



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:23 PM UTC

PDB ID : 1UCX / pdb_00001ucx
Title : Crystal structure of proglycinin C12G mutant
Authors : Utsumi, S.; Adachi, M.
Deposited on : 2003-04-24
Resolution : 3.20 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

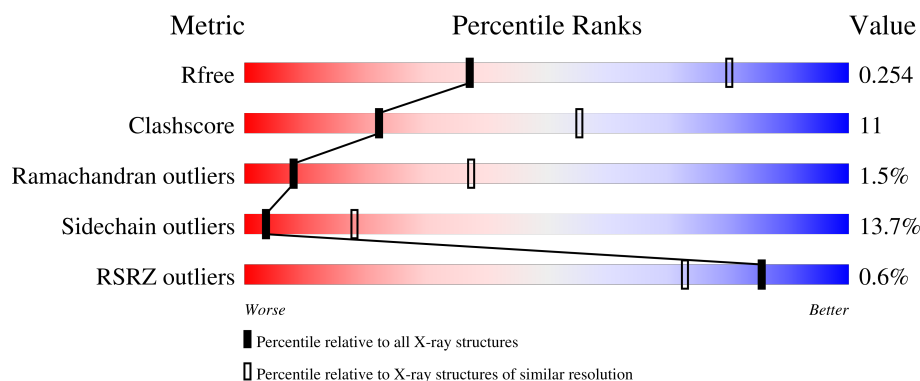
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	48%24%••23%
1	B	476	% 47%23%7%23%
1	C	476	% 45%25%7%•23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8643 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	367	Total	C	N	O	S	0	0	0
			2881	1821	509	540	11			
1	B	367	Total	C	N	O	S	0	0	0
			2881	1821	509	540	11			
1	C	367	Total	C	N	O	S	0	0	0
			2881	1821	509	540	11			

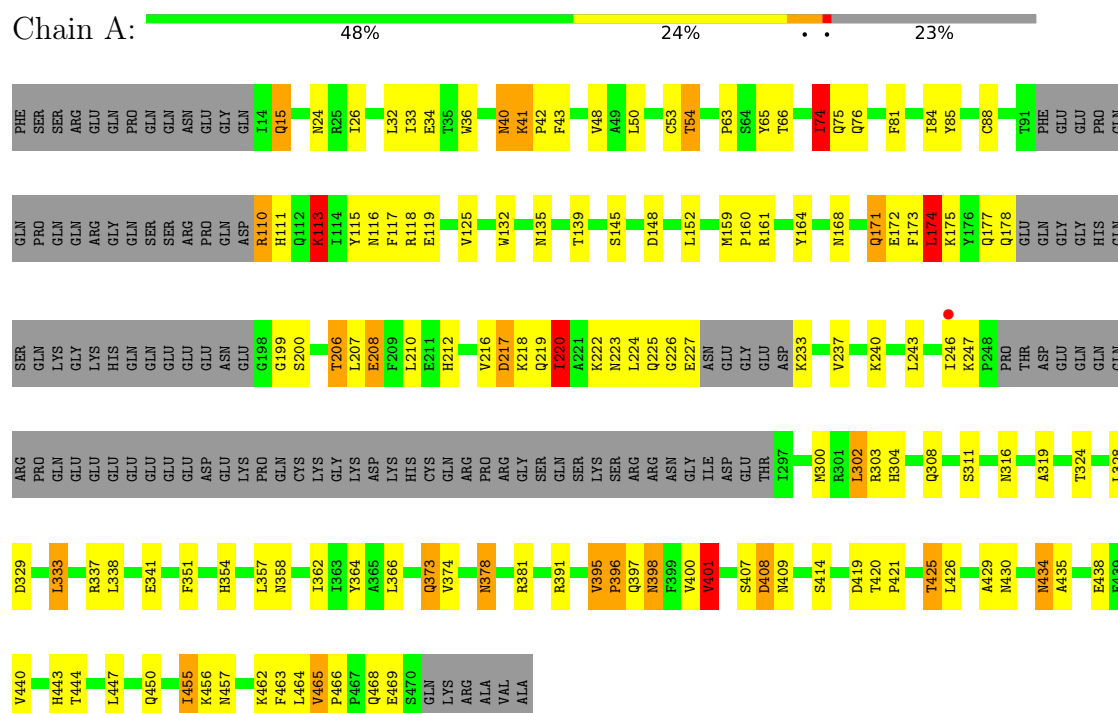
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	CYS	engineered mutation	UNP P04776
B	12	GLY	CYS	engineered mutation	UNP P04776
C	12	GLY	CYS	engineered mutation	UNP P04776

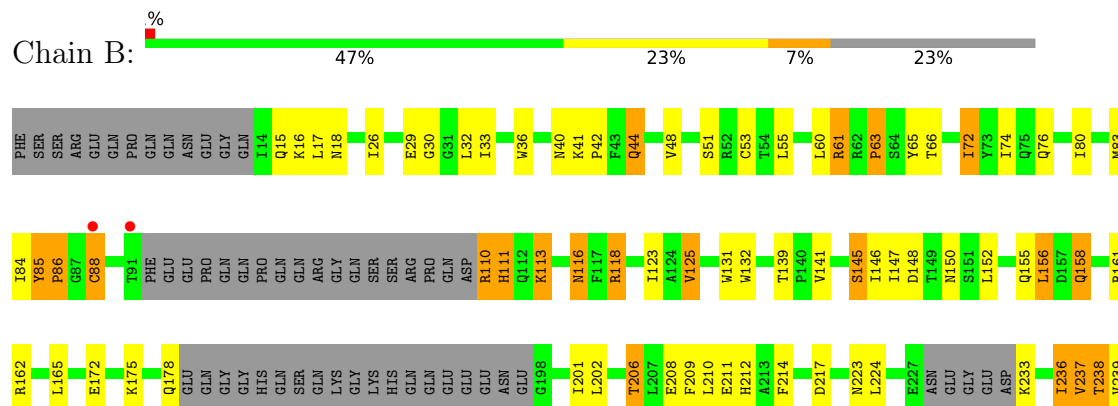
3 Residue-property plots

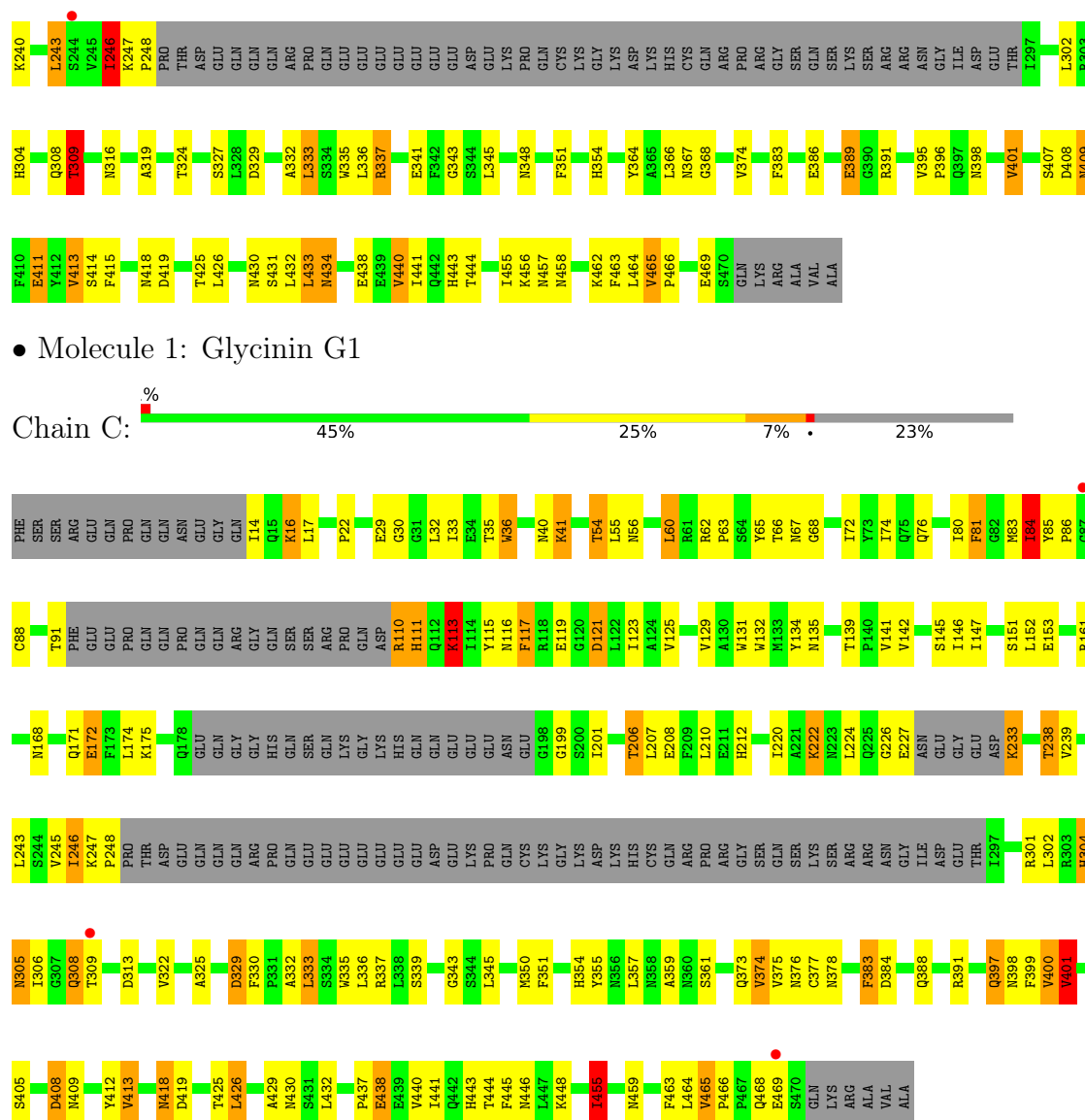
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	115.20Å 115.20Å 147.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 8.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 78.1 (8.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , 0.257 0.184 , 0.254	Depositor DCC
R_{free} test set	3591 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8643	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.89	10/2939 (0.3%)	1.67	54/3982 (1.4%)
1	B	0.86	6/2939 (0.2%)	1.69	50/3982 (1.3%)
1	C	0.89	5/2939 (0.2%)	1.71	65/3982 (1.6%)
All	All	0.88	21/8817 (0.2%)	1.69	169/11946 (1.4%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	HIS	CD2-NE2	-6.91	1.30	1.37
1	C	212	HIS	CD2-NE2	-6.84	1.30	1.37
1	B	443	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	304	HIS	CD2-NE2	-6.73	1.30	1.37
1	C	304	HIS	CD2-NE2	-6.56	1.30	1.37
1	C	111	HIS	CD2-NE2	-6.53	1.30	1.37
1	B	111	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	354	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	443	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	304	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	443	HIS	CD2-NE2	-6.14	1.31	1.37
1	B	212	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	111	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	354	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	212	HIS	CD2-NE2	-5.43	1.31	1.37
1	A	304	HIS	CG-ND1	-5.35	1.32	1.38
1	A	354	HIS	CG-ND1	-5.28	1.32	1.38
1	B	465	VAL	CA-CB	5.27	1.58	1.54
1	A	54	THR	CA-CB	5.23	1.63	1.53
1	A	220	ILE	CA-CB	5.22	1.60	1.54
1	A	74	ILE	CA-CB	5.21	1.59	1.53

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PHE	CA-CB-CG	12.56	126.36	113.80
1	A	408	ASP	CA-CB-CG	-11.11	101.49	112.60
1	C	351	PHE	CA-CB-CG	11.03	124.83	113.80
1	A	351	PHE	CA-CB-CG	10.80	124.60	113.80
1	B	88	CYS	N-CA-C	9.25	122.84	110.08
1	B	457	ASN	N-CA-C	8.71	124.84	114.04
1	A	408	ASP	O-C-N	8.30	133.09	122.87
1	C	117	PHE	CA-CB-CG	8.02	121.82	113.80
1	C	384	ASP	CA-CB-CG	7.86	120.46	112.60
1	B	408	ASP	O-C-N	7.81	133.04	122.57
1	C	408	ASP	O-C-N	7.77	133.13	122.41
1	C	345	LEU	N-CA-C	7.38	120.44	108.41
1	A	206	THR	CA-CB-OG1	-7.34	98.58	109.60
1	B	84	ILE	N-CA-C	7.29	114.01	106.21
1	B	145	SER	N-CA-C	7.14	120.20	108.99
1	A	408	ASP	CA-C-O	7.14	128.55	120.84
1	A	125	VAL	CA-C-N	7.08	127.11	119.89
1	A	125	VAL	C-N-CA	7.08	127.11	119.89
1	A	425	THR	CA-CB-OG1	-7.07	99.00	109.60
1	B	408	ASP	CA-C-O	7.06	128.61	120.98
1	B	212	HIS	CB-CG-CD2	-6.95	122.17	131.20
1	C	359	ALA	N-CA-C	6.76	118.47	108.60
1	B	386	GLU	N-CA-C	6.70	119.82	108.90
1	C	401	VAL	CB-CA-C	-6.62	100.63	110.82
1	B	395	VAL	CA-C-N	6.60	128.09	119.84
1	B	395	VAL	C-N-CA	6.60	128.09	119.84
1	C	408	ASP	CA-CB-CG	-6.60	106.00	112.60
1	A	85	TYR	CA-C-N	6.60	126.10	119.24
1	A	85	TYR	C-N-CA	6.60	126.10	119.24
1	B	348	ASN	N-CA-C	6.51	121.00	113.38
1	A	145	SER	N-CA-C	6.50	119.59	109.52
1	C	125	VAL	CA-C-N	6.49	126.51	119.89
1	C	125	VAL	C-N-CA	6.49	126.51	119.89
1	C	135	ASN	CA-CB-CG	6.46	119.06	112.60
1	B	246	ILE	N-CA-CB	-6.45	100.58	111.23
1	A	212	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	B	125	VAL	CA-C-N	6.43	126.45	119.89
1	B	125	VAL	C-N-CA	6.43	126.45	119.89
1	C	41	LYS	CA-C-N	6.36	125.58	118.97
1	C	41	LYS	C-N-CA	6.36	125.58	118.97
1	C	212	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	429	ALA	N-CA-C	6.27	119.78	111.75
1	C	36	TRP	CG-CD2-CE3	6.26	140.16	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	VAL	N-CA-C	-6.26	98.72	107.80
1	C	113	LYS	N-CA-C	6.25	119.42	110.10
1	C	468	GLN	N-CA-C	6.20	119.69	111.75
1	C	146	ILE	N-CA-C	6.19	117.39	108.48
1	B	116	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	135	ASN	CA-CB-CG	6.11	118.71	112.60
1	B	443	HIS	CA-CB-CG	-6.11	107.69	113.80
1	C	56	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	C	132	TRP	CG-CD2-CE3	6.03	139.93	133.90
1	B	61	ARG	N-CA-C	-6.02	98.92	108.73
1	A	407	SER	CA-C-N	-5.96	114.56	122.85
1	A	407	SER	C-N-CA	-5.96	114.56	122.85
1	B	36	TRP	CG-CD2-CE3	5.92	139.82	133.90
1	C	413	VAL	CB-CA-C	-5.92	102.36	110.77
1	B	389	GLU	N-CA-C	5.91	118.63	110.35
1	B	401	VAL	CB-CA-C	-5.90	101.83	110.62
1	A	132	TRP	CG-CD2-CE3	5.89	139.79	133.90
1	C	413	VAL	N-CA-CB	5.89	119.29	111.64
1	C	121	ASP	N-CA-C	5.88	118.87	110.10
1	B	443	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	B	354	HIS	CB-CG-CD2	-5.86	123.59	131.20
1	B	443	HIS	N-CA-C	5.84	119.59	112.23
1	C	466	PRO	N-CA-C	5.83	117.82	110.70
1	C	245	VAL	O-C-N	5.83	129.17	122.64
1	C	36	TRP	CB-CG-CD1	-5.80	118.20	126.90
1	B	36	TRP	CB-CG-CD1	-5.80	118.20	126.90
1	A	425	THR	CA-CB-CG2	5.77	120.31	110.50
1	A	409	ASN	CA-CB-CG	-5.75	106.85	112.60
1	C	376	ASN	N-CA-C	5.74	118.18	109.63
1	A	36	TRP	CG-CD2-CE3	5.74	139.64	133.90
1	C	304	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	132	TRP	CB-CG-CD1	-5.73	118.31	126.90
1	C	459	ASN	CA-CB-CG	5.72	118.32	112.60
1	B	409	ASN	O-C-N	5.72	130.19	122.59
1	B	131	TRP	CG-CD2-CE3	5.71	139.62	133.90
1	A	41	LYS	CA-C-N	5.71	124.90	118.97
1	A	41	LYS	C-N-CA	5.71	124.90	118.97
1	A	88	CYS	N-CA-C	5.70	118.46	108.82
1	A	465	VAL	CA-C-N	5.69	126.24	120.38
1	A	465	VAL	C-N-CA	5.69	126.24	120.38
1	C	68	GLY	CA-C-N	5.68	125.61	119.76
1	C	68	GLY	C-N-CA	5.68	125.61	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	206	THR	N-CA-CB	-5.67	102.25	110.36
1	B	408	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	457	ASN	N-CA-C	5.65	122.08	113.61
1	C	62	ARG	CA-C-N	5.64	125.92	119.83
1	C	62	ARG	C-N-CA	5.64	125.92	119.83
1	C	443	HIS	CA-CB-CG	-5.64	108.16	113.80
1	C	40	ASN	N-CA-C	-5.63	101.95	110.28
1	C	308	GLN	CB-CG-CD	5.59	122.10	112.60
1	C	465	VAL	CA-C-N	5.57	126.12	120.38
1	C	465	VAL	C-N-CA	5.57	126.12	120.38
1	A	36	TRP	CB-CG-CD1	-5.57	118.55	126.90
1	C	409	ASN	CA-CB-CG	-5.57	107.03	112.60
1	A	132	TRP	CE2-CD2-CG	-5.56	100.53	107.20
1	A	308	GLN	N-CA-C	5.56	118.10	111.71
1	A	88	CYS	CA-C-N	5.55	125.46	119.85
1	A	88	CYS	C-N-CA	5.55	125.46	119.85
1	C	132	TRP	CB-CG-CD1	-5.54	118.59	126.90
1	B	113	LYS	N-CA-C	5.52	118.32	110.10
1	B	238	THR	N-CA-C	5.48	117.65	109.59
1	A	84	ILE	CA-CB-CG2	-5.47	101.19	110.50
1	B	246	ILE	N-CA-C	5.47	120.71	109.34
1	A	455	ILE	CA-CB-CG1	-5.47	101.11	110.40
1	A	113	LYS	N-CA-C	5.41	118.16	110.10
1	C	405	SER	N-CA-C	5.41	117.52	110.43
1	B	217	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	401	VAL	CB-CA-C	-5.38	102.21	110.50
1	C	443	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	B	36	TRP	CE2-CD2-CG	-5.37	100.75	107.20
1	B	401	VAL	N-CA-C	5.37	116.22	108.48
1	A	409	ASN	O-C-N	5.37	129.72	122.59
1	C	145	SER	N-CA-C	5.36	117.92	108.75
1	A	111	HIS	N-CA-C	5.35	117.39	108.99
1	C	408	ASP	CA-C-N	5.31	131.69	121.54
1	C	408	ASP	C-N-CA	5.31	131.69	121.54
1	A	206	THR	CA-CB-CG2	5.29	119.50	110.50
1	B	237	VAL	N-CA-CB	-5.29	104.10	111.41
1	C	329	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	206	THR	CA-CB-OG1	-5.27	101.70	109.60
1	B	41	LYS	CA-C-N	5.26	125.32	119.32
1	B	41	LYS	C-N-CA	5.26	125.32	119.32
1	C	208	GLU	CB-CG-CD	5.26	121.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	C	305	ASN	N-CA-C	5.25	117.28	109.25
1	A	357	LEU	N-CA-C	5.25	117.00	111.28
1	A	174	LEU	N-CA-C	-5.24	105.25	111.69
1	A	398	ASN	N-CA-C	5.22	118.78	112.93
1	C	111	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	C	466	PRO	CA-C-N	5.21	125.12	119.76
1	C	466	PRO	C-N-CA	5.21	125.12	119.76
1	B	386	GLU	CA-C-O	5.20	125.97	120.36
1	B	243	LEU	N-CA-C	5.19	118.00	110.42
1	A	316	ASN	CA-C-N	5.19	124.86	119.56
1	A	316	ASN	C-N-CA	5.19	124.86	119.56
1	C	455	ILE	CA-CB-CG1	-5.18	101.59	110.40
1	A	304	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	C	429	ALA	N-CA-C	5.17	119.90	111.37
1	C	84	ILE	CB-CA-C	-5.16	106.80	112.68
1	C	354	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	378	ASN	CA-CB-CG	5.15	117.75	112.60
1	C	36	TRP	CE2-CD2-CG	-5.15	101.03	107.20
1	C	84	ILE	CA-CB-CG2	-5.14	101.75	110.50
1	C	388	GLN	N-CA-C	5.14	117.35	109.95
1	C	16	LYS	N-CA-C	5.14	116.55	107.61
1	A	395	VAL	CA-C-N	5.13	126.25	119.84
1	A	395	VAL	C-N-CA	5.13	126.25	119.84
1	B	85	TYR	CA-C-N	5.12	126.24	119.84
1	B	85	TYR	C-N-CA	5.12	126.24	119.84
1	A	210	LEU	N-CA-CB	5.11	117.73	110.16
1	A	354	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	304	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	C	383	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	175	LYS	N-CA-CB	-5.05	102.70	110.12
1	C	425	THR	CA-CB-OG1	-5.04	102.03	109.60
1	B	309	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	212	HIS	CB-CG-ND1	5.04	130.26	122.70
1	A	395	VAL	N-CA-C	-5.04	102.21	107.60
1	A	217	ASP	N-CA-C	5.03	117.33	110.55
1	B	337	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	C	399	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	465	VAL	CA-C-N	5.01	125.54	120.38
1	B	465	VAL	C-N-CA	5.01	125.54	120.38
1	B	125	VAL	N-CA-C	5.01	113.11	108.15
1	A	117	PHE	CA-CB-CG	5.01	118.81	113.80

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	2881	0	2847	67	0
1	B	2881	0	2847	67	0
1	C	2881	0	2847	78	0
All	All	8643	0	8541	182	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 11.

All (182) 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:398:ASN:HB3	1:C:65:TYR:HE1	1.39	0.87
1:C:33:ILE:HG21	1:C:172:GLU:HG2	1.65	0.78
1:A:65:TYR:HE1	1:B:398:ASN:HB3	1.50	0.77
1:B:324:THR:HG22	1:B:341:GLU:HG3	1.68	0.76
1:B:367:ASN:HB3	1:B:411:GLU:HG3	1.66	0.76
1:A:168:ASN:HA	1:A:199:GLY:HA2	1.68	0.75
1:B:333:LEU:HD12	1:B:336:LEU:HD12	1.70	0.73
1:A:75:GLN:HG3	1:A:366:LEU:HD22	1.69	0.73
1:A:373:GLN:HG2	1:A:381:ARG:HD2	1.75	0.68
1:B:65:TYR:HE1	1:C:398:ASN:HB3	1.59	0.66
1:A:447:LEU:HD11	1:A:455:ILE:HD12	1.78	0.65
1:A:110:ARG:NH2	1:B:438:GLU:HB2	2.13	0.64
1:C:60:LEU:HD23	1:C:134:TYR:HB2	1.80	0.62
1:B:72:ILE:HA	1:B:145:SER:HB3	1.81	0.62
1:A:395:VAL:HG11	1:A:401:VAL:HG22	1.81	0.61
1:B:374:VAL:HG12	1:B:383:PHE:HB3	1.82	0.61
1:A:430:ASN:ND2	1:A:462:LYS:HE2	2.17	0.59
1:B:201:ILE:HD11	1:C:426:LEU:HD21	1.85	0.59
1:A:110:ARG:HH22	1:B:438:GLU:HB2	1.66	0.59
1:A:400:VAL:HG21	1:C:201:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:VAL:O	1:A:444:THR:HG23	2.03	0.59
1:B:80:ILE:HG22	1:B:116:ASN:HD22	1.69	0.58
1:A:233:LYS:HE2	1:A:237:VAL:HG13	1.83	0.58
1:B:364:TYR:HB3	1:B:413:VAL:HG23	1.85	0.58
1:C:339:SER:HB2	1:C:418:ASN:O	2.04	0.57
1:A:40:ASN:HB3	1:A:42:PRO:HD2	1.86	0.57
1:A:159:MET:SD	1:A:160:PRO:HD2	2.45	0.57
1:B:66:THR:HG22	1:B:161:ARG:O	2.05	0.57
1:B:33:ILE:HG13	1:B:236:ILE:HD11	1.87	0.56
1:C:83:MET:HE3	1:C:129:VAL:HG11	1.86	0.56
1:C:66:THR:HG21	1:C:147:ILE:HD13	1.87	0.56
1:C:239:VAL:HG21	1:C:243:LEU:HD13	1.87	0.56
1:B:368:GLY:O	1:B:389:GLU:HG3	2.05	0.56
1:A:63:PRO:HD3	1:B:444:THR:HG21	1.87	0.56
1:A:302:LEU:H	1:A:302:LEU:HD22	1.71	0.55
1:A:66:THR:HG22	1:A:161:ARG:O	2.06	0.55
1:A:430:ASN:HD21	1:A:462:LYS:HE2	1.71	0.55
1:C:30:GLY:HA3	1:C:238:THR:HG23	1.88	0.54
1:C:207:LEU:HD21	1:C:222:LYS:HD2	1.88	0.54
1:A:333:LEU:HG	1:A:338:LEU:O	2.08	0.54
1:C:116:ASN:HD21	1:C:248:PRO:HD2	1.73	0.54
1:B:214:PHE:CD2	1:B:224:LEU:HD21	2.43	0.54
1:C:32:LEU:HB3	1:C:54:THR:HG23	1.90	0.54
1:C:85:TYR:HB3	1:C:88:CYS:SG	2.48	0.54
1:A:398:ASN:HB3	1:C:65:TYR:CE1	2.31	0.54
1:A:216:VAL:HG11	1:A:220:ILE:HD11	1.89	0.53
1:A:48:VAL:HG21	1:A:362:ILE:HG12	1.90	0.53
1:B:110:ARG:HH12	1:C:438:GLU:H	1.56	0.53
1:C:168:ASN:HD21	1:C:226:GLY:HA3	1.73	0.53
1:B:233:LYS:HB2	1:B:237:VAL:HG22	1.91	0.53
1:B:345:LEU:O	1:B:409:ASN:HA	2.10	0.52
1:C:35:THR:HG21	1:C:172:GLU:HB3	1.92	0.52
1:B:63:PRO:HG3	1:B:132:TRP:HB3	1.90	0.51
1:C:66:THR:HG23	1:C:161:ARG:O	2.09	0.51
1:B:53:CYS:SG	1:B:61:ARG:NH2	2.83	0.51
1:C:74:ILE:HG12	1:C:117:PHE:CD1	2.46	0.51
1:A:341:GLU:HB3	1:A:414:SER:HB3	1.92	0.51
1:A:26:ILE:O	1:A:32:LEU:HD12	2.10	0.51
1:C:374:VAL:CG1	1:C:383:PHE:HB3	2.41	0.51
1:A:113:LYS:HD2	1:A:115:TYR:CZ	2.46	0.51
1:B:156:LEU:HD21	1:C:397:GLN:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:HG22	1:C:119:GLU:HA	1.92	0.51
1:B:33:ILE:HG21	1:B:172:GLU:HG2	1.92	0.50
1:A:81:PHE:HZ	1:A:302:LEU:HD23	1.77	0.50
1:C:113:LYS:HD2	1:C:115:TYR:CZ	2.47	0.50
1:B:434:ASN:O	1:B:456:LYS:HE2	2.11	0.50
1:B:15:GLN:HG3	1:B:16:LYS:N	2.26	0.50
1:B:224:LEU:HD13	1:C:455:ILE:HD13	1.94	0.50
1:A:118:ARG:HH11	1:A:303:ARG:HH22	1.59	0.50
1:C:355:TYR:HE1	1:C:357:LEU:HG	1.77	0.50
1:A:164:TYR:O	1:A:200:SER:HB2	2.12	0.49
1:B:110:ARG:HH12	1:C:438:GLU:HB2	1.77	0.49
1:A:216:VAL:HG12	1:B:458:ASN:ND2	2.26	0.49
1:C:72:ILE:HB	1:C:123:ILE:HB	1.94	0.49
1:C:76:GLN:NE2	1:C:139:THR:HG22	2.28	0.49
1:A:15:GLN:H	1:A:15:GLN:CD	2.21	0.48
1:A:15:GLN:HE22	1:A:41:LYS:HD3	1.77	0.48
1:C:116:ASN:ND2	1:C:248:PRO:HD2	2.28	0.48
1:A:337:ARG:HA	1:A:419:ASP:HB3	1.96	0.48
1:A:438:GLU:HB2	1:C:110:ARG:NH2	2.29	0.48
1:C:14:ILE:HG12	1:C:41:LYS:HD3	1.95	0.48
1:C:76:GLN:HA	1:C:119:GLU:HB3	1.96	0.48
1:B:430:ASN:ND2	1:B:462:LYS:HE2	2.29	0.47
1:B:463:PHE:HD2	1:B:464:LEU:HD13	1.79	0.47
1:A:110:ARG:HH12	1:B:438:GLU:H	1.63	0.47
1:B:83:MET:HE1	1:B:125:VAL:HA	1.95	0.47
1:A:33:ILE:HG23	1:A:53:CYS:SG	2.54	0.47
1:B:343:GLY:O	1:B:411:GLU:HA	2.14	0.47
1:A:434:ASN:O	1:A:456:LYS:HE2	2.14	0.47
1:A:438:GLU:H	1:C:110:ARG:HH12	1.62	0.47
1:A:456:LYS:HZ3	1:C:110:ARG:NH2	2.12	0.47
1:B:165:LEU:HD12	1:B:201:ILE:HD11	1.95	0.47
1:C:80:ILE:HG22	1:C:116:ASN:ND2	2.30	0.47
1:B:118:ARG:NH2	1:B:309:THR:HG21	2.29	0.47
1:C:116:ASN:HD21	1:C:247:LYS:HD3	1.79	0.47
1:B:201:ILE:HD12	1:C:400:VAL:HG21	1.96	0.47
1:C:54:THR:HA	1:C:141:VAL:O	2.14	0.46
1:C:355:TYR:CE1	1:C:357:LEU:HG	2.50	0.46
1:A:24:ASN:O	1:A:34:GLU:HA	2.15	0.46
1:A:364:TYR:CE2	1:A:366:LEU:HD23	2.51	0.46
1:B:110:ARG:NH1	1:C:438:GLU:HB2	2.31	0.46
1:B:17:LEU:HB2	1:B:383:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:VAL:CG1	1:B:383:PHE:HB3	2.45	0.46
1:C:80:ILE:HG22	1:C:116:ASN:HD22	1.80	0.46
1:C:121:ASP:HA	1:C:305:ASN:HA	1.97	0.46
1:A:300:MET:O	1:A:302:LEU:HD13	2.15	0.46
1:A:358:ASN:OD1	1:A:421:PRO:HA	2.16	0.46
1:B:206:THR:HB	1:C:373:GLN:HE22	1.81	0.46
1:C:29:GLU:HB2	1:C:233:LYS:HA	1.98	0.45
1:A:33:ILE:HG21	1:A:172:GLU:HG2	1.98	0.45
1:B:29:GLU:HB2	1:B:233:LYS:HA	1.97	0.45
1:A:76:GLN:HA	1:A:119:GLU:HG2	1.97	0.45
1:A:364:TYR:HE2	1:A:366:LEU:HD23	1.82	0.45
1:B:76:GLN:O	1:B:141:VAL:HA	2.17	0.45
1:B:147:ILE:HD11	1:B:162:ARG:NH2	2.32	0.45
1:B:366:LEU:HB2	1:B:411:GLU:HB2	1.99	0.45
1:A:373:GLN:HE22	1:C:206:THR:HB	1.82	0.45
1:B:40:ASN:O	1:B:44:GLN:HG2	2.17	0.45
1:C:377:CYS:SG	1:C:378:ASN:ND2	2.90	0.45
1:B:30:GLY:HA3	1:B:238:THR:HG23	1.99	0.44
1:B:425:THR:HG23	1:B:431:SER:HA	1.99	0.44
1:A:159:MET:HE2	1:A:177:GLN:HG3	1.99	0.44
1:A:118:ARG:HD3	1:A:303:ARG:HH21	1.82	0.44
1:B:208:GLU:HA	1:B:211:GLU:HB2	1.99	0.44
1:C:301:ARG:NH2	1:C:304:HIS:ND1	2.66	0.44
1:B:327:SER:HB3	1:B:419:ASP:HB2	1.99	0.44
1:A:81:PHE:CE1	1:A:115:TYR:HB2	2.52	0.44
1:C:168:ASN:HA	1:C:199:GLY:HA2	1.99	0.44
1:A:174:LEU:O	1:A:178:GLN:HG2	2.18	0.44
1:C:91:THR:HG23	1:C:111:HIS:O	2.17	0.44
1:B:201:ILE:CD1	1:C:426:LEU:HD21	2.48	0.44
1:B:316:ASN:HB3	1:B:319:ALA:HB3	2.00	0.44
1:C:332:ALA:O	1:C:335:TRP:HB2	2.18	0.44
1:C:374:VAL:HB	1:C:401:VAL:CG1	2.48	0.44
1:B:74:ILE:HD11	1:B:123:ILE:CD1	2.48	0.43
1:C:333:LEU:HD12	1:C:336:LEU:HD12	2.00	0.43
1:A:116:ASN:HD21	1:A:247:LYS:HG2	1.82	0.43
1:A:319:ALA:HB2	1:A:466:PRO:HA	2.00	0.43
1:A:456:LYS:NZ	1:C:110:ARG:NH2	2.66	0.43
1:B:48:VAL:HG12	1:B:148:ASP:HA	2.01	0.43
1:B:201:ILE:HB	1:C:400:VAL:HG21	2.00	0.43
1:A:171:GLN:HE21	1:A:173:PHE:HB2	1.83	0.43
1:B:26:ILE:O	1:B:32:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ILE:HD11	1:C:455:ILE:HG22	2.00	0.43
1:C:445:PHE:O	1:C:446:ASN:HB3	2.17	0.43
1:C:17:LEU:HB2	1:C:383:PHE:HB2	2.01	0.42
1:B:332:ALA:O	1:B:335:TRP:HB2	2.19	0.42
1:B:438:GLU:HA	1:B:441:ILE:HG22	2.01	0.42
1:A:74:ILE:HG22	1:A:119:GLU:HA	2.01	0.42
1:B:85:TYR:HB3	1:B:88:CYS:SG	2.60	0.42
1:C:304:HIS:HB3	1:C:330:PHE:CD2	2.54	0.42
1:A:435:ALA:HB3	1:C:84:ILE:CG2	2.50	0.42
1:A:217:ASP:OD2	1:A:219:GLN:HB2	2.19	0.42
1:C:322:VAL:HG21	1:C:463:PHE:HE2	1.85	0.42
1:C:337:ARG:HD3	1:C:419:ASP:OD1	2.19	0.42
1:C:374:VAL:HB	1:C:401:VAL:HG13	2.01	0.42
1:B:16:LYS:HB2	1:B:16:LYS:HE3	1.83	0.42
1:B:239:VAL:HG11	1:B:243:LEU:HD12	2.02	0.42
1:C:343:GLY:HA3	1:C:412:TYR:CE1	2.55	0.41
1:C:22:PRO:HD3	1:C:36:TRP:CZ2	2.56	0.41
1:C:374:VAL:HA	1:C:400:VAL:O	2.21	0.41
1:B:146:ILE:HD13	1:B:415:PHE:HB3	2.03	0.41
1:B:246:ILE:HG23	1:B:248:PRO:HD3	2.03	0.41
1:B:465:VAL:HA	1:B:466:PRO:HD3	1.92	0.41
1:C:306:ILE:HG21	1:C:325:ALA:HB2	2.02	0.41
1:A:148:ASP:HB2	1:A:338:LEU:HD21	2.02	0.41
1:A:206:THR:HG22	1:A:208:GLU:HG2	2.03	0.41
1:A:233:LYS:HB2	1:A:237:VAL:HG22	2.02	0.41
1:A:243:LEU:HD21	1:B:440:VAL:HG12	2.02	0.41
1:A:444:THR:HG21	1:C:63:PRO:HD3	2.02	0.41
1:B:111:HIS:CD2	1:C:437:PRO:HA	2.56	0.41
1:C:63:PRO:HA	1:C:131:TRP:O	2.21	0.41
1:A:465:VAL:HA	1:A:466:PRO:HD3	1.91	0.41
1:A:447:LEU:CD1	1:A:455:ILE:HD12	2.49	0.40
1:C:66:THR:HG22	1:C:67:ASN:N	2.36	0.40
1:C:85:TYR:HA	1:C:86:PRO:HD2	1.87	0.40
1:C:440:VAL:O	1:C:444:THR:HG23	2.20	0.40
1:A:440:VAL:HG12	1:C:243:LEU:HD21	2.03	0.40
1:C:246:ILE:O	1:C:248:PRO:HD3	2.21	0.40
1:B:433:LEU:HD12	1:B:455:ILE:HG21	2.02	0.40
1:C:350:MET:HB3	1:C:465:VAL:HG13	2.03	0.40
1:A:43:PHE:HD1	1:A:48:VAL:HG23	1.86	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	357/476 (75%)	327 (92%)	24 (7%)	6 (2%)	7	35
1	B	357/476 (75%)	323 (90%)	28 (8%)	6 (2%)	7	35
1	C	357/476 (75%)	328 (92%)	25 (7%)	4 (1%)	11	43
All	All	1071/1428 (75%)	978 (91%)	77 (7%)	16 (2%)	8	37

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	GLN
1	B	246	ILE
1	B	396	PRO
1	C	397	GLN
1	C	246	ILE
1	A	226	GLY
1	A	396	PRO
1	A	397	GLN
1	A	463	PHE
1	B	418	ASN
1	A	240	LYS
1	B	86	PRO
1	B	156	LEU
1	C	418	ASN
1	C	469	GLU
1	A	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	315/413 (76%)	273 (87%)	42 (13%)	4	19
1	B	315/413 (76%)	271 (86%)	44 (14%)	3	17
1	C	315/413 (76%)	272 (86%)	43 (14%)	3	18
All	All	945/1239 (76%)	816 (86%)	129 (14%)	3	18

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	40	ASN
1	A	50	LEU
1	A	54	THR
1	A	74	ILE
1	A	110	ARG
1	A	113	LYS
1	A	139	THR
1	A	152	LEU
1	A	171	GLN
1	A	174	LEU
1	A	175	LYS
1	A	207	LEU
1	A	208	GLU
1	A	218	LYS
1	A	220	ILE
1	A	222	LYS
1	A	223	ASN
1	A	224	LEU
1	A	225	GLN
1	A	227	GLU
1	A	302	LEU
1	A	311	SER
1	A	324	THR
1	A	328	LEU
1	A	329	ASP
1	A	333	LEU
1	A	373	GLN
1	A	374	VAL
1	A	378	ASN
1	A	391	ARG
1	A	396	PRO

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Mol	Chain	Res	Type
1	A	401	VAL
1	A	408	ASP
1	A	420	THR
1	A	425	THR
1	A	426	LEU
1	A	434	ASN
1	A	450	GLN
1	A	464	LEU
1	A	468	GLN
1	A	469	GLU
1	B	18	ASN
1	B	42	PRO
1	B	44	GLN
1	B	51	SER
1	B	55	LEU
1	B	60	LEU
1	B	63	PRO
1	B	72	ILE
1	B	86	PRO
1	B	110	ARG
1	B	113	LYS
1	B	118	ARG
1	B	139	THR
1	B	150	ASN
1	B	152	LEU
1	B	155	GLN
1	B	158	GLN
1	B	178	GLN
1	B	202	LEU
1	B	209	PHE
1	B	210	LEU
1	B	223	ASN
1	B	236	ILE
1	B	240	LYS
1	B	246	ILE
1	B	247	LYS
1	B	302	LEU
1	B	308	GLN
1	B	309	THR
1	B	329	ASP
1	B	333	LEU
1	B	337	ARG

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Mol	Chain	Res	Type
1	B	391	ARG
1	B	401	VAL
1	B	407	SER
1	B	411	GLU
1	B	413	VAL
1	B	414	SER
1	B	426	LEU
1	B	432	LEU
1	B	433	LEU
1	B	434	ASN
1	B	440	VAL
1	B	469	GLU
1	C	16	LYS
1	C	54	THR
1	C	55	LEU
1	C	60	LEU
1	C	81	PHE
1	C	84	ILE
1	C	110	ARG
1	C	113	LYS
1	C	151	SER
1	C	152	LEU
1	C	153	GLU
1	C	171	GLN
1	C	172	GLU
1	C	174	LEU
1	C	175	LYS
1	C	210	LEU
1	C	220	ILE
1	C	222	LYS
1	C	224	LEU
1	C	227	GLU
1	C	233	LYS
1	C	238	THR
1	C	302	LEU
1	C	308	GLN
1	C	309	THR
1	C	313	ASP
1	C	329	ASP
1	C	333	LEU
1	C	361	SER
1	C	374	VAL

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Mol	Chain	Res	Type
1	C	375	VAL
1	C	391	ARG
1	C	400	VAL
1	C	401	VAL
1	C	408	ASP
1	C	413	VAL
1	C	426	LEU
1	C	430	ASN
1	C	432	LEU
1	C	438	GLU
1	C	448	LYS
1	C	455	ILE
1	C	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	39	ASN
1	A	112	GLN
1	A	116	ASN
1	A	135	ASN
1	A	136	ASN
1	A	158	GLN
1	A	171	GLN
1	A	450	GLN
1	A	454	GLN
1	B	37	ASN
1	B	40	ASN
1	B	58	ASN
1	B	75	GLN
1	B	116	ASN
1	B	136	ASN
1	B	171	GLN
1	B	212	HIS
1	B	225	GLN
1	B	308	GLN
1	B	354	HIS
1	B	367	ASN
1	B	378	ASN
1	B	443	HIS
1	B	450	GLN

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Mol	Chain	Res	Type
1	B	451	GLN
1	B	459	ASN
1	C	15	GLN
1	C	18	ASN
1	C	39	ASN
1	C	70	GLN
1	C	75	GLN
1	C	116	ASN
1	C	212	HIS
1	C	223	ASN
1	C	308	GLN
1	C	367	ASN
1	C	378	ASN
1	C	409	ASN
1	C	454	GLN

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 [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	367/476 (77%)	-0.53	1 (0%)	90 81	2, 14, 32, 39	0
1	B	367/476 (77%)	-0.40	3 (0%)	82 67	4, 16, 33, 41	0
1	C	367/476 (77%)	-0.51	3 (0%)	82 67	3, 14, 31, 42	0
All	All	1101/1428 (77%)	-0.48	7 (0%)	85 73	2, 15, 32, 42	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	GLU	3.0
1	A	246	ILE	2.9
1	B	91	THR	2.6
1	C	87	GLY	2.6
1	B	244	SER	2.3
1	B	88	CYS	2.1
1	C	309	THR	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.