL:HG22	1.97	0.47
1:B:213:THR:CG2	2:B:895:HOH:O	2.58	0.47
1:B:13:SER:O	1:B:16:GLN:CB	2.63	0.47
1:B:18:VAL:O	1:B:76:THR:CG2	2.63	0.47
1:A:112:GLN:HB2	1:A:113:PRO:HD2	1.94	0.47
1:B:173:ASN:O	1:B:174:ASN:C	2.56	0.47
1:A:121:LEU:HD12	1:A:137:VAL:O	2.14	0.46
1:B:16:GLN:O	1:B:79:GLY:N	2.46	0.46
1:B:214:GLU:HG2	2:B:758:HOH:O	2.15	0.46
1:A:189:TRP:CZ2	1:A:212:PRO:HA	2.50	0.46
1:B:60:VAL:HG12	1:B:61:PRO:HD2	1.97	0.46
1:B:171:GLN:HE21	1:B:171:GLN:HB2	1.38	0.46
1:A:122:PHE:CZ	1:B:137:VAL:HG23	2.50	0.46
1:B:20:ILE:O	1:B:74:SER:HA	2.16	0.46
1:A:8:PRO:HD2	2:A:625:HOH:O	2.16	0.45
1:B:157:SER:HB2	2:B:735:HOH:O	2.15	0.45
1:A:2:SER:O	1:A:3:ALA:C	2.60	0.45
1:A:159:VAL:HG13	2:A:776:HOH:O	2.17	0.45
1:B:214:GLU:CG	1:B:215:CYS:N	2.79	0.45
1:A:139:LEU:HD11	1:B:181:TYR:CD2	2.50	0.45
1:A:154:ALA:CB	1:A:195:TYR:CE1	3.00	0.45
1:B:187:GLU:HG2	2:B:767:HOH:O	2.17	0.45
1:B:212:PRO:HD3	2:B:589:HOH:O	2.16	0.45
1:A:1:PRO:HB3	1:A:100:VAL:HB	1.98	0.45
1:A:1:PRO:HB3	1:A:100:VAL:CB	2.47	0.45
1:A:98:ASN:HD22	1:A:100:VAL:HG12	1.82	0.45
1:A:32:TYR:O	1:A:34:TYR:N	2.49	0.45
1:A:154:ALA:N	1:A:157:SER:O	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:OE1	1:B:103:THR:O	2.35	0.45
1:A:93:TYR:CD1	1:A:93:TYR:C	2.95	0.45
1:B:154:ALA:N	1:B:157:SER:O	2.50	0.45
1:A:89:TYR:HE2	1:B:45:ALA:HA	1.82	0.44
1:B:16:GLN:CG	1:B:17:SER:H	2.30	0.44
1:A:51:TYR:O	1:A:55:LYS:HB2	2.17	0.44
1:B:107:VAL:O	1:B:107:VAL:HG22	2.17	0.44
1:A:18:VAL:HG13	1:A:80:LEU:HD22	2.00	0.44
1:A:30:GLY:HA2	2:A:768:HOH:O	2.18	0.44
1:B:49:ILE:O	1:B:57:PRO:CD	2.66	0.44
1:B:185:THR:C	1:B:187:GLU:N	2.75	0.44
1:B:13:SER:C	1:B:14:LEU:O	2.58	0.44
1:B:35:VAL:HG11	1:B:73:ALA:CB	2.47	0.44
1:B:196:SER:HB2	1:B:208:LYS:O	2.18	0.44
1:A:93:TYR:CD1	1:A:95:GLY:O	2.72	0.43
1:B:102:GLY:C	1:B:103:THR:O	2.59	0.43
1:B:189:TRP:HA	1:B:189:TRP:CE3	2.53	0.43
1:B:63:ARG:HH11	1:B:63:ARG:HD2	1.40	0.43
1:B:81:GLN:HA	1:B:81:GLN:NE2	2.32	0.43
1:B:119:VAL:CG2	1:B:208:LYS:HG3	2.48	0.43
1:A:32:TYR:HD1	1:A:33:ASN:ND2	1.97	0.43
1:A:143:PHE:CE2	1:A:148:VAL:HG13	2.54	0.43
1:A:45:ALA:HB1	1:A:46:PRO:CD	2.48	0.43
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.86	0.43
1:B:214:GLU:O	1:B:215:CYS:HB3	2.18	0.43
1:A:3:ALA:HA	2:A:607:HOH:O	2.18	0.43
1:B:56:ARG:HD3	1:B:64:PHE:O	2.19	0.43
1:B:173:ASN:ND2	1:B:173:ASN:H	2.17	0.42
1:B:26:SER:HB2	2:B:632:HOH:O	2.18	0.42
1:B:54:ASN:C	1:B:54:ASN:OD1	2.60	0.42
1:B:160:LYS:HD3	1:B:161:ALA:H	1.83	0.42
1:B:64:PHE:CE1	1:B:77:VAL:CG2	2.97	0.42
1:B:56:ARG:CD	1:B:64:PHE:O	2.68	0.42
1:B:140:ILE:CD1	1:B:150:VAL:HG11	2.49	0.42
1:A:32:TYR:HD1	1:A:33:ASN:H	1.67	0.42
1:A:34:TYR:O	1:A:34:TYR:CG	2.72	0.42
1:A:36:SER:HB3	1:A:51:TYR:HA	2.01	0.42
1:A:45:ALA:HA	1:A:46:PRO:HD3	1.82	0.42
1:A:154:ALA:CB	1:A:159:VAL:CG2	2.98	0.42
1:A:116:ASN:HB3	1:A:117:PRO:HD2	2.01	0.42
1:A:44:LYS:HE2	2:A:818:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PHE:CD2	1:B:46:PRO:HD2	2.55	0.41
1:A:165:THR:OG1	1:A:180:SER:HB3	2.20	0.41
1:B:140:ILE:HG21	1:B:199:VAL:HG11	2.02	0.41
1:A:1:PRO:HG3	1:A:98:ASN:ND2	2.35	0.41
1:B:12:GLY:O	1:B:110:LEU:HB2	2.20	0.41
1:B:14:LEU:C	1:B:16:GLN:H	2.28	0.41
1:A:136:LEU:HD21	1:A:210:VAL:CG2	2.49	0.41
1:B:49:ILE:HB	1:B:60:VAL:HG11	2.02	0.41
1:B:61:PRO:HD2	1:B:64:PHE:HD2	1.85	0.41
1:B:168:PRO:HB3	1:B:176:TYR:HB3	2.03	0.41
1:A:16:GLN:HG2	2:A:766:HOH:O	2.20	0.41
1:A:37:TRP:HB2	1:A:50:ILE:HB	2.02	0.41
1:B:48:VAL:HB	2:B:719:HOH:O	2.20	0.41
1:B:198:GLN:HG3	1:B:207:GLU:HB2	2.02	0.41
1:A:24:GLY:HA3	1:A:29:VAL:CA	2.51	0.41
1:A:99:PHE:H	1:A:99:PHE:HD1	1.67	0.41
1:B:144:TYR:HA	1:B:145:PRO:C	2.46	0.41
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.89	0.40
1:A:187:GLU:OE1	1:A:187:GLU:HA	2.20	0.40
1:B:107:VAL:O	1:B:107:VAL:CG2	2.66	0.40
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.87	0.40
1:A:160:LYS:NZ	2:A:775:HOH:O	1.91	0.40
1:A:18:VAL:HG11	1:A:80:LEU:HD22	2.03	0.40
1:A:56:ARG:HA	1:A:57:PRO:HD3	1.87	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)
2:A:769:HOH:O	2:B:820:HOH:O[6_656]	0.99	1.21
2:A:597:HOH:O	2:A:903:HOH:O[6_656]	1.69	0.51
2:A:647:HOH:O	2:B:901:HOH:O[6_656]	1.76	0.44
1:B:216:SER:O	2:A:526:HOH:O[2_545]	1.94	0.26

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	214/216 (99%)	183 (86%)	16 (8%)	15 (7%)	1	0
1	B	214/216 (99%)	189 (88%)	21 (10%)	4 (2%)	6	5
All	All	428/432 (99%)	372 (87%)	37 (9%)	19 (4%)	2	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	29	VAL
1	A	32	TYR
1	A	33	ASN
1	A	96	SER
1	A	214	GLU
1	A	215	CYS
1	A	26	SER
1	A	28	ASN
1	A	95	GLY
1	B	132	ASN
1	B	215	CYS
1	A	58	SER
1	B	2	SER
1	A	93	TYR
1	B	214	GLU
1	A	70	GLY
1	A	156	GLY
1	A	61	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	181/181 (100%)	136 (75%)	45 (25%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	181/181 (100%)	140 (77%)	41 (23%)	1	1
All	All	362/362 (100%)	276 (76%)	86 (24%)	1	0

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	2	SER
1	A	4	LEU
1	A	13	SER
1	A	18	VAL
1	A	23	THR
1	A	25	THR
1	A	26	SER
1	A	28	ASN
1	A	32	TYR
1	A	35	VAL
1	A	36	SER
1	A	44	LYS
1	A	62	ASP
1	A	68	LYS
1	A	72	THR
1	A	75	LEU
1	A	78	SER
1	A	83	GLU
1	A	92	SER
1	A	93	TYR
1	A	98	ASN
1	A	99	PHE
1	A	100	VAL
1	A	103	THR
1	A	109	VAL
1	A	110	LEU
1	A	129	LEU
1	A	133	LYS
1	A	137	VAL
1	A	140	ILE
1	A	141	SER
1	A	153	LYS
1	A	160	LYS
1	A	163	VAL
1	A	167	LYS

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Mol	Chain	Res	Type
1	A	170	LYS
1	A	173	ASN
1	A	182	LEU
1	A	187	GLU
1	A	190	LYS
1	A	191	SER
1	A	202	GLU
1	A	207	GLU
1	A	214	GLU
1	B	2	SER
1	B	11	SER
1	B	16	GLN
1	B	18	VAL
1	B	27	SER
1	B	44	LYS
1	B	49	ILE
1	B	53	VAL
1	B	56	ARG
1	B	60	VAL
1	B	63	ARG
1	B	72	THR
1	B	75	LEU
1	B	76	THR
1	B	78	SER
1	B	81	GLN
1	B	83	GLU
1	B	106	LYS
1	B	107	VAL
1	B	108	THR
1	B	110	LEU
1	B	118	THR
1	B	119	VAL
1	B	126	SER
1	B	139	LEU
1	B	140	ILE
1	B	150	VAL
1	B	153	LYS
1	B	157	SER
1	B	163	VAL
1	B	164	GLU
1	B	166	THR
1	B	167	LYS

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Mol	Chain	Res	Type
1	B	169	SER
1	B	173	ASN
1	B	184	LEU
1	B	187	GLU
1	B	209	THR
1	B	210	VAL
1	B	213	THR
1	B	214	GLU

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	33	ASN
1	A	98	ASN
1	A	112	GLN
1	A	116	ASN
1	A	130	GLN
1	A	171	GLN
1	A	173	ASN
1	A	192	HIS
1	B	81	GLN
1	B	112	GLN
1	B	116	ASN
1	B	132	ASN
1	B	173	ASN
1	B	198	GLN

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

There are no ligands in this entry.

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 [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	216/216 (100%)	-0.82	1 (0%) 87 87	8, 19, 47, 53	0
1	B	216/216 (100%)	-0.82	0 100 100	8, 21, 38, 55	0
All	All	432/432 (100%)	-0.82	1 (0%) 91 91	8, 20, 45, 55	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	VAL	2.4

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.