



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:47 PM UTC

PDB ID : 2Z5C / pdb_00002z5c
Title : Crystal Structure of a Novel Chaperone Complex for Yeast 20S Proteasome Assembly
Authors : Yashiroda, H.; Mizushima, T.; Okamoto, K.; Kameyama, T.; Hayashi, H.; Kishimoto, T.; Kasahara, M.; Kurimoto, E.; Sakata, E.; Suzuki, A.; Hirano, Y.; Murata, S.; Kato, K.; Yamane, T.; Tanaka, K.
Deposited on : 2007-07-03
Resolution : 2.90 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

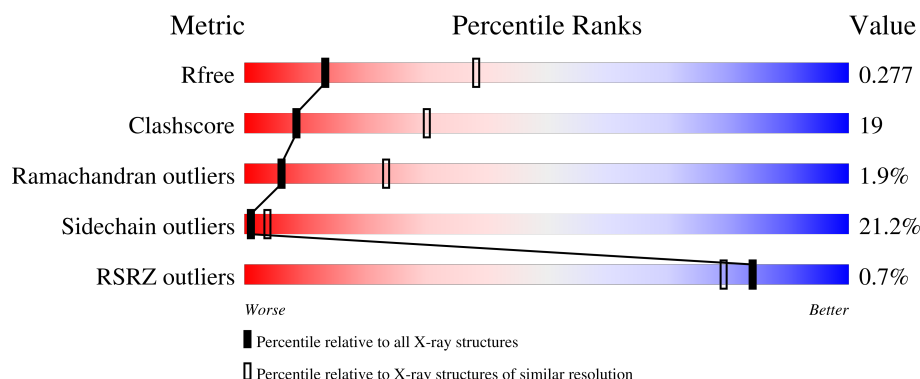
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	151	41% 29% 10% • 18%
1	D	151	41% 28% 12% • 18%
2	B	149	35% 29% 7% • 29%
2	E	149	37% 28% 5% • 29%
3	C	262	41% 25% 6% 28%

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Mol	Chain	Length	Quality of chain
3	F	262	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (41%), yellow (24%), orange (6%), and grey (28%).

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6598 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 Protein YPL144W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			980	623	166	184	7			
1	D	124	Total	C	N	O	S	0	0	0
			980	623	166	184	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q12245
A	-1	SER	-	expression tag	UNP Q12245
A	0	HIS	-	expression tag	UNP Q12245
D	-2	GLY	-	expression tag	UNP Q12245
D	-1	SER	-	expression tag	UNP Q12245
D	0	HIS	-	expression tag	UNP Q12245

- Molecule 2 is a protein called Uncharacterized protein YLR021W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	0	0
			856	557	138	156	5			
2	E	106	Total	C	N	O	S	0	0	0
			856	557	138	156	5			

- Molecule 3 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	189	Total	C	N	O	S	0	0	0
			1463	915	247	295	6			
3	F	189	Total	C	N	O	S	0	0	0
			1463	915	247	295	6			

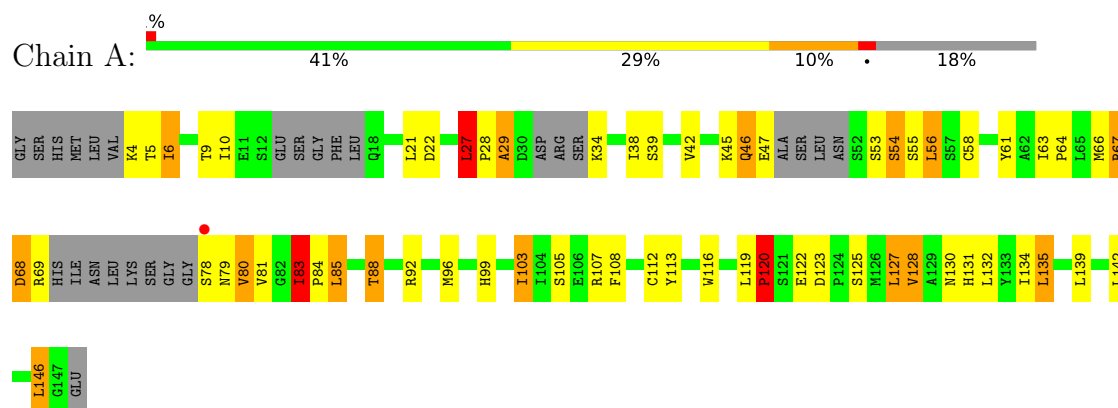
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P32379
C	0	SER	-	expression tag	UNP P32379
F	-1	GLY	-	expression tag	UNP P32379
F	0	SER	-	expression tag	UNP P32379

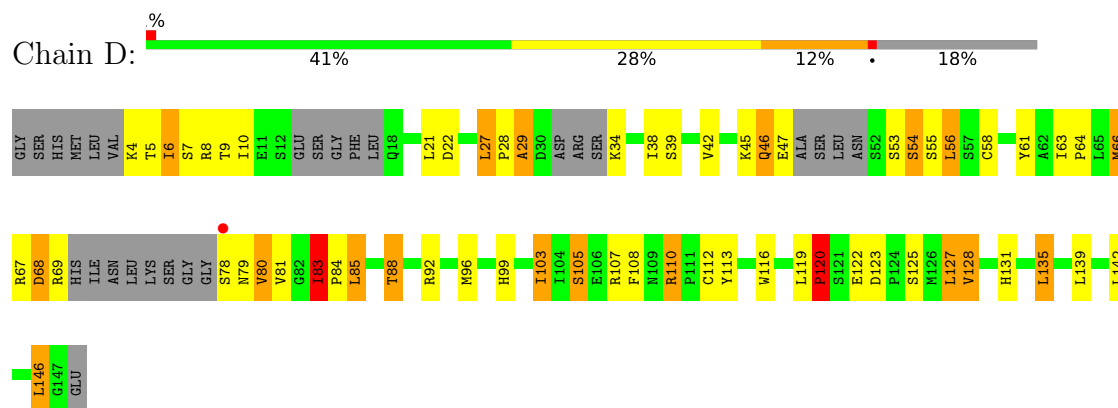
3 Residue-property plots [i](#)

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.

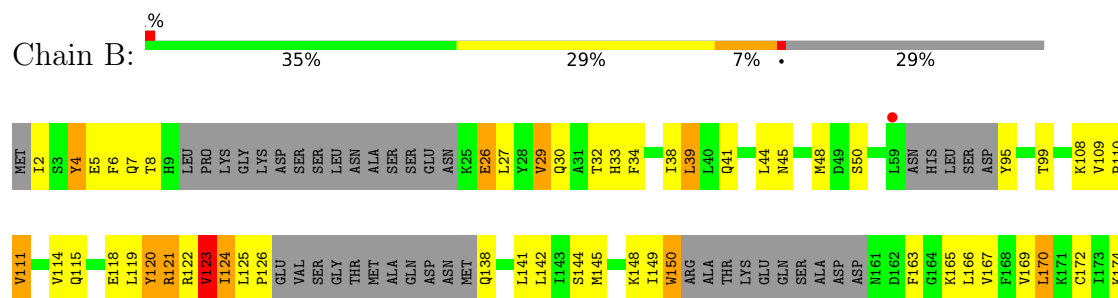
• Molecule 1: Protein YPL144W

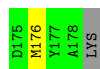


• Molecule 1: Protein YPL144W

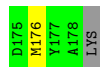
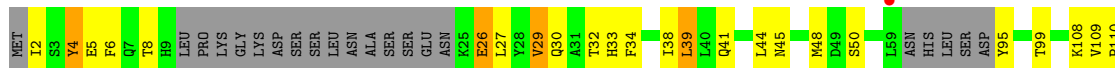


• Molecule 2: Uncharacterized protein YLR021W

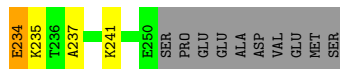
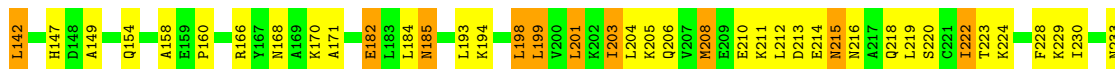
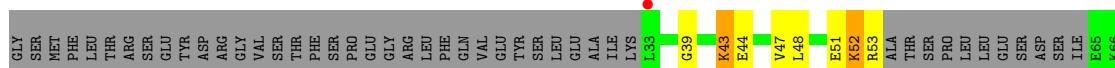




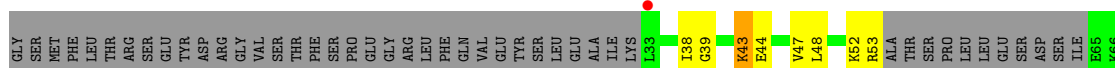
• Molecule 2: Uncharacterized protein YLR021W



• Molecule 3: Proteasome component PUP2



• Molecule 3: Proteasome component PUP2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.69Å 159.18Å 65.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.38 – 2.90 50.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.38-2.90) 98.8 (50.38-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.250 , 0.283 0.245 , 0.277	Depositor DCC
R_{free} test set	1859 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.458 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6598	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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	1.02	1/994 (0.1%)	1.33	13/1341 (1.0%)
1	D	1.01	1/994 (0.1%)	1.31	10/1341 (0.7%)
2	B	0.71	0/869	0.99	1/1169 (0.1%)
2	E	0.73	0/869	0.98	1/1169 (0.1%)
3	C	0.86	0/1478	1.11	4/1987 (0.2%)
3	F	0.86	0/1478	1.13	4/1987 (0.2%)
All	All	0.88	2/6682 (0.0%)	1.15	33/8994 (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	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	ILE	CA-CB	6.19	1.62	1.54
1	A	83	ILE	CA-CB	5.37	1.61	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	PHE	N-CA-C	-9.05	102.02	113.43
2	E	163	PHE	N-CA-C	-9.04	102.04	113.43
1	A	79	ASN	N-CA-C	7.31	119.75	110.33
1	D	54	SER	N-CA-C	7.21	121.19	110.52
1	D	79	ASN	N-CA-C	6.87	119.19	110.33
3	F	142	LEU	N-CA-C	6.86	120.58	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	SER	N-CA-C	6.68	120.41	110.52
1	A	67	ARG	NE-CZ-NH2	6.53	125.08	119.20
3	C	142	LEU	N-CA-C	6.25	119.58	109.40
1	D	120	PRO	CA-C-N	-6.09	112.94	122.49
1	D	120	PRO	C-N-CA	-6.09	112.94	122.49
3	F	149	ALA	N-CA-C	-5.96	105.58	112.92
1	A	120	PRO	CA-C-N	-5.72	113.50	122.49
1	A	120	PRO	C-N-CA	-5.72	113.50	122.49
1	A	67	ARG	CD-NE-CZ	5.70	132.38	124.40
1	A	6	ILE	N-CA-C	5.58	116.03	107.77
1	A	123	ASP	CA-C-N	5.45	126.65	119.84
1	A	123	ASP	C-N-CA	5.45	126.65	119.84
1	A	67	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	A	38	ILE	N-CA-C	-5.38	101.89	109.21
3	C	230	ILE	N-CA-C	-5.36	100.67	108.17
3	C	149	ALA	N-CA-C	-5.33	106.01	112.88
3	F	230	ILE	N-CA-C	-5.32	100.72	108.17
3	C	168	ASN	N-CA-C	-5.26	106.76	114.39
1	D	110	ARG	CA-C-N	-5.20	114.59	119.85
1	D	110	ARG	C-N-CA	-5.20	114.59	119.85
1	D	6	ILE	N-CA-C	5.17	115.43	107.77
3	F	38	ILE	N-CA-C	5.12	115.50	108.12
1	D	123	ASP	CA-C-N	5.09	126.20	119.84
1	D	123	ASP	C-N-CA	5.09	126.20	119.84
1	D	38	ILE	N-CA-C	-5.08	102.30	109.21
1	A	27	LEU	CA-C-N	5.05	124.81	119.76
1	A	27	LEU	C-N-CA	5.05	124.81	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	SER	Peptide
1	D	53	SER	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	980	0	1011	39	0
1	D	980	0	1011	42	1
2	B	856	0	872	39	0
2	E	856	0	872	36	0
3	C	1463	0	1448	51	1
3	F	1463	0	1448	51	0
All	All	6598	0	6662	250	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 19.

All (250) 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:D:68:ASP:OD1	1:D:68:ASP:O	1.72	1.08
1:A:68:ASP:OD1	1:A:68:ASP:O	1.74	1.05
3:F:154:GLN:HE21	3:F:166:ARG:HH22	0.99	0.99
3:C:154:GLN:HE21	3:C:166:ARG:HH22	1.05	0.98
3:C:182:GLU:HG2	3:C:206:GLN:HE22	1.31	0.94
1:A:68:ASP:O	1:A:69:ARG:HG3	1.65	0.94
3:F:182:GLU:HG2	3:F:206:GLN:HE22	1.34	0.92
1:D:68:ASP:O	1:D:69:ARG:HG3	1.71	0.91
3:F:154:GLN:HE21	3:F:166:ARG:NH2	1.69	0.90
3:C:154:GLN:HE21	3:C:166:ARG:NH2	1.71	0.88
3:F:201:LEU:HD12	3:F:212:LEU:HD21	1.57	0.87
3:C:201:LEU:HD12	3:C:212:LEU:HD21	1.58	0.85
3:C:154:GLN:NE2	3:C:166:ARG:HH22	1.79	0.80
3:F:154:GLN:NE2	3:F:166:ARG:HH22	1.78	0.80
3:F:43:LYS:HD3	3:F:43:LYS:H	1.48	0.79
1:D:27:LEU:HB2	1:D:28:PRO:CD	2.13	0.78
3:C:43:LYS:H	3:C:43:LYS:HD3	1.50	0.77
1:A:27:LEU:HB2	1:A:28:PRO:CD	2.14	0.77
2:E:95:TYR:HD1	2:E:114:VAL:HG13	1.51	0.76
2:B:95:TYR:HD1	2:B:114:VAL:HG13	1.51	0.74
1:A:116:TRP:CZ2	1:A:127:LEU:HD11	2.22	0.74
1:D:96:MET:CE	1:D:131:HIS:HA	2.18	0.74
2:E:148:LYS:NZ	3:F:102:TYR:O	2.20	0.74
1:A:96:MET:HE3	1:A:131:HIS:HA	1.70	0.74
1:D:68:ASP:O	1:D:68:ASP:CG	2.31	0.73
1:A:9:THR:HG22	1:A:22:ASP:OD2	1.89	0.73
2:B:148:LYS:NZ	3:C:102:TYR:O	2.22	0.72
1:A:96:MET:CE	1:A:131:HIS:HA	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:MET:HE3	1:D:131:HIS:HA	1.71	0.72
2:E:8:THR:HG21	2:E:172:CYS:SG	2.30	0.71
1:D:116:TRP:CZ2	1:D:127:LEU:HD11	2.25	0.71
1:A:68:ASP:O	1:A:68:ASP:CG	2.34	0.71
2:B:8:THR:HG21	2:B:172:CYS:SG	2.30	0.70
3:C:73:HIS:CD2	3:C:106:ASP:HB3	2.27	0.70
3:F:73:HIS:CD2	3:F:106:ASP:HB3	2.26	0.70
1:D:9:THR:HG22	1:D:22:ASP:OD2	1.92	0.69
2:E:38:ILE:HG22	2:E:39:LEU:N	2.08	0.69
3:F:199:LEU:O	3:F:203:ILE:HG12	1.93	0.68
2:B:8:THR:CG2	2:B:172:CYS:SG	2.82	0.67
3:C:185:ASN:HD22	3:C:185:ASN:C	2.02	0.67
2:E:8:THR:CG2	2:E:172:CYS:SG	2.82	0.67
1:D:27:LEU:HB2	1:D:28:PRO:HD2	1.75	0.67
2:B:38:ILE:HG22	2:B:39:LEU:N	2.10	0.67
3:C:44:GLU:HG3	3:C:193:LEU:HB2	1.76	0.66
3:F:44:GLU:HG3	3:F:193:LEU:HB2	1.78	0.66
3:F:185:ASN:C	3:F:185:ASN:HD22	2.03	0.65
3:C:199:LEU:O	3:C:203:ILE:HG12	1.96	0.65
1:A:27:LEU:HB2	1:A:28:PRO:HD2	1.76	0.65
2:E:109:VAL:HB	2:E:110:PRO:HD3	1.79	0.64
2:E:38:ILE:HG22	2:E:39:LEU:H	1.63	0.64
2:B:38:ILE:HG22	2:B:39:LEU:H	1.64	0.63
1:D:58:CYS:HB2	1:D:88:THR:HG21	1.81	0.63
2:B:109:VAL:HB	2:B:110:PRO:HD3	1.80	0.62
2:E:95:TYR:CD1	2:E:114:VAL:HG13	2.34	0.62
3:F:75:GLY:HA3	3:F:228:PHE:CE1	2.35	0.61
1:D:96:MET:HE2	1:D:131:HIS:ND1	2.15	0.61
1:A:58:CYS:HB2	1:A:88:THR:HG21	1.82	0.61
1:A:99:HIS:ND1	1:A:135:LEU:HD11	2.15	0.60
1:A:4:LYS:HE3	1:A:29:ALA:H	1.65	0.60
3:F:83:ALA:HB2	3:F:86:ARG:HH21	1.66	0.60
3:C:75:GLY:HA3	3:C:228:PHE:CE1	2.37	0.60
2:E:118:GLU:OE2	2:E:118:GLU:HA	2.02	0.59
2:B:95:TYR:CD1	2:B:114:VAL:HG13	2.35	0.59
3:C:182:GLU:HG2	3:C:206:GLN:NE2	2.11	0.59
1:D:68:ASP:OD1	1:D:68:ASP:C	2.45	0.59
1:A:56:LEU:C	1:A:56:LEU:HD12	2.28	0.59
2:B:118:GLU:HA	2:B:118:GLU:OE2	2.03	0.59
3:C:83:ALA:HB2	3:C:86:ARG:HH21	1.68	0.59
1:D:4:LYS:HE3	1:D:29:ALA:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:147:HIS:CE1	3:F:224:LYS:HG3	2.38	0.58
1:D:99:HIS:ND1	1:D:135:LEU:HD11	2.19	0.58
1:D:58:CYS:HB2	1:D:88:THR:CG2	2.34	0.58
3:F:78:MET:HE2	3:F:142:LEU:HD21	1.85	0.58
3:F:142:LEU:HB2	3:F:158:ALA:HB3	1.85	0.58
2:E:6:PHE:HB2	2:E:176:MET:HB3	1.85	0.58
3:C:147:HIS:CE1	3:C:224:LYS:HG3	2.39	0.58
1:A:96:MET:HE2	1:A:131:HIS:ND1	2.19	0.57
3:C:118:ASP:O	3:C:122:ARG:HG3	2.05	0.57
1:A:58:CYS:HB2	1:A:88:THR:CG2	2.34	0.57
1:A:99:HIS:CE1	1:A:103:ILE:HD13	2.39	0.57
1:D:99:HIS:CE1	1:D:103:ILE:HD13	2.40	0.57
3:F:88:MET:HG2	3:F:116:VAL:HG13	1.86	0.57
2:B:6:PHE:HB2	2:B:176:MET:HB3	1.86	0.57
2:E:120:TYR:O	2:E:122:ARG:N	2.38	0.57
1:A:4:LYS:HB3	1:A:27:LEU:O	2.05	0.57
1:A:113:TYR:CE1	2:B:48:MET:HE2	2.40	0.56
1:A:68:ASP:OD1	1:A:68:ASP:C	2.47	0.56
3:F:118:ASP:O	3:F:122:ARG:HG3	2.05	0.56
1:D:56:LEU:HD12	1:D:56:LEU:C	2.30	0.56
3:F:182:GLU:HG2	3:F:206:GLN:NE2	2.13	0.56
3:F:84:ASP:OD1	3:F:84:ASP:N	2.39	0.55
2:E:26:GLU:H	2:E:45:ASN:ND2	2.04	0.55
1:D:105:SER:OG	1:D:110:ARG:O	2.23	0.55
3:C:83:ALA:HA	3:C:86:ARG:HE	1.72	0.55
2:B:120:TYR:O	2:B:122:ARG:N	2.40	0.55
1:D:4:LYS:HB3	1:D:27:LEU:O	2.06	0.55
3:C:142:LEU:HB2	3:C:158:ALA:HB3	1.88	0.55
3:C:88:MET:HG2	3:C:116:VAL:HG13	1.90	0.54
1:A:55:SER:HA	2:B:34:PHE:HB3	1.90	0.53
3:F:213:ASP:C	3:F:215:ASN:H	2.17	0.53
3:C:84:ASP:OD1	3:C:84:ASP:N	2.40	0.53
3:C:78:MET:HE2	3:C:142:LEU:HD21	1.89	0.53
1:D:108:PHE:CD1	1:D:146:LEU:HD23	2.43	0.53
2:E:141:LEU:HD12	2:E:142:LEU:N	2.24	0.53
3:F:220:SER:HB2	3:F:229:LYS:O	2.10	0.52
3:F:123:PHE:CD2	3:F:123:PHE:N	2.73	0.52
3:C:213:ASP:C	3:C:215:ASN:H	2.18	0.52
2:E:38:ILE:CG2	2:E:39:LEU:N	2.73	0.52
3:F:93:ARG:O	3:F:97:VAL:HG23	2.10	0.52
2:B:123:VAL:O	2:B:123:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:GLU:H	2:B:45:ASN:ND2	2.08	0.51
1:D:113:TYR:CE1	2:E:48:MET:HE2	2.46	0.51
2:E:38:ILE:CG2	2:E:39:LEU:H	2.22	0.51
1:A:108:PHE:CD1	1:A:146:LEU:HD23	2.45	0.51
3:C:123:PHE:H	3:C:123:PHE:HD2	1.57	0.51
1:D:63:ILE:HG13	1:D:64:PRO:HD2	1.92	0.51
1:A:45:LYS:HG3	1:A:46:GLN:H	1.75	0.51
2:B:141:LEU:HD12	2:B:142:LEU:N	2.25	0.51
1:D:55:SER:HA	2:E:34:PHE:HB3	1.91	0.51
1:A:83:ILE:HG12	1:A:84:PRO:HD2	1.93	0.51
2:E:99:THR:O	3:F:122:ARG:NH1	2.45	0.50
1:D:99:HIS:ND1	1:D:103:ILE:HD13	2.25	0.50
3:C:123:PHE:CD2	3:C:123:PHE:N	2.72	0.50
2:E:123:VAL:O	2:E:123:VAL:HG13	2.11	0.50
2:B:8:THR:HG22	2:B:172:CYS:SG	2.52	0.50
3:F:83:ALA:HA	3:F:86:ARG:HE	1.76	0.50
2:B:99:THR:O	3:C:122:ARG:NH1	2.45	0.49
3:C:72:ARG:O	3:C:228:PHE:N	2.43	0.49
1:A:45:LYS:HG3	1:A:46:GLN:N	2.28	0.49
1:D:96:MET:HE1	1:D:131:HIS:HA	1.95	0.49
2:E:8:THR:HG22	2:E:172:CYS:SG	2.52	0.49
2:B:32:THR:HG22	2:B:34:PHE:CE2	2.47	0.49
2:E:115:GLN:HG3	2:E:166:LEU:HD21	1.94	0.49
3:C:93:ARG:O	3:C:97:VAL:HG23	2.12	0.49
1:A:63:ILE:HG13	1:A:64:PRO:HD2	1.93	0.49
3:C:220:SER:HB2	3:C:229:LYS:O	2.11	0.49
1:D:83:ILE:HG12	1:D:84:PRO:HD2	1.95	0.49
3:F:67:ILE:HD12	3:F:218:GLN:HE21	1.78	0.48
3:C:205:LYS:HB2	3:C:212:LEU:HD22	1.94	0.48
1:D:34:LYS:O	1:D:34:LYS:HG3	2.13	0.48
2:E:48:MET:HE3	2:E:144:SER:HB3	1.95	0.48
2:B:38:ILE:CG2	2:B:39:LEU:H	2.24	0.48
2:B:38:ILE:CG2	2:B:39:LEU:N	2.74	0.48
3:F:73:HIS:NE2	3:F:106:ASP:HB3	2.28	0.48
1:D:45:LYS:HG3	1:D:46:GLN:H	1.77	0.48
1:A:34:LYS:O	1:A:34:LYS:HG3	2.13	0.48
1:A:6:ILE:HG13	1:A:6:ILE:O	2.13	0.48
1:D:61:TYR:HB2	1:D:85:LEU:HD22	1.95	0.48
1:A:116:TRP:CE2	1:A:127:LEU:HD11	2.49	0.48
3:F:72:ARG:O	3:F:228:PHE:N	2.44	0.48
3:F:83:ALA:CB	3:F:86:ARG:HH21	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ALA:CB	3:C:86:ARG:HH21	2.27	0.47
2:E:44:LEU:HD13	2:E:149:ILE:HG12	1.96	0.47
3:F:204:LEU:O	3:F:208:MET:HB2	2.14	0.47
2:E:32:THR:HG22	2:E:34:PHE:CE2	2.50	0.47
2:E:119:LEU:HG	2:E:124:ILE:HD12	1.96	0.47
3:F:205:LYS:HB2	3:F:212:LEU:HD22	1.96	0.47
1:A:92:ARG:HD2	1:A:128:VAL:HG22	1.97	0.47
2:B:119:LEU:HG	2:B:124:ILE:HD12	1.97	0.47
1:D:6:ILE:O	1:D:6:ILE:HG13	2.13	0.47
3:F:234:GLU:O	3:F:235:LYS:C	2.58	0.47
1:D:116:TRP:CE2	1:D:127:LEU:HD11	2.50	0.47
3:C:204:LEU:O	3:C:208:MET:HB2	2.15	0.47
3:C:73:HIS:NE2	3:C:106:ASP:HB3	2.30	0.47
2:B:48:MET:HE3	2:B:144:SER:HB3	1.96	0.46
3:C:234:GLU:O	3:C:235:LYS:C	2.58	0.46
1:D:42:VAL:O	1:D:116:TRP:CE3	2.67	0.46
3:C:67:ILE:HD12	3:C:218:GLN:HE21	1.80	0.46
1:D:92:ARG:HD2	1:D:128:VAL:HG22	1.97	0.46
1:A:99:HIS:ND1	1:A:103:ILE:HD13	2.30	0.46
2:B:119:LEU:HD11	2:B:174:LYS:HD2	1.98	0.46
3:F:123:PHE:H	3:F:123:PHE:HD2	1.59	0.46
2:E:141:LEU:HD12	2:E:142:LEU:H	1.80	0.46
3:F:185:ASN:C	3:F:185:ASN:ND2	2.70	0.46
1:A:61:TYR:HB2	1:A:85:LEU:HD22	1.97	0.46
2:E:145:MET:HE2	2:E:150:TRP:HE1	1.81	0.46
1:A:45:LYS:CG	1:A:46:GLN:N	2.79	0.45
1:D:45:LYS:HG3	1:D:46:GLN:N	2.31	0.45
3:F:219:LEU:HB3	3:F:231:TYR:CD2	2.51	0.45
3:F:43:LYS:HD3	3:F:43:LYS:N	2.24	0.45
3:F:213:ASP:O	3:F:215:ASN:N	2.50	0.45
3:F:78:MET:CE	3:F:142:LEU:HD21	2.46	0.45
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.81	0.45
2:B:115:GLN:HG3	2:B:166:LEU:HD21	1.99	0.45
1:D:45:LYS:CG	1:D:46:GLN:N	2.79	0.45
2:E:145:MET:CE	2:E:150:TRP:HE1	2.29	0.45
1:A:130:ASN:O	1:A:134:ILE:HG13	2.16	0.44
2:B:29:VAL:HG21	2:B:172:CYS:HB3	1.99	0.44
3:C:71:ASP:OD1	3:C:72:ARG:N	2.45	0.44
1:A:42:VAL:O	1:A:116:TRP:CE3	2.70	0.44
1:A:27:LEU:CB	1:A:28:PRO:CD	2.89	0.44
2:B:141:LEU:HD12	2:B:142:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:ILE:HG22	3:C:228:PHE:HD1	1.82	0.44
2:B:145:MET:HE2	2:B:150:TRP:HE1	1.82	0.43
2:B:4:TYR:CD2	2:B:4:TYR:N	2.87	0.43
2:E:119:LEU:HD11	2:E:174:LYS:HD2	2.00	0.43
2:B:145:MET:CE	2:B:150:TRP:HE1	2.32	0.43
3:C:213:ASP:O	3:C:215:ASN:N	2.51	0.43
2:E:50:SER:O	2:E:144:SER:HA	2.19	0.43
1:A:56:LEU:C	1:A:56:LEU:CD1	2.92	0.43
3:C:78:MET:CE	3:C:142:LEU:HD21	2.47	0.43
3:C:233:ASN:O	3:C:237:ALA:HB2	2.18	0.43
2:E:4:TYR:N	2:E:4:TYR:CD2	2.86	0.43
3:F:89:ILE:O	3:F:93:ARG:HG3	2.18	0.43
3:C:211:LYS:HG2	3:C:212:LEU:H	1.84	0.43
3:C:170:LYS:HG3	3:C:171:ALA:N	2.33	0.42
3:F:233:ASN:O	3:F:237:ALA:HB2	2.19	0.42
2:E:27:LEU:HD21	2:E:169:VAL:HG22	2.01	0.42
2:E:29:VAL:HG21	2:E:172:CYS:HB3	2.00	0.42
2:E:30:GLN:OE1	2:E:41:GLN:NE2	2.52	0.42
1:D:80:VAL:HG21	1:D:105:SER:HB3	2.01	0.42
2:B:123:VAL:O	2:B:123:VAL:CG1	2.66	0.42
1:D:85:LEU:HD12	1:D:85:LEU:HA	1.84	0.42
3:F:78:MET:HE1	3:F:85:ALA:HB1	2.01	0.42
1:A:96:MET:HE1	1:A:131:HIS:HA	1.99	0.42
3:C:201:LEU:HD13	3:C:201:LEU:HA	1.82	0.42
1:D:66:MET:H	1:D:69:ARG:HH21	1.67	0.42
1:D:99:HIS:CE1	1:D:103:ILE:CD1	3.02	0.42
3:F:113:THR:HG23	3:F:144:ILE:HD12	2.02	0.42
3:C:52:LYS:HB3	3:C:216:ASN:HA	2.02	0.42
3:C:185:ASN:C	3:C:185:ASN:ND2	2.69	0.42
1:D:7:SER:O	1:D:8:ARG:HG2	2.19	0.41
3:F:222:ILE:HG22	3:F:228:PHE:HD1	1.84	0.41
2:B:125:LEU:HA	2:B:126:PRO:HA	1.85	0.41
3:F:39:GLY:HA2	3:F:47:VAL:O	2.20	0.41
2:B:30:GLN:OE1	2:B:41:GLN:NE2	2.53	0.41
3:C:44:GLU:O	3:C:193:LEU:HB2	2.21	0.41
3:F:203:ILE:HG12	3:F:203:ILE:H	1.59	0.41
3:C:78:MET:HE1	3:C:85:ALA:HB1	2.02	0.41
1:D:7:SER:C	1:D:8:ARG:HG2	2.45	0.41
3:F:201:LEU:HD13	3:F:201:LEU:HA	1.83	0.41
1:A:80:VAL:HG21	1:A:105:SER:HB3	2.02	0.41
3:C:154:GLN:HG2	3:C:166:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:117:CYS:SG	3:F:164:PHE:HB3	2.61	0.41
2:B:50:SER:O	2:B:144:SER:HA	2.21	0.41
2:E:33:HIS:CE1	2:E:38:ILE:HG12	2.56	0.41
1:D:27:LEU:CB	1:D:28:PRO:CD	2.88	0.41
2:B:44:LEU:HD13	2:B:149:ILE:HG12	2.03	0.41
3:C:39:GLY:HA2	3:C:47:VAL:O	2.21	0.41
2:B:27:LEU:HD21	2:B:169:VAL:HG22	2.02	0.41
2:B:111:VAL:O	2:B:115:GLN:HG2	2.20	0.41
2:B:119:LEU:HD22	2:B:170:LEU:HG	2.03	0.41
3:C:51:GLU:HG3	3:C:208:MET:SD	2.61	0.41
2:E:139:PHE:CD2	2:E:139:PHE:C	2.99	0.41
3:C:140:VAL:HG22	3:C:160:PRO:HB3	2.02	0.41
3:F:44:GLU:O	3:F:193:LEU:HB2	2.21	0.41
3:F:140:VAL:HG22	3:F:160:PRO:HB3	2.02	0.41
2:B:33:HIS:CE1	2:B:38:ILE:HG12	2.56	0.40
3:F:194:LYS:O	3:F:198:LEU:HD12	2.21	0.40
3:C:194:LYS:O	3:C:198:LEU:HD12	2.22	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)
3:C:106:ASP:OD2	1:D:67:ARG:NH2[1_554]	2.06	0.14

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	114/151 (76%)	100 (88%)	11 (10%)	3 (3%)	4 17
1	D	114/151 (76%)	100 (88%)	11 (10%)	3 (3%)	4 17
2	B	96/149 (64%)	83 (86%)	10 (10%)	3 (3%)	3 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	96/149 (64%)	80 (83%)	13 (14%)	3 (3%)	3	14
3	C	181/262 (69%)	167 (92%)	12 (7%)	2 (1%)	11	36
3	F	181/262 (69%)	166 (92%)	14 (8%)	1 (1%)	21	51
All	All	782/1124 (70%)	696 (89%)	71 (9%)	15 (2%)	6	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	ARG
2	B	123	VAL
2	E	121	ARG
2	E	123	VAL
1	A	29	ALA
2	B	120	TYR
1	D	29	ALA
2	E	120	TYR
1	A	122	GLU
3	C	214	GLU
3	F	214	GLU
1	A	120	PRO
1	D	120	PRO
1	D	122	GLU
3	C	74	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/137 (84%)	84 (73%)	31 (27%)	0	1
1	D	115/137 (84%)	85 (74%)	30 (26%)	0	2
2	B	98/135 (73%)	81 (83%)	17 (17%)	2	7
2	E	98/135 (73%)	83 (85%)	15 (15%)	3	9
3	C	155/216 (72%)	124 (80%)	31 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	155/216 (72%)	123 (79%)	32 (21%)	1	4
All	All	736/976 (75%)	580 (79%)	156 (21%)	1	4

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	10	ILE
1	A	21	LEU
1	A	27	LEU
1	A	39	SER
1	A	46	GLN
1	A	47	GLU
1	A	54	SER
1	A	56	LEU
1	A	66	MET
1	A	67	ARG
1	A	68	ASP
1	A	78	SER
1	A	80	VAL
1	A	81	VAL
1	A	83	ILE
1	A	85	LEU
1	A	88	THR
1	A	103	ILE
1	A	107	ARG
1	A	112	CYS
1	A	119	LEU
1	A	120	PRO
1	A	125	SER
1	A	127	LEU
1	A	128	VAL
1	A	132	LEU
1	A	135	LEU
1	A	139	LEU
1	A	142	LEU
1	A	146	LEU
2	B	2	ILE
2	B	4	TYR
2	B	5	GLU
2	B	7	GLN
2	B	26	GLU

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Mol	Chain	Res	Type
2	B	29	VAL
2	B	39	LEU
2	B	108	LYS
2	B	111	VAL
2	B	121	ARG
2	B	123	VAL
2	B	124	ILE
2	B	138	GLN
2	B	150	TRP
2	B	165	LYS
2	B	167	VAL
2	B	170	LEU
3	C	43	LYS
3	C	48	LEU
3	C	52	LYS
3	C	53	ARG
3	C	68	VAL
3	C	70	ILE
3	C	72	ARG
3	C	79	SER
3	C	84	ASP
3	C	87	SER
3	C	111	SER
3	C	114	GLN
3	C	115	SER
3	C	119	LEU
3	C	121	LEU
3	C	123	PHE
3	C	182	GLU
3	C	184	LEU
3	C	185	ASN
3	C	198	LEU
3	C	199	LEU
3	C	201	LEU
3	C	203	ILE
3	C	208	MET
3	C	210	GLU
3	C	215	ASN
3	C	219	LEU
3	C	222	ILE
3	C	223	THR
3	C	234	GLU

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Mol	Chain	Res	Type
3	C	241	LYS
1	D	5	THR
1	D	10	ILE
1	D	21	LEU
1	D	27	LEU
1	D	39	SER
1	D	46	GLN
1	D	47	GLU
1	D	54	SER
1	D	56	LEU
1	D	66	MET
1	D	68	ASP
1	D	78	SER
1	D	80	VAL
1	D	81	VAL
1	D	83	ILE
1	D	85	LEU
1	D	88	THR
1	D	103	ILE
1	D	105	SER
1	D	107	ARG
1	D	112	CYS
1	D	119	LEU
1	D	120	PRO
1	D	125	SER
1	D	127	LEU
1	D	128	VAL
1	D	135	LEU
1	D	139	LEU
1	D	142	LEU
1	D	146	LEU
2	E	2	ILE
2	E	4	TYR
2	E	5	GLU
2	E	26	GLU
2	E	29	VAL
2	E	39	LEU
2	E	108	LYS
2	E	121	ARG
2	E	123	VAL
2	E	124	ILE
2	E	138	GLN

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Mol	Chain	Res	Type
2	E	150	TRP
2	E	165	LYS
2	E	167	VAL
2	E	170	LEU
3	F	43	LYS
3	F	48	LEU
3	F	52	LYS
3	F	53	ARG
3	F	68	VAL
3	F	70	ILE
3	F	72	ARG
3	F	79	SER
3	F	84	ASP
3	F	87	SER
3	F	111	SER
3	F	114	GLN
3	F	115	SER
3	F	119	LEU
3	F	121	LEU
3	F	122	ARG
3	F	123	PHE
3	F	182	GLU
3	F	184	LEU
3	F	185	ASN
3	F	198	LEU
3	F	199	LEU
3	F	201	LEU
3	F	203	ILE
3	F	208	MET
3	F	210	GLU
3	F	215	ASN
3	F	219	LEU
3	F	222	ILE
3	F	223	THR
3	F	234	GLU
3	F	241	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
2	B	33	HIS

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Mol	Chain	Res	Type
2	B	41	GLN
2	B	45	ASN
2	B	96	GLN
3	C	154	GLN
3	C	206	GLN
3	C	215	ASN
3	C	218	GLN
1	D	79	ASN
2	E	7	GLN
2	E	41	GLN
2	E	45	ASN
2	E	96	GLN
3	F	154	GLN
3	F	206	GLN
3	F	215	ASN
3	F	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	124/151 (82%)	-0.85	1 (0%) 82 77	39, 59, 74, 84	0
1	D	124/151 (82%)	-0.80	1 (0%) 82 77	39, 59, 74, 84	0
2	B	106/149 (71%)	-0.80	1 (0%) 81 75	53, 73, 99, 102	0
2	E	106/149 (71%)	-0.65	1 (0%) 81 75	53, 73, 99, 102	0
3	C	189/262 (72%)	-0.88	1 (0%) 87 83	39, 61, 97, 109	0
3	F	189/262 (72%)	-0.84	1 (0%) 87 83	39, 61, 97, 109	0
All	All	838/1124 (74%)	-0.81	6 (0%) 84 79	39, 64, 97, 109	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	SER	4.6
1	D	78	SER	3.5
2	B	59	LEU	3.3
3	C	33	LEU	2.8
2	E	59	LEU	2.5
3	F	33	LEU	2.5

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.