



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:56 AM UTC

PDB ID : 3UUX / pdb_00003uux
Title : Crystal structure of yeast Fis1 in complex with Mdv1 fragment containing N-terminal extension and coiled coil domains
Authors : Zhang, Y.; Chan, N.C.; Gristick, H.; Chan, D.C.
Deposited on : 2011-11-28
Resolution : 3.90 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

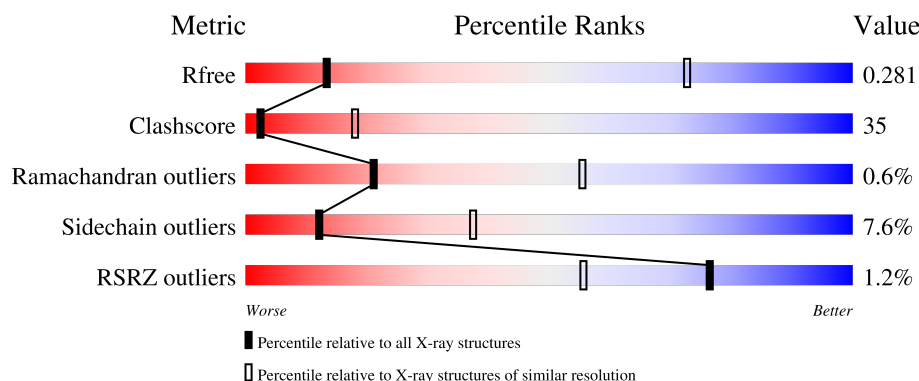
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	129	
1	C	129	
2	B	242	
2	D	242	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4076 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 Mitochondria fission 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1028	654	172	198	4			
1	C	125	Total	C	N	O	S	0	0	0
			1004	638	168	194	4			

- Molecule 2 is a protein called Mitochondrial division protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1013	641	164	206	2			
2	D	135	Total	C	N	O	S	0	0	0
			1031	651	169	209	2			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	MET	-	expression tag	UNP P47025
B	74	GLY	-	expression tag	UNP P47025
B	75	SER	-	expression tag	UNP P47025
B	76	SER	-	expression tag	UNP P47025
B	77	HIS	-	expression tag	UNP P47025
B	78	HIS	-	expression tag	UNP P47025
B	79	HIS	-	expression tag	UNP P47025
B	80	HIS	-	expression tag	UNP P47025
B	81	HIS	-	expression tag	UNP P47025
B	82	HIS	-	expression tag	UNP P47025
B	83	SER	-	expression tag	UNP P47025
B	84	SER	-	expression tag	UNP P47025
B	85	GLY	-	expression tag	UNP P47025
B	86	LEU	-	expression tag	UNP P47025
B	87	VAL	-	expression tag	UNP P47025
B	88	PRO	-	expression tag	UNP P47025

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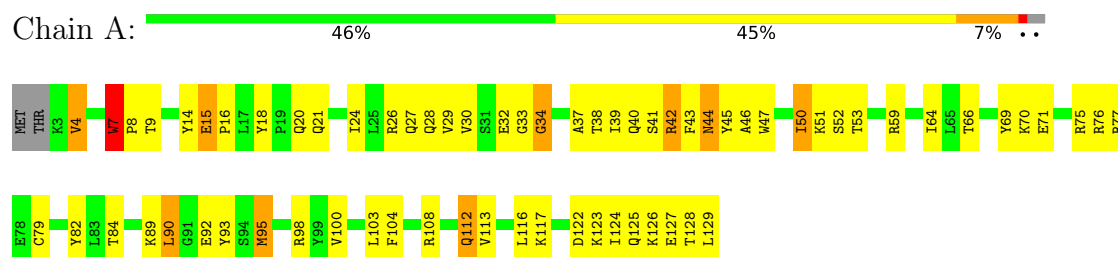
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Chain	Residue	Modelled	Actual	Comment	Reference
B	89	ARG	-	expression tag	UNP P47025
B	90	GLY	-	expression tag	UNP P47025
B	91	SER	-	expression tag	UNP P47025
B	92	HIS	-	expression tag	UNP P47025
B	93	MET	-	expression tag	UNP P47025
B	215	ALA	LYS	engineered mutation	UNP P47025
B	216	ALA	LYS	engineered mutation	UNP P47025
D	73	MET	-	expression tag	UNP P47025
D	74	GLY	-	expression tag	UNP P47025
D	75	SER	-	expression tag	UNP P47025
D	76	SER	-	expression tag	UNP P47025
D	77	HIS	-	expression tag	UNP P47025
D	78	HIS	-	expression tag	UNP P47025
D	79	HIS	-	expression tag	UNP P47025
D	80	HIS	-	expression tag	UNP P47025
D	81	HIS	-	expression tag	UNP P47025
D	82	HIS	-	expression tag	UNP P47025
D	83	SER	-	expression tag	UNP P47025
D	84	SER	-	expression tag	UNP P47025
D	85	GLY	-	expression tag	UNP P47025
D	86	LEU	-	expression tag	UNP P47025
D	87	VAL	-	expression tag	UNP P47025
D	88	PRO	-	expression tag	UNP P47025
D	89	ARG	-	expression tag	UNP P47025
D	90	GLY	-	expression tag	UNP P47025
D	91	SER	-	expression tag	UNP P47025
D	92	HIS	-	expression tag	UNP P47025
D	93	MET	-	expression tag	UNP P47025
D	215	ALA	LYS	engineered mutation	UNP P47025
D	216	ALA	LYS	engineered mutation	UNP P47025

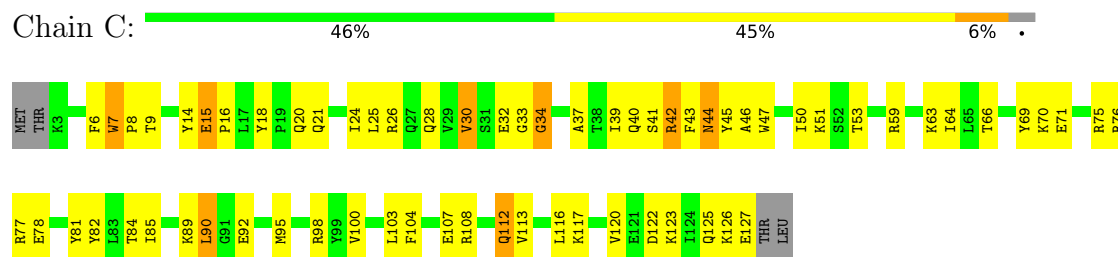
3 Residue-property plots [i](#)

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.

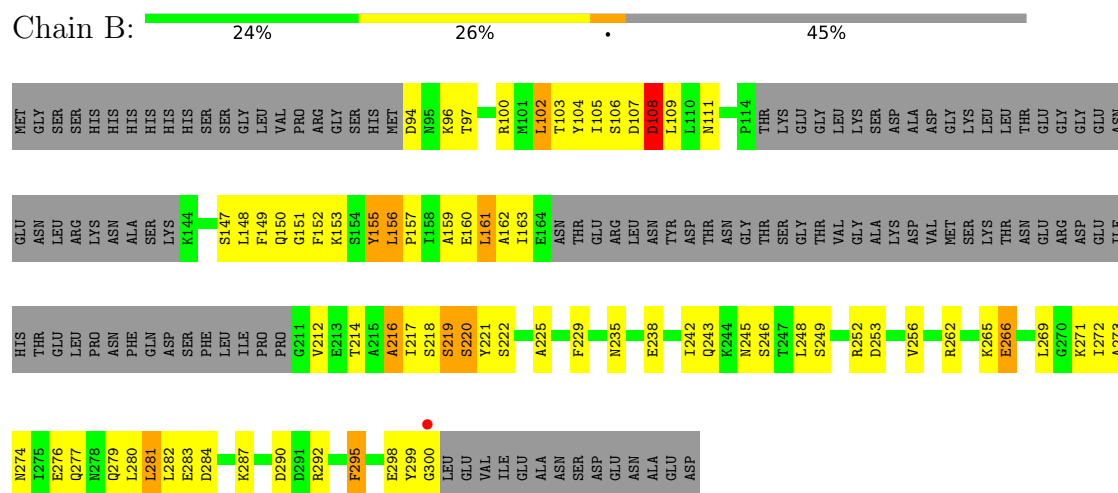
• Molecule 1: Mitochondria fission 1 protein



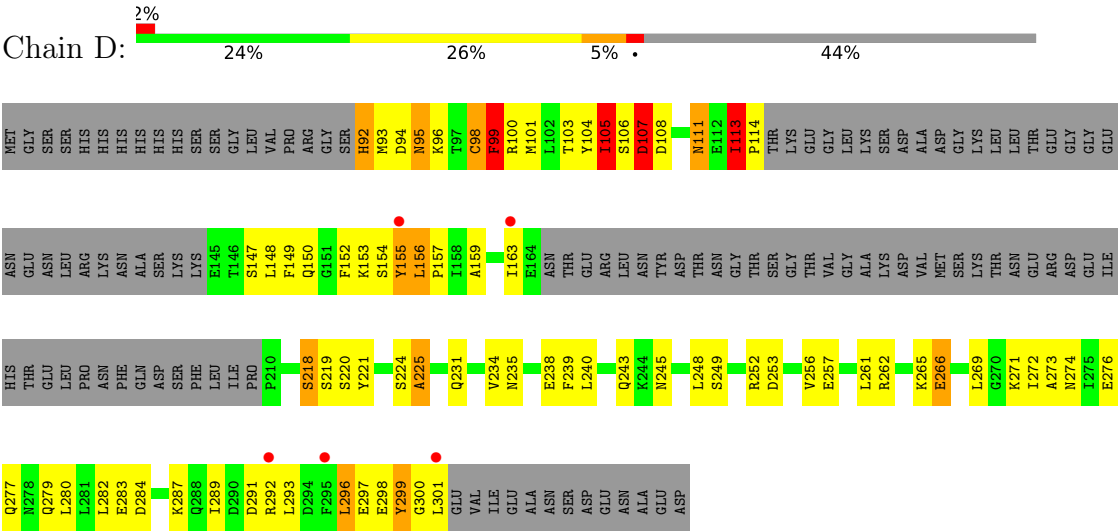
• Molecule 1: Mitochondria fission 1 protein



• Molecule 2: Mitochondrial division protein 1



• Molecule 2: Mitochondrial division protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.68Å 174.68Å 167.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.51 – 3.90 123.51 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (123.51-3.90) 98.6 (123.51-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.94Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.270 , 0.284 0.266 , 0.281	Depositor DCC
R_{free} test set	1178 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	122.5	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 112.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.028 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4076	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	1.12	3/1048 (0.3%)	1.24	5/1417 (0.4%)
1	C	1.05	3/1024 (0.3%)	1.21	4/1388 (0.3%)
2	B	1.29	5/1023 (0.5%)	1.38	10/1382 (0.7%)
2	D	1.64	14/1042 (1.3%)	1.45	10/1407 (0.7%)
All	All	1.30	25/4137 (0.6%)	1.32	29/5594 (0.5%)

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
2	B	0	1
2	D	0	1
All	All	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	225	ALA	C-O	21.54	1.49	1.23
2	B	225	ALA	C-O	-14.37	1.05	1.24
2	D	218	SER	CB-OG	11.95	1.66	1.42
1	C	127	GLU	C-O	8.75	1.41	1.23
2	D	163	ILE	CA-CB	8.47	1.64	1.54
2	D	99	PHE	C-O	8.23	1.34	1.24
2	B	225	ALA	CA-CB	7.99	1.66	1.53
2	B	212	VAL	CA-CB	7.82	1.63	1.53
2	D	113	ILE	CG1-CD1	7.78	1.82	1.51
2	D	92	HIS	CG-CD2	7.50	1.44	1.35
1	C	44	ASN	CB-CG	-6.84	1.34	1.52
1	A	127	GLU	C-O	6.82	1.33	1.24
2	D	99	PHE	CA-C	6.49	1.61	1.52
2	B	163	ILE	CA-CB	5.90	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	94	ASP	N-CA	5.90	1.53	1.46
2	B	216	ALA	C-N	5.61	1.41	1.33
2	D	92	HIS	ND1-CE1	5.58	1.38	1.32
1	A	44	ASN	CB-CG	-5.52	1.38	1.52
2	D	92	HIS	CE1-NE2	5.50	1.38	1.32
1	A	44	ASN	N-CA	-5.32	1.39	1.46
2	D	113	ILE	CA-CB	5.32	1.61	1.54
2	D	224	SER	C-O	5.20	1.30	1.24
2	D	225	ALA	C-N	5.15	1.41	1.33
1	C	30	VAL	CA-CB	5.11	1.59	1.54
2	D	219	SER	N-CA	5.03	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	107	ASP	N-CA-C	-15.97	93.71	114.31
2	B	106	SER	N-CA-C	9.57	125.66	112.93
2	B	221	TYR	N-CA-C	8.10	123.37	113.17
1	C	44	ASN	CB-CA-C	-7.93	94.63	110.42
2	D	221	TYR	N-CA-C	7.36	120.35	111.82
2	D	106	SER	N-CA-C	7.00	125.70	110.80
2	D	111	ASN	N-CA-C	6.89	119.54	109.07
2	B	220	SER	N-CA-C	6.50	120.15	110.52
2	D	155	TYR	N-CA-C	6.41	118.35	111.36
2	D	219	SER	N-CA-C	5.95	117.77	111.28
2	B	290	ASP	N-CA-C	-5.93	104.90	111.36
1	A	50	ILE	N-CA-C	-5.85	104.82	110.72
2	B	222	SER	CA-C-N	-5.59	112.85	119.84
2	B	222	SER	C-N-CA	-5.59	112.85	119.84
2	B	219	SER	N-CA-C	5.57	119.33	112.54
1	C	42	ARG	N-CA-C	-5.51	105.35	111.36
2	D	98	CYS	CA-CB-SG	-5.40	101.99	114.40
2	B	155	TYR	N-CA-C	5.32	117.16	111.36
2	D	105	ILE	CB-CA-C	-5.27	102.70	110.82
2	B	111	ASN	N-CA-C	5.25	119.27	111.87
1	A	4	VAL	N-CA-C	5.23	116.11	108.58
1	C	120	VAL	N-CA-C	-5.22	105.62	110.53
1	A	42	ARG	N-CA-C	-5.21	105.68	111.36
2	B	108	ASP	N-CA-C	-5.18	105.53	111.07
2	D	107	ASP	CA-C-O	5.17	124.51	118.77
1	C	50	ILE	N-CA-C	-5.15	105.37	110.62
2	D	291	ASP	N-CA-C	5.11	117.75	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	TRP	CA-C-N	5.03	124.94	119.76
1	A	7	TRP	C-N-CA	5.03	124.94	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	220	SER	Peptide
2	D	225	ALA	Mainchain

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	1028	0	1001	76	0
1	C	1004	0	961	74	0
2	B	1013	0	975	72	0
2	D	1031	0	986	107	2
All	All	4076	0	3923	279	2

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 35.

All (279) 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)
2:D:113:ILE:CG1	2:D:113:ILE:CD1	1.82	1.54
2:D:218:SER:CB	2:D:218:SER:OG	1.66	1.39
1:C:77:ARG:NH2	2:D:114:PRO:HD3	1.46	1.26
1:C:59:ARG:HD2	2:D:99:PHE:HD1	1.02	1.15
1:A:126:LYS:HB3	2:D:104:TYR:CE2	1.86	1.10
2:D:99:PHE:CE2	2:D:103:THR:HG21	1.93	1.04
1:C:59:ARG:HD2	2:D:99:PHE:CD1	1.94	1.03
1:C:59:ARG:CD	2:D:99:PHE:HD1	1.72	1.02
2:D:113:ILE:HD13	2:D:114:PRO:N	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HH22	2:D:114:PRO:HD3	1.02	0.99
1:C:77:ARG:HH22	2:D:114:PRO:CD	1.76	0.98
2:D:99:PHE:C	2:D:99:PHE:HD2	1.73	0.96
1:A:126:LYS:HB3	2:D:104:TYR:CD2	2.05	0.92
1:C:59:ARG:HG2	1:C:90:LEU:HD11	1.53	0.90
1:A:44:ASN:HB2	2:B:152:PHE:HD1	1.38	0.88
1:C:28:GLN:HG2	2:D:155:TYR:OH	1.73	0.88
1:A:59:ARG:HG2	1:A:90:LEU:HD11	1.55	0.87
2:B:214:THR:O	2:B:229:PHE:HZ	1.55	0.86
1:A:4:VAL:HG11	2:B:153:LYS:HG3	1.56	0.86
2:D:113:ILE:HD13	2:D:113:ILE:C	2.00	0.86
1:A:43:PHE:CD2	2:B:148:LEU:HG	2.11	0.85
2:D:99:PHE:C	2:D:99:PHE:CD2	2.52	0.85
2:D:269:LEU:O	2:D:272:ILE:HG12	1.76	0.84
2:B:298:GLU:OE1	2:B:298:GLU:HA	1.78	0.83
2:D:99:PHE:HE2	2:D:103:THR:HG21	1.41	0.83
2:D:99:PHE:CE2	2:D:103:THR:CG2	2.62	0.83
2:B:269:LEU:O	2:B:272:ILE:HG12	1.79	0.82
1:C:77:ARG:NH2	2:D:114:PRO:CD	2.36	0.82
2:B:272:ILE:HG13	2:B:273:ALA:N	1.91	0.82
2:D:99:PHE:HE2	2:D:103:THR:CG2	1.93	0.81
2:D:92:HIS:CG	2:D:93:MET:H	1.99	0.81
2:D:99:PHE:HD2	2:D:99:PHE:O	1.65	0.80
2:B:214:THR:OG1	2:B:229:PHE:HE2	1.65	0.80
2:D:272:ILE:HG13	2:D:273:ALA:N	1.96	0.78
2:B:214:THR:HG1	2:B:229:PHE:HE2	1.33	0.77
2:D:293:LEU:O	2:D:297:GLU:HG2	1.85	0.75
1:A:7:TRP:HD1	1:A:8:PRO:HD2	1.52	0.75
2:D:108:ASP:O	2:D:111:ASN:OD1	2.05	0.74
2:D:113:ILE:HD13	2:D:114:PRO:CD	2.17	0.73
1:C:46:ALA:HB2	1:C:64:ILE:CG2	2.19	0.73
1:C:59:ARG:CD	2:D:99:PHE:CD1	2.61	0.73
1:A:41:SER:HA	1:A:44:ASN:OD1	1.89	0.72
1:A:46:ALA:HB2	1:A:64:ILE:CG2	2.19	0.72
1:C:78:GLU:OE2	2:D:148:LEU:HB2	1.89	0.72
2:B:147:SER:HB3	2:B:150:GLN:HG3	1.71	0.72
2:D:147:SER:HB3	2:D:150:GLN:HG3	1.71	0.72
2:D:272:ILE:O	2:D:276:GLU:HB2	1.89	0.72
1:C:46:ALA:HB2	1:C:64:ILE:HG21	1.73	0.71
2:D:249:SER:HA	2:D:252:ARG:NH1	2.06	0.71
1:A:8:PRO:HB3	2:B:149:PHE:CE1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:OE1	2:B:100:ARG:CD	2.40	0.70
1:C:92:GLU:OE1	2:D:100:ARG:NE	2.24	0.70
2:B:253:ASP:O	2:B:256:VAL:HG12	1.92	0.70
1:A:126:LYS:CB	2:D:104:TYR:CE2	2.73	0.70
1:A:112:GLN:HE21	1:A:112:GLN:H	1.40	0.69
2:D:107:ASP:OD2	2:D:107:ASP:C	2.34	0.69
2:B:105:ILE:HG13	2:B:109:LEU:HD11	1.74	0.69
1:A:46:ALA:HB2	1:A:64:ILE:HG21	1.75	0.68
1:C:43:PHE:CD2	2:D:148:LEU:HG	2.28	0.68
2:D:92:HIS:CG	2:D:93:MET:N	2.62	0.67
2:D:253:ASP:O	2:D:256:VAL:HG12	1.94	0.67
2:B:96:LYS:O	2:B:100:ARG:HG3	1.94	0.67
2:B:272:ILE:O	2:B:276:GLU:HB2	1.95	0.66
2:D:292:ARG:O	2:D:296:LEU:HG	1.96	0.66
1:A:69:TYR:CZ	1:A:76:ARG:HD3	2.30	0.66
1:A:125:GLN:HG3	1:A:126:LYS:N	2.09	0.66
1:C:69:TYR:CZ	1:C:76:ARG:HD3	2.31	0.65
2:D:155:TYR:C	2:D:155:TYR:CD2	2.74	0.65
2:D:289:ILE:HG22	2:D:292:ARG:HH22	1.61	0.65
1:A:7:TRP:CD1	1:A:8:PRO:HD2	2.32	0.65
2:B:298:GLU:C	2:B:299:TYR:HD2	2.04	0.65
2:D:113:ILE:CD1	2:D:113:ILE:C	2.70	0.65
1:C:41:SER:HA	1:C:44:ASN:OD1	1.97	0.65
1:C:7:TRP:HD1	1:C:8:PRO:HD2	1.62	0.64
2:D:245:ASN:HA	2:D:248:LEU:HB3	1.80	0.64
1:A:93:TYR:CE1	1:A:123:LYS:HD2	2.33	0.64
1:A:126:LYS:C	2:D:104:TYR:HE2	2.06	0.64
1:A:124:ILE:O	1:A:128:THR:HG23	1.99	0.63
2:D:113:ILE:CD1	2:D:113:ILE:CB	2.75	0.63
1:A:39:ILE:HG13	1:A:40:GLN:H	1.64	0.62
1:A:84:THR:HG21	1:A:100:VAL:HB	1.81	0.62
2:B:155:TYR:C	2:B:155:TYR:CD2	2.78	0.61
1:A:39:ILE:HG13	1:A:40:GLN:N	2.16	0.61
1:C:84:THR:HG21	1:C:100:VAL:HB	1.81	0.61
1:C:18:TYR:O	1:C:21:GLN:N	2.33	0.61
2:D:99:PHE:HE2	2:D:103:THR:HG1	1.48	0.61
1:C:15:GLU:O	1:C:15:GLU:HG2	2.00	0.60
1:C:39:ILE:HG13	1:C:40:GLN:H	1.67	0.60
2:D:113:ILE:CD1	2:D:114:PRO:HD2	2.32	0.60
1:A:18:TYR:O	1:A:21:GLN:N	2.34	0.59
2:D:92:HIS:CD2	2:D:93:MET:N	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HG13	1:C:40:GLN:N	2.18	0.58
2:B:249:SER:HA	2:B:252:ARG:NH1	2.19	0.58
1:A:8:PRO:HB3	2:B:149:PHE:CD1	2.38	0.58
2:B:245:ASN:HA	2:B:248:LEU:HB3	1.86	0.58
1:C:6:PHE:CD1	2:D:147:SER:HB2	2.39	0.58
2:D:299:TYR:N	2:D:299:TYR:CD2	2.70	0.58
1:C:77:ARG:HH21	2:D:114:PRO:HD3	1.58	0.58
2:B:105:ILE:O	2:B:109:LEU:HD13	2.04	0.57
2:D:218:SER:CB	2:D:218:SER:HG	2.09	0.57
2:D:92:HIS:CD2	2:D:93:MET:H	2.21	0.57
2:D:280:LEU:HA	2:D:283:GLU:OE2	2.05	0.57
1:A:44:ASN:HB2	2:B:152:PHE:CD1	2.29	0.57
1:A:50:ILE:O	1:A:89:LYS:NZ	2.31	0.56
1:A:93:TYR:CZ	1:A:123:LYS:HD2	2.40	0.56
1:C:112:GLN:H	1:C:112:GLN:HE21	1.52	0.56
1:A:92:GLU:OE1	2:B:100:ARG:HD2	2.05	0.56
1:A:15:GLU:O	1:A:15:GLU:HG2	2.04	0.56
2:B:272:ILE:HG13	2:B:273:ALA:H	1.69	0.56
1:C:43:PHE:O	1:C:46:ALA:N	2.39	0.56
1:A:28:GLN:NE2	1:A:32:GLU:HG3	2.21	0.56
1:C:16:PRO:HG3	1:C:53:THR:HG23	1.87	0.56
1:A:42:ARG:NH2	1:A:71:GLU:OE1	2.35	0.55
1:A:103:LEU:HD21	1:A:113:VAL:HG22	1.88	0.55
2:B:298:GLU:OE1	2:B:298:GLU:CA	2.48	0.55
2:B:262:ARG:O	2:B:265:LYS:HB3	2.06	0.55
1:C:77:ARG:HD3	1:C:107:GLU:OE2	2.06	0.55
2:B:280:LEU:HA	2:B:283:GLU:OE2	2.06	0.55
2:D:272:ILE:HG13	2:D:273:ALA:H	1.71	0.55
2:D:113:ILE:CD1	2:D:114:PRO:CD	2.85	0.55
1:A:15:GLU:O	1:A:51:LYS:HG2	2.07	0.55
1:A:16:PRO:HG3	1:A:53:THR:HG23	1.89	0.55
1:A:40:GLN:HG2	2:B:243:GLN:HE22	1.72	0.54
1:A:28:GLN:HE21	1:A:32:GLU:HG3	1.72	0.54
1:A:92:GLU:OE1	2:B:100:ARG:NE	2.40	0.54
1:C:43:PHE:O	1:C:44:ASN:C	2.51	0.54
1:C:7:TRP:CD1	1:C:8:PRO:HD2	2.43	0.54
2:B:104:TYR:C	2:B:105:ILE:HG23	2.33	0.54
1:A:39:ILE:HD12	1:A:75:ARG:HD2	1.90	0.53
1:A:43:PHE:CE2	2:B:148:LEU:HG	2.43	0.53
2:D:113:ILE:CG1	2:D:114:PRO:HD2	2.38	0.53
2:B:295:PHE:C	2:B:295:PHE:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:ASP:OD2	2:D:108:ASP:N	2.42	0.52
1:A:28:GLN:HG2	2:B:155:TYR:OH	2.10	0.52
1:C:7:TRP:CD1	1:C:81:TYR:CD2	2.97	0.52
2:D:99:PHE:HE2	2:D:103:THR:CB	2.22	0.52
1:C:28:GLN:NE2	1:C:32:GLU:HG3	2.25	0.52
1:C:15:GLU:O	1:C:51:LYS:HG2	2.10	0.51
1:A:20:GLN:O	1:A:24:ILE:HG12	2.11	0.51
2:D:99:PHE:HE2	2:D:103:THR:OG1	1.92	0.51
2:D:113:ILE:HG12	2:D:114:PRO:HD2	1.90	0.51
2:D:300:GLY:O	2:D:301:LEU:CB	2.57	0.51
1:C:78:GLU:OE2	2:D:148:LEU:CB	2.56	0.51
1:C:76:ARG:O	1:C:77:ARG:C	2.53	0.51
2:D:95:ASN:HB3	2:D:96:LYS:CB	2.41	0.51
1:C:32:GLU:HB3	1:C:37:ALA:HA	1.91	0.51
1:C:77:ARG:HH22	2:D:114:PRO:CG	2.24	0.51
1:C:66:THR:O	1:C:70:LYS:HG3	2.11	0.51
1:A:32:GLU:HB3	1:A:37:ALA:HA	1.92	0.51
1:C:14:TYR:CZ	1:C:89:LYS:HD2	2.46	0.51
2:D:272:ILE:O	2:D:276:GLU:N	2.44	0.51
2:B:271:LYS:O	2:B:274:ASN:HB3	2.11	0.51
1:C:40:GLN:HG2	2:D:243:GLN:HE22	1.76	0.51
1:A:39:ILE:HD12	1:A:75:ARG:CD	2.41	0.50
1:C:63:LYS:HA	2:D:103:THR:HG22	1.93	0.50
2:B:298:GLU:O	2:B:299:TYR:HD2	1.95	0.50
2:D:105:ILE:HG22	2:D:108:ASP:HB3	1.93	0.50
1:A:126:LYS:O	2:D:104:TYR:HE2	1.95	0.49
2:B:276:GLU:O	2:B:279:GLN:HG2	2.11	0.49
1:C:20:GLN:O	1:C:24:ILE:HG12	2.11	0.49
1:C:76:ARG:HH11	2:D:111:ASN:HB2	1.76	0.49
2:D:155:TYR:CD2	2:D:155:TYR:O	2.65	0.49
2:B:269:LEU:O	2:B:269:LEU:HD23	2.12	0.49
2:D:235:ASN:O	2:D:238:GLU:HG2	2.11	0.49
2:B:108:ASP:O	2:B:109:LEU:C	2.52	0.49
2:B:102:LEU:HB2	2:B:103:THR:HG23	1.94	0.49
2:D:98:CYS:HA	2:D:101:MET:HE3	1.94	0.49
2:B:153:LYS:O	2:B:157:PRO:HD2	2.13	0.48
1:C:8:PRO:HB3	2:D:149:PHE:CE1	2.49	0.48
2:D:269:LEU:O	2:D:269:LEU:HD23	2.13	0.48
2:B:214:THR:O	2:B:229:PHE:CZ	2.48	0.48
2:B:298:GLU:O	2:B:299:TYR:CD2	2.66	0.48
1:C:39:ILE:HD12	1:C:75:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:SER:HA	2:D:252:ARG:HH12	1.78	0.48
2:B:292:ARG:CZ	2:B:292:ARG:HB3	2.43	0.48
1:C:108:ARG:NH1	1:C:108:ARG:HB2	2.29	0.48
1:C:28:GLN:HE21	1:C:32:GLU:HG3	1.79	0.47
2:D:98:CYS:O	2:D:99:PHE:C	2.56	0.47
1:A:32:GLU:OE1	1:A:38:THR:N	2.44	0.47
1:A:108:ARG:NH1	1:A:108:ARG:HB2	2.29	0.47
2:B:272:ILE:O	2:B:276:GLU:N	2.47	0.47
1:A:43:PHE:CG	2:B:148:LEU:HG	2.49	0.47
1:A:76:ARG:O	1:A:77:ARG:C	2.56	0.47
2:B:271:LYS:HA	2:B:274:ASN:HB3	1.97	0.47
1:C:103:LEU:HD21	1:C:113:VAL:HG22	1.95	0.47
2:D:266:GLU:HA	2:D:269:LEU:HB3	1.95	0.47
2:D:271:LYS:O	2:D:274:ASN:HB3	2.15	0.47
2:B:281:LEU:C	2:B:281:LEU:HD23	2.40	0.47
1:A:66:THR:O	1:A:70:LYS:HG3	2.15	0.46
1:C:47:TRP:NE1	1:C:51:LYS:HD2	2.30	0.46
2:D:147:SER:HB3	2:D:150:GLN:CG	2.44	0.46
1:C:43:PHE:CG	2:D:148:LEU:HG	2.50	0.46
2:B:155:TYR:CD2	2:B:155:TYR:O	2.69	0.46
1:C:125:GLN:HG3	1:C:126:LYS:N	2.31	0.46
2:D:269:LEU:O	2:D:272:ILE:CG1	2.56	0.46
1:C:82:TYR:CE2	2:D:148:LEU:HD23	2.49	0.46
1:A:79:CYS:HA	1:A:82:TYR:HD2	1.80	0.46
2:D:276:GLU:O	2:D:279:GLN:HG2	2.16	0.46
2:B:160:GLU:C	2:B:162:ALA:N	2.74	0.46
2:D:292:ARG:CZ	2:D:292:ARG:HB3	2.44	0.46
2:D:99:PHE:CZ	2:D:103:THR:HG21	2.48	0.46
2:D:153:LYS:O	2:D:157:PRO:HD2	2.15	0.46
2:B:216:ALA:C	2:B:218:SER:H	2.24	0.45
2:B:298:GLU:C	2:B:299:TYR:CD2	2.90	0.45
1:C:104:PHE:O	1:C:108:ARG:HA	2.16	0.45
1:A:125:GLN:O	1:A:128:THR:N	2.39	0.45
2:B:277:GLN:O	2:B:280:LEU:HB3	2.16	0.45
1:A:92:GLU:OE1	2:B:100:ARG:HG2	2.17	0.45
2:D:262:ARG:O	2:D:265:LYS:HB3	2.17	0.45
2:D:298:GLU:HB2	2:D:299:TYR:CD2	2.52	0.45
2:D:156:LEU:HD22	2:D:159:ALA:HB3	1.98	0.45
1:A:26:ARG:HB2	1:A:45:TYR:CE1	2.52	0.45
2:B:299:TYR:O	2:B:300:GLY:C	2.59	0.45
1:C:26:ARG:O	1:C:30:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:CE2	2:D:148:LEU:HG	2.52	0.45
2:B:214:THR:OG1	2:B:229:PHE:CE2	2.52	0.45
1:A:52:SER:OG	1:A:53:THR:N	2.50	0.45
1:C:33:GLY:O	1:C:34:GLY:C	2.60	0.45
1:A:123:LYS:CE	1:C:98:ARG:HH12	2.29	0.44
2:D:154:SER:O	2:D:157:PRO:HG2	2.17	0.44
2:D:239:PHE:HD2	2:D:240:LEU:HD12	1.80	0.44
2:D:277:GLN:O	2:D:280:LEU:HB3	2.17	0.44
2:B:105:ILE:HD13	2:B:105:ILE:HG21	1.52	0.44
1:A:47:TRP:NE1	1:A:51:LYS:HD2	2.32	0.44
1:C:14:TYR:CE1	1:C:89:LYS:HD2	2.52	0.44
2:B:235:ASN:O	2:B:238:GLU:HG2	2.18	0.44
1:A:90:LEU:HD23	1:A:90:LEU:O	2.17	0.44
1:A:122:ASP:O	1:A:123:LYS:C	2.59	0.44
1:C:6:PHE:CE1	2:D:147:SER:HB2	2.53	0.44
2:D:152:PHE:CD2	2:D:152:PHE:C	2.95	0.44
1:C:42:ARG:NH2	1:C:71:GLU:OE1	2.45	0.43
1:C:59:ARG:HB3	2:D:99:PHE:CD1	2.52	0.43
1:C:116:LEU:O	1:C:117:LYS:C	2.60	0.43
2:D:271:LYS:HA	2:D:274:ASN:HB3	2.00	0.43
1:A:104:PHE:O	1:A:108:ARG:HA	2.18	0.43
2:D:284:ASP:O	2:D:287:LYS:HB3	2.19	0.43
2:B:266:GLU:HA	2:B:269:LEU:HB3	1.99	0.43
2:B:94:ASP:O	2:B:97:THR:N	2.44	0.43
2:B:160:GLU:C	2:B:162:ALA:H	2.27	0.43
1:C:25:LEU:HD21	2:D:156:LEU:HD21	2.01	0.43
1:A:116:LEU:O	1:A:117:LYS:C	2.60	0.43
1:C:43:PHE:C	1:C:45:TYR:N	2.73	0.43
1:A:40:GLN:HB2	2:B:246:SER:OG	2.19	0.43
1:A:43:PHE:O	1:A:46:ALA:N	2.52	0.42
1:C:90:LEU:HD23	1:C:90:LEU:O	2.20	0.42
1:A:123:LYS:HE3	1:C:98:ARG:HH12	1.83	0.42
1:C:122:ASP:O	1:C:123:LYS:C	2.63	0.42
1:A:123:LYS:HZ1	1:C:98:ARG:HH12	1.68	0.42
1:A:104:PHE:CD1	1:A:117:LYS:HD2	2.54	0.41
2:B:97:THR:HA	2:B:100:ARG:HG3	2.02	0.41
1:C:69:TYR:CE1	1:C:76:ARG:HB3	2.55	0.41
2:D:155:TYR:C	2:D:155:TYR:HD2	2.26	0.41
1:A:39:ILE:HD12	1:A:75:ARG:NE	2.34	0.41
2:B:104:TYR:C	2:B:105:ILE:CG2	2.93	0.41
2:B:161:LEU:HD23	2:B:161:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:LYS:HA	2:B:274:ASN:CB	2.50	0.41
2:B:284:ASP:O	2:B:287:LYS:HB3	2.21	0.41
1:A:26:ARG:O	1:A:30:VAL:HG23	2.21	0.41
1:A:39:ILE:O	1:A:40:GLN:C	2.63	0.41
1:A:95:MET:O	1:A:98:ARG:HB3	2.20	0.41
2:B:156:LEU:N	2:B:157:PRO:HD2	2.36	0.41
1:C:85:ILE:HD12	1:C:85:ILE:HG23	1.75	0.41
1:A:26:ARG:O	1:A:27:GLN:C	2.64	0.41
1:A:126:LYS:HA	1:A:129:LEU:HG	2.03	0.41
1:C:39:ILE:HD12	1:C:75:ARG:CD	2.50	0.41
1:C:76:ARG:NH1	2:D:111:ASN:HB2	2.36	0.41
2:D:231:GLN:HA	2:D:234:VAL:HG12	2.02	0.41
1:A:33:GLY:O	1:A:34:GLY:C	2.64	0.41
2:D:238:GLU:HG3	2:D:239:PHE:N	2.35	0.41
1:C:7:TRP:NE1	1:C:81:TYR:CG	2.89	0.40
1:A:14:TYR:CE1	1:A:89:LYS:HD2	2.56	0.40
1:A:38:THR:O	1:A:39:ILE:C	2.63	0.40
2:B:108:ASP:OD2	2:B:108:ASP:N	2.54	0.40
1:A:26:ARG:O	1:A:29:VAL:N	2.55	0.40
2:B:105:ILE:HG13	2:B:109:LEU:CD1	2.47	0.40
2:B:156:LEU:HD22	2:B:159:ALA:HB3	2.03	0.40
2:D:257:GLU:O	2:D:261:LEU:HB2	2.20	0.40
2:B:151:GLY:HA2	2:B:242:ILE:HG21	2.04	0.40
2:D:245:ASN:HA	2:D:248:LEU:CB	2.47	0.40

All (2) 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)
2:D:98:CYS:SG	2:D:98:CYS:SG[5_555]	1.04	1.16
2:D:218:SER:OG	2:D:292:ARG:NH2[5_555]	1.82	0.38

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	125/129 (97%)	118 (94%)	6 (5%)	1 (1%)	16	50
1	C	123/129 (95%)	115 (94%)	7 (6%)	1 (1%)	16	50
2	B	126/242 (52%)	118 (94%)	7 (6%)	1 (1%)	16	50
2	D	129/242 (53%)	119 (92%)	10 (8%)	0	100	100
All	All	503/742 (68%)	470 (93%)	30 (6%)	3 (1%)	21	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLY
1	C	34	GLY
2	B	217	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	109/116 (94%)	103 (94%)	6 (6%)	19	45
1	C	105/116 (90%)	99 (94%)	6 (6%)	18	44
2	B	110/217 (51%)	100 (91%)	10 (9%)	9	31
2	D	111/217 (51%)	100 (90%)	11 (10%)	7	28
All	All	435/666 (65%)	402 (92%)	33 (8%)	12	37

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TRP
1	A	9	THR
1	A	15	GLU
1	A	90	LEU
1	A	95	MET

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Mol	Chain	Res	Type
1	A	112	GLN
2	B	102	LEU
2	B	107	ASP
2	B	108	ASP
2	B	156	LEU
2	B	161	LEU
2	B	219	SER
2	B	266	GLU
2	B	281	LEU
2	B	282	LEU
2	B	295	PHE
1	C	7	TRP
1	C	9	THR
1	C	15	GLU
1	C	90	LEU
1	C	95	MET
1	C	112	GLN
2	D	95	ASN
2	D	99	PHE
2	D	105	ILE
2	D	107	ASP
2	D	113	ILE
2	D	156	LEU
2	D	220	SER
2	D	266	GLU
2	D	282	LEU
2	D	296	LEU
2	D	299	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	109	ASN
1	A	112	GLN
2	B	231	GLN
2	B	243	GLN
1	C	28	GLN
1	C	109	ASN
1	C	112	GLN
2	D	92	HIS
2	D	243	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 [i](#)

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	127/129 (98%)	-0.04	0	100 100	101, 123, 134, 138	0
1	C	125/129 (96%)	0.00	0	100 100	108, 124, 135, 145	0
2	B	132/242 (54%)	0.07	1 (0%)	82 64	104, 128, 138, 145	0
2	D	135/242 (55%)	0.42	5 (3%)	45 32	108, 133, 146, 152	0
All	All	519/742 (69%)	0.12	6 (1%)	76 55	101, 127, 142, 152	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	295	PHE	3.1
2	B	300	GLY	2.8
2	D	301	LEU	2.6
2	D	155	TYR	2.4
2	D	292	ARG	2.3
2	D	163	ILE	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.