



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:33 pm BST

PDB ID : 5OWV
Title : An oligomerised bacterial dynamin pair provides a mechanism for the long-range sensing and tethering of membranes
Authors : Liu, J.W.; Noel, J.K.; Low, H.H.
Deposited on : 2017-09-04
Resolution : 3.72 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

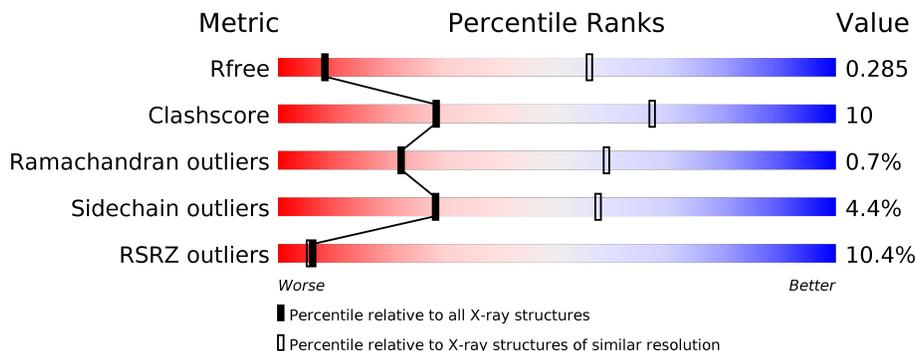
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.72 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}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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 on 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	732	 10% 77% 18% • 5%
1	B	732	 9% 65% 14% • 20%
2	C	614	 10% 74% 21% • •
2	D	614	 9% 68% 25% • •

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 19375 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 GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	699	Total	C	N	O	S	0	0	0
			5021	3179	858	970	14			
1	B	587	Total	C	N	O	S	0	0	0
			4436	2828	739	855	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	729	LYS	-	expression tag	UNP A0A1D9BJX7
A	730	LEU	-	expression tag	UNP A0A1D9BJX7
A	731	HIS	-	expression tag	UNP A0A1D9BJX7
A	732	HIS	-	expression tag	UNP A0A1D9BJX7
B	729	LYS	-	expression tag	UNP A0A1D9BJX7
B	730	LEU	-	expression tag	UNP A0A1D9BJX7
B	731	HIS	-	expression tag	UNP A0A1D9BJX7
B	732	HIS	-	expression tag	UNP A0A1D9BJX7

- Molecule 2 is a protein called GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	598	Total	C	N	O	S	0	0	0
			4959	3206	799	943	11			
2	D	598	Total	C	N	O	S	0	0	0
			4959	3206	799	943	11			

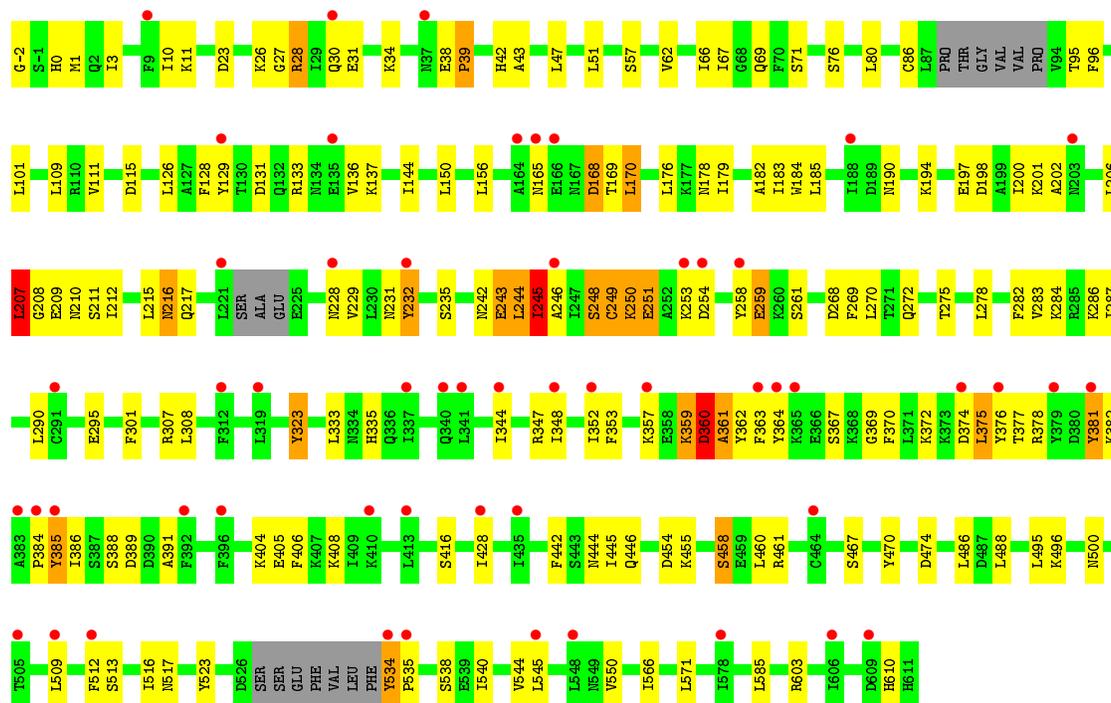
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A1D9BKH6
C	-1	SER	-	expression tag	UNP A0A1D9BKH6
C	0	HIS	-	expression tag	UNP A0A1D9BKH6
C	610	HIS	-	expression tag	UNP A0A1D9BKH6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	611	HIS	-	expression tag	UNP A0A1D9BKH6
D	-2	GLY	-	expression tag	UNP A0A1D9BKH6
D	-1	SER	-	expression tag	UNP A0A1D9BKH6
D	0	HIS	-	expression tag	UNP A0A1D9BKH6
D	610	HIS	-	expression tag	UNP A0A1D9BKH6
D	611	HIS	-	expression tag	UNP A0A1D9BKH6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.59Å 226.06Å 317.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.13 – 3.72 106.13 – 3.72	Depositor EDS
% Data completeness (in resolution range)	99.5 (106.13-3.72) 99.5 (106.13-3.72)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.67Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.259 , 0.286 0.258 , 0.285	Depositor DCC
R_{free} test set	4195 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	147.9	Xtrriage
Anisotropy	0.583	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 202.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19375	wwPDB-VP
Average B, all atoms (Å ²)	212.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 [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	0.26	0/5069	0.47	1/6846 (0.0%)
1	B	0.26	0/4480	0.46	0/6024
2	C	0.29	0/5044	0.53	2/6771 (0.0%)
2	D	0.29	0/5044	0.55	1/6771 (0.0%)
All	All	0.27	0/19637	0.51	4/26412 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
2	C	0	6
2	D	0	5
All	All	0	18

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	207	LEU	CA-CB-CG	8.76	135.44	115.30
2	C	244	LEU	CA-CB-CG	-6.75	99.78	115.30
1	A	264	LEU	CB-CG-CD2	-5.71	101.29	111.00
2	C	5	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	196	THR	Peptide
1	A	255	LEU	Peptide
1	B	196	THR	Peptide
1	B	255	LEU	Peptide
1	B	433	LEU	Peptide
1	B	84	PHE	Peptide
2	C	244	LEU	Peptide
2	C	248	SER	Peptide
2	C	249	CYS	Peptide
2	C	259	GLU	Peptide
2	C	359	LYS	Peptide
2	C	95	THR	Peptide
2	D	248	SER	Peptide
2	D	259	GLU	Peptide
2	D	359	LYS	Peptide
2	D	360	ASP	Peptide
2	D	95	THR	Peptide

5.2 Too-close contacts [i](#)

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	5021	0	4509	86	0
1	B	4436	0	4219	73	0
2	C	4959	0	5000	103	0
2	D	4959	0	5000	134	0
All	All	19375	0	18728	375	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 10.

All (375) 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:C:364:TYR:CE1	2:D:364:TYR:CE2	2.00	1.46
2:C:364:TYR:CE1	2:D:364:TYR:CD2	2.22	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:TYR:HE1	2:D:364:TYR:CD2	1.59	1.14
1:B:263:GLU:OE2	1:B:265:LYS:NZ	1.92	1.00
2:D:202:ALA:HB3	2:D:207:LEU:HD22	1.50	0.94
2:C:364:TYR:OH	2:D:364:TYR:O	1.87	0.92
2:C:364:TYR:CE1	2:D:364:TYR:HE2	1.76	0.88
2:D:364:TYR:HB3	2:D:378:ARG:HA	1.56	0.88
2:C:361:ALA:HB1	2:C:381:TYR:HB3	1.57	0.86
1:A:84:PHE:HE2	1:A:118:ILE:HG23	1.41	0.84
2:C:364:TYR:CZ	2:D:364:TYR:CE2	2.65	0.83
1:B:403:MET:HB3	1:B:416:SER:HB2	1.59	0.82
2:C:364:TYR:CZ	2:D:364:TYR:CD2	2.68	0.82
2:D:375:LEU:HD12	2:D:376:TYR:H	1.43	0.81
2:C:364:TYR:HB3	2:C:378:ARG:HA	1.61	0.81
1:A:16:LEU:HD13	1:A:74:ILE:HD11	1.64	0.80
2:C:364:TYR:CD1	2:D:364:TYR:HE2	2.00	0.80
2:C:366:GLU:H	2:C:376:TYR:HD1	1.30	0.79
2:C:364:TYR:CD1	2:D:364:TYR:CE2	2.69	0.78
1:A:183:LEU:HD22	1:A:287:LEU:HD13	1.67	0.77
2:C:182:ALA:HB3	2:C:207:LEU:HD22	1.68	0.76
1:B:20:ALA:HB2	1:B:78:ASN:HB2	1.67	0.76
2:C:364:TYR:HE1	2:D:364:TYR:HD2	1.26	0.75
2:D:243:GLU:OE2	2:D:243:GLU:HA	1.85	0.75
2:C:364:TYR:CB	2:C:378:ARG:HA	2.17	0.74
1:A:100:ILE:HD11	2:D:10:ILE:HA	1.69	0.74
2:C:377:THR:HG22	2:D:374:ASP:HB3	1.69	0.73
2:D:202:ALA:CB	2:D:207:LEU:HD22	2.19	0.72
2:D:364:TYR:CB	2:D:378:ARG:HA	2.19	0.72
1:B:167:ILE:HD11	1:B:326:LEU:HD11	1.73	0.71
2:C:384:PRO:HB3	2:C:534:TYR:CD2	2.26	0.70
1:A:334:THR:O	1:A:337:ASP:N	2.23	0.70
1:A:84:PHE:CE2	1:A:118:ILE:HG23	2.27	0.70
2:D:133:ARG:HB2	2:D:136:VAL:HG22	1.74	0.70
1:B:266:ASN:ND2	1:B:266:ASN:O	2.24	0.69
2:D:115:ASP:OD2	2:D:137:LYS:NZ	2.24	0.69
1:A:288:GLU:HA	1:A:291:LYS:HB3	1.74	0.69
1:A:184:LYS:HE2	1:A:417:LEU:HD11	1.73	0.69
1:B:217:LYS:HD3	1:B:256:ILE:HG23	1.75	0.69
2:D:34:LYS:HG3	2:D:51:LEU:HB3	1.76	0.68
1:A:167:ILE:HD11	1:A:326:LEU:HD11	1.75	0.68
1:B:63:ARG:NH1	2:D:446:GLN:O	2.26	0.68
1:B:22:PHE:CD2	1:B:75:CYS:HB2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:GLU:OE1	2:D:603:ARG:NH1	2.27	0.68
1:A:171:MET:SD	1:A:196:THR:HG21	2.34	0.67
1:B:183:LEU:HD22	1:B:287:LEU:HD13	1.77	0.67
1:A:334:THR:HB	1:A:337:ASP:HB2	1.76	0.67
1:B:318:ARG:O	1:B:320:SER:N	2.26	0.67
2:C:43:ALA:HB1	2:C:47:LEU:HD23	1.75	0.67
2:D:150:LEU:HD11	2:D:270:LEU:HB3	1.75	0.66
2:D:367:SER:N	2:D:375:LEU:HD13	2.10	0.66
2:D:202:ALA:O	2:D:207:LEU:HD23	1.96	0.65
2:D:126:LEU:HD22	2:D:144:ILE:HD11	1.79	0.65
2:C:295:GLU:OE1	2:C:603:ARG:NH1	2.29	0.65
2:D:216:ASN:HD22	2:D:217:GLN:H	1.45	0.64
2:D:534:TYR:HB2	2:D:535:PRO:HD3	1.78	0.64
2:D:216:ASN:HD21	2:D:250:LYS:HB3	1.63	0.64
1:A:310:GLU:OE2	1:A:314:ASN:ND2	2.30	0.64
2:C:229:VAL:HA	2:C:232:TYR:CD2	2.33	0.64
2:C:229:VAL:HA	2:C:232:TYR:HD2	1.62	0.64
2:D:62:VAL:HG21	2:D:275:THR:HB	1.80	0.64
2:C:150:LEU:HD11	2:C:270:LEU:HB3	1.80	0.63
2:D:229:VAL:HA	2:D:232:TYR:HD2	1.63	0.63
1:A:20:ALA:HB2	1:A:78:ASN:HB2	1.81	0.63
2:D:229:VAL:HA	2:D:232:TYR:CD2	2.33	0.63
2:C:491:GLU:HG3	2:D:488:LEU:HD22	1.81	0.63
1:A:220:TRP:CH2	1:A:237:ILE:HD11	2.34	0.63
1:A:197:ALA:HB3	1:A:308:GLN:OE1	1.99	0.63
1:B:223:ILE:HA	1:B:306:VAL:HG21	1.81	0.63
2:D:228:ASN:HA	2:D:231:ASN:ND2	2.13	0.63
2:C:42:HIS:HB3	2:C:455:LYS:HB3	1.81	0.62
1:B:334:THR:O	1:B:337:ASP:N	2.31	0.62
2:D:101:LEU:HB2	2:D:156:LEU:HB2	1.81	0.62
2:D:347:ARG:NH2	2:D:405:GLU:OE1	2.33	0.62
2:D:458:SER:HA	2:D:461:ARG:HH11	1.64	0.62
2:D:369:GLY:H	2:D:375:LEU:HD22	1.64	0.62
2:D:284:LYS:HE2	2:D:610:HIS:HB2	1.82	0.62
1:A:454:LEU:HD11	1:A:717:LEU:HB3	1.83	0.61
2:D:215:LEU:O	2:D:248:SER:HA	2.00	0.61
1:B:173:ALA:HA	1:B:328:ASN:HB2	1.83	0.60
2:C:178:ASN:HA	2:C:282:PHE:CZ	2.36	0.60
2:C:66:ILE:HD13	2:C:183:ILE:HB	1.83	0.60
1:A:352:LYS:HG2	1:A:393:LYS:O	2.00	0.60
2:D:216:ASN:ND2	2:D:250:LYS:HB3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ALA:HB3	1:B:308:GLN:OE1	2.01	0.60
2:C:169:THR:HG21	2:C:201:LYS:HA	1.84	0.60
2:C:67:ILE:HD11	2:C:206:LEU:HD22	1.84	0.60
1:A:223:ILE:HA	1:A:306:VAL:HG21	1.84	0.60
2:C:388:SER:HA	2:C:509:LEU:HG	1.84	0.60
2:C:534:TYR:HB2	2:C:535:PRO:HD3	1.84	0.59
2:C:0:HIS:HA	2:C:3:ILE:HD12	1.85	0.59
2:D:43:ALA:HB1	2:D:47:LEU:HD23	1.84	0.59
2:C:364:TYR:OH	2:D:364:TYR:CD2	2.55	0.59
2:D:375:LEU:CD1	2:D:376:TYR:H	2.16	0.59
2:D:352:ILE:HD12	2:D:509:LEU:HD13	1.85	0.59
2:C:110:ARG:HB3	2:C:143:HIS:HB2	1.86	0.58
2:C:226:LEU:HD23	2:C:226:LEU:H	1.68	0.58
2:C:264:GLN:O	2:C:268:ASP:HB2	2.04	0.58
2:C:218:LYS:HD3	2:C:249:CYS:SG	2.44	0.58
2:D:69:GLN:NE2	2:D:194:LYS:HD2	2.18	0.58
1:B:390:LEU:O	1:B:393:LYS:HB3	2.04	0.57
2:D:202:ALA:CB	2:D:206:LEU:HB3	2.34	0.57
1:B:454:LEU:HD21	1:B:721:GLU:HB2	1.86	0.57
1:A:62:LEU:HD21	1:A:72:ALA:HB2	1.85	0.57
2:D:513:SER:O	2:D:517:ASN:ND2	2.35	0.57
2:D:202:ALA:HB2	2:D:206:LEU:HB3	1.87	0.57
2:C:447:LYS:HD2	2:C:452:GLN:HB2	1.85	0.57
1:B:184:LYS:HE2	1:B:417:LEU:HD11	1.87	0.57
2:C:250:LYS:O	2:C:251:GLU:HG3	2.05	0.57
1:A:709:GLU:O	1:A:713:LYS:HG2	2.05	0.57
1:B:100:ILE:HD11	2:C:10:ILE:HA	1.85	0.56
2:D:207:LEU:HD11	2:D:242:ASN:HD21	1.70	0.56
2:C:347:ARG:NH2	2:C:405:GLU:OE1	2.39	0.56
2:C:391:ALA:HB3	2:C:509:LEU:HD21	1.87	0.56
1:A:352:LYS:HA	1:A:393:LYS:HG2	1.86	0.56
1:B:352:LYS:HG2	1:B:393:LYS:O	2.05	0.56
1:A:313:THR:O	1:A:317:LEU:HB3	2.06	0.56
1:A:16:LEU:HD13	1:A:74:ILE:CD1	2.35	0.56
2:D:361:ALA:CB	2:D:381:TYR:HB3	2.36	0.56
1:B:345:LEU:HD21	1:B:394:ILE:HD11	1.88	0.55
1:B:120:GLN:HB3	1:B:434:TYR:HD2	1.71	0.55
2:D:348:ILE:O	2:D:352:ILE:HG12	2.05	0.55
1:A:328:ASN:HB3	1:A:331:GLN:HG2	1.86	0.55
2:D:249:CYS:HB2	2:D:261:SER:O	2.06	0.55
1:A:77:LEU:HD21	1:A:106:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:215:LEU:O	2:C:248:SER:HA	2.06	0.55
2:D:0:HIS:HA	2:D:3:ILE:HD12	1.87	0.55
2:C:79:ASN:OD1	2:C:86:CYS:N	2.39	0.55
2:D:244:LEU:HD12	2:D:244:LEU:O	2.07	0.55
1:B:288:GLU:HA	1:B:291:LYS:HB3	1.89	0.54
2:D:386:ILE:HG21	2:D:513:SER:HA	1.89	0.54
2:D:208:GLY:O	2:D:209:GLU:OE1	2.26	0.54
1:A:363:LEU:HD12	1:A:368:LEU:HD13	1.88	0.54
2:D:391:ALA:HB3	2:D:509:LEU:HD21	1.89	0.54
1:A:213:TYR:HB2	1:A:280:LYS:HB3	1.90	0.54
2:C:386:ILE:HG21	2:C:513:SER:HA	1.90	0.53
2:D:333:LEU:HD11	2:D:416:SER:HB3	1.89	0.53
2:D:178:ASN:HA	2:D:282:PHE:CZ	2.43	0.53
2:D:361:ALA:HB3	2:D:381:TYR:HB3	1.89	0.53
1:A:164:ASN:HD22	1:A:320:SER:HA	1.72	0.53
1:A:241:ASP:O	1:A:244:VAL:HG22	2.09	0.53
2:D:286:LYS:O	2:D:290:LEU:HG	2.09	0.53
2:C:357:LYS:N	2:C:385:TYR:O	2.42	0.52
1:B:124:PHE:HB2	1:B:434:TYR:CD1	2.44	0.52
2:D:170:LEU:HD23	2:D:170:LEU:H	1.75	0.52
1:A:318:ARG:O	1:A:320:SER:N	2.42	0.52
2:C:495:LEU:O	2:C:500:ASN:ND2	2.41	0.52
1:A:115:VAL:O	1:A:116:GLN:HB2	2.09	0.52
2:C:26:LYS:HD2	2:C:280:GLU:HG2	1.91	0.52
2:C:61:ASN:HB3	2:C:155:THR:HG23	1.91	0.52
1:A:345:LEU:HD21	1:A:394:ILE:HD11	1.92	0.52
2:D:197:GLU:HA	2:D:200:ILE:HG13	1.92	0.52
1:A:403:MET:HB3	1:A:416:SER:HB2	1.92	0.52
2:C:225:GLU:HG3	2:C:226:LEU:HD23	1.92	0.52
2:D:86:CYS:HB3	2:D:126:LEU:HD23	1.92	0.52
1:B:22:PHE:HD2	1:B:75:CYS:HB2	1.71	0.51
1:B:233:LEU:O	1:B:237:ILE:HG12	2.09	0.51
1:B:170:VAL:HG21	1:B:334:THR:HG21	1.92	0.51
2:D:202:ALA:O	2:D:207:LEU:CD2	2.58	0.51
2:D:208:GLY:C	2:D:209:GLU:OE1	2.49	0.51
2:D:388:SER:HA	2:D:509:LEU:HG	1.93	0.51
1:B:95:LYS:O	1:B:98:GLU:HB2	2.11	0.51
1:B:72:ALA:HA	1:B:75:CYS:SG	2.50	0.51
2:D:404:LYS:O	2:D:408:LYS:HG2	2.11	0.51
1:A:62:LEU:HD13	1:A:69:MET:HE1	1.93	0.51
1:A:96:ILE:HG23	1:A:389:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:PRO:HG3	2:D:534:TYR:CE2	2.46	0.50
1:A:63:ARG:NH1	2:C:446:GLN:O	2.44	0.50
2:D:245:ILE:HG23	2:D:246:ALA:O	2.11	0.50
1:A:187:PHE:CE1	1:A:287:LEU:HD11	2.46	0.50
1:A:22:PHE:CD2	1:A:75:CYS:HB3	2.47	0.50
2:D:183:ILE:HD11	2:D:270:LEU:HD11	1.94	0.50
1:B:213:TYR:HB2	1:B:280:LYS:HB2	1.93	0.50
1:B:324:ILE:HD11	1:B:429:LEU:HD21	1.93	0.50
1:A:205:GLY:O	1:A:286:HIS:NE2	2.45	0.50
1:A:264:LEU:HD13	1:A:267:PHE:CD1	2.47	0.50
1:B:124:PHE:HB2	1:B:434:TYR:HB2	1.92	0.50
2:C:111:VAL:HG21	2:C:129:TYR:CD2	2.47	0.50
1:A:224:LEU:O	1:A:227:SER:OG	2.25	0.50
1:A:86:SER:HB3	1:A:90:LEU:HB2	1.94	0.50
1:B:171:MET:SD	1:B:196:THR:HG21	2.51	0.50
2:D:202:ALA:HB1	2:D:207:LEU:N	2.27	0.50
2:D:169:THR:OG1	2:D:201:LYS:HA	2.12	0.50
2:D:301:PHE:CE1	2:D:460:LEU:HD22	2.47	0.50
1:B:197:ALA:HB1	1:B:300:PRO:HB3	1.94	0.49
2:C:108:PHE:HB2	2:C:145:PHE:HB2	1.94	0.49
2:C:367:SER:OG	2:C:377:THR:N	2.44	0.49
2:D:216:ASN:HD22	2:D:217:GLN:N	2.10	0.49
2:D:369:GLY:H	2:D:375:LEU:CD2	2.25	0.49
1:B:8:ILE:O	1:B:41:LYS:HB3	2.13	0.49
2:D:357:LYS:N	2:D:385:TYR:O	2.46	0.49
2:C:165:ASN:HB3	2:C:168:ASP:HB2	1.95	0.49
2:D:442:PHE:HA	2:D:445:ILE:HG12	1.94	0.49
2:D:367:SER:OG	2:D:377:THR:N	2.45	0.49
2:C:212:ILE:HD11	2:C:269:PHE:CG	2.48	0.48
1:B:224:LEU:O	1:B:227:SER:OG	2.25	0.48
1:B:227:SER:O	1:B:234:LYS:HB2	2.14	0.48
2:C:251:GLU:O	2:C:261:SER:OG	2.22	0.48
1:A:240:LEU:HD11	1:A:277:LEU:HD21	1.95	0.48
1:B:18:PHE:HA	1:B:74:ILE:HG21	1.96	0.48
2:D:28:ARG:HD2	2:D:28:ARG:N	2.27	0.48
1:A:447:LYS:HD3	1:A:728:ASP:HB2	1.95	0.48
1:B:303:ASP:CG	1:B:304:ASP:H	2.15	0.48
2:C:357:LYS:HB2	2:C:385:TYR:CD2	2.49	0.48
2:C:215:LEU:HB3	2:C:248:SER:HB3	1.96	0.48
2:C:364:TYR:HB2	2:C:378:ARG:HA	1.94	0.48
1:A:227:SER:O	1:A:234:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:496:LYS:HE3	2:D:495:LEU:HD22	1.96	0.48
1:A:141:LEU:HD22	1:A:713:LYS:HD2	1.95	0.47
1:B:341:LEU:O	1:B:345:LEU:HG	2.15	0.47
2:C:169:THR:OG1	2:C:201:LYS:HG2	2.13	0.47
1:B:62:LEU:HD21	1:B:72:ALA:HB2	1.96	0.47
1:A:447:LYS:CD	1:A:728:ASP:HB2	2.44	0.47
1:A:390:LEU:O	1:A:393:LYS:HB3	2.14	0.47
1:A:324:ILE:HD13	1:A:425:PHE:HZ	1.80	0.47
2:D:66:ILE:HD11	2:D:156:LEU:HD22	1.96	0.47
2:D:26:LYS:HE2	2:D:30:GLN:CD	2.35	0.47
1:A:341:LEU:O	1:A:345:LEU:HG	2.14	0.47
1:B:217:LYS:HB2	1:B:256:ILE:HA	1.96	0.47
2:C:466:ALA:HB3	2:C:470:TYR:HE2	1.80	0.47
2:C:308:LEU:HB2	2:C:438:PHE:CE2	2.49	0.47
1:A:90:LEU:HD12	1:A:110:ILE:HG21	1.97	0.47
1:B:321:ASP:OD2	1:B:438:LYS:NZ	2.33	0.47
2:C:101:LEU:HB2	2:C:156:LEU:HB2	1.97	0.47
2:C:308:LEU:HD23	2:C:585:LEU:HD21	1.96	0.47
2:C:268:ASP:O	2:C:272:GLN:HG2	2.15	0.47
2:C:389:ASP:O	2:C:393:LEU:HD13	2.14	0.47
2:D:250:LYS:HD2	2:D:251:GLU:N	2.29	0.47
1:B:62:LEU:HD13	1:B:69:MET:HE1	1.97	0.46
1:A:303:ASP:CG	1:A:304:ASP:H	2.19	0.46
2:C:361:ALA:HB2	2:C:383:ALA:CB	2.45	0.46
2:D:-2:GLY:O	2:D:1:MET:HG2	2.16	0.46
1:B:180:ASN:OD1	1:B:187:PHE:N	2.44	0.46
1:B:41:LYS:O	1:B:41:LYS:HG2	2.13	0.46
1:A:713:LYS:O	1:A:717:LEU:HG	2.16	0.46
1:A:173:ALA:HA	1:A:328:ASN:HB2	1.98	0.45
1:A:334:THR:O	1:A:336:LYS:N	2.49	0.45
1:A:80:PHE:CZ	1:A:110:ILE:HG23	2.51	0.45
1:B:264:LEU:HD13	1:B:267:PHE:HD1	1.80	0.45
2:D:323:TYR:CE2	2:D:571:LEU:HB2	2.50	0.45
2:C:337:ILE:HG12	2:C:413:LEU:HD13	1.97	0.45
2:D:182:ALA:O	2:D:211:SER:HB3	2.17	0.45
1:A:32:GLU:O	1:A:36:ILE:HG12	2.16	0.45
1:B:264:LEU:HD13	1:B:267:PHE:CD1	2.51	0.45
1:A:197:ALA:HB1	1:A:300:PRO:HB3	1.98	0.45
1:B:324:ILE:HD13	1:B:425:PHE:HZ	1.81	0.45
2:C:525:LEU:HA	2:C:525:LEU:HD12	1.78	0.45
1:B:32:GLU:O	1:B:36:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:ALA:O	2:C:211:SER:OG	2.21	0.45
2:C:67:ILE:HD11	2:C:206:LEU:CD2	2.46	0.45
2:D:190:ASN:ND2	2:D:235:SER:OG	2.50	0.45
1:B:212:ILE:HD13	1:B:281:ILE:HG12	1.99	0.45
1:B:83:GLY:HA2	1:B:118:ILE:HG21	1.99	0.45
2:C:203:ASN:C	2:C:205:GLU:H	2.21	0.45
1:B:334:THR:O	1:B:336:LYS:N	2.50	0.45
2:C:286:LYS:O	2:C:290:LEU:HG	2.17	0.45
2:D:384:PRO:HB2	2:D:516:ILE:HG23	1.99	0.45
2:C:232:TYR:O	2:C:236:VAL:HG23	2.16	0.45
2:D:165:ASN:OD1	2:D:168:ASP:N	2.49	0.44
1:A:212:ILE:HB	1:A:261:LEU:HB2	1.99	0.44
1:A:288:GLU:HG3	1:A:289:PHE:N	2.32	0.44
2:D:283:VAL:O	2:D:287:ILE:HG13	2.17	0.44
1:A:124:PHE:HB2	1:A:434:TYR:HB2	1.98	0.44
1:B:263:GLU:HG3	1:B:264:LEU:N	2.33	0.44
2:C:311:GLN:NE2	2:C:434:GLU:HB3	2.32	0.44
1:A:167:ILE:HA	1:A:324:ILE:O	2.18	0.44
1:A:271:LYS:HE2	1:A:271:LYS:HB3	1.79	0.44
1:B:56:LEU:O	1:B:60:ILE:HG13	2.17	0.44
2:D:301:PHE:HE1	2:D:460:LEU:HD22	1.82	0.44
2:D:458:SER:HA	2:D:461:ARG:NH1	2.31	0.44
1:A:324:ILE:HD11	1:A:429:LEU:HD21	1.99	0.44
1:A:9:TRP:HA	1:A:41:LYS:HB3	2.00	0.44
1:B:167:ILE:HA	1:B:324:ILE:O	2.16	0.44
2:D:176:LEU:HD12	2:D:179:ILE:HD11	1.98	0.44
2:D:245:ILE:HG23	2:D:246:ALA:N	2.31	0.44
2:D:216:ASN:ND2	2:D:249:CYS:O	2.51	0.44
1:A:354:LEU:HD11	1:A:397:LEU:HG	2.00	0.44
2:D:210:ASN:HB2	2:D:278:LEU:HD21	1.99	0.44
2:D:359:LYS:HG2	2:D:360:ASP:H	1.82	0.44
2:D:361:ALA:O	2:D:362:TYR:HD1	2.01	0.44
2:D:495:LEU:O	2:D:500:ASN:ND2	2.51	0.44
1:A:124:PHE:HB2	1:A:434:TYR:CD1	2.52	0.43
2:C:249:CYS:O	2:C:250:LYS:HB2	2.18	0.43
2:C:25:PHE:CE2	2:C:27:GLY:HA3	2.53	0.43
2:C:364:TYR:OH	2:D:364:TYR:CG	2.71	0.43
2:D:212:ILE:HD11	2:D:269:PHE:CG	2.52	0.43
1:A:297:VAL:HG11	1:A:315:GLU:HG2	1.99	0.43
2:C:518:GLU:O	2:C:521:VAL:HG12	2.18	0.43
2:C:495:LEU:HD22	2:D:496:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:SER:OG	2:C:377:THR:HG23	2.18	0.43
2:D:27:GLY:C	2:D:28:ARG:HD2	2.38	0.43
1:B:12:GLU:HG3	1:B:41:LYS:HG3	2.01	0.43
2:C:244:LEU:HD22	2:C:269:PHE:HD1	1.84	0.43
2:D:512:PHE:CE2	2:D:540:ILE:HA	2.53	0.43
1:B:328:ASN:HB3	1:B:331:GLN:HG2	2.01	0.43
1:B:3:GLU:O	1:B:7:LYS:HG3	2.18	0.43
2:D:34:LYS:O	2:D:38:GLU:HG3	2.17	0.43
1:A:168:THR:HG23	1:A:325:HIS:CD2	2.54	0.43
2:C:27:GLY:C	2:C:28:ARG:HD2	2.39	0.43
2:D:253:LYS:O	2:D:254:ASP:HB2	2.19	0.43
1:A:90:LEU:CD1	1:A:110:ILE:HD13	2.49	0.43
1:A:187:PHE:HZ	1:A:285:SER:HG	1.67	0.43
1:A:721:GLU:HA	1:A:724:LEU:HD12	2.01	0.43
1:B:333:LEU:HD13	1:B:375:THR:HA	2.00	0.43
2:C:28:ARG:HD2	2:C:28:ARG:N	2.34	0.43
2:C:488:LEU:HD23	2:D:488:LEU:HD23	2.01	0.43
2:D:344:ILE:HG12	2:D:406:PHE:CD1	2.53	0.42
2:D:359:LYS:HG2	2:D:360:ASP:N	2.34	0.42
1:A:98:GLU:HA	1:A:101:SER:O	2.19	0.42
1:A:56:LEU:O	1:A:60:ILE:HG13	2.19	0.42
1:A:96:ILE:HG23	1:A:389:ASN:ND2	2.34	0.42
2:D:308:LEU:HD23	2:D:585:LEU:HD21	2.01	0.42
1:B:325:HIS:HB3	1:B:355:ILE:HD13	2.01	0.42
2:D:357:LYS:HB2	2:D:385:TYR:CD2	2.54	0.42
1:A:90:LEU:HD11	1:A:110:ILE:HD13	2.00	0.42
1:A:89:ASP:O	1:A:92:LYS:HB2	2.19	0.42
1:B:79:LEU:HD23	1:B:85:ILE:HG22	2.02	0.42
1:A:333:LEU:HG	1:A:338:ALA:HB2	2.01	0.42
2:D:111:VAL:HG21	2:D:129:TYR:CD2	2.55	0.42
2:C:428:ILE:HA	2:C:428:ILE:HD13	1.84	0.42
1:A:211:LYS:HA	1:A:261:LEU:O	2.20	0.42
1:A:65:ASP:OD1	1:A:68:SER:N	2.27	0.42
1:B:203:SER:OG	1:B:204:TYR:N	2.53	0.42
1:B:9:TRP:CE3	1:B:41:LYS:HB2	2.55	0.42
2:C:333:LEU:HD12	2:C:333:LEU:HA	1.92	0.42
2:D:76:SER:O	2:D:80:LEU:HG	2.20	0.42
1:B:170:VAL:HG23	1:B:302:LEU:HD11	2.02	0.42
2:C:348:ILE:HB	2:C:544:VAL:HG11	2.02	0.42
2:C:67:ILE:HA	2:C:159:THR:OG1	2.20	0.42
1:B:207:SER:OG	1:B:208:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HB2	1:B:18:PHE:CE2	2.55	0.42
2:D:348:ILE:HB	2:D:544:VAL:HG11	2.02	0.42
2:D:545:LEU:HG	2:D:550:VAL:HB	2.01	0.42
2:C:71:SER:O	2:C:71:SER:OG	2.35	0.41
2:D:202:ALA:HB1	2:D:207:LEU:H	1.83	0.41
2:D:250:LYS:O	2:D:251:GLU:HB3	2.21	0.41
2:D:372:LYS:HD3	2:D:372:LYS:N	2.36	0.41
1:B:287:LEU:O	1:B:291:LYS:N	2.44	0.41
1:A:324:ILE:HD13	1:A:425:PHE:CZ	2.55	0.41
1:A:14:GLN:O	1:A:16:LEU:HG	2.21	0.41
2:D:428:ILE:HD13	2:D:428:ILE:HA	1.85	0.41
2:C:364:TYR:HB2	2:C:377:THR:O	2.21	0.41
2:C:512:PHE:CE2	2:C:540:ILE:HA	2.55	0.41
1:A:254:PRO:N	1:A:259:ILE:HG12	2.35	0.41
2:D:442:PHE:HD1	2:D:445:ILE:HG13	1.85	0.41
1:B:181:ALA:HB1	1:B:404:ALA:HB3	2.03	0.41
1:B:87:LYS:HB3	1:B:87:LYS:HE2	1.94	0.41
1:B:95:LYS:O	1:B:98:GLU:CB	2.69	0.41
2:C:176:LEU:HD12	2:C:179:ILE:HD11	2.03	0.41
2:C:454:ASP:OD1	2:C:454:ASP:N	2.51	0.41
2:D:67:ILE:HD11	2:D:206:LEU:HD12	2.03	0.41
1:A:24:ASP:C	1:A:26:SER:H	2.24	0.41
2:C:466:ALA:HB3	2:C:470:TYR:CE2	2.55	0.41
2:D:11:LYS:HD2	2:D:11:LYS:HA	1.82	0.41
2:D:42:HIS:HB3	2:D:455:LYS:HB3	2.02	0.41
2:D:486:LEU:HD23	2:D:566:ILE:HD12	2.02	0.41
2:C:323:TYR:HA	2:C:326:PHE:HB3	2.03	0.41
2:C:408:LYS:O	2:C:412:GLU:HG2	2.21	0.41
2:D:28:ARG:NE	2:D:31:GLU:OE2	2.54	0.41
1:A:171:MET:HG3	1:A:302:LEU:HB2	2.02	0.40
2:D:184:TRP:CH2	2:D:198:ASP:HA	2.56	0.40
2:D:268:ASP:O	2:D:272:GLN:HG2	2.21	0.40
2:D:445:ILE:HD13	2:D:445:ILE:HA	1.94	0.40
1:B:106:ILE:H	1:B:106:ILE:HG13	1.73	0.40
1:B:364:SER:O	1:B:367:ASP:HB2	2.21	0.40
2:D:109:LEU:HD22	2:D:126:LEU:HA	2.04	0.40
2:D:467:SER:HA	2:D:470:TYR:HB2	2.03	0.40
1:B:175:LYS:H	1:B:175:LYS:HG2	1.78	0.40
2:C:42:HIS:ND1	2:C:455:LYS:HD3	2.36	0.40
2:C:62:VAL:HG21	2:C:275:THR:HB	2.03	0.40
2:C:384:PRO:HB3	2:C:534:TYR:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:ASN:O	2:C:83:GLY:N	2.54	0.40
1:A:221:GLN:O	1:A:224:LEU:HG	2.22	0.40
2:C:61:ASN:N	2:C:61:ASN:OD1	2.54	0.40
2:D:38:GLU:N	2:D:39:PRO:HD3	2.37	0.40

There are no symmetry-related clashes.

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	685/732 (94%)	627 (92%)	54 (8%)	4 (1%)	25	61
1	B	569/732 (78%)	514 (90%)	53 (9%)	2 (0%)	34	69
2	C	590/614 (96%)	526 (89%)	59 (10%)	5 (1%)	19	56
2	D	590/614 (96%)	533 (90%)	50 (8%)	7 (1%)	13	48
All	All	2434/2692 (90%)	2200 (90%)	216 (9%)	18 (1%)	22	59

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	245	ILE
2	D	245	ILE
2	D	360	ASP
2	D	361	ALA
1	A	319	GLU
1	B	335	GLN
1	A	197	ALA
1	A	335	GLN
1	B	197	ALA
2	C	244	LEU
2	C	96	PHE

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Mol	Chain	Res	Type
2	D	39	PRO
2	C	39	PRO
2	C	249	CYS
2	D	96	PHE
2	D	249	CYS
2	D	523	TYR
1	A	115	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/683 (66%)	434 (97%)	14 (3%)	40	65
1	B	440/683 (64%)	429 (98%)	11 (2%)	47	70
2	C	555/569 (98%)	529 (95%)	26 (5%)	26	56
2	D	555/569 (98%)	519 (94%)	36 (6%)	17	48
All	All	1998/2504 (80%)	1911 (96%)	87 (4%)	28	57

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	44	TYR
1	A	46	ARG
1	A	61	ASP
1	A	103	ASN
1	A	171	MET
1	A	187	PHE
1	A	241	ASP
1	A	264	LEU
1	A	308	GLN
1	A	316	TYR
1	A	349	ARG
1	A	350	LEU
1	A	459	SER

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Mol	Chain	Res	Type
1	B	22	PHE
1	B	61	ASP
1	B	171	MET
1	B	187	PHE
1	B	266	ASN
1	B	308	GLN
1	B	316	TYR
1	B	318	ARG
1	B	333	LEU
1	B	351	SER
1	B	446	TYR
2	C	-1	SER
2	C	14	GLU
2	C	25	PHE
2	C	28	ARG
2	C	57	SER
2	C	71	SER
2	C	170	LEU
2	C	194	LYS
2	C	232	TYR
2	C	258	TYR
2	C	259	GLU
2	C	324	GLU
2	C	359	LYS
2	C	363	PHE
2	C	375	LEU
2	C	381	TYR
2	C	382	LYS
2	C	385	TYR
2	C	397	TYR
2	C	444	ASN
2	C	454	ASP
2	C	458	SER
2	C	474	ASP
2	C	513	SER
2	C	514	ARG
2	C	534	TYR
2	D	23	ASP
2	D	28	ARG
2	D	57	SER
2	D	71	SER
2	D	128	PHE

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Mol	Chain	Res	Type
2	D	131	ASP
2	D	168	ASP
2	D	170	LEU
2	D	185	LEU
2	D	207	LEU
2	D	216	ASN
2	D	232	TYR
2	D	243	GLU
2	D	244	LEU
2	D	245	ILE
2	D	250	LYS
2	D	251	GLU
2	D	258	TYR
2	D	259	GLU
2	D	307	ARG
2	D	323	TYR
2	D	335	HIS
2	D	353	PHE
2	D	363	PHE
2	D	370	PHE
2	D	375	LEU
2	D	381	TYR
2	D	382	LYS
2	D	385	TYR
2	D	389	ASP
2	D	444	ASN
2	D	454	ASP
2	D	458	SER
2	D	474	ASP
2	D	534	TYR
2	D	538	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
2	C	311	GLN
2	D	69	GLN
2	D	216	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	699/732 (95%)	0.57	74 (10%) 6 5	101, 234, 464, 550	0
1	B	587/732 (80%)	0.67	68 (11%) 4 4	100, 213, 427, 486	0
2	C	598/614 (97%)	0.76	63 (10%) 6 5	101, 165, 310, 428	0
2	D	598/614 (97%)	0.72	54 (9%) 9 7	101, 170, 307, 448	0
All	All	2482/2692 (92%)	0.67	259 (10%) 6 5	100, 191, 424, 550	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	221	LEU	9.7
2	C	368	LYS	7.4
2	C	367	SER	7.2
2	C	377	THR	6.6
1	A	591	ASP	6.4
1	A	664	ASN	6.4
1	A	677	HIS	6.3
2	C	220	LYS	6.2
1	B	717	LEU	5.7
1	A	195	GLU	5.7
2	C	164	ALA	5.7
1	B	195	GLU	5.7
1	A	434	TYR	5.6
1	B	583	SER	5.6
1	A	577	GLU	5.5
1	B	713	LYS	5.4
2	C	381	TYR	5.3
1	B	434	TYR	5.3
2	D	228	ASN	5.3
1	A	435	ALA	5.3
1	A	578	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	731	HIS	5.2
1	A	574	LYS	5.2
2	D	166	GLU	5.2
2	D	203	ASN	5.2
1	A	724	LEU	5.1
2	C	380	ASP	5.1
1	A	676	LYS	5.0
2	C	369	GLY	5.0
1	B	714	ILE	4.9
1	B	245	ASN	4.9
1	B	254	PRO	4.7
1	A	245	ASN	4.6
1	A	700	ASP	4.6
2	D	384	PRO	4.5
2	C	30	GLN	4.4
1	B	679	GLU	4.4
1	A	673	ASP	4.4
1	A	541	GLN	4.4
1	A	595	ASN	4.3
1	A	275	SER	4.2
2	D	253	LYS	4.2
2	D	363	PHE	4.2
1	A	210	ALA	4.2
1	A	610	SER	4.1
1	A	492	LEU	4.0
2	D	535	PRO	4.0
1	A	540	ALA	4.0
1	B	210	ALA	4.0
2	C	352	ILE	3.9
1	B	587	ASP	3.9
2	D	164	ALA	3.9
2	D	221	LEU	3.9
1	A	496	ALA	3.9
2	C	219	ASP	3.8
1	B	499	GLU	3.8
2	C	172	THR	3.8
2	C	363	PHE	3.8
1	B	411	LEU	3.7
1	B	85	ILE	3.7
2	D	396	PHE	3.6
1	A	439	SER	3.6
2	D	258	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	174	ASP	3.5
1	A	141	LEU	3.5
1	A	609	ASP	3.5
2	C	37	ASN	3.5
1	B	306	VAL	3.5
1	A	158	PHE	3.5
2	D	135	GLU	3.5
1	B	495	GLU	3.4
2	C	231	ASN	3.4
1	B	504	ILE	3.4
1	B	672	ASN	3.4
1	A	727	ALA	3.4
2	C	163	ASN	3.3
2	C	348	ILE	3.3
1	A	544	ASN	3.3
2	C	26	LYS	3.3
1	B	496	ALA	3.3
2	D	505	THR	3.3
2	C	22	ASP	3.3
2	D	534	TYR	3.2
1	A	491	THR	3.2
1	A	728	ASP	3.2
2	C	129	TYR	3.2
2	C	173	LEU	3.2
1	B	16	LEU	3.1
1	B	147	LEU	3.1
2	D	509	LEU	3.1
2	C	94	VAL	3.1
2	D	37	ASN	3.1
1	A	276	ALA	3.0
1	B	362	LEU	3.0
1	B	457	ILE	3.0
2	C	370	PHE	3.0
1	A	598	GLU	3.0
1	A	450	LEU	3.0
1	A	138	LEU	3.0
1	B	446	TYR	3.0
2	C	190	ASN	3.0
1	A	443	LEU	3.0
2	D	348	ILE	3.0
2	C	382	LYS	2.9
1	B	86	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	312	PHE	2.9
2	C	228	ASN	2.9
2	D	165	ASN	2.9
1	A	703	ILE	2.9
1	A	184	LYS	2.8
1	A	499	GLU	2.8
1	B	329	ALA	2.8
2	D	337	ILE	2.8
2	C	162	LEU	2.8
1	B	106	ILE	2.8
1	B	460	GLU	2.8
1	B	215	TRP	2.8
1	B	584	LEU	2.8
1	B	363	LEU	2.7
1	B	209	GLU	2.7
1	A	316	TYR	2.7
2	C	379	TYR	2.7
2	C	396	PHE	2.7
2	D	381	TYR	2.7
2	C	70	PHE	2.7
2	D	383	ALA	2.7
2	D	344	ILE	2.7
1	A	1	MET	2.7
2	D	246	ALA	2.7
2	C	33	CYS	2.6
1	B	453	GLU	2.6
1	B	382	ARG	2.6
2	C	362	TYR	2.6
1	A	341	LEU	2.6
1	B	103	ASN	2.6
1	A	429	LEU	2.6
1	B	710	ASN	2.6
2	C	498	PHE	2.6
1	A	661	LEU	2.6
1	A	163	PHE	2.6
1	A	453	GLU	2.5
2	C	378	ARG	2.5
2	D	379	TYR	2.5
1	A	215	TRP	2.5
1	A	704	LEU	2.5
1	B	413	SER	2.5
2	C	384	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	498	ASP	2.5
1	B	158	PHE	2.5
2	D	340	GLN	2.5
1	A	182	LEU	2.5
2	D	548	LEU	2.5
2	C	544	VAL	2.5
1	B	269	SER	2.5
2	D	392	PHE	2.5
2	D	352	ILE	2.5
1	A	594	ASP	2.5
1	B	461	TYR	2.5
1	A	345	LEU	2.5
1	B	450	LEU	2.5
2	C	218	LYS	2.4
1	B	345	LEU	2.4
2	C	592	LEU	2.4
1	B	716	LYS	2.4
1	B	273	LYS	2.4
1	A	254	PRO	2.4
1	B	294	ILE	2.4
1	A	47	TYR	2.4
1	B	454	LEU	2.4
2	D	30	GLN	2.4
2	C	501	TYR	2.4
1	B	236	PHE	2.4
2	D	357	LYS	2.4
2	D	319	LEU	2.4
2	D	254	ASP	2.4
1	A	382	ARG	2.4
2	C	330	ILE	2.4
2	D	188	ILE	2.4
2	D	365	LYS	2.4
2	D	232	TYR	2.4
1	A	379	LEU	2.3
1	A	190	VAL	2.3
1	A	214	PHE	2.3
2	D	578	ILE	2.3
1	A	128	PHE	2.3
2	C	263	PHE	2.3
1	A	457	ILE	2.3
1	B	206	LYS	2.3
2	D	606	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	144	ASP	2.3
1	A	708	GLU	2.3
1	B	435	ALA	2.3
1	A	714	ILE	2.3
1	B	357	LEU	2.3
2	D	413	LEU	2.3
2	D	9	PHE	2.3
1	A	383	LEU	2.3
2	D	512	PHE	2.3
1	B	270	ALA	2.2
2	C	244	LEU	2.2
2	C	361	ALA	2.2
1	B	151	LEU	2.2
2	D	428	ILE	2.2
1	B	138	LEU	2.2
1	B	394	ILE	2.2
2	C	253	LYS	2.2
2	D	435	ILE	2.2
2	D	341	LEU	2.2
1	A	463	MET	2.2
2	C	283	VAL	2.2
2	C	388	SER	2.2
2	D	291	CYS	2.2
1	A	362	LEU	2.2
1	A	110	ILE	2.2
1	B	456	ASN	2.2
2	C	217	GLN	2.2
2	D	410	LYS	2.2
2	C	364	TYR	2.2
1	A	236	PHE	2.2
1	A	404	ALA	2.2
2	C	435	ILE	2.2
2	C	535	PRO	2.1
2	C	312	PHE	2.1
2	C	291	CYS	2.1
2	D	545	LEU	2.1
1	B	137	GLU	2.1
1	A	587	ASP	2.1
2	C	166	GLU	2.1
1	B	675	LEU	2.1
2	C	323	TYR	2.1
1	A	84	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	570	GLU	2.1
1	B	668	PHE	2.1
1	B	720	LEU	2.1
2	C	471	PHE	2.1
2	D	376	TYR	2.1
1	A	416	SER	2.1
2	C	195	SER	2.1
1	A	147	LEU	2.1
2	C	298	ASN	2.1
2	C	534	TYR	2.1
1	A	124	PHE	2.1
2	D	609	ASP	2.1
1	B	170	VAL	2.1
2	D	129	TYR	2.1
2	D	385	TYR	2.1
2	D	464	CYS	2.0
1	B	458	LEU	2.0
2	C	111	VAL	2.0
2	C	464	CYS	2.0
1	B	333	LEU	2.0
1	B	383	LEU	2.0
2	C	326	PHE	2.0
1	B	429	LEU	2.0
1	A	304	ASP	2.0
1	B	47	TYR	2.0
2	D	364	TYR	2.0
2	D	374	ASP	2.0
1	A	333	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.