



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 02:15 PM UTC

PDB ID : 3UW6 / pdb_00003uw6
Title : Crystal Structure of Engineered Protein, Northeast Structural Genomics Consortium Target OR120
Authors : Seetharaman, J.; Lew, S.; Nivon, L.; Baker, D.; Bjelic, S.; Ciccocanti, C.; Sahdev, S.; Xiao, R.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-11-30
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
Mogul	:	2022.3.0, CSD as543be (2022)
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

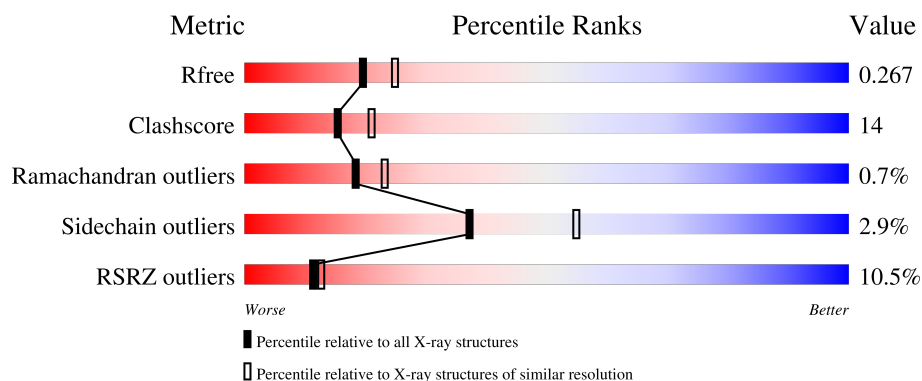
1 Overall quality at a glance

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))
R_{free}	180053	6319 (2.30-2.30)
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	390	8% 71% 21% • 5%
1	B	390	9% 68% 23% • 5%
1	C	390	12% 67% 25% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8977 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 Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	Se	0	0	0
			2929	1876	520	519	4	10			
1	B	371	Total	C	N	O	S	Se	0	0	0
			2914	1867	516	518	4	9			
1	C	370	Total	C	N	O	S	Se	0	0	0
			2900	1858	515	514	4	9			

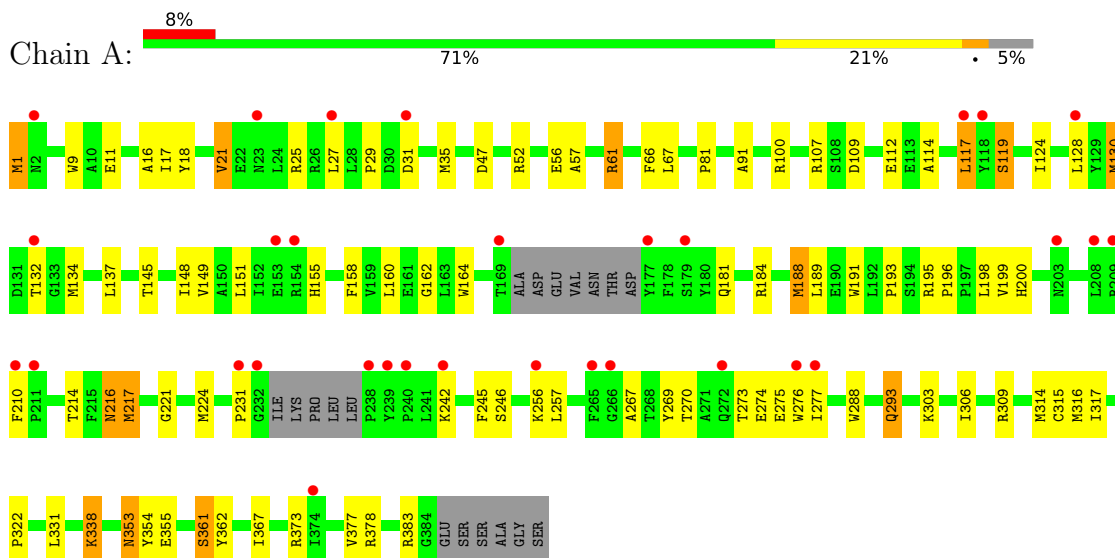
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	80	Total	O	0	0
			80	80		
2	C	74	Total	O	0	0
			74	74		

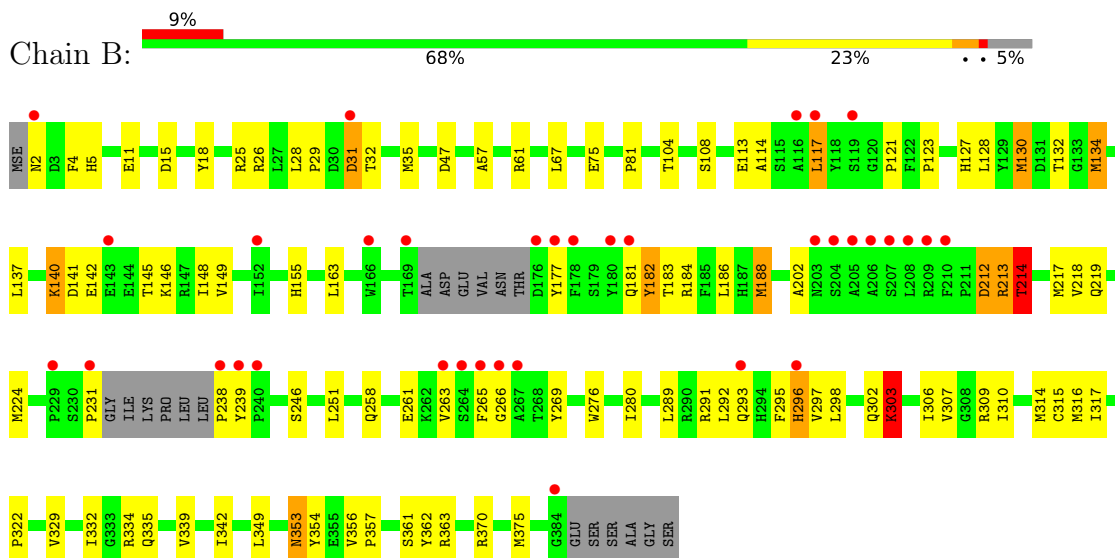
3 Residue-property plots [i](#)

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

• Molecule 1: Alanine racemase

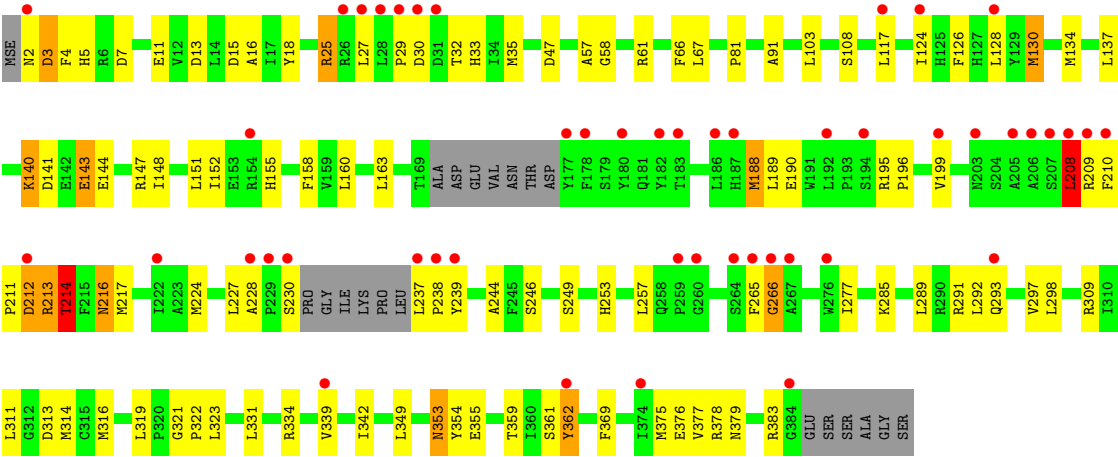


• Molecule 1: Alanine racemase



• Molecule 1: Alanine racemase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.35Å 112.35Å 237.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.47 – 2.30 30.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.47-2.30) 97.1 (30.47-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 2.14Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.259 0.231 , 0.267	Depositor DCC
R_{free} test set	12039 reflections (7.48%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8977	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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	0.72	13/2995 (0.4%)	0.94	12/4051 (0.3%)
1	B	1.07	31/2980 (1.0%)	0.93	13/4035 (0.3%)
1	C	1.35	62/2965 (2.1%)	0.99	19/4014 (0.5%)
All	All	1.08	106/8940 (1.2%)	0.95	44/12100 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	379	ASN	C-O	-18.43	1.02	1.24
1	B	213	ARG	CA-CB	-18.02	1.23	1.53
1	C	376	GLU	C-O	-15.27	1.05	1.23
1	C	377	VAL	C-O	-14.14	1.08	1.24
1	B	213	ARG	C-O	-13.78	1.06	1.24
1	B	214	THR	C-O	-13.77	1.06	1.24
1	C	378	ARG	C-O	-13.51	1.08	1.24
1	C	3	ASP	C-O	-13.38	1.06	1.23
1	A	119	SER	C-O	-13.06	1.07	1.24
1	B	303	LYS	CB-CG	-12.95	1.13	1.52
1	C	4	PHE	C-O	-11.92	1.08	1.23
1	B	296	HIS	C-O	-11.88	1.08	1.23
1	B	214	THR	CB-CG2	-11.83	1.13	1.52
1	B	212	ASP	C-O	-11.80	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	LYS	CA-CB	-10.74	1.37	1.53
1	B	303	LYS	C-O	-10.64	1.11	1.24
1	C	379	ASN	CG-ND2	-10.56	1.11	1.33
1	C	3	ASP	CB-CG	-10.43	1.25	1.52
1	C	3	ASP	CG-OD2	-10.33	1.05	1.25
1	B	212	ASP	CA-C	-10.30	1.43	1.52
1	C	208	LEU	N-CA	-10.15	1.33	1.46
1	C	213	ARG	C-O	-9.89	1.12	1.23
1	C	377	VAL	CA-CB	-9.65	1.42	1.54
1	C	211	PRO	CA-C	-9.62	1.38	1.52
1	C	211	PRO	C-O	-9.37	1.11	1.24
1	C	3	ASP	CG-OD1	-9.37	1.07	1.25
1	C	378	ARG	CZ-NH2	-9.32	1.21	1.33
1	A	224	MSE	SE-CE	-9.30	1.67	1.95
1	C	379	ASN	CA-C	-9.28	1.41	1.52
1	C	379	ASN	CG-OD1	-9.14	1.06	1.23
1	A	217	MSE	SE-CE	-9.09	1.68	1.95
1	B	212	ASP	CG-OD2	-8.97	1.08	1.25
1	C	2	ASN	C-O	-8.91	1.05	1.23
1	B	213	ARG	CA-C	-8.88	1.40	1.52
1	C	214	THR	CA-CB	-8.84	1.38	1.53
1	C	35	MSE	SE-CE	-8.69	1.69	1.95
1	C	377	VAL	CB-CG2	-8.30	1.25	1.52
1	B	214	THR	N-CA	-8.23	1.35	1.46
1	B	303	LYS	CG-CD	-8.15	1.28	1.52
1	A	119	SER	CA-CB	-8.13	1.42	1.54
1	C	214	THR	C-O	-8.11	1.13	1.24
1	A	35	MSE	SE-CE	-8.04	1.71	1.95
1	B	35	MSE	SE-CE	-7.91	1.71	1.95
1	B	303	LYS	N-CA	-7.89	1.36	1.46
1	C	211	PRO	N-CA	-7.85	1.37	1.47
1	C	376	GLU	CD-OE1	-7.73	1.10	1.25
1	C	4	PHE	CD2-CE2	-7.63	1.15	1.38
1	C	376	GLU	CD-OE2	-7.51	1.11	1.25
1	B	224	MSE	SE-CE	-7.47	1.73	1.95
1	C	378	ARG	CZ-NH1	-7.47	1.22	1.32
1	C	210	PHE	CA-C	-7.42	1.43	1.52
1	C	130	MSE	SE-CE	-7.40	1.73	1.95
1	C	214	THR	CB-CG2	-7.36	1.28	1.52
1	C	208	LEU	C-O	-7.35	1.14	1.24
1	C	4	PHE	CD1-CE1	-7.32	1.16	1.38
1	B	295	PHE	C-N	-7.17	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	379	ASN	N-CA	-7.14	1.37	1.46
1	B	212	ASP	CG-OD1	-7.11	1.11	1.25
1	A	119	SER	CA-C	-7.07	1.42	1.52
1	C	377	VAL	C-N	-7.04	1.24	1.33
1	C	4	PHE	CE2-CZ	-6.90	1.18	1.38
1	B	212	ASP	C-N	-6.88	1.24	1.33
1	C	188	MSE	SE-CE	-6.86	1.74	1.95
1	C	209	ARG	C-O	-6.86	1.15	1.23
1	C	314	MSE	SE-CE	-6.77	1.75	1.95
1	C	377	VAL	CB-CG1	-6.76	1.30	1.52
1	C	212	ASP	CA-C	-6.68	1.43	1.52
1	C	4	PHE	CG-CD2	-6.58	1.25	1.38
1	C	2	ASN	CG-OD1	-6.43	1.11	1.23
1	B	188	MSE	SE-CE	-6.41	1.76	1.95
1	C	224	MSE	SE-CE	-6.26	1.76	1.95
1	C	3	ASP	CA-CB	-6.21	1.43	1.53
1	C	4	PHE	CE1-CZ	-6.20	1.20	1.38
1	A	130	MSE	SE-CE	-6.19	1.76	1.95
1	C	378	ARG	CB-CG	-6.16	1.33	1.52
1	B	217	MSE	SE-CE	-6.07	1.77	1.95
1	C	378	ARG	N-CA	-6.07	1.39	1.46
1	C	214	THR	N-CA	-5.99	1.38	1.46
1	C	208	LEU	CA-C	-5.96	1.44	1.52
1	A	134	MSE	SE-CE	-5.91	1.77	1.95
1	B	314	MSE	SE-CE	-5.84	1.77	1.95
1	B	134	MSE	SE-CE	-5.78	1.78	1.95
1	C	209	ARG	CA-C	-5.77	1.45	1.53
1	B	375	MSE	SE-CE	-5.75	1.78	1.95
1	B	303	LYS	CA-C	-5.70	1.45	1.52
1	B	213	ARG	C-N	-5.70	1.26	1.33
1	B	302	GLN	C-N	-5.62	1.25	1.33
1	B	130	MSE	SE-CE	-5.60	1.78	1.95
1	C	208	LEU	CA-CB	-5.60	1.44	1.53
1	A	316	MSE	SE-CE	-5.54	1.78	1.95
1	C	212	ASP	C-O	-5.47	1.17	1.24
1	B	130	MSE	CG-SE	-5.37	1.79	1.95
1	C	134	MSE	SE-CE	-5.36	1.79	1.95
1	C	188	MSE	CG-SE	-5.35	1.79	1.95
1	A	188	MSE	CG-SE	-5.29	1.79	1.95
1	A	188	MSE	SE-CE	-5.27	1.79	1.95
1	C	376	GLU	C-N	-5.25	1.26	1.33
1	C	375	MSE	SE-CE	-5.22	1.79	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	MSE	CG-SE	-5.22	1.79	1.95
1	C	134	MSE	CG-SE	-5.21	1.79	1.95
1	C	2	ASN	CA-CB	-5.19	1.43	1.53
1	A	314	MSE	SE-CE	-5.15	1.79	1.95
1	C	4	PHE	CG-CD1	-5.10	1.28	1.38
1	B	188	MSE	CG-SE	-5.09	1.80	1.95
1	C	378	ARG	CA-CB	-5.06	1.46	1.53
1	A	1	MSE	SE-CE	-5.02	1.80	1.95

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PRO	N-CA-CB	10.64	109.89	102.65
1	A	378	ARG	N-CA-CB	-9.39	96.03	110.77
1	A	377	VAL	N-CA-C	-9.19	94.77	108.46
1	B	303	LYS	N-CA-C	8.62	123.47	109.76
1	C	213	ARG	N-CA-C	8.25	121.12	108.42
1	B	361	SER	N-CA-C	8.20	120.90	110.33
1	A	378	ARG	N-CA-C	-7.93	95.34	108.34
1	C	361	SER	N-CA-C	7.69	120.51	110.43
1	B	183	THR	N-CA-C	-7.36	103.34	111.36
1	C	2	ASN	N-CA-C	7.29	131.43	111.00
1	C	209	ARG	N-CA-C	-7.00	101.96	112.04
1	A	355	GLU	N-CA-C	6.53	119.40	111.82
1	B	289	LEU	N-CA-C	6.50	118.69	110.24
1	C	376	GLU	N-CA-C	6.47	118.39	108.42
1	B	231	PRO	N-CA-CB	6.40	110.04	103.00
1	C	3	ASP	N-CA-C	6.33	119.89	110.52
1	A	377	VAL	CB-CA-C	-6.06	101.17	110.50
1	C	355	GLU	N-CA-C	5.97	118.58	111.71
1	A	47	ASP	N-CA-C	5.96	117.47	110.97
1	B	5	HIS	N-CA-C	5.93	119.75	111.56
1	C	4	PHE	N-CA-C	5.89	118.80	109.50
1	C	377	VAL	O-C-N	-5.84	116.96	123.26
1	C	378	ARG	N-CA-C	5.79	117.85	108.41
1	C	67	LEU	N-CA-C	5.78	118.04	111.11
1	C	211	PRO	N-CA-C	-5.74	100.65	112.47
1	C	378	ARG	CG-CD-NE	5.67	124.48	112.00
1	C	289	LEU	N-CA-C	5.66	117.60	110.24
1	A	119	SER	CA-CB-OG	-5.55	100.00	111.10
1	B	295	PHE	O-C-N	-5.49	116.26	122.68
1	A	67	LEU	N-CA-C	5.43	117.62	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	ASP	N-CA-C	5.40	116.86	110.97
1	B	155	HIS	CA-C-N	5.36	124.97	119.56
1	B	155	HIS	C-N-CA	5.36	124.97	119.56
1	C	5	HIS	N-CA-C	5.34	118.93	111.56
1	A	361	SER	N-CA-C	5.33	122.15	110.80
1	C	293	GLN	N-CA-C	5.30	118.84	112.38
1	C	210	PHE	O-C-N	5.24	126.65	121.57
1	B	67	LEU	N-CA-C	5.22	119.99	111.37
1	B	108	SER	N-CA-C	-5.22	105.76	111.82
1	B	140	LYS	N-CA-C	5.11	119.79	113.50
1	B	47	ASP	N-CA-C	5.06	117.19	111.02
1	A	245	PHE	N-CA-C	5.03	117.10	108.90
1	A	293	GLN	N-CA-C	5.02	118.17	111.75
1	C	266	GLY	N-CA-C	-5.01	108.10	114.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	TYR	Sidechain
1	B	362	TYR	Sidechain
1	C	213	ARG	Peptide
1	C	362	TYR	Sidechain

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	2929	0	2900	68	0
1	B	2914	0	2865	74	0
1	C	2900	0	2861	99	1
2	A	80	0	0	4	1
2	B	80	0	0	1	0
2	C	74	0	0	2	0
All	All	8977	0	8626	235	1

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 14.

All (235) 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:B:296:HIS:ND1	1:B:303:LYS:HE2	1.20	1.46
1:B:296:HIS:CE1	1:B:303:LYS:HE2	1.72	1.23
1:C:91:ALA:HA	1:C:117:LEU:CD2	1.71	1.19
1:C:208:LEU:CD2	1:C:239:TYR:OH	1.94	1.15
1:B:296:HIS:ND1	1:B:303:LYS:CE	2.13	1.11
1:B:296:HIS:CE1	1:B:303:LYS:CE	2.39	1.06
1:C:91:ALA:HA	1:C:117:LEU:HD21	1.38	1.04
1:B:296:HIS:CE1	1:B:303:LYS:NZ	2.38	0.92
1:C:199:VAL:H	1:C:216:ASN:HD21	1.15	0.90
1:C:208:LEU:HD21	1:C:239:TYR:OH	1.70	0.90
1:C:91:ALA:HA	1:C:117:LEU:HD23	1.52	0.89
1:A:25:ARG:O	1:A:25:ARG:HD3	1.74	0.88
1:A:353:ASN:HD22	1:A:354:TYR:H	1.16	0.88
1:C:128:LEU:HD21	1:C:148:ILE:HG21	1.54	0.87
1:A:216:ASN:HD22	1:A:216:ASN:H	1.18	0.87
1:A:199:VAL:H	1:A:216:ASN:HD21	1.20	0.86
1:A:132:THR:HG23	1:A:184:ARG:CG	2.07	0.84
1:A:17:ILE:O	1:A:21:VAL:HG12	1.79	0.83
1:B:25:ARG:O	1:B:25:ARG:HD3	1.78	0.82
1:A:132:THR:HG22	1:A:132:THR:O	1.76	0.82
1:A:130:MSE:HE3	1:A:188:MSE:HB3	1.64	0.80
1:A:353:ASN:HD22	1:A:354:TYR:N	1.82	0.78
1:C:208:LEU:HD22	1:C:239:TYR:OH	1.82	0.77
1:B:296:HIS:HE1	1:B:303:LYS:NZ	1.82	0.75
1:C:322:PRO:O	1:C:323:LEU:HD12	1.85	0.75
1:C:128:LEU:CD2	1:C:148:ILE:HG21	2.16	0.75
1:A:114:ALA:HA	1:A:117:LEU:HD22	1.68	0.75
1:C:353:ASN:HD22	1:C:354:TYR:H	1.35	0.74
1:C:91:ALA:CA	1:C:117:LEU:CD2	2.61	0.74
1:C:163:LEU:HG	1:C:196:PRO:HG3	1.70	0.73
1:B:212:ASP:OD1	1:B:214:THR:CG2	2.36	0.72
1:A:132:THR:HG21	1:A:181:GLN:HA	1.72	0.72
1:C:216:ASN:H	1:C:216:ASN:HD22	1.36	0.71
1:C:91:ALA:CA	1:C:117:LEU:HD21	2.19	0.71
1:B:266:GLY:HA3	1:B:309:ARG:HB2	1.72	0.71
1:C:208:LEU:HD21	1:C:239:TYR:HH	1.55	0.71
1:B:332:ILE:HD13	1:B:342:ILE:HD13	1.72	0.71
1:B:130:MSE:SE	1:B:163:LEU:HD21	2.41	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:THR:O	1:B:184:ARG:HG2	1.91	0.70
1:A:216:ASN:H	1:A:216:ASN:ND2	1.88	0.70
1:B:334:ARG:HB2	1:B:339:VAL:HG12	1.75	0.68
1:A:52:ARG:HD2	2:A:400:HOH:O	1.93	0.68
1:A:132:THR:HG23	1:A:184:ARG:HB3	1.75	0.68
1:A:132:THR:CG2	1:A:184:ARG:HB3	2.24	0.68
1:C:195:ARG:NH2	1:C:199:VAL:HG21	2.08	0.68
1:C:124:ILE:HD13	1:C:126:PHE:CZ	2.29	0.68
1:B:353:ASN:HD22	1:B:354:TYR:H	1.43	0.67
1:A:91:ALA:HA	1:A:117:LEU:HD11	1.76	0.67
1:C:29:PRO:HG2	1:C:32:THR:HG23	1.77	0.67
1:A:61:ARG:HG3	1:A:81:PRO:HB2	1.76	0.67
1:C:321:GLY:O	1:C:323:LEU:HD13	1.95	0.67
1:A:107:ARG:NH1	1:A:109:ASP:HB2	2.10	0.66
1:A:256:LYS:HD3	1:A:276:TRP:CZ2	2.31	0.66
1:B:296:HIS:HE1	1:B:303:LYS:HZ1	1.43	0.65
1:C:199:VAL:H	1:C:216:ASN:ND2	1.90	0.65
1:B:297:VAL:HG11	1:B:329:VAL:CG1	2.27	0.65
1:B:212:ASP:O	1:B:213:ARG:CB	2.30	0.64
1:A:353:ASN:ND2	1:A:354:TYR:H	1.94	0.64
1:A:132:THR:HG23	1:A:184:ARG:CB	2.28	0.64
1:A:199:VAL:H	1:A:216:ASN:ND2	1.96	0.62
1:C:147:ARG:O	1:C:151:LEU:HD23	2.00	0.62
1:C:353:ASN:HD22	1:C:354:TYR:N	1.98	0.61
1:C:216:ASN:HD22	1:C:216:ASN:N	1.95	0.61
1:C:334:ARG:HB2	1:C:339:VAL:HG12	1.82	0.61
1:C:322:PRO:C	1:C:323:LEU:HD12	2.26	0.60
1:A:61:ARG:HD2	1:A:217:MSE:HE1	1.82	0.60
1:B:353:ASN:HD22	1:B:354:TYR:N	1.99	0.60
1:C:216:ASN:H	1:C:216:ASN:ND2	2.00	0.60
1:A:132:THR:O	1:A:132:THR:CG2	2.48	0.60
1:A:257:LEU:HD11	1:A:277:ILE:HD12	1.84	0.59
1:B:145:THR:O	1:B:149:VAL:HG23	2.02	0.59
1:C:27:LEU:HD21	1:C:238:PRO:HG2	1.83	0.59
1:B:114:ALA:HA	1:B:117:LEU:CD2	2.33	0.58
1:B:291:ARG:HE	1:C:291:ARG:NE	2.01	0.58
1:A:100:ARG:HG3	1:A:100:ARG:HH11	1.68	0.58
1:B:363:ARG:HG2	1:C:66:PHE:HZ	1.67	0.58
1:C:128:LEU:HD21	1:C:148:ILE:CG2	2.29	0.58
1:B:184:ARG:O	1:B:188:MSE:HG3	2.03	0.58
1:C:124:ILE:HG23	1:C:124:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LEU:HD21	1:C:316:MSE:HE1	1.87	0.57
1:B:296:HIS:CE1	1:B:303:LYS:HZ3	2.22	0.57
1:C:297:VAL:CG2	1:C:331:LEU:HD13	2.34	0.57
1:B:61:ARG:HG2	1:B:81:PRO:HB2	1.86	0.57
1:B:251:LEU:HD21	1:B:317:ILE:HD11	1.87	0.56
1:C:208:LEU:CD2	1:C:239:TYR:HH	2.09	0.56
1:C:266:GLY:HA3	1:C:309:ARG:HB2	1.85	0.56
1:C:297:VAL:HG22	1:C:298:LEU:H	1.71	0.56
1:B:291:ARG:NE	1:C:291:ARG:NE	2.54	0.56
1:C:227:LEU:HD21	1:C:342:ILE:HD12	1.88	0.56
1:B:356:VAL:HB	1:B:357:PRO:HD3	1.87	0.56
1:C:297:VAL:HG23	1:C:331:LEU:HD13	1.87	0.55
1:A:216:ASN:HD22	1:A:216:ASN:N	1.83	0.55
1:A:130:MSE:CE	1:A:188:MSE:HB3	2.36	0.55
1:C:163:LEU:HD12	1:C:163:LEU:O	2.07	0.55
1:A:132:THR:HG23	1:A:184:ARG:HG3	1.87	0.55
1:C:128:LEU:HG	1:C:160:LEU:HD11	1.90	0.54
1:A:52:ARG:O	1:A:56:GLU:HG3	2.06	0.54
1:A:353:ASN:ND2	1:A:354:TYR:N	2.55	0.54
1:B:212:ASP:OD1	1:B:214:THR:HG23	2.07	0.54
1:C:238:PRO:HG2	1:C:239:TYR:HD1	1.73	0.53
1:A:27:LEU:C	1:A:27:LEU:HD23	2.33	0.53
1:B:142:GLU:O	1:B:146:LYS:HG2	2.08	0.53
1:A:267:ALA:HB2	1:A:309:ARG:HD2	1.91	0.53
1:C:141:ASP:OD2	1:C:143:GLU:HB2	2.09	0.53
1:B:114:ALA:HA	1:B:117:LEU:HD22	1.90	0.53
1:C:292:LEU:HG	1:C:349:LEU:HD21	1.90	0.52
1:A:269:TYR:OH	1:A:275:GLU:OE2	2.24	0.52
1:A:293:GLN:O	1:A:306:ILE:O	2.27	0.52
1:B:297:VAL:HG12	1:B:298:LEU:N	2.22	0.52
1:A:184:ARG:O	1:A:188:MSE:HG3	2.09	0.52
1:B:263:VAL:HG23	1:B:269:TYR:HB3	1.92	0.52
1:B:266:GLY:C	1:B:309:ARG:HD2	2.34	0.52
1:A:124:ILE:HD12	2:A:409:HOH:O	2.09	0.52
1:A:315:CYS:HB2	2:A:401:HOH:O	2.09	0.51
1:A:160:LEU:HD22	1:A:196:PRO:HB3	1.91	0.51
1:C:309:ARG:HG2	1:C:309:ARG:HH11	1.76	0.51
1:A:128:LEU:HD11	1:A:148:ILE:HG21	1.92	0.51
1:B:291:ARG:C	1:B:293:GLN:H	2.19	0.51
1:B:181:GLN:O	1:B:182:TYR:HB2	2.10	0.51
1:C:316:MSE:SE	1:C:316:MSE:N	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ILE:HG21	1:B:310:ILE:HD11	1.93	0.50
1:C:33:HIS:O	1:C:217:MSE:HA	2.12	0.50
1:A:117:LEU:C	1:A:117:LEU:HD23	2.37	0.50
1:B:75:GLU:OE1	1:C:383:ARG:HA	2.11	0.50
1:C:195:ARG:HH22	1:C:199:VAL:HG21	1.75	0.50
1:B:28:LEU:HD11	1:B:218:VAL:HG21	1.94	0.50
1:C:297:VAL:HG22	1:C:298:LEU:N	2.26	0.50
1:A:29:PRO:HG2	1:A:31:ASP:OD1	2.13	0.49
1:C:237:LEU:N	1:C:238:PRO:HD2	2.27	0.49
1:B:32:THR:HG21	1:B:218:VAL:HG13	1.94	0.49
1:C:25:ARG:HG3	1:C:58:GLY:HA3	1.94	0.49
1:B:113:GLU:O	1:B:117:LEU:HD22	2.13	0.48
1:B:128:LEU:HB2	1:B:163:LEU:HD23	1.95	0.48
1:C:130:MSE:HE3	1:C:188:MSE:HE2	1.94	0.48
1:C:103:LEU:HD12	1:C:124:ILE:HD11	1.94	0.48
1:B:18:TYR:CD1	1:B:57:ALA:HB2	2.49	0.48
1:B:238:PRO:HG2	1:B:239:TYR:CD1	2.49	0.47
1:A:288:TRP:CE2	1:A:331:LEU:HD23	2.49	0.47
1:C:199:VAL:HG23	1:C:199:VAL:O	2.15	0.47
1:C:11:GLU:HB2	1:C:246:SER:OG	2.15	0.47
1:C:334:ARG:CB	1:C:339:VAL:HG12	2.45	0.47
1:C:128:LEU:O	1:C:163:LEU:HA	2.14	0.47
1:C:257:LEU:HD11	1:C:277:ILE:HD12	1.95	0.47
1:A:132:THR:HG23	1:A:184:ARG:HG2	1.94	0.47
1:A:25:ARG:HD3	1:A:25:ARG:C	2.34	0.46
1:A:155:HIS:HB3	1:A:158:PHE:HB2	1.96	0.46
1:B:128:LEU:HD21	1:B:148:ILE:HG21	1.98	0.46
1:B:297:VAL:CG1	1:B:329:VAL:CG1	2.94	0.46
1:C:334:ARG:HB2	1:C:334:ARG:HH11	1.80	0.46
1:B:316:MSE:SE	1:B:316:MSE:N	2.98	0.46
1:A:303:LYS:HE2	1:A:338:LYS:HG3	1.97	0.46
1:A:61:ARG:CD	1:A:217:MSE:HE1	2.46	0.46
1:B:29:PRO:C	1:B:31:ASP:H	2.24	0.46
1:C:11:GLU:HG2	1:C:369:PHE:HE1	1.80	0.46
1:B:140:LYS:HG3	1:B:141:ASP:OD1	2.16	0.46
1:A:107:ARG:HH12	1:A:109:ASP:HB2	1.80	0.46
1:B:128:LEU:HB2	1:B:163:LEU:CD2	2.47	0.46
1:C:152:ILE:HG23	1:C:158:PHE:HB3	1.98	0.45
1:A:195:ARG:NH2	1:A:214:THR:O	2.49	0.45
1:A:1:MSE:HG2	1:A:383:ARG:HB2	1.98	0.45
1:C:3:ASP:OD2	1:C:3:ASP:N	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ILE:HG23	1:C:126:PHE:CE2	2.52	0.45
1:A:91:ALA:CA	1:A:117:LEU:HD11	2.45	0.45
1:B:15:ASP:OD2	1:B:370:ARG:HD2	2.16	0.45
1:B:202:ALA:HB2	1:B:219:GLN:OE1	2.17	0.45
1:B:266:GLY:CA	1:B:309:ARG:HB2	2.44	0.45
1:C:353:ASN:HD22	1:C:353:ASN:N	2.15	0.45
1:A:164:TRP:HA	1:A:200:HIS:O	2.17	0.44
1:A:9:TRP:CD1	1:A:367:ILE:HD12	2.52	0.44
1:B:137:LEU:HB2	1:C:253:HIS:CD2	2.52	0.44
1:B:182:TYR:O	1:B:186:LEU:HG	2.17	0.44
1:B:269:TYR:CE2	1:B:307:VAL:HB	2.52	0.44
1:C:7:ASP:O	1:C:249:SER:HA	2.17	0.44
1:A:162:GLY:HA2	1:A:198:LEU:O	2.18	0.44
1:B:26:ARG:HH11	1:B:26:ARG:HB3	1.83	0.44
1:C:16:ALA:HB3	1:C:244:ALA:HB2	2.00	0.44
1:C:362:TYR:N	1:C:362:TYR:CD1	2.84	0.44
1:C:140:LYS:H	1:C:140:LYS:HD3	1.82	0.44
1:B:276:TRP:CE3	1:B:322:PRO:HB3	2.53	0.44
1:C:238:PRO:HG2	1:C:239:TYR:CD1	2.53	0.44
1:A:188:MSE:HA	1:A:191:TRP:CD2	2.53	0.44
1:C:155:HIS:HB3	1:C:158:PHE:HB2	2.00	0.44
1:B:296:HIS:CD2	1:B:296:HIS:H	2.34	0.43
1:C:32:THR:HA	1:C:216:ASN:O	2.18	0.43
1:C:61:ARG:HG2	1:C:61:ARG:HH11	1.83	0.43
1:C:124:ILE:CG2	1:C:126:PHE:CE2	3.02	0.43
1:B:104:THR:HA	1:B:127:HIS:O	2.18	0.43
1:B:263:VAL:HG23	1:B:263:VAL:O	2.19	0.43
1:C:13:ASP:OD1	1:C:15:ASP:HB2	2.18	0.43
1:C:334:ARG:HB2	1:C:334:ARG:NH1	2.33	0.43
1:A:306:ILE:HA	1:A:317:ILE:HG22	2.00	0.43
1:B:276:TRP:CZ3	1:B:322:PRO:HB3	2.53	0.43
1:B:26:ARG:HB3	1:B:26:ARG:NH1	2.33	0.43
1:C:61:ARG:HD3	1:C:81:PRO:HB2	2.00	0.43
1:A:137:LEU:C	1:A:137:LEU:HD12	2.43	0.43
1:A:276:TRP:CZ2	1:A:322:PRO:HB3	2.54	0.43
1:C:195:ARG:NH2	1:C:214:THR:O	2.51	0.43
1:C:29:PRO:HG2	1:C:32:THR:CG2	2.47	0.43
1:C:353:ASN:N	1:C:353:ASN:ND2	2.65	0.43
1:C:237:LEU:N	1:C:238:PRO:CD	2.82	0.43
1:B:25:ARG:HD3	1:B:25:ARG:C	2.41	0.42
1:B:280:ILE:HD11	1:B:315:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HG	1:B:349:LEU:HD21	1.99	0.42
1:A:257:LEU:CD1	1:A:277:ILE:HD12	2.50	0.42
1:C:18:TYR:CD1	1:C:57:ALA:HB2	2.55	0.42
1:C:25:ARG:O	1:C:25:ARG:HD3	2.19	0.42
1:C:27:LEU:HD12	1:C:27:LEU:N	2.34	0.42
1:C:108:SER:HB3	1:C:144:GLU:HG3	2.00	0.42
1:B:4:PHE:HB2	2:C:399:HOH:O	2.19	0.42
1:B:134:MSE:HE1	1:B:177:TYR:CZ	2.55	0.42
1:A:18:TYR:CD1	1:A:57:ALA:HB2	2.55	0.42
1:A:273:THR:OG1	1:A:274:GLU:N	2.52	0.42
1:C:353:ASN:ND2	1:C:354:TYR:H	2.11	0.42
1:C:359:THR:HB	2:C:413:HOH:O	2.20	0.42
1:C:228:ALA:C	1:C:230:SER:H	2.27	0.42
1:C:311:LEU:CD2	1:C:316:MSE:HE1	2.50	0.41
1:A:11:GLU:HB2	1:A:246:SER:OG	2.20	0.41
1:B:11:GLU:HB2	1:B:246:SER:OG	2.20	0.41
1:C:124:ILE:O	1:C:124:ILE:CG2	2.67	0.41
1:C:319:LEU:HD13	1:C:323:LEU:HB2	2.02	0.41
1:A:16:ALA:HB1	1:A:242:LYS:HG3	2.02	0.41
1:C:285:LYS:HE2	1:C:313:ASP:OD1	2.20	0.41
1:A:145:THR:O	1:A:149:VAL:HG23	2.20	0.41
1:B:29:PRO:C	1:B:31:ASP:N	2.78	0.41
1:B:258:GLN:O	1:B:261:GLU:HB2	2.21	0.41
1:B:363:ARG:HG2	1:C:66:PHE:CZ	2.52	0.41
1:C:189:LEU:HD23	1:C:189:LEU:O	2.21	0.41
1:A:66:PHE:HB2	2:A:398:HOH:O	2.20	0.40
1:A:373:ARG:NH1	1:A:373:ARG:HB2	2.35	0.40
1:B:332:ILE:HD13	1:B:342:ILE:CD1	2.46	0.40
1:C:137:LEU:C	1:C:137:LEU:HD12	2.45	0.40
1:C:297:VAL:HG21	1:C:331:LEU:HD13	2.03	0.40
1:A:112:GLU:HG2	1:A:151:LEU:HD11	2.03	0.40
1:B:123:PRO:HB3	2:B:469:HOH:O	2.20	0.40
1:C:353:ASN:ND2	1:C:354:TYR:N	2.68	0.40

All (1) 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)
1:C:117:LEU:CD1	2:A:443:HOH:O[8_654]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/390 (94%)	355 (97%)	9 (2%)	2 (0%)	24	31
1	B	365/390 (94%)	347 (95%)	16 (4%)	2 (0%)	24	31
1	C	364/390 (93%)	351 (96%)	9 (2%)	4 (1%)	11	13
All	All	1095/1170 (94%)	1053 (96%)	34 (3%)	8 (1%)	18	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	PHE
1	C	212	ASP
1	C	214	THR
1	B	182	TYR
1	C	265	PHE
1	C	30	ASP
1	A	221	GLY
1	A	193	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	304/314 (97%)	293 (96%)	11 (4%)	31	47
1	B	300/314 (96%)	292 (97%)	8 (3%)	39	58
1	C	299/314 (95%)	292 (98%)	7 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	903/942 (96%)	877 (97%)	26 (3%)	37 55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	61	ARG
1	A	117	LEU
1	A	119	SER
1	A	189	LEU
1	A	210	PHE
1	A	216	ASN
1	A	270	THR
1	A	338	LYS
1	A	353	ASN
1	A	361	SER
1	B	2	ASN
1	B	31	ASP
1	B	117	LEU
1	B	121	PRO
1	B	214	THR
1	B	303	LYS
1	B	335	GLN
1	B	353	ASN
1	C	25	ARG
1	C	140	LYS
1	C	143	GLU
1	C	190	GLU
1	C	208	LEU
1	C	216	ASN
1	C	353	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	99	GLN
1	A	203	ASN
1	A	216	ASN
1	A	253	HIS
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	293	GLN
1	A	348	HIS
1	A	353	ASN
1	B	5	HIS
1	B	157	HIS
1	B	203	ASN
1	B	258	GLN
1	B	293	GLN
1	B	296	HIS
1	B	302	GLN
1	B	348	HIS
1	B	353	ASN
1	C	23	ASN
1	C	33	HIS
1	C	99	GLN
1	C	125	HIS
1	C	216	ASN
1	C	253	HIS
1	C	272	GLN
1	C	353	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	362/390 (92%)	0.52	31 (8%)	16 17	20, 37, 64, 78	0
1	B	362/390 (92%)	0.55	35 (9%)	13 15	23, 39, 66, 82	0
1	C	361/390 (92%)	0.76	48 (13%)	7 8	25, 44, 74, 82	0
All	All	1085/1170 (92%)	0.61	114 (10%)	11 13	20, 40, 69, 82	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	SER	7.5
1	A	232	GLY	6.6
1	C	117	LEU	6.1
1	C	210	PHE	6.1
1	C	206	ALA	5.3
1	C	237	LEU	5.2
1	A	238	PRO	5.2
1	C	265	PHE	5.1
1	B	176	ASP	5.1
1	A	265	PHE	5.0
1	B	266	GLY	4.7
1	C	230	SER	4.6
1	C	177	TYR	4.6
1	B	239	TYR	4.1
1	B	208	LEU	4.1
1	A	210	PHE	4.0
1	B	231	PRO	4.0
1	C	260	GLY	4.0
1	A	203	ASN	3.7
1	C	207	SER	3.7
1	A	169	THR	3.6
1	C	27	LEU	3.6
1	B	210	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	208	LEU	3.5
1	B	238	PRO	3.4
1	A	239	TYR	3.4
1	C	209	ARG	3.4
1	A	208	LEU	3.3
1	B	229	PRO	3.3
1	B	265	PHE	3.3
1	C	266	GLY	3.2
1	A	2	ASN	3.2
1	C	128	LEU	3.2
1	B	293	GLN	3.1
1	B	267	ALA	3.1
1	C	29	PRO	3.1
1	B	209	ARG	3.1
1	B	205	ALA	3.1
1	C	26	ARG	3.0
1	B	117	LEU	3.0
1	C	229	PRO	3.0
1	C	124	ILE	3.0
1	A	209	ARG	3.0
1	C	183	THR	2.9
1	A	240	PRO	2.9
1	A	27	LEU	2.9
1	C	205	ALA	2.9
1	B	169	THR	2.9
1	A	117	LEU	2.9
1	C	264	SER	2.8
1	A	177	TYR	2.8
1	B	116	ALA	2.8
1	C	2	ASN	2.8
1	A	231	PRO	2.7
1	B	206	ALA	2.7
1	C	180	TYR	2.7
1	C	228	ALA	2.7
1	B	178	PHE	2.7
1	A	211	PRO	2.7
1	C	267	ALA	2.7
1	B	263	VAL	2.7
1	A	31	ASP	2.7
1	B	180	TYR	2.6
1	C	30	ASP	2.6
1	C	222	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	166	TRP	2.6
1	C	186	LEU	2.6
1	A	153	GLU	2.6
1	A	276	TRP	2.6
1	C	384	GLY	2.6
1	B	203	ASN	2.5
1	C	194	SER	2.5
1	A	266	GLY	2.5
1	B	181	GLN	2.5
1	B	264	SER	2.5
1	C	362	TYR	2.5
1	C	203	ASN	2.5
1	B	119	SER	2.5
1	C	182	TYR	2.5
1	B	177	TYR	2.4
1	B	2	ASN	2.4
1	C	154	ARG	2.4
1	A	277	ILE	2.4
1	A	23	ASN	2.4
1	C	212	ASP	2.4
1	C	238	PRO	2.4
1	A	179	SER	2.4
1	A	374	ILE	2.3
1	B	152	ILE	2.3
1	A	118	TYR	2.3
1	A	272	GLN	2.3
1	C	293	GLN	2.3
1	A	154	ARG	2.3
1	C	259	PRO	2.2
1	B	384	GLY	2.2
1	C	199	VAL	2.2
1	B	240	PRO	2.2
1	B	296	HIS	2.2
1	B	143	GLU	2.1
1	C	178	PHE	2.1
1	C	374	ILE	2.1
1	C	187	HIS	2.1
1	C	276	TRP	2.1
1	C	239	TYR	2.1
1	A	132	THR	2.1
1	C	31	ASP	2.1
1	A	242	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	256	LYS	2.0
1	C	28	LEU	2.0
1	C	192	LEU	2.0
1	C	339	VAL	2.0
1	B	204	SER	2.0
1	A	128	LEU	2.0
1	B	31	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.