



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:20 AM UTC

PDB ID : 2DYM / pdb_00002dym
Title : The crystal structure of Saccharomyces cerevisiae Atg5- Atg16(1-46) complex
Authors : Matsushita, M.; Suzuki, N.N.; Inagaki, F.
Deposited on : 2006-09-15
Resolution : 2.20 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:

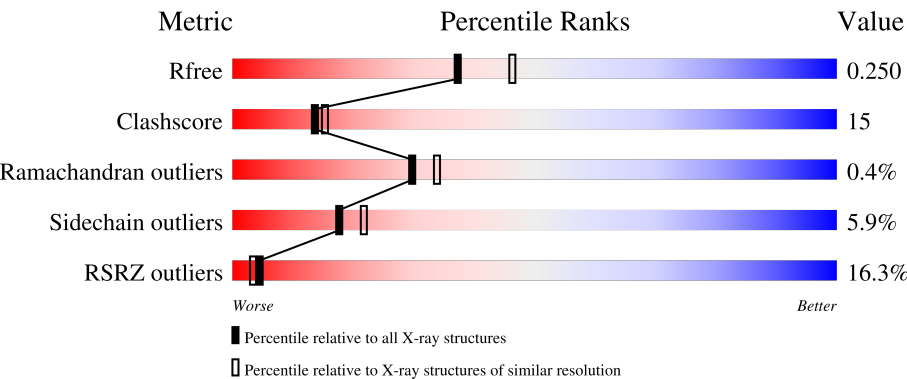
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	297	12% 62%21%•14%
1	C	297	17% 58%23%•15%
1	E	297	14% 58%22%•17%
1	G	297	17% 65%19%•12%
2	B	46	2% 35%15%•48%

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Mol	Chain	Length	Quality of chain
2	D	46	48% 48%
2	F	46	2% 43% 7% 48%
2	H	46	2% 43% 9% 48%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9196 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 Autophagy protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2041	1339	339	353	10			
1	C	251	Total	C	N	O	S	0	0	0
			1989	1306	327	345	11			
1	E	247	Total	C	N	O	S	0	0	0
			1970	1298	326	336	10			
1	G	262	Total	C	N	O	S	0	0	0
			2064	1355	339	359	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q12380
A	-1	ALA	-	cloning artifact	UNP Q12380
A	0	HIS	-	cloning artifact	UNP Q12380
C	-2	GLY	-	cloning artifact	UNP Q12380
C	-1	ALA	-	cloning artifact	UNP Q12380
C	0	HIS	-	cloning artifact	UNP Q12380
E	-2	GLY	-	cloning artifact	UNP Q12380
E	-1	ALA	-	cloning artifact	UNP Q12380
E	0	HIS	-	cloning artifact	UNP Q12380
G	-2	GLY	-	cloning artifact	UNP Q12380
G	-1	ALA	-	cloning artifact	UNP Q12380
G	0	HIS	-	cloning artifact	UNP Q12380

- Molecule 2 is a protein called Autophagy protein 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	S	0	0	0
			202	124	38	39	1			
2	D	24	Total	C	N	O	S	0	0	0
			203	124	38	40	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	24	Total	C	N	O	S	0	0	0
			203	124	38	40	1			
2	H	24	Total	C	N	O	S	0	0	0
			203	124	38	40	1			

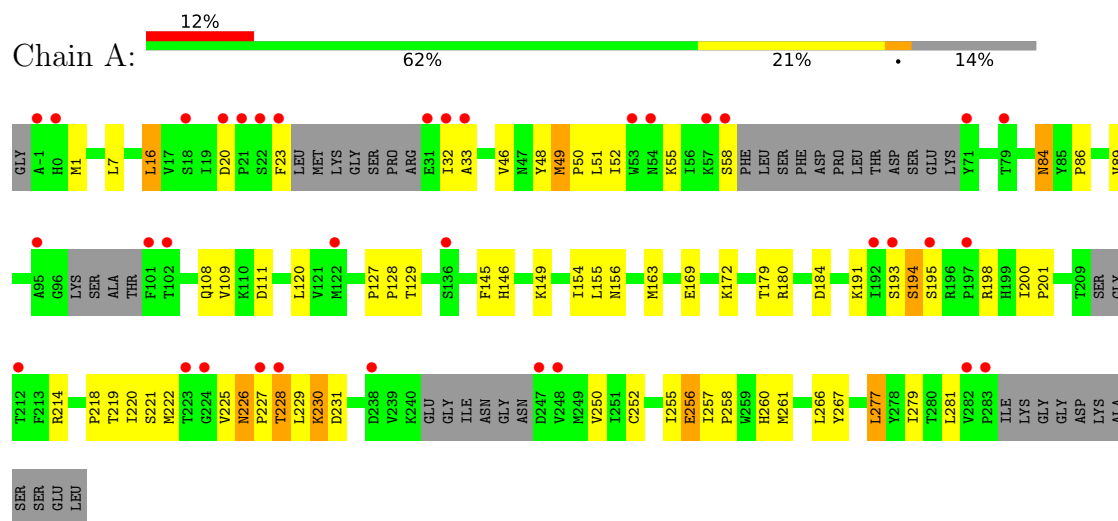
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	8	Total	O	0	0
			8	8		
3	C	61	Total	O	0	0
			61	61		
3	D	12	Total	O	0	0
			12	12		
3	E	73	Total	O	0	0
			73	73		
3	F	15	Total	O	0	0
			15	15		
3	G	65	Total	O	0	0
			65	65		
3	H	11	Total	O	0	0
			11	11		

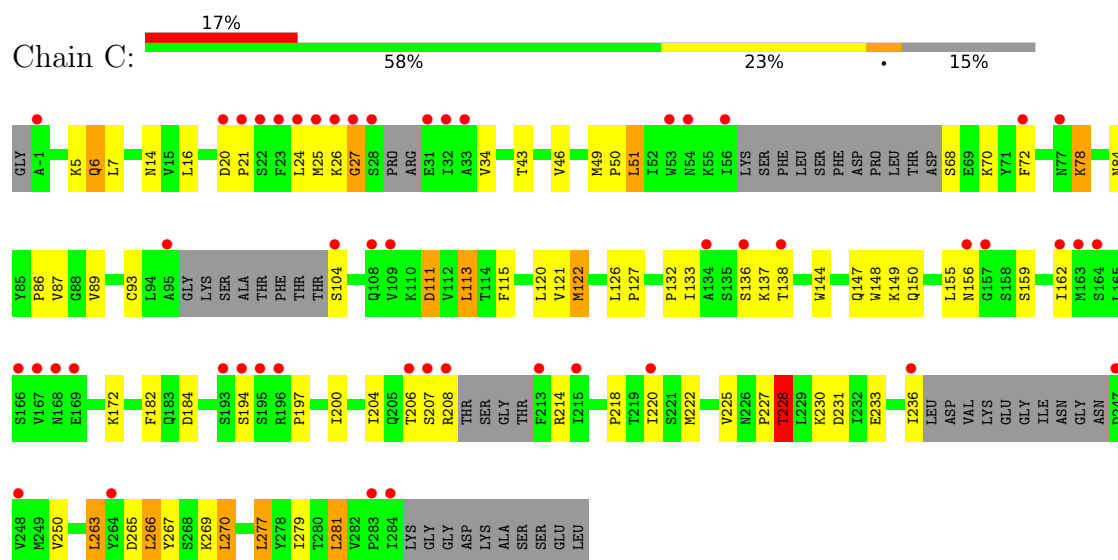
3 Residue-property plots [i](#)

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: Autophagy protein 5

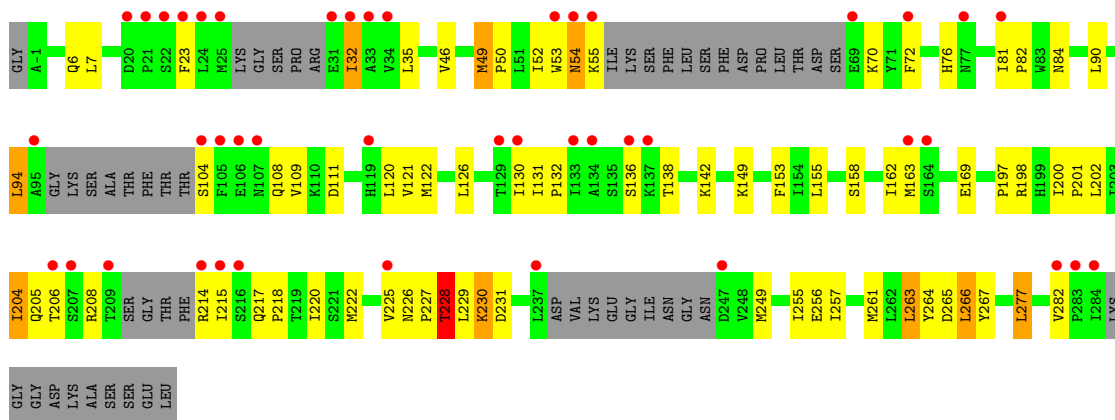


• Molecule 1: Autophagy protein 5

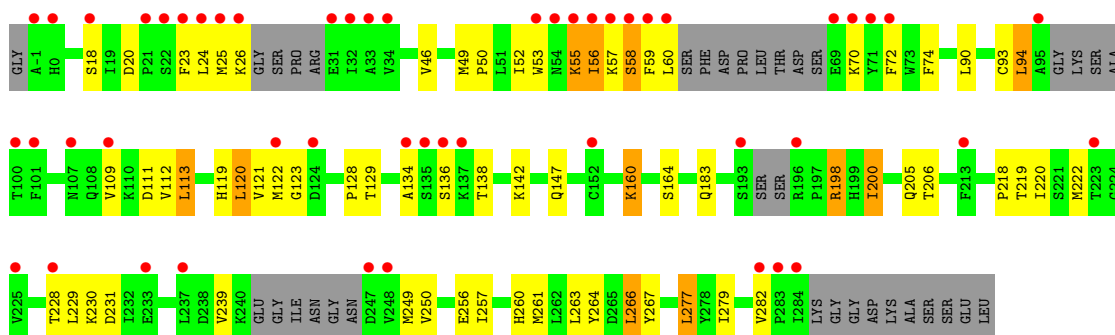


• Molecule 1: Autophagy protein 5

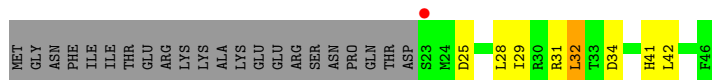
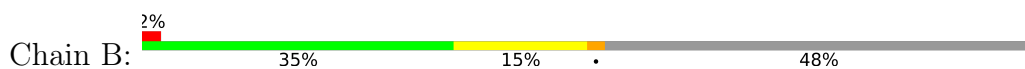




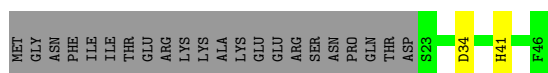
• Molecule 1: Autophagy protein 5



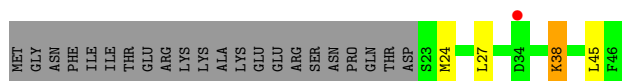
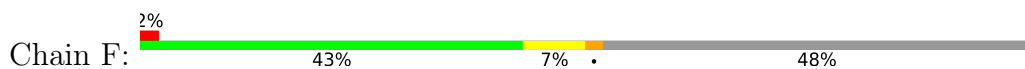
• Molecule 2: Autophagy protein 16



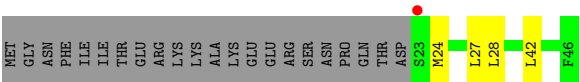
• Molecule 2: Autophagy protein 16



• Molecule 2: Autophagy protein 16



• Molecule 2: Autophagy protein 16



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.35Å 104.42Å 112.15Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	49.38 – 2.20 49.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.38-2.20) 96.5 (49.38-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.250 0.219 , 0.250	Depositor DCC
R_{free} test set	7451 reflections (8.47%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9196	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7741e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/2095	1.00	13/2850 (0.5%)
1	C	0.39	0/2041	0.92	5/2777 (0.2%)
1	E	0.41	0/2022	0.96	9/2751 (0.3%)
1	G	0.38	0/2118	0.94	6/2888 (0.2%)
2	B	0.44	0/203	0.74	0/271
2	D	0.40	0/204	0.79	0/272
2	F	0.41	0/204	0.81	1/272 (0.4%)
2	H	0.38	0/204	0.74	0/272
All	All	0.40	0/9091	0.94	34/12353 (0.3%)

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

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	32	ILE	N-CA-C	-12.60	100.36	112.83
1	A	32	ILE	N-CA-C	-9.99	103.38	113.47
1	G	55	LYS	N-CA-C	-7.75	100.30	110.53
1	A	198	ARG	N-CA-C	-7.57	102.38	111.69
1	G	198	ARG	N-CA-C	-7.48	102.49	111.69
1	E	111	ASP	N-CA-C	6.62	120.68	111.74
1	E	206	THR	N-CA-C	-6.59	100.21	110.17
1	A	194	SER	N-CA-C	6.52	120.07	110.30
1	A	128	PRO	N-CA-C	6.50	122.43	113.65
1	A	228	THR	N-CA-C	-6.31	100.87	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASP	N-CA-C	6.12	120.00	111.74
1	E	228	THR	N-CA-C	-6.08	101.20	110.14
1	G	111	ASP	N-CA-C	5.83	119.70	112.24
1	A	111	ASP	N-CA-C	5.82	119.59	111.74
1	A	127	PRO	CA-C-N	5.77	125.63	119.28
1	A	127	PRO	C-N-CA	5.77	125.63	119.28
1	G	129	THR	N-CA-C	5.70	120.08	113.18
1	C	137	LYS	N-CA-C	-5.69	106.23	112.72
1	A	33	ALA	N-CA-C	-5.55	106.35	113.23
2	F	24	MET	N-CA-C	-5.45	105.42	111.36
1	A	129	THR	N-CA-C	5.45	119.93	113.28
1	G	57	LYS	N-CA-C	-5.43	105.82	113.20
1	E	130	ILE	N-CA-C	5.42	116.66	108.96
1	E	226	ASN	CA-C-N	5.36	125.30	119.78
1	E	226	ASN	C-N-CA	5.36	125.30	119.78
1	A	193	SER	N-CA-C	5.33	117.42	109.59
1	C	270	LEU	N-CA-C	5.31	119.73	112.88
1	A	226	ASN	CA-C-N	5.31	125.32	119.90
1	A	226	ASN	C-N-CA	5.31	125.32	119.90
1	E	217	GLN	CA-C-N	5.28	125.18	119.85
1	E	217	GLN	C-N-CA	5.28	125.18	119.85
1	C	14	ASN	N-CA-C	-5.24	101.43	109.76
1	C	228	THR	N-CA-C	-5.21	102.34	110.42
1	G	128	PRO	N-CA-C	5.00	120.12	113.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	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	2041	0	2013	53	0
1	C	1989	0	1948	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1970	0	1956	59	0
1	G	2064	0	2005	66	0
2	B	202	0	196	5	0
2	D	203	0	199	3	0
2	F	203	0	199	3	0
2	H	203	0	199	7	0
3	A	76	0	0	4	0
3	B	8	0	0	0	0
3	C	61	0	0	1	0
3	D	12	0	0	0	0
3	E	73	0	0	0	0
3	F	15	0	0	0	0
3	G	65	0	0	0	0
3	H	11	0	0	0	0
All	All	9196	0	8715	256	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 15.

All (256) 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:E:70:LYS:HG2	1:E:122:MET:HE2	1.35	1.04
1:G:49:MET:HE2	1:G:49:MET:HA	1.43	0.97
1:E:49:MET:HE2	1:E:49:MET:HA	1.53	0.91
1:C:228:THR:HG22	1:C:231:ASP:H	1.40	0.87
1:E:205:GLN:HG2	1:E:215:ILE:HG12	1.57	0.85
1:C:70:LYS:HG2	1:C:122:MET:HE2	1.61	0.83
1:E:228:THR:HG22	1:E:231:ASP:H	1.44	0.80
1:C:266:LEU:HD13	1:C:277:LEU:HD11	1.63	0.80
1:C:206:THR:HG23	1:C:206:THR:O	1.79	0.80
1:A:218:PRO:HB2	1:A:220:ILE:HD11	1.66	0.77
1:G:20:ASP:HB3	1:G:23:PHE:HD1	1.49	0.77
1:C:200:ILE:HD13	1:C:222:MET:HG3	1.69	0.76
1:E:49:MET:CE	1:E:52:ILE:HD12	2.18	0.74
1:A:86:PRO:HG2	1:A:89:VAL:CG2	2.18	0.73
1:C:86:PRO:HG2	1:C:89:VAL:CG2	2.19	0.71
1:A:1:MET:HE3	3:A:296:HOH:O	1.89	0.71
1:C:200:ILE:HG12	1:C:263:LEU:HD22	1.74	0.70
1:A:49:MET:HA	1:A:49:MET:HE2	1.71	0.70
1:E:204:ILE:N	1:E:204:ILE:HD12	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ILE:HD13	1:C:222:MET:CG	2.24	0.68
1:C:204:ILE:HD13	1:C:236:ILE:HA	1.77	0.67
1:G:200:ILE:HD13	1:G:222:MET:CG	2.25	0.67
1:A:225:VAL:HG23	1:A:227:PRO:HD3	1.76	0.66
1:G:228:THR:HG22	1:G:231:ASP:CG	2.20	0.66
1:C:78:LYS:HE2	1:C:78:LYS:HA	1.76	0.66
1:A:86:PRO:HG2	1:A:89:VAL:HG21	1.78	0.66
1:A:20:ASP:HB3	1:A:23:PHE:CE1	2.31	0.66
1:G:55:LYS:O	1:G:56:ILE:HB	1.95	0.66
2:B:25:ASP:O	2:B:29:ILE:HG12	1.95	0.66
1:G:228:THR:HG22	1:G:231:ASP:H	1.61	0.66
1:E:218:PRO:HB2	1:E:220:ILE:HD11	1.77	0.65
1:G:49:MET:HA	1:G:49:MET:CE	2.22	0.65
1:G:206:THR:HG23	1:G:239:VAL:HG12	1.78	0.65
1:G:24:LEU:CD2	1:G:56:ILE:HG23	2.27	0.65
1:A:84:ASN:H	1:A:84:ASN:HD22	1.44	0.65
1:A:145:PHE:HE1	1:A:163:MET:HE1	1.60	0.64
1:E:149:LYS:HA	1:E:162:ILE:HG21	1.80	0.64
1:C:206:THR:CG2	1:C:214:ARG:HB3	2.27	0.63
1:G:261:MET:HE1	2:H:28:LEU:HD11	1.80	0.63
1:G:200:ILE:HD13	1:G:222:MET:HG3	1.80	0.63
1:C:49:MET:CE	1:C:133:ILE:HD13	2.28	0.63
1:E:136:SER:HB2	1:E:138:THR:HG22	1.79	0.62
1:A:155:LEU:HB3	1:A:194:SER:CB	2.30	0.62
1:G:109:VAL:HG23	1:G:112:VAL:HG23	1.81	0.62
1:C:250:VAL:HG13	1:C:279:ILE:HG23	1.81	0.62
1:A:228:THR:HG22	1:A:231:ASP:CG	2.25	0.62
1:C:228:THR:HG23	1:C:230:LYS:H	1.66	0.61
1:A:49:MET:HA	1:A:49:MET:CE	2.31	0.61
1:G:56:ILE:HG22	1:G:56:ILE:O	2.00	0.60
1:G:56:ILE:C	1:G:58:SER:H	2.09	0.60
1:G:219:THR:C	1:G:220:ILE:HD12	2.27	0.60
1:G:250:VAL:HG13	1:G:279:ILE:HG23	1.83	0.60
1:E:228:THR:HG23	1:E:230:LYS:H	1.66	0.60
1:G:218:PRO:HB2	1:G:220:ILE:HD11	1.83	0.60
1:G:20:ASP:HB3	1:G:23:PHE:CD1	2.34	0.59
1:G:261:MET:HE3	2:H:24:MET:CG	2.33	0.59
1:E:53:TRP:C	1:E:55:LYS:H	2.11	0.59
1:C:200:ILE:HG21	1:C:263:LEU:HD21	1.84	0.58
1:C:218:PRO:HB2	1:C:220:ILE:HD11	1.84	0.58
1:G:228:THR:CG2	1:G:231:ASP:H	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:TYR:HA	1:G:277:LEU:HG	1.83	0.58
1:A:261:MET:HE1	2:B:28:LEU:HD11	1.84	0.58
1:E:200:ILE:HG13	1:E:263:LEU:HD13	1.85	0.58
1:C:200:ILE:CD1	1:C:222:MET:HG3	2.32	0.58
1:C:236:ILE:HG22	1:C:281:LEU:HD21	1.84	0.58
1:C:86:PRO:HG2	1:C:89:VAL:HG21	1.86	0.57
1:A:156:ASN:OD1	1:A:194:SER:CB	2.51	0.57
1:C:149:LYS:HG3	1:C:159:SER:HB2	1.87	0.57
1:C:206:THR:HG22	1:C:214:ARG:HB3	1.87	0.57
1:E:228:THR:HG23	1:E:230:LYS:N	2.20	0.57
1:A:172:LYS:HE3	1:A:184:ASP:CG	2.29	0.57
1:C:46:VAL:HA	1:C:49:MET:HG2	1.87	0.57
1:A:255:ILE:HD13	2:B:32:LEU:HD13	1.87	0.56
1:G:59:PHE:O	1:G:60:LEU:CB	2.53	0.56
1:C:149:LYS:HA	1:C:162:ILE:HG21	1.87	0.56
1:A:218:PRO:HB2	1:A:220:ILE:CD1	2.35	0.56
1:G:49:MET:HB2	1:G:50:PRO:HD3	1.86	0.56
1:A:51:LEU:C	1:A:51:LEU:HD23	2.31	0.56
1:G:23:PHE:CE1	1:G:122:MET:HB2	2.41	0.56
1:G:25:MET:HE2	1:G:58:SER:HA	1.88	0.56
1:G:138:THR:HB	1:G:142:LYS:HE3	1.88	0.56
1:C:104:SER:HA	2:D:34:ASP:OD1	2.07	0.55
1:G:266:LEU:HD13	1:G:277:LEU:HD11	1.89	0.55
2:H:27:LEU:C	2:H:27:LEU:HD23	2.32	0.55
1:C:228:THR:HG22	1:C:231:ASP:N	2.15	0.55
1:G:55:LYS:O	1:G:56:ILE:CB	2.54	0.55
1:A:180:ARG:HD3	3:A:306:HOH:O	2.05	0.55
1:C:172:LYS:HE3	1:C:184:ASP:CG	2.32	0.55
1:E:49:MET:HA	1:E:49:MET:CE	2.32	0.55
1:G:25:MET:HE2	1:G:58:SER:CA	2.37	0.55
1:A:220:ILE:N	1:A:220:ILE:HD12	2.22	0.54
1:C:70:LYS:CG	1:C:122:MET:HE2	2.33	0.54
1:E:126:LEU:HD22	1:E:132:PRO:HB3	1.89	0.54
1:C:51:LEU:HD23	1:C:51:LEU:C	2.33	0.54
1:A:108:GLN:NE2	3:A:362:HOH:O	2.31	0.54
1:C:49:MET:HE2	1:C:133:ILE:HD13	1.90	0.54
1:C:206:THR:O	1:C:206:THR:CG2	2.52	0.54
1:G:228:THR:HG23	1:G:230:LYS:H	1.73	0.54
1:E:72:PHE:CE2	1:E:122:MET:HE3	2.42	0.54
1:A:145:PHE:CE1	1:A:163:MET:HE1	2.42	0.54
1:G:256:GLU:C	1:G:257:ILE:HD12	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD21	1:A:250:VAL:HG11	1.91	0.53
1:A:250:VAL:HG13	1:A:279:ILE:HG23	1.91	0.53
1:C:49:MET:HB2	1:C:50:PRO:HD3	1.91	0.53
1:E:149:LYS:HE2	1:E:163:MET:SD	2.48	0.53
1:G:200:ILE:CD1	1:G:222:MET:HG3	2.38	0.53
1:C:220:ILE:HG21	1:C:263:LEU:CD1	2.39	0.53
1:A:84:ASN:H	1:A:84:ASN:ND2	2.06	0.52
1:G:160:LYS:HD3	1:G:164:SER:OG	2.09	0.52
1:A:179:THR:O	1:A:180:ARG:HB2	2.09	0.52
1:E:23:PHE:CZ	1:E:122:MET:HB3	2.44	0.52
1:C:230:LYS:O	1:C:233:GLU:HG2	2.10	0.52
1:E:228:THR:CG2	1:E:231:ASP:H	2.19	0.52
1:C:111:ASP:HA	2:D:41:HIS:HE1	1.75	0.52
1:E:267:TYR:HA	1:E:277:LEU:HG	1.92	0.52
1:G:134:ALA:O	1:G:136:SER:N	2.43	0.52
1:G:49:MET:CE	1:G:74:PHE:HZ	2.23	0.52
1:A:109:VAL:HG21	1:E:109:VAL:HG21	1.92	0.52
1:E:32:ILE:O	1:E:32:ILE:HG22	2.09	0.51
1:E:222:MET:HE2	1:E:264:TYR:HB2	1.92	0.51
1:C:225:VAL:HG23	1:C:227:PRO:HD3	1.93	0.51
1:G:228:THR:HG23	1:G:230:LYS:N	2.26	0.51
1:A:252:CYS:SG	1:A:277:LEU:HD21	2.51	0.51
1:C:86:PRO:HG2	1:C:89:VAL:HG23	1.91	0.51
1:G:46:VAL:HA	1:G:49:MET:HG2	1.92	0.51
1:G:90:LEU:O	1:G:94:LEU:HB2	2.11	0.51
1:A:221:SER:O	1:A:222:MET:HE2	2.11	0.51
1:C:148:TRP:HB3	1:C:162:ILE:HD12	1.93	0.51
1:E:49:MET:HB2	1:E:50:PRO:HD3	1.93	0.51
1:A:20:ASP:HB3	1:A:23:PHE:CD1	2.47	0.50
1:C:49:MET:HE3	1:C:133:ILE:HG21	1.94	0.50
1:C:113:LEU:HD12	2:H:42:LEU:HD13	1.93	0.50
1:G:25:MET:O	1:G:26:LYS:C	2.55	0.50
1:E:90:LEU:O	1:E:94:LEU:HB2	2.11	0.50
1:C:155:LEU:HD22	1:C:197:PRO:HB3	1.94	0.50
2:B:41:HIS:CD2	2:B:42:LEU:HG	2.47	0.49
1:E:220:ILE:HD12	1:E:220:ILE:N	2.26	0.49
1:A:49:MET:HE3	1:A:52:ILE:HD12	1.93	0.49
1:C:230:LYS:O	1:C:230:LYS:HD3	2.12	0.49
1:C:126:LEU:HD22	1:C:132:PRO:HB3	1.95	0.49
1:C:84:ASN:H	1:C:84:ASN:HD22	1.61	0.48
1:E:50:PRO:O	1:E:54:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:PHE:HE2	1:E:122:MET:HE3	1.76	0.48
1:E:138:THR:OG1	1:E:142:LYS:HE2	2.12	0.48
1:E:256:GLU:C	1:E:257:ILE:HD12	2.39	0.48
1:C:72:PHE:HE2	1:C:122:MET:HE3	1.79	0.48
2:F:27:LEU:C	2:F:27:LEU:HD23	2.39	0.48
1:A:228:THR:HG23	1:A:230:LYS:N	2.29	0.48
1:C:6:GLN:HG2	1:C:182:PHE:CE2	2.49	0.48
1:C:206:THR:HG21	1:C:214:ARG:HB3	1.95	0.48
1:E:76:HIS:HB3	1:E:81:ILE:HD11	1.96	0.48
1:E:225:VAL:HG22	1:E:227:PRO:HG3	1.97	0.47
1:C:51:LEU:HD23	1:C:51:LEU:O	2.14	0.47
1:E:155:LEU:HD22	1:E:197:PRO:HB3	1.95	0.47
1:A:256:GLU:C	1:A:257:ILE:HD12	2.40	0.47
1:A:146:HIS:O	1:A:149:LYS:HB3	2.14	0.47
1:A:49:MET:N	1:A:50:PRO:HD2	2.29	0.47
1:E:214:ARG:HH21	1:E:214:ARG:HG2	1.79	0.47
1:G:49:MET:CE	1:G:52:ILE:HD12	2.45	0.47
1:E:208:ARG:HG3	1:E:208:ARG:HH11	1.78	0.47
1:A:222:MET:HE1	1:A:227:PRO:HD2	1.97	0.46
1:C:84:ASN:H	1:C:84:ASN:ND2	2.13	0.46
1:G:228:THR:H	1:G:231:ASP:HB2	1.80	0.46
1:G:249:MET:HB3	1:G:282:VAL:HG23	1.96	0.46
1:E:84:ASN:HB3	1:E:131:ILE:HD11	1.97	0.46
1:C:220:ILE:N	1:C:220:ILE:HD12	2.30	0.46
1:E:255:ILE:HG13	1:E:257:ILE:CD1	2.46	0.46
1:A:194:SER:O	1:A:195:SER:C	2.58	0.46
1:G:218:PRO:HB2	1:G:220:ILE:CD1	2.45	0.46
1:A:219:THR:C	1:A:220:ILE:HD12	2.41	0.45
1:C:220:ILE:HG21	1:C:263:LEU:HD11	1.97	0.45
1:E:84:ASN:ND2	1:E:84:ASN:H	2.15	0.45
1:C:51:LEU:C	1:C:51:LEU:CD2	2.90	0.45
1:C:93:CYS:O	1:C:208:ARG:N	2.49	0.45
1:G:93:CYS:HB3	1:G:205:GLN:NE2	2.31	0.45
1:G:267:TYR:HD1	1:G:277:LEU:HB2	1.81	0.45
1:G:198:ARG:HH21	1:G:198:ARG:HG3	1.82	0.45
1:C:113:LEU:HD13	1:C:115:PHE:CD2	2.52	0.45
1:C:72:PHE:CE2	1:C:122:MET:HE3	2.52	0.44
1:G:18:SER:OG	1:G:119:HIS:ND1	2.49	0.44
1:A:46:VAL:HA	1:A:49:MET:HG2	2.00	0.44
1:E:153:PHE:HD1	1:E:158:SER:HA	1.82	0.44
1:G:138:THR:CB	1:G:142:LYS:HE3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:GLN:CD	1:G:183:GLN:H	2.25	0.44
1:G:250:VAL:HG13	1:G:279:ILE:CG2	2.46	0.44
1:C:25:MET:C	1:C:27:GLY:H	2.26	0.44
1:E:104:SER:O	1:E:108:GLN:N	2.50	0.44
1:C:16:LEU:HD11	1:C:34:VAL:CG1	2.48	0.44
1:C:197:PRO:O	1:C:222:MET:HB2	2.17	0.44
1:G:49:MET:HE3	1:G:74:PHE:HZ	1.81	0.44
1:C:20:ASP:OD1	1:C:21:PRO:HD2	2.18	0.43
1:G:72:PHE:HA	1:G:121:VAL:O	2.17	0.43
1:G:260:HIS:CE1	2:H:24:MET:HE1	2.53	0.43
1:A:258:PRO:HB3	1:A:260:HIS:CE1	2.53	0.43
1:C:156:ASN:OD1	1:C:194:SER:CB	2.67	0.43
1:E:136:SER:C	1:E:138:THR:H	2.26	0.43
1:A:226:ASN:N	1:A:227:PRO:HD3	2.33	0.43
1:E:53:TRP:C	1:E:55:LYS:N	2.77	0.43
1:A:16:LEU:HD11	2:F:45:LEU:HD21	2.00	0.43
1:A:169:GLU:OE1	1:A:191:LYS:HE3	2.18	0.43
1:C:136:SER:CB	1:C:138:THR:HG22	2.48	0.43
1:G:20:ASP:HB2	1:G:120:LEU:O	2.18	0.43
1:C:68:SER:C	1:C:70:LYS:H	2.27	0.43
1:C:126:LEU:HD12	1:C:127:PRO:HD2	2.01	0.43
1:C:207:SER:O	1:C:208:ARG:C	2.62	0.43
1:G:229:LEU:HD21	1:G:250:VAL:HG11	2.01	0.43
1:A:228:THR:HG23	1:A:230:LYS:H	1.84	0.43
1:C:43:THR:O	1:C:87:VAL:HG23	2.19	0.43
1:E:121:VAL:HG12	1:E:122:MET:N	2.32	0.43
1:G:53:TRP:O	1:G:55:LYS:O	2.37	0.42
1:G:222:MET:HE2	1:G:264:TYR:HB2	2.01	0.42
1:C:269:LYS:C	1:C:270:LEU:HD23	2.44	0.42
1:E:121:VAL:CG1	1:E:122:MET:N	2.82	0.42
1:G:109:VAL:HG23	1:G:112:VAL:CG2	2.47	0.42
1:E:46:VAL:HA	1:E:49:MET:HG2	2.01	0.42
1:E:201:PRO:HD2	1:E:267:TYR:CE1	2.54	0.42
1:C:267:TYR:HA	1:C:277:LEU:HG	2.01	0.42
1:E:228:THR:HG22	1:E:231:ASP:CG	2.44	0.42
1:A:154:ILE:HD13	3:A:345:HOH:O	2.18	0.42
1:E:49:MET:HE1	1:E:52:ILE:HD12	1.95	0.42
1:E:249:MET:HB3	1:E:282:VAL:HG23	2.01	0.42
1:A:51:LEU:HD21	1:A:55:LYS:HE2	2.02	0.42
1:C:228:THR:CG2	1:C:230:LYS:H	2.32	0.42
1:G:249:MET:HB3	1:G:282:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PRO:HB2	1:C:220:ILE:CD1	2.50	0.41
1:E:35:LEU:HD13	1:E:55:LYS:HD2	2.01	0.41
1:G:113:LEU:HD23	2:H:42:LEU:HB2	2.02	0.41
1:E:81:ILE:HA	1:E:82:PRO:HD3	1.88	0.41
1:E:204:ILE:N	1:E:204:ILE:CD1	2.79	0.41
1:A:51:LEU:HD23	1:A:51:LEU:O	2.20	0.41
1:A:86:PRO:HG2	1:A:89:VAL:HG23	1.98	0.41
1:A:256:GLU:HG2	2:B:31:ARG:NH1	2.35	0.41
1:G:70:LYS:HA	1:G:123:GLY:O	2.20	0.41
1:A:20:ASP:HB3	1:A:23:PHE:HE1	1.84	0.41
1:C:5:LYS:NZ	3:C:345:HOH:O	2.54	0.41
1:E:49:MET:N	1:E:50:PRO:CD	2.83	0.41
1:G:261:MET:HE3	2:H:24:MET:HG2	2.01	0.41
1:C:144:TRP:O	1:C:147:GLN:HB2	2.21	0.41
1:E:222:MET:C	1:E:225:VAL:HG12	2.46	0.41
1:G:25:MET:CE	1:G:58:SER:HB3	2.49	0.41
1:C:228:THR:O	1:C:231:ASP:HB2	2.21	0.41
1:E:225:VAL:CG2	1:E:227:PRO:HG3	2.50	0.41
1:E:202:LEU:HG	1:E:204:ILE:HD11	2.03	0.41
1:A:257:ILE:HA	1:A:258:PRO:HD3	1.92	0.41
1:E:218:PRO:O	1:E:220:ILE:HD12	2.20	0.41
2:F:38:LYS:CB	2:F:38:LYS:NZ	2.83	0.41
1:G:121:VAL:HG12	1:G:122:MET:N	2.36	0.41
1:A:201:PRO:HD2	1:A:267:TYR:CE1	2.56	0.40
1:C:68:SER:C	1:C:70:LYS:N	2.79	0.40
1:E:204:ILE:HD13	1:E:218:PRO:CD	2.52	0.40
1:E:266:LEU:HD13	1:E:277:LEU:HD11	2.03	0.40
1:G:56:ILE:C	1:G:58:SER:N	2.76	0.40
1:C:111:ASP:HA	2:D:41:HIS:CE1	2.55	0.40
1:C:121:VAL:HG12	1:C:122:MET:N	2.36	0.40
1:A:252:CYS:HB3	1:A:257:ILE:CD1	2.51	0.40
1:G:198:ARG:HG3	1:G:198:ARG:NH2	2.37	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	242/297 (82%)	235 (97%)	7 (3%)	0	100	100
1	C	239/297 (80%)	229 (96%)	8 (3%)	2 (1%)	16	16
1	E	235/297 (79%)	226 (96%)	8 (3%)	1 (0%)	30	34
1	G	250/297 (84%)	243 (97%)	6 (2%)	1 (0%)	30	34
2	B	22/46 (48%)	22 (100%)	0	0	100	100
2	D	22/46 (48%)	22 (100%)	0	0	100	100
2	F	22/46 (48%)	22 (100%)	0	0	100	100
2	H	22/46 (48%)	22 (100%)	0	0	100	100
All	All	1054/1372 (77%)	1021 (97%)	29 (3%)	4 (0%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	26	LYS
1	E	54	ASN
1	G	56	ILE
1	C	27	GLY

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	223/271 (82%)	210 (94%)	13 (6%)	18	22
1	C	214/271 (79%)	199 (93%)	15 (7%)	14	16
1	E	214/271 (79%)	198 (92%)	16 (8%)	12	14
1	G	221/271 (82%)	211 (96%)	10 (4%)	24	33
2	B	22/43 (51%)	20 (91%)	2 (9%)	9	9
2	D	23/43 (54%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	23/43 (54%)	22 (96%)	1 (4%)	26	35
2	H	23/43 (54%)	23 (100%)	0	100	100
All	All	963/1256 (77%)	906 (94%)	57 (6%)	18	22

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	16	LEU
1	A	49	MET
1	A	58	SER
1	A	84	ASN
1	A	120	LEU
1	A	200	ILE
1	A	214	ARG
1	A	230	LYS
1	A	256	GLU
1	A	266	LEU
1	A	277	LEU
1	A	281	LEU
2	B	32	LEU
2	B	34	ASP
1	C	6	GLN
1	C	7	LEU
1	C	24	LEU
1	C	51	LEU
1	C	78	LYS
1	C	113	LEU
1	C	120	LEU
1	C	122	MET
1	C	150	GLN
1	C	228	THR
1	C	263	LEU
1	C	265	ASP
1	C	266	LEU
1	C	277	LEU
1	C	281	LEU
1	E	6	GLN
1	E	7	LEU
1	E	49	MET
1	E	94	LEU

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Mol	Chain	Res	Type
1	E	120	LEU
1	E	169	GLU
1	E	198	ARG
1	E	204	ILE
1	E	228	THR
1	E	229	LEU
1	E	230	LYS
1	E	261	MET
1	E	263	LEU
1	E	265	ASP
1	E	266	LEU
1	E	277	LEU
2	F	38	LYS
1	G	58	SER
1	G	94	LEU
1	G	113	LEU
1	G	120	LEU
1	G	147	GLN
1	G	160	LYS
1	G	200	ILE
1	G	263	LEU
1	G	266	LEU
1	G	277	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	47	ASN
1	A	84	ASN
1	A	108	GLN
1	A	146	HIS
1	A	150	GLN
1	A	190	ASN
1	A	205	GLN
1	A	217	GLN
1	A	226	ASN
1	A	260	HIS
1	C	6	GLN
1	C	10	ASN
1	C	47	ASN
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	107	ASN
1	C	190	ASN
1	C	205	GLN
1	C	217	GLN
1	C	226	ASN
2	D	41	HIS
1	E	6	GLN
1	E	10	ASN
1	E	47	ASN
1	E	84	ASN
1	E	168	ASN
1	E	190	ASN
1	E	205	GLN
1	E	217	GLN
1	E	226	ASN
1	E	260	HIS
1	G	6	GLN
1	G	10	ASN
1	G	47	ASN
1	G	76	HIS
1	G	84	ASN
1	G	108	GLN
1	G	147	GLN
1	G	156	ASN
1	G	190	ASN
1	G	205	GLN
1	G	217	GLN
1	G	226	ASN
1	G	260	HIS

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	254/297 (85%)	0.69	35 (13%) 6 5	23, 41, 67, 86	0
1	C	251/297 (84%)	1.01	50 (19%) 3 2	26, 47, 74, 89	0
1	E	247/297 (83%)	0.80	43 (17%) 4 3	24, 42, 70, 83	0
1	G	262/297 (88%)	0.91	50 (19%) 3 2	24, 44, 75, 92	0
2	B	24/46 (52%)	0.25	1 (4%) 40 37	24, 37, 52, 59	0
2	D	24/46 (52%)	0.31	0 100 100	26, 38, 52, 55	0
2	F	24/46 (52%)	0.17	1 (4%) 40 37	25, 36, 45, 53	0
2	H	24/46 (52%)	0.51	1 (4%) 40 37	29, 39, 58, 69	0
All	All	1110/1372 (80%)	0.81	181 (16%) 4 3	23, 42, 71, 92	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	MET	5.5
1	G	54	ASN	5.3
1	C	284	ILE	5.1
1	G	26	LYS	5.0
1	E	104	SER	4.9
1	C	25	MET	4.9
1	A	247	ASP	4.8
1	C	213	PHE	4.8
1	C	247	ASP	4.5
1	G	69	GLU	4.4
1	G	70	LYS	4.4
1	E	107	ASN	4.4
1	C	136	SER	4.3
1	G	59	PHE	4.3
1	G	56	ILE	4.3
1	C	56	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	GLU	4.2
1	A	102	THR	4.2
1	E	284	ILE	4.1
1	G	25	MET	4.1
1	A	101	PHE	4.1
1	C	194	SER	4.1
1	E	209	THR	4.0
1	G	247	ASP	4.0
1	A	58	SER	4.0
1	C	22	SER	4.0
2	B	23	SER	4.0
1	A	21	PRO	3.9
1	A	31	GLU	3.9
1	G	124	ASP	3.9
1	G	237	LEU	3.9
1	G	60	LEU	3.8
1	C	195	SER	3.8
1	G	284	ILE	3.8
1	C	208	ARG	3.7
1	C	72	PHE	3.7
1	C	28	SER	3.7
1	G	100	THR	3.6
1	E	31	GLU	3.6
1	C	32	ILE	3.6
1	E	206	THR	3.6
1	C	95	ALA	3.6
1	E	72	PHE	3.6
1	A	23	PHE	3.6
1	A	283	PRO	3.4
1	E	22	SER	3.4
1	A	248	VAL	3.4
1	C	196	ARG	3.3
1	G	101	PHE	3.3
1	E	106	GLU	3.3
1	A	32	ILE	3.2
1	E	282	VAL	3.2
1	G	21	PRO	3.2
1	C	23	PHE	3.2
1	E	55	LYS	3.2
1	G	53	TRP	3.2
1	C	206	THR	3.2
1	G	0	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	21	PRO	3.2
1	A	57	LYS	3.1
1	G	193	SER	3.1
1	C	134	ALA	3.1
1	G	24	LEU	3.1
1	G	32	ILE	3.1
1	E	129	THR	3.1
1	C	167	VAL	3.1
1	C	24	LEU	3.1
1	E	136	SER	3.0
1	G	135	SER	3.0
1	G	23	PHE	3.0
1	A	212	THR	3.0
1	G	223	THR	3.0
1	G	58	SER	3.0
1	C	168	ASN	3.0
1	C	-1	ALA	3.0
1	E	32	ILE	3.0
1	C	26	LYS	3.0
1	E	54	ASN	3.0
1	E	247	ASP	3.0
1	C	162	ILE	2.9
1	E	24	LEU	2.9
1	C	248	VAL	2.9
1	A	195	SER	2.9
1	C	27	GLY	2.9
1	A	-1	ALA	2.9
1	G	33	ALA	2.9
1	G	134	ALA	2.9
1	G	233	GLU	2.9
1	A	136	SER	2.8
1	E	33	ALA	2.8
1	C	77	ASN	2.8
1	G	57	LYS	2.8
1	G	196	ARG	2.8
1	E	283	PRO	2.8
1	C	163	MET	2.8
1	E	134	ALA	2.8
1	A	0	HIS	2.7
1	A	224	GLY	2.7
1	E	216	SER	2.7
1	C	33	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	71	TYR	2.7
1	E	105	PHE	2.7
1	A	54	ASN	2.7
1	G	31	GLU	2.6
1	C	193	SER	2.6
1	C	207	SER	2.6
1	A	238	ASP	2.6
1	C	109	VAL	2.6
1	G	283	PRO	2.6
1	E	119	HIS	2.6
1	A	228	THR	2.6
1	E	133	ILE	2.6
1	A	197	PRO	2.6
1	A	22	SER	2.6
1	C	164	SER	2.6
1	C	215	ILE	2.6
1	G	136	SER	2.6
1	G	95	ALA	2.5
1	G	107	ASN	2.5
2	F	34	ASP	2.5
1	G	228	THR	2.5
1	G	-1	ALA	2.5
1	E	69	GLU	2.5
1	C	236	ILE	2.5
1	E	23	PHE	2.4
1	E	164	SER	2.4
1	E	207	SER	2.4
1	C	220	ILE	2.4
1	E	215	ILE	2.4
1	G	55	LYS	2.4
1	G	137	LYS	2.4
1	C	54	ASN	2.4
1	C	283	PRO	2.4
1	C	138	THR	2.4
1	E	225	VAL	2.4
1	A	71	TYR	2.4
1	C	108	GLN	2.4
1	E	130	ILE	2.4
1	C	53	TRP	2.4
2	H	23	SER	2.4
1	G	213	PHE	2.4
1	G	282	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	20	ASP	2.3
1	A	227	PRO	2.3
1	E	21	PRO	2.3
1	E	137	LYS	2.3
1	C	157	GLY	2.3
1	A	95	ALA	2.3
1	C	156	ASN	2.3
1	E	34	VAL	2.3
1	G	152	CYS	2.2
1	E	214	ARG	2.2
1	C	169	GLU	2.2
1	C	264	TYR	2.2
1	G	109	VAL	2.2
1	E	95	ALA	2.2
1	A	53	TRP	2.2
1	E	81	ILE	2.2
1	A	33	ALA	2.2
1	A	18	SER	2.2
1	G	22	SER	2.2
1	E	237	LEU	2.2
1	C	166	SER	2.2
1	A	223	THR	2.1
1	A	192	ILE	2.1
1	G	225	VAL	2.1
1	G	248	VAL	2.1
1	G	72	PHE	2.1
1	C	104	SER	2.1
1	E	163	MET	2.1
1	E	20	ASP	2.1
1	A	282	VAL	2.1
1	G	34	VAL	2.1
1	A	193	SER	2.1
1	G	18	SER	2.1
1	E	53	TRP	2.1
1	G	122	MET	2.0
1	A	20	ASP	2.0
1	A	122	MET	2.0
1	A	79	THR	2.0
1	E	77	ASN	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.