



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:33 PM UTC

PDB ID : 1UD1 / pdb_00001ud1
Title : Crystal structure of proglycinin mutant C88S
Authors : Utsumi, S.; Adachi, M.
Deposited on : 2003-04-24
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	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

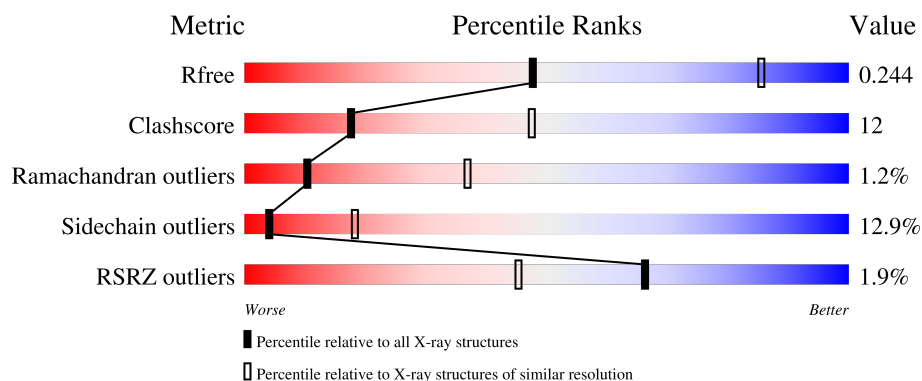
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	476	2% 45% 25% 7% 23%
1	B	476	% 41% 28% 7% 23%
1	C	476	% 43% 28% 5% 23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8649 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 Glycinin G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2883	1821	510	541	11			
1	B	366	Total	C	N	O	S	0	0	0
			2883	1821	510	541	11			
1	C	366	Total	C	N	O	S	0	0	0
			2883	1821	510	541	11			

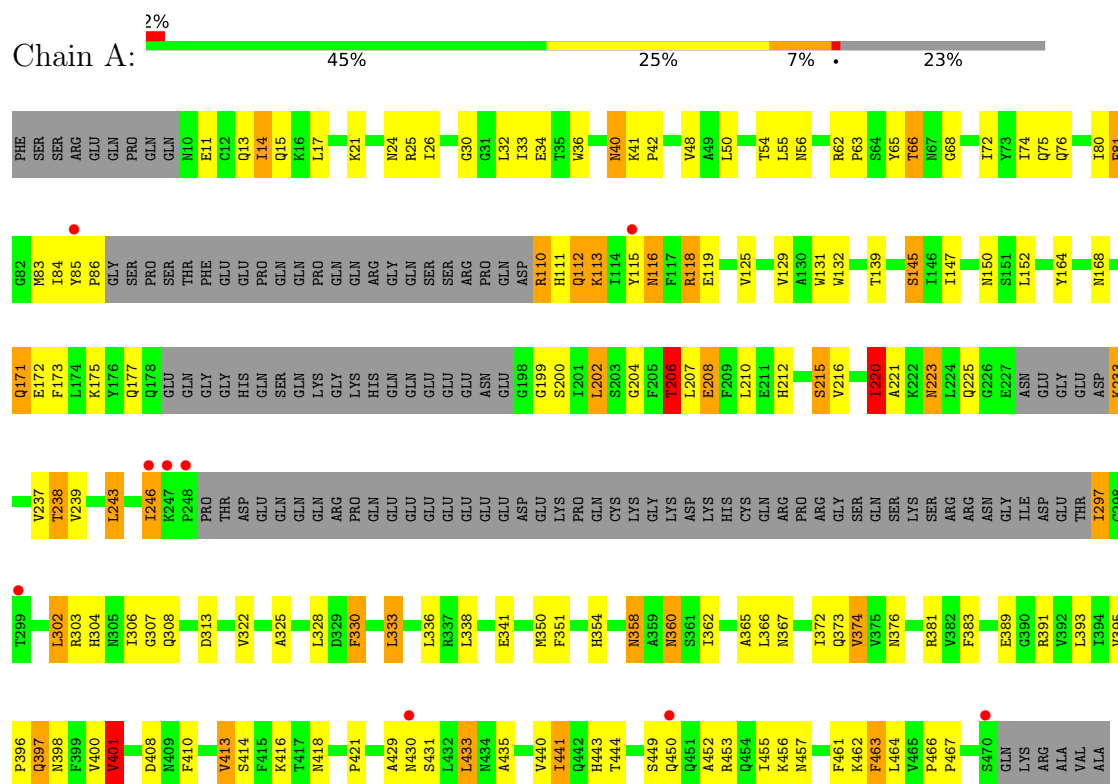
There are 3 discrepancies between the modelled and reference sequences:

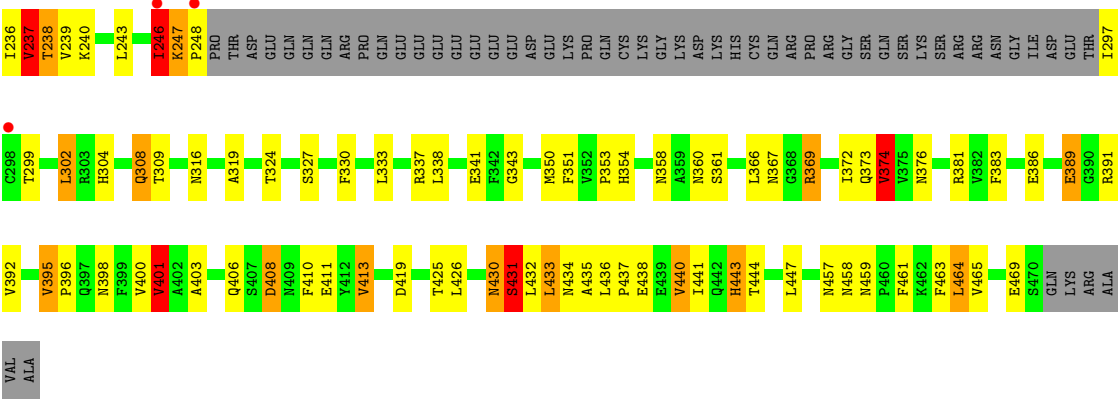
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	SER	CYS	engineered mutation	UNP P04776
B	88	SER	CYS	engineered mutation	UNP P04776
C	88	SER	CYS	engineered mutation	UNP P04776

3 Residue-property plots

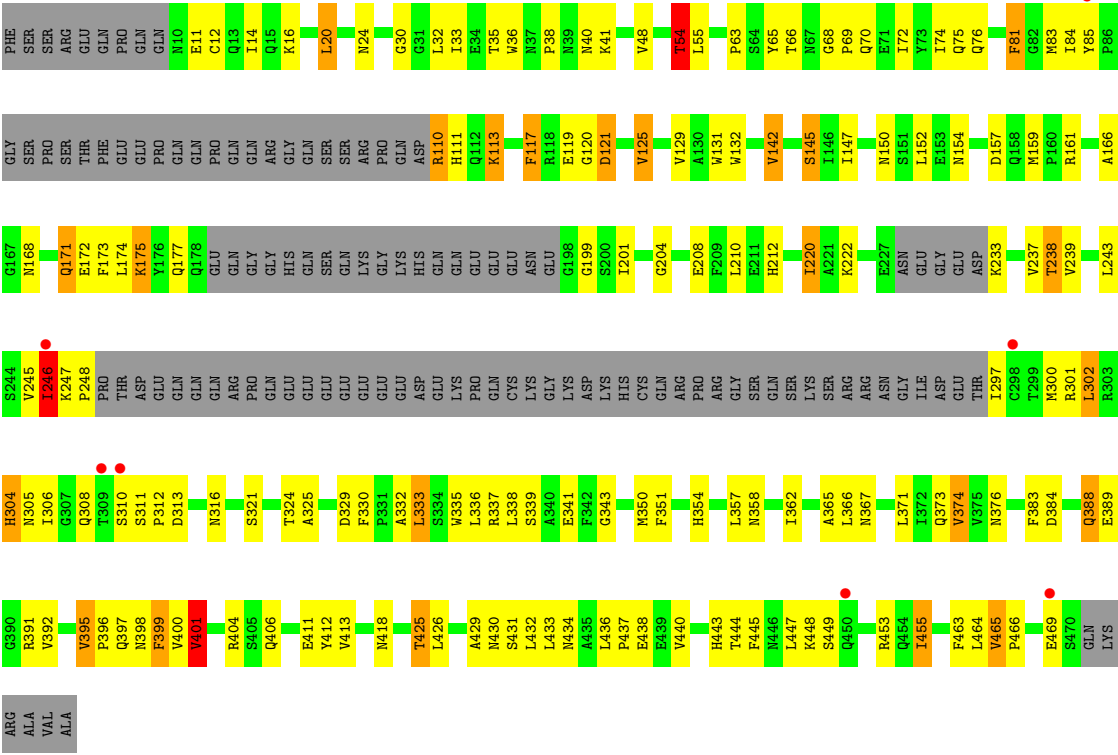
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycinin G1





• Molecule 1: Glycinin G1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	114.34Å 114.34Å 145.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10 8.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.10) 83.0 (8.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.193 , 0.253 0.193 , 0.244	Depositor DCC
R_{free} test set	4408 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8649	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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	0.91	8/2940 (0.3%)	1.70	52/3982 (1.3%)
1	B	0.88	7/2940 (0.2%)	1.71	54/3982 (1.4%)
1	C	0.93	7/2940 (0.2%)	1.74	56/3982 (1.4%)
All	All	0.91	22/8820 (0.2%)	1.72	162/11946 (1.4%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	HIS	CD2-NE2	-6.92	1.30	1.37
1	B	443	HIS	CD2-NE2	-6.92	1.30	1.37
1	C	212	HIS	CD2-NE2	-6.82	1.30	1.37
1	C	304	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	443	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	111	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	111	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	304	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	443	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	354	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	111	HIS	CD2-NE2	-6.09	1.31	1.37
1	C	354	HIS	CD2-NE2	-5.90	1.31	1.37
1	B	304	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	212	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	374	VAL	CA-CB	5.63	1.61	1.54
1	B	212	HIS	CD2-NE2	-5.56	1.31	1.37
1	C	54	THR	CA-CB	5.55	1.61	1.53
1	A	220	ILE	CA-CB	5.43	1.60	1.54
1	A	304	HIS	CG-ND1	-5.40	1.32	1.38
1	A	354	HIS	CG-ND1	-5.18	1.32	1.38
1	B	354	HIS	CG-ND1	-5.09	1.32	1.38
1	C	304	HIS	CG-ND1	-5.03	1.32	1.38

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	PHE	CA-CB-CG	14.53	128.33	113.80
1	A	351	PHE	CA-CB-CG	13.39	127.19	113.80
1	B	351	PHE	CA-CB-CG	12.91	126.71	113.80
1	C	401	VAL	CB-CA-C	-8.78	97.47	110.81
1	C	329	ASP	CA-CB-CG	8.17	120.77	112.60
1	B	408	ASP	O-C-N	-8.07	112.79	122.63
1	C	117	PHE	CA-CB-CG	7.95	121.75	113.80
1	B	84	ILE	N-CA-C	7.75	114.50	106.21
1	C	154	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	B	246	ILE	N-CA-C	7.55	121.42	110.09
1	C	431	SER	N-CA-C	7.50	119.63	110.41
1	B	237	VAL	N-CA-C	7.46	118.81	107.77
1	C	443	HIS	CA-CB-CG	-7.43	106.37	113.80
1	A	113	LYS	N-CA-C	7.25	120.34	109.25
1	C	384	ASP	CA-CB-CG	7.24	119.84	112.60
1	A	41	LYS	CA-C-N	7.08	126.34	118.97
1	A	41	LYS	C-N-CA	7.08	126.34	118.97
1	B	237	VAL	N-CA-CB	-7.05	102.23	111.82
1	B	431	SER	N-CA-C	7.00	125.71	110.80
1	A	429	ALA	N-CA-C	6.98	120.68	111.75
1	C	145	SER	N-CA-C	6.97	119.77	109.24
1	B	11	GLU	N-CA-C	6.96	119.75	111.33
1	C	376	ASN	N-CA-C	6.89	120.76	109.94
1	C	425	THR	CA-CB-OG1	-6.87	99.29	109.60
1	B	386	GLU	N-CA-C	6.82	120.29	108.76
1	A	461	PHE	N-CA-C	6.81	121.40	109.96
1	B	413	VAL	CB-CA-C	-6.81	101.23	110.42
1	A	111	HIS	N-CA-C	6.79	118.11	108.74
1	A	376	ASN	N-CA-C	6.74	120.62	109.96
1	B	401	VAL	CB-CA-C	-6.73	100.46	110.82
1	A	413	VAL	CB-CA-C	-6.67	100.68	110.62
1	A	221	ALA	N-CA-C	-6.65	103.51	111.69
1	A	125	VAL	CA-C-N	6.53	126.56	119.90
1	A	125	VAL	C-N-CA	6.53	126.56	119.90
1	A	62	ARG	CA-C-N	6.49	126.87	119.93
1	A	62	ARG	C-N-CA	6.49	126.87	119.93
1	B	413	VAL	N-CA-CB	6.48	120.63	111.82
1	A	457	ASN	N-CA-C	6.42	123.24	113.61
1	B	166	ALA	N-CA-C	6.39	118.66	109.14
1	B	212	HIS	CB-CG-CD2	-6.32	122.99	131.20
1	C	304	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	C	40	ASN	N-CA-C	-6.28	100.28	110.20
1	C	395	VAL	N-CA-C	-6.27	101.34	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	413	VAL	CB-CA-C	-6.25	101.90	110.77
1	C	121	ASP	N-CA-C	6.21	119.24	110.23
1	C	36	TRP	CG-CD2-CE3	6.21	140.11	133.90
1	B	395	VAL	CA-C-N	6.21	127.60	119.84
1	B	395	VAL	C-N-CA	6.21	127.60	119.84
1	C	212	HIS	CB-CG-CD2	-6.19	123.16	131.20
1	A	431	SER	N-CA-C	6.13	118.23	110.33
1	C	113	LYS	N-CA-C	6.13	119.09	109.96
1	C	388	GLN	N-CA-C	6.07	118.69	109.95
1	B	457	ASN	N-CA-C	6.04	122.36	114.75
1	B	206	THR	N-CA-CB	-5.99	101.19	110.29
1	C	443	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	C	166	ALA	N-CA-C	5.94	118.10	109.07
1	C	20	LEU	N-CA-C	5.93	119.75	110.32
1	B	360	ASN	N-CA-C	-5.92	101.73	110.48
1	B	125	VAL	CA-C-N	5.91	125.92	119.89
1	B	125	VAL	C-N-CA	5.91	125.92	119.89
1	C	142	VAL	N-CA-C	-5.91	99.12	107.75
1	A	441	ILE	N-CA-C	-5.90	104.76	110.72
1	B	358	ASN	N-CA-C	5.90	119.73	111.30
1	A	354	HIS	CB-CG-CD2	-5.89	123.55	131.20
1	A	401	VAL	CB-CA-C	-5.88	101.44	110.50
1	A	145	SER	N-CA-C	5.85	117.68	108.96
1	A	443	HIS	CA-CB-CG	-5.85	107.95	113.80
1	A	330	PHE	CA-CB-CG	5.84	119.64	113.80
1	C	41	LYS	CB-CG-CD	-5.81	97.93	111.30
1	C	36	TRP	CB-CG-CD1	-5.81	118.19	126.90
1	C	237	VAL	N-CA-CB	-5.76	100.84	111.91
1	A	206	THR	CA-CB-OG1	-5.76	100.96	109.60
1	B	24	ASN	CA-CB-CG	5.76	118.36	112.60
1	B	351	PHE	N-CA-C	-5.75	99.86	109.24
1	A	212	HIS	CB-CG-CD2	-5.73	123.76	131.20
1	B	41	LYS	CA-C-N	5.72	127.00	119.84
1	B	41	LYS	C-N-CA	5.72	127.00	119.84
1	A	36	TRP	CB-CG-CD1	-5.71	118.33	126.90
1	C	443	HIS	N-CA-C	5.70	120.08	113.18
1	B	308	GLN	CA-C-N	5.70	127.92	120.28
1	B	308	GLN	C-N-CA	5.70	127.92	120.28
1	B	131	TRP	CG-CD2-CE3	5.68	139.58	133.90
1	C	413	VAL	N-CA-CB	5.67	119.01	111.64
1	C	125	VAL	CA-C-N	5.63	125.64	119.89
1	C	125	VAL	C-N-CA	5.63	125.64	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	111	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	B	304	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	397	GLN	N-CA-C	5.61	122.75	110.80
1	C	465	VAL	CA-C-N	5.60	126.14	120.38
1	C	465	VAL	C-N-CA	5.60	126.14	120.38
1	C	313	ASP	N-CA-C	-5.59	105.10	111.14
1	B	376	ASN	N-CA-C	5.56	117.92	109.63
1	C	68	GLY	CA-C-N	5.56	125.32	119.76
1	C	68	GLY	C-N-CA	5.56	125.32	119.76
1	C	358	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	A	14	ILE	CA-C-O	5.54	126.63	120.59
1	A	443	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	A	246	ILE	N-CA-C	5.53	120.85	109.34
1	B	111	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	A	68	GLY	CA-C-N	5.51	125.78	119.83
1	A	68	GLY	C-N-CA	5.51	125.78	119.83
1	C	316	ASN	CA-C-O	5.50	123.88	119.59
1	A	358	ASN	N-CA-C	5.50	119.16	111.30
1	A	36	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	C	131	TRP	CG-CD2-CE3	5.49	139.38	133.90
1	C	399	PHE	CA-CB-CG	5.49	119.28	113.80
1	B	389	GLU	N-CA-C	5.48	117.36	110.24
1	B	461	PHE	N-CA-C	5.48	118.99	110.17
1	B	354	HIS	CB-CG-CD2	-5.47	124.08	131.20
1	C	246	ILE	N-CA-C	5.47	120.72	109.34
1	B	369	ARG	CB-CG-CD	-5.46	98.73	111.30
1	A	131	TRP	CG-CD2-CE3	5.45	139.35	133.90
1	B	246	ILE	O-C-N	5.43	127.43	122.65
1	A	21	LYS	O-C-N	-5.42	117.69	121.65
1	A	116	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	56	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	C	425	THR	CA-CB-CG2	5.37	119.63	110.50
1	C	466	PRO	CA-C-N	5.36	125.28	119.76
1	C	466	PRO	C-N-CA	5.36	125.28	119.76
1	B	113	LYS	N-CA-C	5.31	117.39	109.59
1	A	413	VAL	N-CA-C	-5.30	100.85	108.48
1	A	56	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	175	LYS	CA-CB-CG	5.28	124.66	114.10
1	B	430	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	360	ASN	N-CA-C	-5.25	101.71	110.17
1	C	14	ILE	N-CA-C	5.25	115.87	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	SER	CA-C-O	5.24	124.90	119.97
1	B	157	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	132	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	A	365	ALA	CA-C-O	5.23	126.55	120.49
1	C	337	ARG	N-CA-C	-5.22	104.69	111.74
1	A	132	TRP	CE2-CD2-CG	-5.21	100.94	107.20
1	C	208	GLU	CB-CG-CD	5.21	121.45	112.60
1	C	354	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	B	400	VAL	N-CA-CB	-5.20	105.05	110.72
1	A	413	VAL	N-CA-CB	5.20	120.43	111.39
1	B	330	PHE	CA-C-N	5.17	124.78	119.56
1	B	330	PHE	C-N-CA	5.17	124.78	119.56
1	C	404	ARG	N-CA-C	-5.17	100.48	108.90
1	B	20	LEU	N-CA-C	5.16	118.36	110.20
1	C	36	TRP	CE2-CD2-CG	-5.16	101.00	107.20
1	C	247	LYS	N-CA-C	-5.15	102.08	109.24
1	B	61	ARG	N-CA-C	-5.14	100.14	108.52
1	B	465	VAL	CA-C-N	5.14	125.68	120.38
1	B	465	VAL	C-N-CA	5.14	125.68	120.38
1	A	40	ASN	O-C-N	-5.14	116.99	122.85
1	A	131	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	A	466	PRO	CA-C-N	5.12	125.11	119.89
1	A	466	PRO	C-N-CA	5.12	125.11	119.89
1	A	410	PHE	N-CA-C	-5.10	100.20	108.41
1	C	212	HIS	N-CA-C	5.08	116.90	111.36
1	A	206	THR	CA-CB-CG2	5.07	119.12	110.50
1	B	131	TRP	CB-CG-CD1	-5.07	119.30	126.90
1	B	158	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	410	PHE	N-CA-C	-5.05	101.07	109.46
1	C	132	TRP	CG-CD2-CE3	5.05	138.95	133.90
1	B	413	VAL	N-CA-C	-5.04	100.31	107.77
1	B	36	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	C	120	GLY	N-CA-C	-5.03	108.20	113.58
1	A	132	TRP	CB-CG-CD1	-5.03	119.36	126.90
1	A	177	GLN	N-CA-C	-5.02	105.72	111.14

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	2883	0	2845	78	0
1	B	2883	0	2845	101	0
1	C	2883	0	2845	74	0
All	All	8649	0	8535	213	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 12.

All (213) 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:33:ILE:HG21	1:C:172:GLU:HG2	1.54	0.90
1:B:65:TYR:HE1	1:C:398:ASN:HB3	1.46	0.79
1:A:168:ASN:HA	1:A:199:GLY:HA2	1.66	0.77
1:A:398:ASN:HB3	1:C:65:TYR:HE1	1.50	0.76
1:B:206:THR:HB	1:C:373:GLN:HE22	1.51	0.74
1:B:25:ARG:HG2	1:B:32:LEU:HD11	1.70	0.73
1:C:395:VAL:HG11	1:C:401:VAL:HG22	1.72	0.71
1:A:65:TYR:HE1	1:B:398:ASN:HB3	1.55	0.71
1:B:116:ASN:HD21	1:B:247:LYS:HA	1.58	0.68
1:A:33:ILE:HG21	1:A:172:GLU:HG2	1.74	0.68
1:A:112:GLN:HB2	1:B:435:ALA:HB1	1.75	0.67
1:B:75:GLN:HG3	1:B:366:LEU:HD22	1.76	0.67
1:A:341:GLU:HB3	1:A:414:SER:HB3	1.76	0.67
1:B:66:THR:HG22	1:B:161:ARG:O	1.94	0.67
1:A:233:LYS:HB2	1:A:237:VAL:HG22	1.76	0.66
1:B:324:THR:HG22	1:B:341:GLU:HG3	1.78	0.66
1:C:447:LEU:HD11	1:C:455:ILE:HD12	1.78	0.66
1:B:81:PHE:CE1	1:B:115:TYR:HB2	2.30	0.65
1:C:168:ASN:HA	1:C:199:GLY:HA2	1.77	0.65
1:B:246:ILE:HG23	1:B:248:PRO:HD3	1.79	0.65
1:A:75:GLN:HG3	1:A:366:LEU:HD22	1.79	0.64
1:B:239:VAL:HG11	1:B:243:LEU:HD12	1.79	0.64
1:B:118:ARG:NH2	1:B:309:THR:HG21	2.13	0.64
1:B:425:THR:HG21	1:B:430:ASN:ND2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HH22	1:B:309:THR:HG21	1.63	0.63
1:B:374:VAL:HG13	1:B:383:PHE:HB3	1.82	0.62
1:B:33:ILE:HG21	1:B:172:GLU:HG2	1.81	0.61
1:C:75:GLN:HG3	1:C:366:LEU:HD22	1.84	0.60
1:C:306:ILE:HG21	1:C:325:ALA:HB2	1.84	0.60
1:C:66:THR:HG23	1:C:161:ARG:O	2.02	0.60
1:B:437:PRO:HB2	1:B:440:VAL:HG13	1.84	0.59
1:A:74:ILE:HG22	1:A:119:GLU:HA	1.84	0.59
1:B:353:PRO:HA	1:B:401:VAL:O	2.02	0.59
1:B:425:THR:HG21	1:B:430:ASN:CG	2.28	0.58
1:B:438:GLU:O	1:B:441:ILE:HG22	2.03	0.58
1:B:302:LEU:HD22	1:B:302:LEU:H	1.69	0.58
1:B:63:PRO:HG3	1:B:132:TRP:HB3	1.85	0.58
1:A:373:GLN:HG2	1:A:381:ARG:HD2	1.86	0.57
1:B:333:LEU:HG	1:B:338:LEU:O	2.04	0.57
1:A:449:SER:O	1:A:453:ARG:HG3	2.05	0.56
1:C:239:VAL:HG21	1:C:243:LEU:HD13	1.87	0.56
1:A:395:VAL:HG11	1:A:401:VAL:HG22	1.87	0.56
1:C:300:MET:HE2	1:C:332:ALA:HA	1.88	0.55
1:B:316:ASN:HB3	1:B:319:ALA:HB3	1.88	0.55
1:A:206:THR:HG23	1:A:208:GLU:HG2	1.87	0.55
1:C:333:LEU:HG	1:C:338:LEU:O	2.07	0.55
1:C:300:MET:HE1	1:C:335:TRP:CD1	2.42	0.55
1:A:216:VAL:HG12	1:B:458:ASN:ND2	2.21	0.55
1:A:440:VAL:O	1:A:444:THR:HG23	2.06	0.55
1:A:306:ILE:HG21	1:A:325:ALA:HB2	1.88	0.54
1:B:25:ARG:HG3	1:B:34:GLU:HG2	1.89	0.54
1:B:77:GLY:HA3	1:B:141:VAL:HG22	1.89	0.54
1:C:54:THR:HB	1:C:142:VAL:HG22	1.89	0.54
1:A:83:MET:HE3	1:A:129:VAL:HG11	1.88	0.54
1:B:147:ILE:HD11	1:B:162:ARG:NH2	2.23	0.54
1:A:455:ILE:HG13	1:C:220:ILE:HD11	1.90	0.53
1:C:83:MET:HE2	1:C:302:LEU:HG	1.90	0.53
1:A:215:SER:HB3	1:B:459:ASN:HB2	1.91	0.53
1:A:81:PHE:HE2	1:A:83:MET:SD	2.32	0.52
1:B:425:THR:HG23	1:B:431:SER:HA	1.91	0.52
1:A:81:PHE:CE1	1:A:115:TYR:HB2	2.44	0.52
1:C:343:GLY:O	1:C:411:GLU:HA	2.10	0.52
1:C:433:LEU:HA	1:C:436:LEU:HD12	1.91	0.52
1:A:430:ASN:ND2	1:A:462:LYS:HE2	2.25	0.51
1:B:28:SER:HB3	1:B:236:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:HA	1:B:141:VAL:O	2.10	0.51
1:A:243:LEU:HD21	1:B:440:VAL:HG12	1.91	0.51
1:C:30:GLY:HA3	1:C:238:THR:HG23	1.91	0.51
1:C:85:TYR:CZ	1:C:297:ILE:HG12	2.45	0.51
1:A:85:TYR:CZ	1:A:297:ILE:HG12	2.46	0.51
1:A:302:LEU:H	1:A:302:LEU:HD22	1.76	0.51
1:A:367:ASN:HA	1:A:389:GLU:HG2	1.93	0.51
1:B:233:LYS:HB2	1:B:237:VAL:CG2	2.40	0.50
1:B:201:ILE:HD12	1:C:400:VAL:HG21	1.93	0.50
1:A:83:MET:HE2	1:A:302:LEU:HG	1.94	0.50
1:B:233:LYS:HB2	1:B:237:VAL:HG22	1.93	0.50
1:B:343:GLY:O	1:B:411:GLU:HA	2.12	0.50
1:A:223:ASN:HB3	1:B:447:LEU:HD21	1.94	0.49
1:B:27:GLU:HG3	1:B:32:LEU:HD13	1.94	0.49
1:C:159:MET:HE2	1:C:177:GLN:HB2	1.95	0.49
1:C:449:SER:O	1:C:453:ARG:HG3	2.12	0.49
1:C:324:THR:HG22	1:C:341:GLU:HG3	1.95	0.48
1:A:444:THR:HG21	1:C:63:PRO:HD3	1.95	0.48
1:A:374:VAL:HG13	1:A:383:PHE:HB3	1.95	0.48
1:A:204:GLY:O	1:B:381:ARG:HD3	2.13	0.48
1:A:206:THR:HB	1:B:373:GLN:HE22	1.77	0.48
1:B:74:ILE:HG22	1:B:119:GLU:HA	1.94	0.48
1:A:216:VAL:HG12	1:B:458:ASN:HD22	1.79	0.48
1:A:306:ILE:CG2	1:A:325:ALA:HB2	2.43	0.48
1:A:330:PHE:CD2	1:A:333:LEU:HD22	2.48	0.48
1:B:30:GLY:HA3	1:B:238:THR:HG23	1.95	0.48
1:C:121:ASP:HA	1:C:305:ASN:HA	1.95	0.48
1:C:367:ASN:HA	1:C:389:GLU:HG2	1.95	0.48
1:A:233:LYS:HE2	1:A:237:VAL:HG13	1.96	0.48
1:B:203:SER:HB3	1:B:226:GLY:HA3	1.95	0.48
1:C:76:GLN:HA	1:C:119:GLU:HB3	1.96	0.48
1:A:322:VAL:HG21	1:A:463:PHE:CE2	2.49	0.48
1:A:171:GLN:HE21	1:A:173:PHE:HB2	1.80	0.47
1:B:63:PRO:HD3	1:C:444:THR:HG21	1.96	0.47
1:C:365:ALA:HB3	1:C:388:GLN:O	2.14	0.47
1:B:81:PHE:HE2	1:B:83:MET:SD	2.37	0.47
1:C:339:SER:HB2	1:C:418:ASN:O	2.14	0.47
1:A:239:VAL:HG13	1:B:443:HIS:CE1	2.49	0.47
1:B:20:LEU:HB2	1:B:392:VAL:HG12	1.97	0.47
1:B:433:LEU:HA	1:B:436:LEU:HD12	1.97	0.47
1:C:83:MET:HE3	1:C:129:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:LEU:HB2	1:C:406:GLN:NE2	2.29	0.47
1:C:302:LEU:H	1:C:302:LEU:HD22	1.80	0.47
1:A:14:ILE:HG21	1:A:17:LEU:CD2	2.45	0.47
1:A:65:TYR:CE1	1:B:398:ASN:HB3	2.42	0.47
1:C:343:GLY:HA3	1:C:412:TYR:CE1	2.50	0.46
1:C:374:VAL:CG1	1:C:383:PHE:HB3	2.46	0.46
1:A:360:ASN:O	1:A:416:LYS:HA	2.15	0.46
1:A:435:ALA:HB3	1:C:84:ILE:HG23	1.98	0.46
1:A:164:TYR:O	1:A:200:SER:HB2	2.16	0.46
1:A:63:PRO:HD3	1:B:444:THR:HG21	1.97	0.46
1:B:64:SER:HB2	1:B:162:ARG:HG2	1.98	0.46
1:A:358:ASN:OD1	1:A:421:PRO:HA	2.15	0.46
1:B:373:GLN:HA	1:B:383:PHE:O	2.16	0.46
1:B:440:VAL:O	1:B:444:THR:HG23	2.16	0.45
1:C:396:PRO:HD2	1:C:399:PHE:CD2	2.51	0.45
1:A:30:GLY:HA3	1:A:238:THR:HG23	1.98	0.45
1:A:76:GLN:HA	1:A:119:GLU:HG2	1.98	0.45
1:A:110:ARG:HH12	1:B:438:GLU:H	1.62	0.45
1:A:333:LEU:HD12	1:A:336:LEU:HD12	1.98	0.45
1:B:85:TYR:CZ	1:B:297:ILE:HG12	2.52	0.45
1:C:301:ARG:NH2	1:C:304:HIS:ND1	2.65	0.45
1:A:381:ARG:HD3	1:C:204:GLY:O	2.17	0.45
1:B:62:ARG:HG2	1:C:444:THR:HG22	1.98	0.45
1:A:80:ILE:HG22	1:A:116:ASN:HD22	1.81	0.45
1:B:35:THR:HG22	1:B:51:SER:HB2	1.98	0.45
1:B:201:ILE:CD1	1:C:426:LEU:HD21	2.47	0.45
1:B:369:ARG:HE	1:B:406:GLN:NE2	2.15	0.45
1:A:333:LEU:HG	1:A:338:LEU:O	2.17	0.45
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.81	0.45
1:B:76:GLN:O	1:B:141:VAL:HA	2.15	0.44
1:C:333:LEU:HD12	1:C:336:LEU:HD12	1.99	0.44
1:B:367:ASN:HA	1:B:389:GLU:HG2	1.99	0.44
1:A:85:TYR:HA	1:A:86:PRO:HD2	1.84	0.44
1:C:48:VAL:HG21	1:C:362:ILE:HG12	2.00	0.44
1:A:13:GLN:HE21	1:C:159:MET:HG3	1.82	0.43
1:A:433:LEU:O	1:A:441:ILE:HD11	2.18	0.43
1:A:430:ASN:HD21	1:A:462:LYS:HE2	1.83	0.43
1:B:53:CYS:SG	1:B:61:ARG:NH2	2.86	0.43
1:C:81:PHE:CZ	1:C:83:MET:SD	3.11	0.43
1:A:11:GLU:HG3	1:C:157:ASP:HB3	2.00	0.43
1:A:456:LYS:NZ	1:C:110:ARG:NH2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HB3	1:B:54:THR:HG23	2.00	0.43
1:C:246:ILE:O	1:C:248:PRO:HD3	2.19	0.43
1:A:24:ASN:O	1:A:34:GLU:HA	2.18	0.43
1:A:216:VAL:HG11	1:A:220:ILE:HD11	2.01	0.43
1:B:33:ILE:HG21	1:B:172:GLU:CG	2.47	0.43
1:C:69:PRO:HB3	1:C:336:LEU:HD22	2.01	0.43
1:A:84:ILE:HG21	1:B:432:LEU:HA	2.01	0.43
1:B:206:THR:HB	1:C:373:GLN:NE2	2.28	0.43
1:C:70:GLN:HB3	1:C:125:VAL:HB	2.01	0.43
1:C:72:ILE:HG23	1:C:145:SER:HB3	2.00	0.43
1:B:374:VAL:CG1	1:B:383:PHE:HB3	2.48	0.42
1:C:171:GLN:HE21	1:C:173:PHE:HB2	1.84	0.42
1:A:40:ASN:HB3	1:A:42:PRO:HD2	2.01	0.42
1:A:452:ALA:O	1:A:456:LYS:HG3	2.19	0.42
1:B:86:PRO:HG2	1:C:357:LEU:HD11	2.00	0.42
1:B:395:VAL:HG21	1:B:401:VAL:HG11	2.00	0.42
1:C:330:PHE:O	1:C:333:LEU:HB2	2.19	0.42
1:A:400:VAL:HG21	1:C:201:ILE:HB	2.01	0.42
1:B:76:GLN:HA	1:B:119:GLU:HB3	2.01	0.42
1:B:80:ILE:HG22	1:B:116:ASN:ND2	2.35	0.42
1:B:438:GLU:C	1:B:441:ILE:HG22	2.44	0.42
1:C:66:THR:HG21	1:C:147:ILE:HD13	2.02	0.42
1:A:66:THR:HG21	1:A:147:ILE:HD13	2.02	0.42
1:B:214:PHE:CD2	1:B:224:LEU:HD21	2.54	0.42
1:C:24:ASN:HB3	1:C:35:THR:OG1	2.20	0.42
1:B:206:THR:HG22	1:B:209:PHE:H	1.84	0.42
1:B:24:ASN:HB3	1:B:35:THR:OG1	2.20	0.42
1:B:327:SER:HB3	1:B:419:ASP:HB2	2.01	0.42
1:A:13:GLN:NE2	1:C:159:MET:HG3	2.35	0.42
1:A:26:ILE:HD11	1:A:172:GLU:HA	2.01	0.42
1:B:156:LEU:HA	1:C:12:CYS:SG	2.60	0.42
1:B:441:ILE:HD13	1:B:441:ILE:HG21	1.85	0.42
1:A:48:VAL:HG21	1:A:362:ILE:HG12	2.01	0.42
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.77	0.42
1:B:68:GLY:N	1:B:127:THR:HG23	2.34	0.42
1:B:247:LYS:HZ2	1:B:247:LYS:HG2	1.58	0.42
1:C:350:MET:HB3	1:C:465:VAL:HG13	2.02	0.42
1:B:57:ARG:HG2	1:B:58:ASN:OD1	2.20	0.42
1:B:110:ARG:HH12	1:C:438:GLU:H	1.68	0.42
1:B:159:MET:HE3	1:B:160:PRO:O	2.20	0.42
1:B:168:ASN:HA	1:B:199:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HB3	1:C:54:THR:HG23	2.02	0.42
1:A:84:ILE:HD11	1:B:436:LEU:HD21	2.01	0.41
1:B:207:LEU:O	1:B:211:GLU:HG3	2.19	0.41
1:A:440:VAL:HG12	1:C:243:LEU:HD21	2.02	0.41
1:B:201:ILE:HD11	1:C:426:LEU:HD21	2.01	0.41
1:A:313:ASP:HB2	1:A:322:VAL:O	2.20	0.41
1:B:70:GLN:HE22	1:B:162:ARG:HH22	1.67	0.41
1:B:166:ALA:HB2	1:C:445:PHE:CE1	2.55	0.41
1:B:463:PHE:HD2	1:B:464:LEU:HD13	1.86	0.41
1:C:74:ILE:HG12	1:C:117:PHE:CD1	2.56	0.41
1:B:426:LEU:HD13	1:B:432:LEU:HD22	2.03	0.41
1:C:437:PRO:HB2	1:C:440:VAL:HG22	2.02	0.41
1:A:25:ARG:HG2	1:A:32:LEU:HD11	2.02	0.41
1:A:118:ARG:HH11	1:A:303:ARG:NH2	2.19	0.41
1:B:63:PRO:HB2	1:B:165:LEU:HD22	2.03	0.41
1:B:163:PHE:CZ	1:C:398:ASN:HB2	2.56	0.41
1:B:463:PHE:CD2	1:B:464:LEU:HD13	2.56	0.41
1:B:35:THR:HG21	1:B:172:GLU:HB3	2.03	0.40
1:C:20:LEU:HB2	1:C:392:VAL:HG13	2.02	0.40
1:C:312:PRO:HB3	1:C:321:SER:HB2	2.03	0.40
1:A:72:ILE:HG23	1:A:145:SER:HB3	2.03	0.40
1:B:11:GLU:HA	1:B:41:LYS:HE2	2.03	0.40
1:B:372:ILE:HG12	1:B:403:ALA:CB	2.52	0.40
1:A:398:ASN:HB3	1:C:65:TYR:CE1	2.40	0.40
1:A:372:ILE:HG21	1:A:393:LEU:CD2	2.52	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	356/476 (75%)	331 (93%)	19 (5%)	6 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	356/476 (75%)	324 (91%)	29 (8%)	3 (1%)	16	47
1	C	356/476 (75%)	326 (92%)	26 (7%)	4 (1%)	11	39
All	All	1068/1428 (75%)	981 (92%)	74 (7%)	13 (1%)	10	37

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	ILE
1	B	396	PRO
1	B	431	SER
1	A	397	GLN
1	C	397	GLN
1	A	463	PHE
1	B	156	LEU
1	C	429	ALA
1	C	463	PHE
1	A	418	ASN
1	A	307	GLY
1	A	396	PRO
1	C	246	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/414 (76%)	273 (87%)	42 (13%)	4	17
1	B	315/414 (76%)	269 (85%)	46 (15%)	3	14
1	C	315/414 (76%)	281 (89%)	34 (11%)	6	25
All	All	945/1242 (76%)	823 (87%)	122 (13%)	4	18

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN

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Mol	Chain	Res	Type
1	A	50	LEU
1	A	54	THR
1	A	55	LEU
1	A	66	THR
1	A	81	PHE
1	A	110	ARG
1	A	112	GLN
1	A	113	LYS
1	A	118	ARG
1	A	139	THR
1	A	150	ASN
1	A	152	LEU
1	A	171	GLN
1	A	175	LYS
1	A	202	LEU
1	A	206	THR
1	A	207	LEU
1	A	208	GLU
1	A	210	LEU
1	A	215	SER
1	A	220	ILE
1	A	223	ASN
1	A	225	GLN
1	A	233	LYS
1	A	238	THR
1	A	243	LEU
1	A	297	ILE
1	A	302	LEU
1	A	308	GLN
1	A	328	LEU
1	A	333	LEU
1	A	350	MET
1	A	374	VAL
1	A	391	ARG
1	A	401	VAL
1	A	408	ASP
1	A	413	VAL
1	A	433	LEU
1	A	450	GLN
1	A	464	LEU
1	A	467	PRO
1	B	18	ASN

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Mol	Chain	Res	Type
1	B	26	ILE
1	B	27	GLU
1	B	28	SER
1	B	40	ASN
1	B	50	LEU
1	B	54	THR
1	B	55	LEU
1	B	60	LEU
1	B	67	ASN
1	B	74	ILE
1	B	110	ARG
1	B	113	LYS
1	B	118	ARG
1	B	150	ASN
1	B	158	GLN
1	B	165	LEU
1	B	171	GLN
1	B	202	LEU
1	B	206	THR
1	B	208	GLU
1	B	209	PHE
1	B	210	LEU
1	B	223	ASN
1	B	225	GLN
1	B	237	VAL
1	B	238	THR
1	B	240	LYS
1	B	246	ILE
1	B	247	LYS
1	B	299	THR
1	B	302	LEU
1	B	308	GLN
1	B	337	ARG
1	B	350	MET
1	B	361	SER
1	B	374	VAL
1	B	391	ARG
1	B	401	VAL
1	B	408	ASP
1	B	413	VAL
1	B	433	LEU
1	B	434	ASN

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Mol	Chain	Res	Type
1	B	440	VAL
1	B	464	LEU
1	B	469	GLU
1	C	11	GLU
1	C	16	LYS
1	C	38	PRO
1	C	54	THR
1	C	55	LEU
1	C	81	PHE
1	C	110	ARG
1	C	113	LYS
1	C	150	ASN
1	C	152	LEU
1	C	171	GLN
1	C	174	LEU
1	C	175	LYS
1	C	210	LEU
1	C	220	ILE
1	C	222	LYS
1	C	233	LYS
1	C	238	THR
1	C	245	VAL
1	C	302	LEU
1	C	308	GLN
1	C	311	SER
1	C	333	LEU
1	C	374	VAL
1	C	391	ARG
1	C	401	VAL
1	C	425	THR
1	C	430	ASN
1	C	432	LEU
1	C	434	ASN
1	C	448	LYS
1	C	455	ILE
1	C	464	LEU
1	C	469	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN

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Mol	Chain	Res	Type
1	A	75	GLN
1	A	116	ASN
1	A	169	GLN
1	A	171	GLN
1	A	177	GLN
1	A	378	ASN
1	A	397	GLN
1	A	450	GLN
1	A	454	GLN
1	B	10	ASN
1	B	37	ASN
1	B	40	ASN
1	B	116	ASN
1	B	135	ASN
1	B	354	HIS
1	B	378	ASN
1	B	451	GLN
1	B	459	ASN
1	C	75	GLN
1	C	116	ASN
1	C	136	ASN
1	C	158	GLN
1	C	177	GLN
1	C	223	ASN
1	C	308	GLN
1	C	367	ASN
1	C	378	ASN
1	C	458	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

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

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	366/476 (76%)	-0.43	9 (2%) 58 37	3, 15, 37, 47	0
1	B	366/476 (76%)	-0.35	5 (1%) 73 53	4, 19, 37, 50	0
1	C	366/476 (76%)	-0.42	7 (1%) 66 45	3, 15, 36, 47	0
All	All	1098/1428 (76%)	-0.40	21 (1%) 66 45	3, 16, 37, 50	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	3.6
1	A	246	ILE	3.5
1	A	470	SER	3.4
1	B	85	TYR	3.2
1	C	310	SER	3.1
1	A	299	THR	3.0
1	B	246	ILE	2.9
1	C	450	GLN	2.8
1	C	469	GLU	2.7
1	A	85	TYR	2.7
1	A	430	ASN	2.7
1	A	450	GLN	2.5
1	C	85	TYR	2.5
1	B	248	PRO	2.4
1	A	115	TYR	2.4
1	C	298	CYS	2.4
1	A	247	LYS	2.4
1	C	309	THR	2.2
1	B	178	GLN	2.2
1	B	298	CYS	2.1
1	C	246	ILE	2.1

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.