



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:00 AM UTC

PDB ID : 2I00 / pdb_00002i00
Title : Crystal structure of acetyltransferase (GNAT family) from *Enterococcus faecalis*
Authors : Zhang, R.; Zhou, M.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-08-09
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

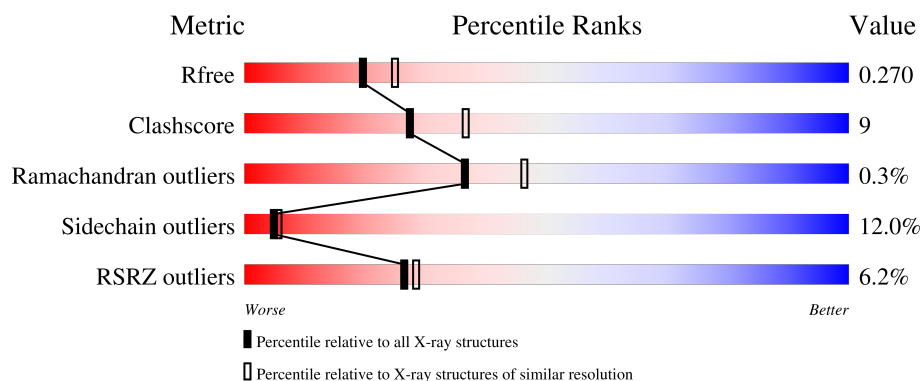
1 Overall quality at a glance

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))
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	406	4% 73% 20% 5% .
1	B	406	9% 75% 19% . .
1	C	406	2% 72% 20% 5% .
1	D	406	4% 70% 23% . .
1	E	406	3% 74% 20% . .

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Mol	Chain	Length	Quality of chain
1	F	406	13% 75% 18% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20278 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 Acetyltransferase, GNAT family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3318	2157	539	611	11			
1	B	396	Total	C	N	O	S	0	0	0
			3310	2151	538	610	11			
1	C	398	Total	C	N	O	S	0	0	0
			3327	2162	541	613	11			
1	D	396	Total	C	N	O	S	0	0	0
			3310	2151	538	610	11			
1	E	396	Total	C	N	O	S	0	0	0
			3310	2151	538	610	11			
1	F	398	Total	C	N	O	S	0	0	0
			3327	2162	541	613	11			

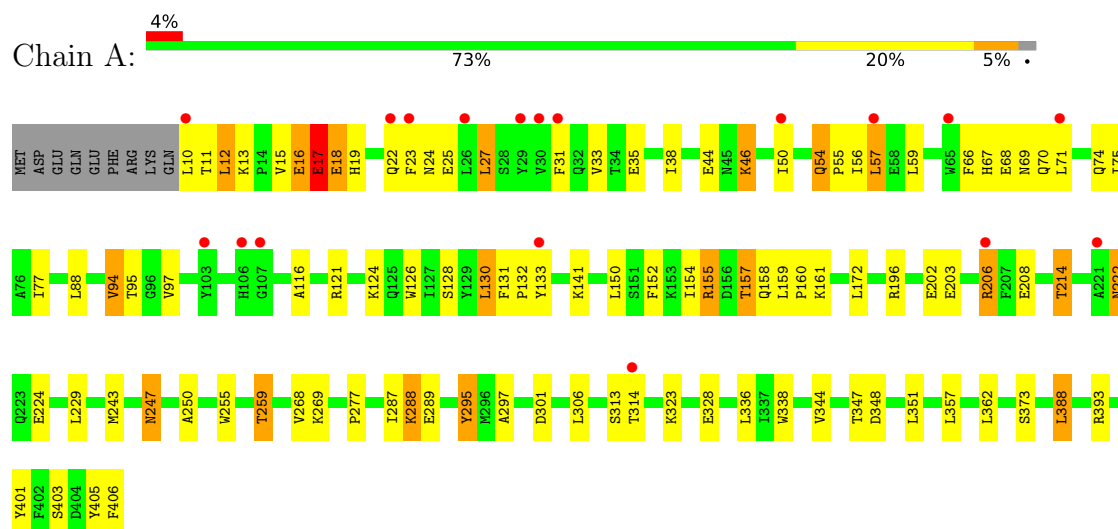
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	80	Total	O	0	0
			80	80		
2	C	48	Total	O	0	0
			48	48		
2	D	59	Total	O	0	0
			59	59		
2	E	57	Total	O	0	0
			57	57		
2	F	42	Total	O	0	0
			42	42		

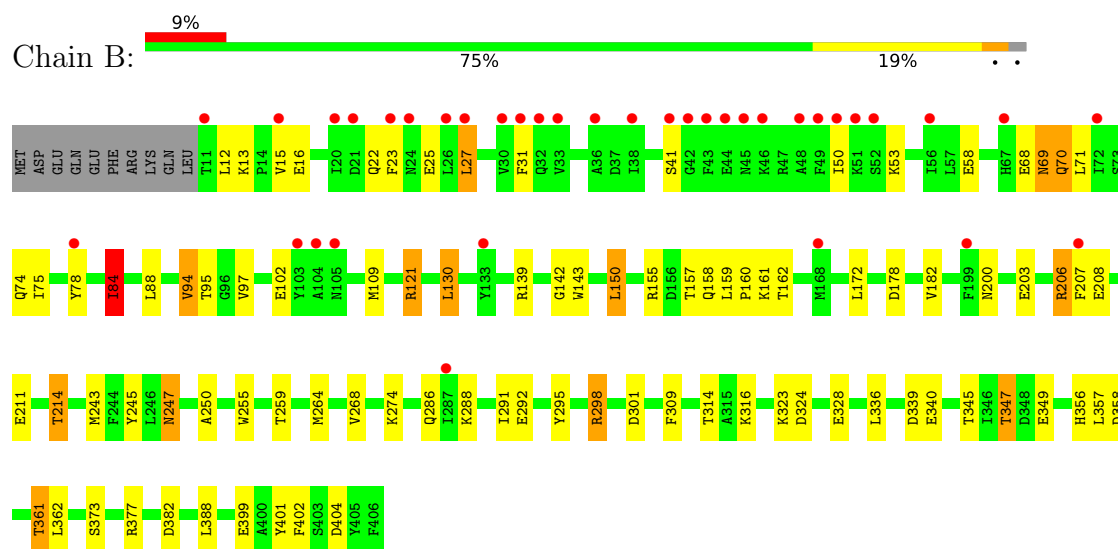
3 Residue-property plots

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: Acetyltransferase, GNAT family

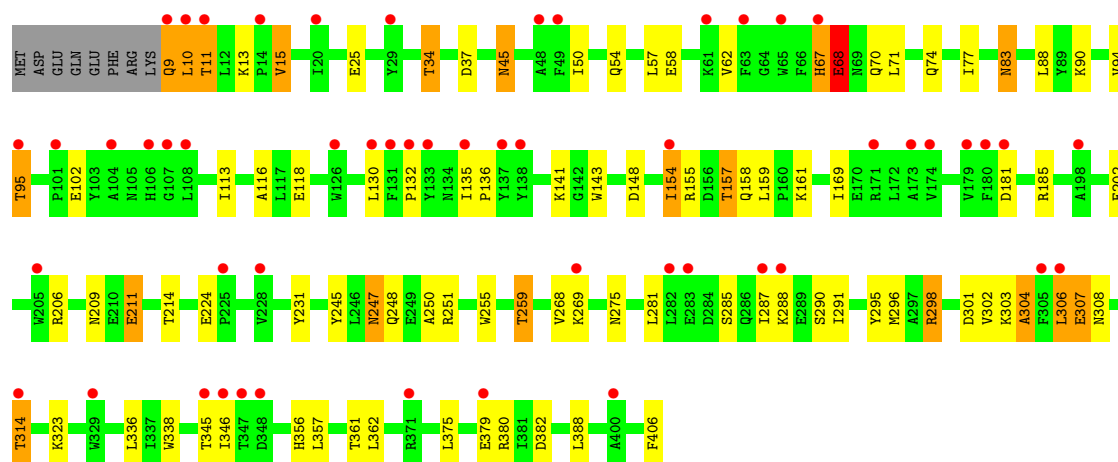
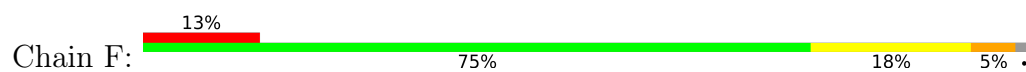


• Molecule 1: Acetyltransferase, GNAT family



• Molecule 1: Acetyltransferase, GNAT family





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.41Å 177.09Å 104.43Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	41.92 – 2.30 41.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.92-2.30) 98.8 (41.92-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.270 (Not available) , 0.270	Depositor DCC
R_{free} test set	6834 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.4	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	0.94	EDS
Total number of atoms	20278	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	1/3417 (0.0%)	0.95	1/4642 (0.0%)
1	B	0.83	0/3409	0.95	1/4631 (0.0%)
1	C	0.80	0/3426	0.93	3/4654 (0.1%)
1	D	0.82	0/3409	0.92	1/4631 (0.0%)
1	E	0.79	1/3409 (0.0%)	0.93	0/4631
1	F	0.77	1/3426 (0.0%)	0.89	1/4654 (0.0%)
All	All	0.82	3/20496 (0.0%)	0.93	7/27843 (0.0%)

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	C	0	1
1	E	0	1
1	F	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	304	ALA	CA-CB	-5.33	1.45	1.53
1	A	94	VAL	CA-CB	5.25	1.60	1.54
1	E	15	VAL	CA-CB	5.02	1.60	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	380	ARG	N-CA-C	-7.48	105.06	114.56
1	B	84	ILE	CB-CA-C	5.82	118.56	110.99
1	A	94	VAL	N-CA-CB	5.35	116.36	110.53
1	D	306	LEU	N-CA-C	5.30	117.81	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	TYR	N-CA-C	5.28	116.68	109.18
1	F	231	TYR	N-CA-C	5.11	116.57	108.96
1	C	95	THR	CB-CA-C	-5.07	99.89	111.95

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	9	GLN	Peptide
1	E	67	HIS	Peptide
1	F	67	HIS	Peptide
1	F	68	GLU	Peptide

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	3318	0	3181	69	0
1	B	3310	0	3170	48	0
1	C	3327	0	3189	62	0
1	D	3310	0	3170	64	0
1	E	3310	0	3170	58	0
1	F	3327	0	3189	68	0
2	A	90	0	0	6	0
2	B	80	0	0	2	0
2	C	48	0	0	4	0
2	D	59	0	0	8	0
2	E	57	0	0	5	0
2	F	42	0	0	7	0
All	All	20278	0	19069	356	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 9.

All (356) 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:18:GLU:HG2	2:A:487:HOH:O	1.41	1.18
1:F:13:LYS:NZ	1:F:68:GLU:OE1	1.85	1.09
1:F:11:THR:CG2	1:F:68:GLU:HG3	1.87	1.03
2:C:446:HOH:O	1:D:371:ARG:HG3	1.68	0.93
1:F:379:GLU:OE2	2:F:420:HOH:O	1.88	0.92
1:B:358:ASP:OD1	1:B:361:THR:HG23	1.68	0.92
1:F:11:THR:HG21	1:F:68:GLU:HG3	1.55	0.88
1:A:222:ASN:ND2	2:A:412:HOH:O	2.07	0.85
1:F:209:ASN:HD21	1:F:211:GLU:HG2	1.43	0.83
1:E:55:PRO:O	1:E:58:GLU:HG3	1.81	0.79
1:E:155:ARG:H	1:E:158:GLN:HE21	1.31	0.78
1:A:155:ARG:H	1:A:158:GLN:HE21	1.31	0.78
1:F:248:GLN:NE2	1:F:251:ARG:HH21	1.81	0.78
1:A:405:TYR:O	1:A:406:PHE:C	2.22	0.78
1:E:248:GLN:NE2	1:E:251:ARG:HH21	1.82	0.77
1:B:78:TYR:OH	1:B:200:ASN:ND2	2.18	0.77
1:D:67:HIS:O	1:D:68:GLU:C	2.30	0.75
1:E:97:VAL:HG21	1:E:138:TYR:OH	1.87	0.74
1:C:154:ILE:HD11	1:C:159:LEU:HD23	1.69	0.74
1:F:224:GLU:HG2	2:F:407:HOH:O	1.86	0.74
1:C:358:ASP:OD1	1:C:361:THR:HG23	1.88	0.73
1:F:209:ASN:ND2	1:F:211:GLU:HG2	2.03	0.73
1:E:358:ASP:OD1	1:E:361:THR:HG23	1.89	0.72
1:B:288:LYS:O	2:B:469:HOH:O	2.08	0.71
1:F:154:ILE:HD12	1:F:158:GLN:HB2	1.73	0.71
1:C:9:GLN:CA	1:C:10:LEU:HB2	2.21	0.71
1:B:358:ASP:OD1	1:B:361:THR:CG2	2.37	0.71
1:F:34:THR:HG22	1:F:37:ASP:H	1.56	0.70
1:D:155:ARG:H	1:D:158:GLN:HE21	1.40	0.69
1:F:157:THR:CG2	2:F:435:HOH:O	2.41	0.69
1:C:200:ASN:HA	2:C:441:HOH:O	1.91	0.69
1:B:27:LEU:O	1:B:31:PHE:HB2	1.92	0.69
1:B:75:ILE:HD12	1:B:109:MET:HE1	1.75	0.69
1:D:160:PRO:O	1:D:259:THR:HG21	1.93	0.69
1:E:160:PRO:O	1:E:259:THR:HG21	1.93	0.69
1:A:214:THR:CG2	2:A:438:HOH:O	2.41	0.68
1:D:67:HIS:HB3	1:D:70:GLN:HB3	1.75	0.68
1:E:406:PHE:O	2:E:453:HOH:O	2.11	0.68
1:C:9:GLN:HA	1:C:10:LEU:HB2	1.76	0.67
1:A:206:ARG:HB3	1:A:206:ARG:NH1	2.10	0.67
1:F:255:TRP:O	1:F:259:THR:HG23	1.95	0.67
1:D:295:TYR:OH	1:D:405:TYR:O	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:HD21	1:B:268:VAL:HG21	1.76	0.67
1:D:88:LEU:HD13	1:D:188:ARG:NH2	2.09	0.67
1:D:159:LEU:HD21	1:D:268:VAL:HG21	1.77	0.66
1:D:314:THR:O	1:D:393:ARG:NH1	2.27	0.66
1:C:9:GLN:HB2	1:C:10:LEU:HB2	1.78	0.66
1:B:243:MET:HE3	1:B:245:TYR:CE2	2.31	0.66
1:D:243:MET:HE1	1:D:255:TRP:HE1	1.61	0.66
1:E:405:TYR:O	1:E:406:PHE:O	2.14	0.66
1:B:84:ILE:HD11	1:B:309:PHE:CE1	2.31	0.66
1:D:288:LYS:O	2:D:462:HOH:O	2.12	0.65
1:C:398:GLN:HB2	2:D:463:HOH:O	1.96	0.65
1:C:9:GLN:HA	1:C:10:LEU:HG	1.78	0.65
1:A:24:ASN:OD1	1:A:54:GLN:NE2	2.30	0.65
1:E:159:LEU:HD13	1:E:259:THR:HA	1.78	0.65
1:B:155:ARG:H	1:B:158:GLN:HE21	1.45	0.64
1:B:243:MET:HE3	1:B:245:TYR:HE2	1.62	0.64
1:F:356:HIS:HB2	1:F:382:ASP:HB3	1.80	0.64
1:A:214:THR:HG22	2:A:438:HOH:O	1.97	0.64
1:C:9:GLN:CB	1:C:10:LEU:HB2	2.28	0.64
1:B:160:PRO:O	1:B:259:THR:HG21	1.98	0.63
1:C:141:LYS:O	1:C:298:ARG:NH1	2.32	0.63
1:B:94:VAL:HG22	1:B:130:LEU:HD23	1.81	0.62
1:F:302:VAL:CG1	1:F:306:LEU:HD22	2.29	0.62
1:F:45:ASN:N	1:F:45:ASN:HD22	1.96	0.62
1:B:150:LEU:HD11	1:B:291:ILE:HD12	1.81	0.62
1:A:295:TYR:OH	1:A:405:TYR:O	2.14	0.62
1:B:23:PHE:HA	1:B:74:GLN:HE22	1.65	0.62
1:A:31:PHE:HB3	1:A:46:LYS:NZ	2.14	0.62
1:B:214:THR:HG22	2:B:432:HOH:O	2.00	0.62
1:C:160:PRO:O	1:C:259:THR:HG21	2.00	0.61
1:A:222:ASN:N	1:A:222:ASN:OD1	2.33	0.61
1:A:222:ASN:CG	2:A:412:HOH:O	2.39	0.61
1:C:255:TRP:O	1:C:259:THR:HG23	2.01	0.61
1:E:22:GLN:HE22	1:E:70:GLN:HA	1.65	0.61
1:B:102:GLU:OE1	1:D:171:ARG:NH2	2.34	0.61
1:D:358:ASP:OD1	1:D:361:THR:HG23	2.01	0.60
1:C:94:VAL:HG13	1:C:130:LEU:HG	1.83	0.60
1:C:306:LEU:HB3	1:C:346:ILE:CD1	2.31	0.60
1:E:248:GLN:HE22	1:E:251:ARG:HH21	1.49	0.60
1:F:77:ILE:HD11	1:F:116:ALA:HB1	1.83	0.59
1:E:155:ARG:N	1:E:158:GLN:HE21	1.98	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:HG22	1:A:348:ASP:H	1.68	0.59
1:B:159:LEU:HB3	1:B:259:THR:HG22	1.85	0.59
1:E:121:ARG:HD2	1:E:301:ASP:OD2	2.03	0.59
1:F:287:ILE:HG23	2:F:434:HOH:O	2.02	0.59
1:A:247:ASN:C	1:A:247:ASN:HD22	2.10	0.58
1:C:9:GLN:HA	1:C:10:LEU:CB	2.32	0.58
1:F:11:THR:CG2	1:F:68:GLU:CG	2.72	0.58
1:A:33:VAL:HG13	1:A:38:ILE:HD11	1.85	0.58
1:B:203:GLU:OE1	1:B:206:ARG:NH2	2.36	0.58
1:B:347:THR:HG21	1:B:349:GLU:OE2	2.04	0.57
1:B:75:ILE:HD12	1:B:109:MET:CE	2.34	0.57
1:D:380:ARG:HG2	1:D:380:ARG:HH21	1.69	0.57
1:B:214:THR:HG21	1:E:29:TYR:HE2	1.70	0.57
1:E:157:THR:CG2	2:E:433:HOH:O	2.52	0.57
1:B:13:LYS:NZ	1:B:69:ASN:HD21	2.02	0.57
1:A:121:ARG:HD2	1:A:301:ASP:OD2	2.05	0.56
1:E:285:SER:HB2	1:F:135:ILE:HG21	1.88	0.56
1:F:155:ARG:H	1:F:158:GLN:HE21	1.53	0.56
1:D:380:ARG:HH21	1:D:380:ARG:CG	2.18	0.56
1:A:152:PHE:HB3	1:A:289:GLU:HG2	1.88	0.56
1:B:247:ASN:C	1:B:247:ASN:HD22	2.12	0.56
1:C:18:GLU:HB2	2:C:449:HOH:O	2.05	0.56
1:A:160:PRO:O	1:A:259:THR:HG21	2.05	0.56
1:C:306:LEU:HB3	1:C:346:ILE:HD12	1.87	0.55
1:D:380:ARG:HG2	1:D:380:ARG:NH2	2.21	0.55
1:D:255:TRP:O	1:D:259:THR:HG23	2.07	0.55
1:F:302:VAL:HG13	1:F:306:LEU:HD22	1.89	0.55
1:A:23:PHE:HA	1:A:74:GLN:HE22	1.72	0.54
1:C:95:THR:CG2	1:C:406:PHE:C	2.79	0.54
1:D:336:LEU:HD22	1:D:346:ILE:CD1	2.38	0.54
1:E:218:TYR:OH	1:E:249:GLU:OE1	2.24	0.54
1:E:26:LEU:HD13	1:E:74:GLN:NE2	2.22	0.54
1:E:135:ILE:HG21	1:F:285:SER:HB2	1.89	0.54
1:E:75:ILE:HD12	1:E:109:MET:CE	2.38	0.54
1:A:247:ASN:ND2	1:A:250:ALA:H	2.06	0.54
1:B:53:LYS:HG2	1:B:206:ARG:CZ	2.38	0.54
1:B:247:ASN:ND2	1:B:250:ALA:H	2.06	0.54
1:F:141:LYS:O	1:F:298:ARG:NH1	2.40	0.54
1:E:155:ARG:H	1:E:158:GLN:NE2	2.04	0.53
1:C:47:ARG:HA	1:C:50:ILE:HD13	1.89	0.53
1:D:247:ASN:ND2	1:D:250:ALA:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:CE2	1:A:57:LEU:HD11	2.43	0.53
1:D:319:HIS:HD2	1:D:351:LEU:O	1.91	0.53
1:E:154:ILE:HD11	1:E:159:LEU:HA	1.89	0.53
1:A:31:PHE:HB3	1:A:46:LYS:HZ1	1.74	0.53
1:A:255:TRP:O	1:A:259:THR:HG23	2.09	0.53
1:E:405:TYR:O	1:E:406:PHE:C	2.51	0.53
1:F:306:LEU:HB3	1:F:346:ILE:HG12	1.89	0.53
1:E:159:LEU:HD21	1:E:268:VAL:HG21	1.91	0.53
1:E:247:ASN:C	1:E:247:ASN:HD22	2.16	0.53
1:F:181:ASP:O	1:F:185:ARG:HG3	2.08	0.53
1:F:247:ASN:ND2	1:F:250:ALA:H	2.06	0.53
1:A:46:LYS:O	1:A:50:ILE:HG12	2.09	0.53
1:A:77:ILE:HD11	1:A:116:ALA:HB1	1.91	0.53
1:E:255:TRP:O	1:E:259:THR:HG23	2.08	0.52
1:C:121:ARG:HD2	1:C:301:ASP:OD2	2.10	0.52
1:C:361:THR:HG21	1:C:380:ARG:HG3	1.91	0.52
1:E:298:ARG:NH2	1:E:324:ASP:OD2	2.41	0.52
1:F:314:THR:HG1	1:F:338:TRP:CG	2.28	0.52
1:F:83:ASN:OD1	1:F:83:ASN:C	2.53	0.52
1:F:303:LYS:O	1:F:307:GLU:HG2	2.08	0.52
1:A:351:LEU:HD12	1:A:351:LEU:O	2.09	0.52
1:A:157:THR:CG2	2:A:470:HOH:O	2.57	0.52
1:C:9:GLN:CA	1:C:10:LEU:CB	2.87	0.52
1:A:130:LEU:HD22	1:A:131:PHE:O	2.10	0.51
1:C:32:GLN:O	1:C:32:GLN:HG3	2.10	0.51
1:D:358:ASP:OD1	1:D:361:THR:CG2	2.58	0.51
1:D:368:ASN:HD22	1:D:398:GLN:C	2.18	0.51
1:C:9:GLN:HA	1:C:10:LEU:CG	2.39	0.51
1:C:95:THR:HG22	1:C:406:PHE:C	2.36	0.51
1:B:243:MET:HE1	1:B:255:TRP:HE1	1.75	0.51
1:C:155:ARG:H	1:C:158:GLN:HE21	1.57	0.51
1:B:102:GLU:OE2	1:D:171:ARG:NH1	2.44	0.51
1:C:83:ASN:OD1	1:C:83:ASN:C	2.53	0.51
1:D:200:ASN:HA	2:D:436:HOH:O	2.10	0.51
1:D:83:ASN:C	1:D:83:ASN:OD1	2.52	0.51
1:F:302:VAL:O	1:F:306:LEU:HB2	2.10	0.51
1:D:67:HIS:O	1:D:68:GLU:O	2.29	0.51
1:D:248:GLN:NE2	1:D:251:ARG:HH21	2.08	0.51
1:D:241:LYS:NZ	2:D:454:HOH:O	2.30	0.50
1:F:281:LEU:HA	2:F:440:HOH:O	2.10	0.50
1:A:124:LYS:HA	1:A:126:TRP:CH2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:THR:HG22	1:C:37:ASP:H	1.77	0.50
1:C:22:GLN:HE22	1:C:70:GLN:HA	1.76	0.50
1:C:356:HIS:HB2	1:C:382:ASP:HB3	1.93	0.50
1:B:13:LYS:HZ3	1:B:69:ASN:HD21	1.58	0.49
1:D:356:HIS:HB2	1:D:382:ASP:HB3	1.94	0.49
1:B:356:HIS:HB2	1:B:382:ASP:HB3	1.94	0.49
1:A:347:THR:HG22	1:A:348:ASP:N	2.28	0.49
1:E:22:GLN:NE2	1:E:70:GLN:HA	2.26	0.49
1:E:356:HIS:HB2	1:E:382:ASP:HB3	1.93	0.49
1:A:68:GLU:OE1	1:A:69:ASN:ND2	2.46	0.49
1:E:75:ILE:HD12	1:E:109:MET:HE3	1.94	0.49
1:D:361:THR:HG21	2:D:409:HOH:O	2.12	0.49
1:F:15:VAL:HG22	1:F:62:VAL:HB	1.95	0.49
1:A:206:ARG:HB3	1:A:206:ARG:HH11	1.78	0.48
1:D:159:LEU:HB3	1:D:259:THR:HG22	1.95	0.48
1:F:302:VAL:HG12	1:F:306:LEU:HD22	1.93	0.48
1:C:97:VAL:HG12	1:C:109:MET:HE1	1.95	0.48
1:C:398:GLN:CB	2:D:463:HOH:O	2.59	0.48
1:C:77:ILE:HD11	1:C:116:ALA:HB1	1.95	0.48
1:D:171:ARG:NH1	2:D:413:HOH:O	2.46	0.48
1:F:302:VAL:CG1	1:F:306:LEU:CD2	2.91	0.48
1:C:84:ILE:O	1:C:84:ILE:HG13	2.13	0.48
1:B:298:ARG:NH2	1:B:324:ASP:OD2	2.46	0.48
1:D:97:VAL:HG21	1:D:138:TYR:OH	2.12	0.48
1:B:22:GLN:HE22	1:B:70:GLN:HA	1.78	0.48
1:D:68:GLU:HA	1:D:69:ASN:HA	1.53	0.48
1:E:247:ASN:ND2	1:E:250:ALA:H	2.11	0.48
1:C:298:ARG:NH2	1:C:324:ASP:OD2	2.47	0.48
1:D:405:TYR:O	1:D:406:PHE:C	2.57	0.48
1:B:68:GLU:HA	1:B:69:ASN:HA	1.71	0.47
1:D:22:GLN:HE22	1:D:71:LEU:H	1.62	0.47
1:B:121:ARG:HD2	1:B:301:ASP:OD2	2.13	0.47
1:D:23:PHE:HA	1:D:74:GLN:HE22	1.79	0.47
1:C:401:TYR:OH	1:C:403:SER:OG	2.33	0.47
1:F:302:VAL:HG12	1:F:306:LEU:CD2	2.44	0.47
1:A:13:LYS:NZ	1:A:69:ASN:HD21	2.13	0.47
1:A:159:LEU:HD21	1:A:268:VAL:HG21	1.96	0.47
1:A:288:LYS:NZ	1:B:292:GLU:OE1	2.46	0.47
1:F:148:ASP:OD2	1:F:275:ASN:ND2	2.47	0.47
1:F:155:ARG:H	1:F:158:GLN:NE2	2.11	0.47
1:D:128:SER:O	1:D:297:ALA:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:LEU:O	1:F:380:ARG:HB3	2.15	0.47
1:F:95:THR:CG2	1:F:406:PHE:C	2.87	0.47
1:F:143:TRP:CD1	1:F:298:ARG:HB2	2.50	0.47
1:C:347:THR:HG21	1:C:349:GLU:OE2	2.15	0.46
1:A:66:PHE:HA	1:A:70:GLN:O	2.16	0.46
1:D:65:TRP:CD1	1:D:108:LEU:HB3	2.50	0.46
1:F:247:ASN:HD22	1:F:250:ALA:H	1.61	0.46
1:A:12:LEU:HD12	1:A:12:LEU:C	2.40	0.46
1:A:214:THR:HG21	1:C:29:TYR:HE2	1.80	0.46
1:C:288:LYS:HD2	1:C:288:LYS:N	2.31	0.46
1:F:245:TYR:CZ	1:F:251:ARG:HG3	2.50	0.46
1:A:16:GLU:O	1:A:17:GLU:C	2.58	0.46
1:A:133:TYR:CD2	1:A:133:TYR:C	2.92	0.46
1:A:401:TYR:OH	1:A:403:SER:OG	2.12	0.46
1:B:264:MET:HE1	1:E:101:PRO:HG3	1.97	0.46
1:C:398:GLN:CG	2:D:463:HOH:O	2.63	0.46
1:D:94:VAL:HG13	1:D:130:LEU:HD23	1.98	0.46
1:F:159:LEU:HD21	1:F:268:VAL:HG21	1.98	0.46
1:D:101:PRO:HG3	1:E:264:MET:HE1	1.98	0.45
1:E:88:LEU:HD13	1:E:188:ARG:CZ	2.46	0.45
1:D:121:ARG:HD2	1:D:301:ASP:OD2	2.16	0.45
1:E:150:LEU:HD11	1:E:291:ILE:HG13	1.98	0.45
1:A:141:LYS:HD2	1:A:141:LYS:N	2.31	0.45
1:F:95:THR:HG21	1:F:406:PHE:C	2.42	0.45
1:F:281:LEU:CA	2:F:440:HOH:O	2.65	0.45
1:A:56:ILE:HD11	1:A:203:GLU:HG3	1.98	0.45
1:F:132:PRO:HB3	1:F:296:MET:SD	2.57	0.45
1:D:243:MET:HE3	1:D:245:TYR:HE2	1.81	0.45
1:F:247:ASN:HD22	1:F:247:ASN:C	2.25	0.45
1:C:43:PHE:CZ	1:C:52:SER:HB3	2.51	0.45
1:C:117:LEU:HD23	1:C:120:MET:HE3	1.99	0.45
1:E:51:LYS:O	1:E:54:GLN:HB2	2.17	0.45
1:F:77:ILE:HD11	1:F:116:ALA:CB	2.47	0.45
1:D:70:GLN:O	1:D:72:ILE:HG23	2.17	0.44
1:D:185:ARG:O	1:D:189:GLN:HG2	2.17	0.44
1:A:75:ILE:HG13	1:A:97:VAL:HG12	1.99	0.44
1:E:205:TRP:HB3	1:E:210:GLU:HG2	1.99	0.44
1:A:196:ARG:NH2	1:A:403:SER:HB2	2.31	0.44
1:D:11:THR:HG23	1:D:66:PHE:HB2	1.99	0.44
1:A:16:GLU:O	1:A:19:HIS:N	2.48	0.44
1:C:17:GLU:HA	1:C:20:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:LEU:C	1:E:12:LEU:HD12	2.43	0.44
1:E:154:ILE:HG13	1:E:158:GLN:HB2	2.00	0.44
1:E:157:THR:HG23	2:E:433:HOH:O	2.14	0.44
1:E:284:ASP:HA	1:F:136:PRO:HD3	2.00	0.44
1:E:347:THR:HG22	1:E:348:ASP:N	2.33	0.44
1:F:306:LEU:HD12	1:F:306:LEU:HA	1.79	0.44
1:A:155:ARG:H	1:A:158:GLN:NE2	2.08	0.43
1:F:375:LEU:O	1:F:380:ARG:CB	2.66	0.43
1:D:406:PHE:C	1:D:406:PHE:CD2	2.96	0.43
1:D:75:ILE:HD12	1:D:109:MET:CE	2.48	0.43
1:A:229:LEU:HD13	1:A:243:MET:HE2	2.01	0.43
1:D:95:THR:HG23	1:D:406:PHE:O	2.19	0.43
1:D:336:LEU:HD22	1:D:346:ILE:HD12	2.00	0.43
1:E:17:GLU:HA	1:E:20:ILE:HG12	2.00	0.43
1:F:336:LEU:HD22	1:F:346:ILE:HG13	2.00	0.43
1:C:24:ASN:HD21	1:C:54:GLN:HE21	1.66	0.43
1:E:102:GLU:OE1	1:E:102:GLU:N	2.42	0.43
1:A:16:GLU:H	1:A:19:HIS:HD2	1.66	0.43
1:B:178:ASP:O	1:B:182:VAL:HG23	2.19	0.43
1:A:313:SER:HB3	1:A:393:ARG:HG2	2.01	0.43
1:E:139:ARG:HA	1:E:143:TRP:O	2.18	0.43
1:D:209:ASN:O	1:D:210:GLU:C	2.62	0.43
1:F:155:ARG:N	1:F:158:GLN:HE21	2.16	0.43
1:C:16:GLU:HB3	2:C:449:HOH:O	2.18	0.43
1:C:68:GLU:HA	1:C:69:ASN:HA	1.78	0.43
1:D:319:HIS:CE1	1:D:354:ALA:HB2	2.54	0.42
1:A:31:PHE:HB3	1:A:46:LYS:HZ3	1.83	0.42
1:A:154:ILE:HG22	1:A:287:ILE:HG21	2.01	0.42
1:B:373:SER:O	1:B:377:ARG:HB2	2.20	0.42
1:C:284:ASP:HA	1:D:136:PRO:HD3	2.01	0.42
1:D:299:ILE:CD1	1:D:362:LEU:HD13	2.50	0.42
1:F:304:ALA:O	1:F:308:ASN:OD1	2.38	0.42
1:D:247:ASN:HD22	1:D:247:ASN:C	2.27	0.42
1:E:26:LEU:HD23	1:E:26:LEU:O	2.19	0.42
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.89	0.42
1:B:27:LEU:O	1:B:31:PHE:CB	2.66	0.42
1:B:84:ILE:HD11	1:B:309:PHE:HE1	1.82	0.42
1:D:221:ALA:O	1:D:222:ASN:CB	2.67	0.42
1:C:95:THR:HG23	1:C:406:PHE:HD2	1.84	0.42
1:A:68:GLU:HA	1:A:69:ASN:HA	1.69	0.42
1:C:286:GLN:HG3	1:D:135:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:GLN:HA	1:F:10:LEU:HA	1.85	0.42
1:A:27:LEU:HD22	1:A:31:PHE:HD2	1.84	0.42
1:A:401:TYR:CZ	1:A:403:SER:OG	2.70	0.42
1:B:139:ARG:HA	1:B:143:TRP:O	2.18	0.42
1:C:347:THR:HB	1:C:349:GLU:H	1.85	0.42
1:A:128:SER:O	1:A:297:ALA:HA	2.19	0.42
1:B:142:GLY:HA3	1:B:298:ARG:NH1	2.34	0.42
1:A:23:PHE:CZ	1:A:57:LEU:HD11	2.55	0.41
1:C:339:ASP:C	1:C:339:ASP:OD2	2.62	0.41
1:D:141:LYS:N	1:D:141:LYS:HD2	2.35	0.41
1:A:54:GLN:N	1:A:55:PRO:CD	2.83	0.41
1:C:137:TYR:O	1:C:141:LYS:HG2	2.20	0.41
1:E:34:THR:HG22	1:E:36:ALA:N	2.36	0.41
1:F:10:LEU:HA	2:F:444:HOH:O	2.19	0.41
1:A:401:TYR:CD2	1:A:401:TYR:C	2.98	0.41
1:B:211:GLU:OE2	1:B:211:GLU:HA	2.20	0.41
1:F:15:VAL:O	1:F:15:VAL:HG23	2.18	0.41
1:F:77:ILE:CD1	1:F:116:ALA:HB1	2.47	0.41
1:F:307:GLU:HG2	1:F:307:GLU:H	1.77	0.41
1:A:22:GLN:HE22	1:A:70:GLN:HA	1.84	0.41
1:B:401:TYR:CD2	1:B:401:TYR:C	2.98	0.41
1:D:36:ALA:O	1:D:39:GLU:HB3	2.21	0.41
1:F:67:HIS:CD2	1:F:67:HIS:C	2.97	0.41
1:F:15:VAL:O	1:F:15:VAL:CG2	2.69	0.41
1:A:74:GLN:HE21	1:A:74:GLN:HB3	1.67	0.41
1:C:11:THR:HG23	1:C:66:PHE:HB2	2.03	0.41
1:C:302:VAL:HG13	1:C:306:LEU:HD22	2.03	0.41
1:E:88:LEU:CD1	1:E:188:ARG:CZ	2.99	0.41
1:F:143:TRP:NE1	1:F:298:ARG:HB2	2.36	0.41
1:A:10:LEU:HD23	1:A:67:HIS:HA	2.01	0.41
1:A:132:PRO:HG2	1:B:286:GLN:HE22	1.86	0.41
1:A:314:THR:HG1	1:A:338:TRP:CG	2.37	0.41
1:C:401:TYR:CD2	1:C:401:TYR:C	2.98	0.41
1:A:150:LEU:HD23	1:A:277:PRO:HA	2.03	0.41
1:C:84:ILE:HG12	1:C:89:TYR:CE1	2.55	0.41
1:C:167:GLY:HA3	1:C:219:TYR:O	2.21	0.41
1:C:229:LEU:HD11	1:C:240:ILE:HG12	2.02	0.41
1:C:247:ASN:ND2	1:C:250:ALA:H	2.19	0.41
1:D:34:THR:HG22	1:D:36:ALA:H	1.84	0.41
1:D:92:GLY:O	1:D:128:SER:OG	2.36	0.41
1:E:75:ILE:HD12	1:E:109:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:GLN:HE22	1:E:251:ARG:HD3	1.86	0.41
1:F:301:ASP:HB3	1:F:304:ALA:HB3	2.03	0.41
1:A:206:ARG:HB3	1:A:206:ARG:CZ	2.51	0.41
1:B:339:ASP:OD1	1:B:339:ASP:C	2.63	0.41
1:D:54:GLN:N	1:D:55:PRO:CD	2.84	0.41
1:F:181:ASP:OD1	1:F:181:ASP:C	2.63	0.41
1:C:178:ASP:O	1:C:182:VAL:HG23	2.21	0.40
1:C:317:PRO:HG3	1:C:337:ILE:HG13	2.03	0.40
1:D:15:VAL:HG22	1:D:62:VAL:HB	2.03	0.40
1:D:88:LEU:HD11	1:D:195:ILE:CD1	2.51	0.40
1:E:90:LYS:CE	1:E:123:ASP:O	2.69	0.40
1:F:202:GLU:O	1:F:206:ARG:HB3	2.21	0.40
1:F:248:GLN:NE2	1:F:251:ARG:NH2	2.58	0.40
1:B:402:PHE:CZ	1:B:404:ASP:HB2	2.56	0.40
1:E:151:SER:O	1:E:289:GLU:HA	2.21	0.40
1:B:41:SER:HB3	1:B:207:PHE:HA	2.02	0.40
1:E:53:LYS:NZ	2:E:419:HOH:O	2.51	0.40
1:E:97:VAL:HG21	1:E:138:TYR:HH	1.84	0.40
1:E:305:PHE:CD2	1:E:305:PHE:C	2.99	0.40
1:E:345:THR:HG23	2:E:409:HOH:O	2.19	0.40
1:E:401:TYR:CD2	1:E:401:TYR:C	3.00	0.40
1:F:11:THR:HG22	1:F:68:GLU:HG3	1.92	0.40
1:A:27:LEU:O	1:A:31:PHE:HB2	2.21	0.40
1:A:373:SER:HA	1:A:388:LEU:HD11	2.03	0.40
1:C:247:ASN:HD22	1:C:249:GLU:H	1.68	0.40
1:E:247:ASN:HD22	1:E:250:ALA:H	1.69	0.40
1:F:54:GLN:O	1:F:58:GLU:HG3	2.21	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	395/406 (97%)	382 (97%)	12 (3%)	1 (0%)	36	46
1	B	394/406 (97%)	377 (96%)	17 (4%)	0	100	100
1	C	396/406 (98%)	382 (96%)	13 (3%)	1 (0%)	36	46
1	D	394/406 (97%)	378 (96%)	13 (3%)	3 (1%)	16	20
1	E	394/406 (97%)	379 (96%)	14 (4%)	1 (0%)	36	46
1	F	396/406 (98%)	369 (93%)	27 (7%)	0	100	100
All	All	2369/2436 (97%)	2267 (96%)	96 (4%)	6 (0%)	36	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	D	222	ASN
1	C	10	LEU
1	D	68	GLU
1	D	210	GLU
1	E	212	GLU

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	355/364 (98%)	314 (88%)	41 (12%)	5	6
1	B	354/364 (97%)	312 (88%)	42 (12%)	5	6
1	C	356/364 (98%)	310 (87%)	46 (13%)	4	4
1	D	354/364 (97%)	310 (88%)	44 (12%)	4	5
1	E	354/364 (97%)	316 (89%)	38 (11%)	6	8
1	F	356/364 (98%)	311 (87%)	45 (13%)	4	5
All	All	2129/2184 (98%)	1873 (88%)	256 (12%)	5	5

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	12	LEU
1	A	15	VAL
1	A	16	GLU
1	A	17	GLU
1	A	18	GLU
1	A	25	GLU
1	A	27	LEU
1	A	35	GLU
1	A	44	GLU
1	A	46	LYS
1	A	54	GLN
1	A	57	LEU
1	A	59	LEU
1	A	71	LEU
1	A	88	LEU
1	A	94	VAL
1	A	95	THR
1	A	130	LEU
1	A	155	ARG
1	A	157	THR
1	A	161	LYS
1	A	172	LEU
1	A	202	GLU
1	A	206	ARG
1	A	208	GLU
1	A	214	THR
1	A	222	ASN
1	A	224	GLU
1	A	247	ASN
1	A	259	THR
1	A	269	LYS
1	A	288	LYS
1	A	295	TYR
1	A	323	LYS
1	A	328	GLU
1	A	336	LEU
1	A	344	VAL
1	A	357	LEU
1	A	362	LEU
1	A	388	LEU
1	B	12	LEU
1	B	15	VAL

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Mol	Chain	Res	Type
1	B	16	GLU
1	B	25	GLU
1	B	27	LEU
1	B	50	ILE
1	B	58	GLU
1	B	69	ASN
1	B	70	GLN
1	B	71	LEU
1	B	84	ILE
1	B	88	LEU
1	B	94	VAL
1	B	95	THR
1	B	97	VAL
1	B	121	ARG
1	B	130	LEU
1	B	150	LEU
1	B	157	THR
1	B	161	LYS
1	B	162	THR
1	B	172	LEU
1	B	206	ARG
1	B	208	GLU
1	B	214	THR
1	B	247	ASN
1	B	274	LYS
1	B	295	TYR
1	B	298	ARG
1	B	314	THR
1	B	316	LYS
1	B	323	LYS
1	B	328	GLU
1	B	336	LEU
1	B	340	GLU
1	B	345	THR
1	B	347	THR
1	B	357	LEU
1	B	361	THR
1	B	362	LEU
1	B	388	LEU
1	B	399	GLU
1	C	11	THR
1	C	12	LEU

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Mol	Chain	Res	Type
1	C	15	VAL
1	C	16	GLU
1	C	25	GLU
1	C	34	THR
1	C	46	LYS
1	C	50	ILE
1	C	54	GLN
1	C	56	ILE
1	C	57	LEU
1	C	59	LEU
1	C	70	GLN
1	C	71	LEU
1	C	74	GLN
1	C	77	ILE
1	C	84	ILE
1	C	88	LEU
1	C	90	LYS
1	C	94	VAL
1	C	95	THR
1	C	121	ARG
1	C	130	LEU
1	C	150	LEU
1	C	154	ILE
1	C	157	THR
1	C	161	LYS
1	C	208	GLU
1	C	214	THR
1	C	224	GLU
1	C	247	ASN
1	C	259	THR
1	C	269	LYS
1	C	292	GLU
1	C	295	TYR
1	C	306	LEU
1	C	314	THR
1	C	328	GLU
1	C	336	LEU
1	C	345	THR
1	C	346	ILE
1	C	347	THR
1	C	357	LEU
1	C	361	THR

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Mol	Chain	Res	Type
1	C	362	LEU
1	C	388	LEU
1	D	15	VAL
1	D	18	GLU
1	D	20	ILE
1	D	26	LEU
1	D	32	GLN
1	D	33	VAL
1	D	35	GLU
1	D	39	GLU
1	D	46	LYS
1	D	50	ILE
1	D	57	LEU
1	D	59	LEU
1	D	71	LEU
1	D	77	ILE
1	D	88	LEU
1	D	94	VAL
1	D	95	THR
1	D	105	ASN
1	D	114	GLN
1	D	130	LEU
1	D	157	THR
1	D	161	LYS
1	D	168	MET
1	D	172	LEU
1	D	211	GLU
1	D	214	THR
1	D	224	GLU
1	D	247	ASN
1	D	251	ARG
1	D	264	MET
1	D	269	LYS
1	D	295	TYR
1	D	314	THR
1	D	316	LYS
1	D	328	GLU
1	D	336	LEU
1	D	344	VAL
1	D	345	THR
1	D	357	LEU
1	D	361	THR

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Mol	Chain	Res	Type
1	D	362	LEU
1	D	380	ARG
1	D	388	LEU
1	D	403	SER
1	E	11	THR
1	E	12	LEU
1	E	15	VAL
1	E	25	GLU
1	E	32	GLN
1	E	46	LYS
1	E	57	LEU
1	E	59	LEU
1	E	70	GLN
1	E	71	LEU
1	E	88	LEU
1	E	94	VAL
1	E	95	THR
1	E	114	GLN
1	E	130	LEU
1	E	154	ILE
1	E	157	THR
1	E	161	LYS
1	E	172	LEU
1	E	210	GLU
1	E	211	GLU
1	E	214	THR
1	E	247	ASN
1	E	251	ARG
1	E	259	THR
1	E	269	LYS
1	E	295	TYR
1	E	298	ARG
1	E	314	THR
1	E	323	LYS
1	E	328	GLU
1	E	336	LEU
1	E	345	THR
1	E	357	LEU
1	E	361	THR
1	E	362	LEU
1	E	380	ARG
1	E	388	LEU

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Mol	Chain	Res	Type
1	F	9	GLN
1	F	10	LEU
1	F	11	THR
1	F	15	VAL
1	F	25	GLU
1	F	34	THR
1	F	45	ASN
1	F	50	ILE
1	F	57	LEU
1	F	68	GLU
1	F	70	GLN
1	F	71	LEU
1	F	74	GLN
1	F	83	ASN
1	F	88	LEU
1	F	90	LYS
1	F	94	VAL
1	F	95	THR
1	F	102	GLU
1	F	113	ILE
1	F	118	GLU
1	F	130	LEU
1	F	154	ILE
1	F	157	THR
1	F	161	LYS
1	F	169	ILE
1	F	211	GLU
1	F	214	THR
1	F	247	ASN
1	F	259	THR
1	F	269	LYS
1	F	288	LYS
1	F	290	SER
1	F	291	ILE
1	F	295	TYR
1	F	298	ARG
1	F	306	LEU
1	F	307	GLU
1	F	314	THR
1	F	323	LYS
1	F	345	THR
1	F	357	LEU

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Mol	Chain	Res	Type
1	F	361	THR
1	F	362	LEU
1	F	388	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	22	GLN
1	A	24	ASN
1	A	54	GLN
1	A	69	ASN
1	A	70	GLN
1	A	74	GLN
1	A	158	GLN
1	A	247	ASN
1	A	319	HIS
1	B	22	GLN
1	B	69	ASN
1	B	70	GLN
1	B	74	GLN
1	B	158	GLN
1	B	247	ASN
1	B	286	GLN
1	B	308	ASN
1	B	319	HIS
1	B	398	GLN
1	C	9	GLN
1	C	22	GLN
1	C	24	ASN
1	C	54	GLN
1	C	70	GLN
1	C	74	GLN
1	C	114	GLN
1	C	158	GLN
1	C	176	HIS
1	C	247	ASN
1	C	248	GLN
1	C	319	HIS
1	D	19	HIS
1	D	22	GLN
1	D	24	ASN

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Mol	Chain	Res	Type
1	D	32	GLN
1	D	54	GLN
1	D	67	HIS
1	D	69	ASN
1	D	70	GLN
1	D	74	GLN
1	D	158	GLN
1	D	239	HIS
1	D	247	ASN
1	D	248	GLN
1	D	286	GLN
1	D	319	HIS
1	E	22	GLN
1	E	24	ASN
1	E	74	GLN
1	E	105	ASN
1	E	158	GLN
1	E	190	ASN
1	E	247	ASN
1	E	248	GLN
1	E	319	HIS
1	F	22	GLN
1	F	24	ASN
1	F	45	ASN
1	F	69	ASN
1	F	70	GLN
1	F	74	GLN
1	F	158	GLN
1	F	209	ASN
1	F	247	ASN
1	F	248	GLN
1	F	252	ASN
1	F	286	GLN
1	F	308	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	397/406 (97%)	0.28	18 (4%) 38 40	22, 44, 79, 87	0
1	B	396/406 (97%)	0.52	37 (9%) 14 16	22, 47, 101, 116	0
1	C	398/406 (98%)	0.46	9 (2%) 61 63	23, 52, 69, 75	0
1	D	396/406 (97%)	0.58	17 (4%) 40 41	22, 51, 83, 88	0
1	E	396/406 (97%)	0.41	13 (3%) 49 51	23, 51, 68, 71	0
1	F	398/406 (98%)	1.11	53 (13%) 7 8	25, 62, 86, 96	0
All	All	2381/2436 (97%)	0.56	147 (6%) 26 28	22, 51, 82, 116	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	PHE	6.1
1	F	282	LEU	5.0
1	A	221	ALA	5.0
1	B	48	ALA	4.8
1	B	46	LYS	4.6
1	B	49	PHE	4.4
1	B	43	PHE	4.0
1	A	29	TYR	4.0
1	B	50	ILE	3.9
1	B	11	THR	3.8
1	B	33	VAL	3.7
1	D	96	GLY	3.6
1	D	29	TYR	3.6
1	F	138	TYR	3.5
1	F	133	TYR	3.5
1	F	135	ILE	3.5
1	B	31	PHE	3.5
1	E	282	LEU	3.3
1	B	133	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	133	TYR	3.3
1	B	44	GLU	3.2
1	B	103	TYR	3.2
1	D	50	ILE	3.2
1	F	306	LEU	3.1
1	F	10	LEU	3.1
1	B	45	ASN	3.1
1	D	207	PHE	3.0
1	B	78	TYR	2.9
1	F	49	PHE	2.9
1	F	287	ILE	2.9
1	C	207	PHE	2.9
1	E	174	VAL	2.9
1	F	104	ALA	2.9
1	E	133	TYR	2.8
1	F	179	VAL	2.8
1	B	24	ASN	2.8
1	A	206	ARG	2.8
1	B	15	VAL	2.8
1	B	20	ILE	2.7
1	B	287	ILE	2.7
1	B	32	GLN	2.7
1	F	95	THR	2.7
1	E	103	TYR	2.7
1	B	51	LYS	2.7
1	D	11	THR	2.7
1	D	103	TYR	2.6
1	F	14	PRO	2.6
1	F	180	PHE	2.6
1	F	329	TRP	2.6
1	D	174	VAL	2.6
1	C	205	TRP	2.6
1	D	65	TRP	2.6
1	E	41	SER	2.6
1	E	67	HIS	2.5
1	D	221	ALA	2.5
1	F	101	PRO	2.5
1	E	11	THR	2.5
1	B	41	SER	2.5
1	B	56	ILE	2.5
1	F	283	GLU	2.5
1	F	348	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	314	THR	2.5
1	B	52	SER	2.5
1	B	38	ILE	2.5
1	F	205	TRP	2.5
1	A	133	TYR	2.5
1	C	185	ARG	2.4
1	F	305	PHE	2.4
1	B	67	HIS	2.4
1	B	30	VAL	2.4
1	F	65	TRP	2.4
1	B	26	LEU	2.4
1	C	133	TYR	2.4
1	C	221	ALA	2.4
1	F	314	THR	2.4
1	A	31	PHE	2.4
1	F	269	LYS	2.4
1	F	108	LEU	2.4
1	B	42	GLY	2.4
1	F	400	ALA	2.4
1	F	228	VAL	2.4
1	E	138	TYR	2.3
1	D	49	PHE	2.3
1	F	346	ILE	2.3
1	A	65	TRP	2.3
1	F	67	HIS	2.3
1	F	9	GLN	2.3
1	F	173	ALA	2.3
1	E	169	ILE	2.3
1	B	27	LEU	2.3
1	D	138	TYR	2.3
1	F	379	GLU	2.3
1	A	23	PHE	2.2
1	F	63	PHE	2.2
1	A	106	HIS	2.2
1	B	36	ALA	2.2
1	F	288	LYS	2.2
1	F	345	THR	2.2
1	C	57	LEU	2.2
1	F	11	THR	2.2
1	F	137	TYR	2.2
1	D	351	LEU	2.2
1	F	171	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	371	ARG	2.2
1	E	314	THR	2.2
1	F	29	TYR	2.1
1	B	105	ASN	2.1
1	F	174	VAL	2.1
1	A	107	GLY	2.1
1	A	71	LEU	2.1
1	F	20	ILE	2.1
1	E	283	GLU	2.1
1	F	126	TRP	2.1
1	F	132	PRO	2.1
1	F	107	GLY	2.1
1	B	104	ALA	2.1
1	F	61	LYS	2.1
1	A	57	LEU	2.1
1	D	44	GLU	2.1
1	D	286	GLN	2.1
1	F	106	HIS	2.1
1	B	207	PHE	2.1
1	E	184	ALA	2.1
1	E	168	MET	2.1
1	D	88	LEU	2.1
1	F	130	LEU	2.1
1	A	50	ILE	2.1
1	C	50	ILE	2.1
1	D	72	ILE	2.1
1	F	181	ASP	2.1
1	A	103	TYR	2.1
1	A	30	VAL	2.1
1	B	199	PHE	2.1
1	F	131	PHE	2.1
1	F	347	THR	2.0
1	A	10	LEU	2.0
1	B	21	ASP	2.0
1	C	105	ASN	2.0
1	B	168	MET	2.0
1	F	48	ALA	2.0
1	F	198	ALA	2.0
1	A	22	GLN	2.0
1	A	26	LEU	2.0
1	C	282	LEU	2.0
1	B	72	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	154	ILE	2.0
1	F	225	PRO	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.