



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:04 PM UTC

PDB ID : 8J8Q / pdb_00008j8q
Title : Structure of the four-component Paf1 complex from *Saccharomyces eubayanus*
Authors : Wang, Z.; Qin, Y.; Zhou, Y.; Cao, Y.
Deposited on : 2023-05-02
Resolution : 3.11 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
Mogul : 2022.3.0, CSD as543be (2022)
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

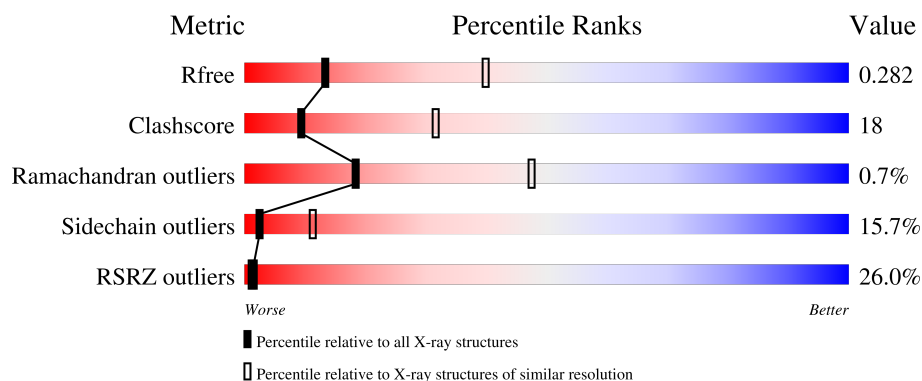
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	C	907	
2	P	111	
3	R	77	
4	A	81	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8756 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 CTR9-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	866	Total	C	N	O	S	Se	0	0	0
			7031	4489	1184	1338	6	14			

- Molecule 2 is a protein called PAF1-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	98	Total	C	N	O	Se	0	0	0
			784	502	130	150	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	0	SER	-	expression tag	UNP A0A0L8RM45

- Molecule 3 is a protein called RTF1-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	69	Total	C	N	O	Se	0	0	0
			594	373	107	112	2			

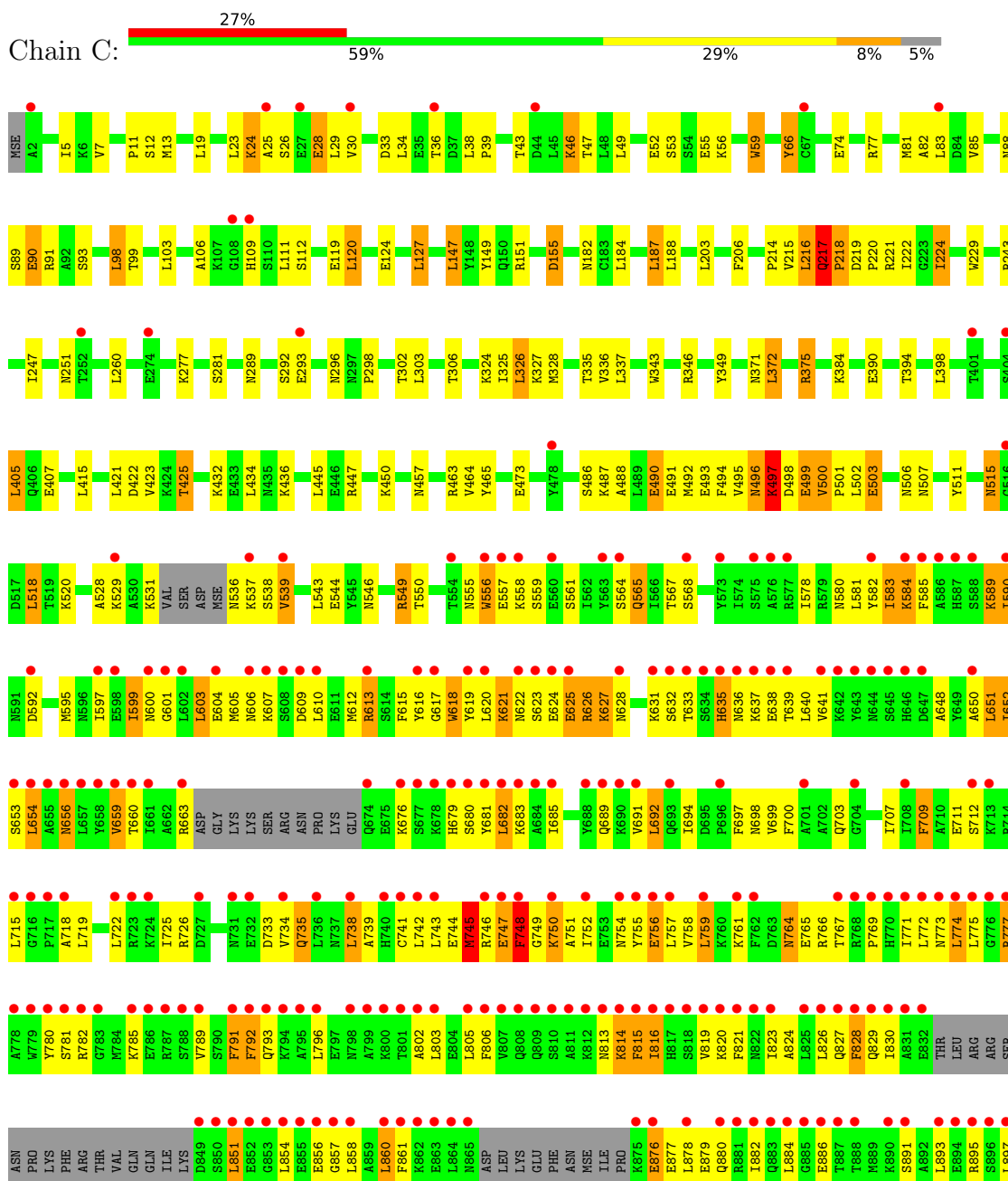
- Molecule 4 is a protein called CDC73-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	44	Total	C	N	O	Se	0	0	0
			347	218	63	65	1			

3 Residue-property plots [i](#)

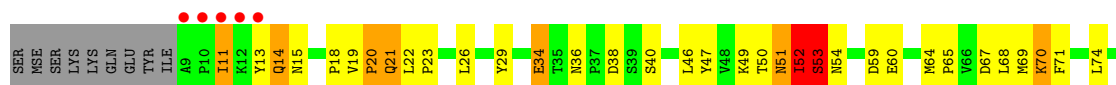
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CTR9-like protein





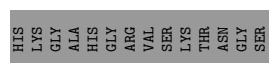
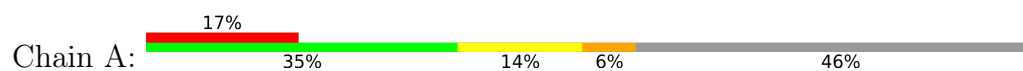
• Molecule 2: PAF1-like protein



• Molecule 3: RTF1-like protein



• Molecule 4: CDC73-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.63Å 89.17Å 128.07Å 90.00° 97.08° 90.00°	Depositor
Resolution (Å)	27.07 – 3.11 27.07 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.7 (27.07-3.11) 98.8 (27.07-3.11)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.237 , 0.278 0.253 , 0.282	Depositor DCC
R_{free} test set	1428 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8756	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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	C	0.61	18/7144 (0.3%)	0.73	25/9608 (0.3%)
2	P	1.00	9/798 (1.1%)	0.85	4/1082 (0.4%)
3	R	0.14	0/597	0.41	0/783
4	A	0.15	0/350	0.41	0/470
All	All	0.62	27/8889 (0.3%)	0.71	29/11943 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	LEU	CA-C	-9.81	1.40	1.52
2	P	53	SER	CA-C	-8.53	1.40	1.52
2	P	54	ASN	C-O	-7.33	1.14	1.24
1	C	219	ASP	C-O	-6.90	1.15	1.24
1	C	13	MSE	CA-C	-6.88	1.43	1.52
1	C	746	ARG	C-O	-6.76	1.19	1.24
2	P	51	ASN	C-O	-6.70	1.16	1.24
1	C	216	LEU	C-O	-6.65	1.15	1.23
2	P	52	ILE	CA-C	-6.44	1.45	1.53
1	C	59	TRP	C-O	-6.41	1.16	1.24
2	P	53	SER	C-O	-6.29	1.15	1.24
1	C	90	GLU	N-CA	-6.08	1.38	1.46
1	C	490	GLU	CA-C	-5.72	1.45	1.52
1	C	88	ASN	C-O	-5.66	1.16	1.24
1	C	38	LEU	CA-C	-5.61	1.45	1.52
2	P	54	ASN	CG-OD1	-5.52	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	86	PHE	C-O	-5.50	1.16	1.23
1	C	217	GLN	C-O	-5.44	1.18	1.24
2	P	51	ASN	CG-OD1	-5.37	1.13	1.23
1	C	59	TRP	CA-C	-5.28	1.46	1.52
1	C	219	ASP	CG-OD2	-5.24	1.15	1.25
1	C	618	TRP	CB-CG	-5.21	1.34	1.50
1	C	219	ASP	CB-CG	-5.15	1.39	1.52
1	C	12	SER	CA-C	-5.15	1.46	1.52
1	C	33	ASP	C-O	-5.09	1.17	1.24
2	P	50	THR	C-O	-5.08	1.17	1.24
1	C	85	VAL	C-O	-5.06	1.18	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	51	ASN	N-CA-C	18.06	130.40	111.07
1	C	748	PHE	N-CA-C	16.34	129.09	111.28
1	C	26	SER	N-CA-C	16.11	133.44	111.54
1	C	217	GLN	C-N-CD	-13.56	90.77	120.60
1	C	90	GLU	N-CA-C	-12.73	98.22	113.88
1	C	622	ASN	N-CA-C	11.84	123.74	111.07
1	C	217	GLN	CA-C-N	11.30	154.13	127.00
1	C	217	GLN	C-N-CA	11.30	154.13	127.00
1	C	498	ASP	CA-C-N	-9.17	108.09	122.67
1	C	498	ASP	C-N-CA	-9.17	108.09	122.67
1	C	497	LYS	N-CA-C	7.99	122.46	112.87
1	C	36	THR	N-CA-C	7.47	122.62	112.68
1	C	217	GLN	N-CA-C	-7.46	98.00	109.64
1	C	34	LEU	N-CA-C	7.33	121.66	112.87
2	P	54	ASN	N-CA-C	-7.16	104.42	113.02
1	C	217	GLN	CB-CA-C	-6.98	101.23	109.47
1	C	745	MSE	N-CA-C	6.87	118.84	111.36
1	C	499	GLU	N-CA-C	6.74	120.81	112.59
1	C	25	ALA	N-CA-C	6.60	120.19	111.28
1	C	625	GLU	N-CA-C	6.58	124.80	110.80
1	C	623	SER	N-CA-C	6.41	124.44	110.80
1	C	500	VAL	CB-CA-C	-6.04	103.74	110.68
1	C	85	VAL	CB-CA-C	-5.80	101.78	111.29
1	C	490	GLU	CB-CA-C	-5.64	101.99	110.90
2	P	52	ILE	N-CA-CB	-5.43	104.88	111.94
1	C	36	THR	CB-CA-C	-5.34	101.33	110.24
2	P	53	SER	N-CA-C	5.26	119.32	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ASN	N-CA-C	5.22	121.93	110.80
1	C	626	ARG	N-CA-C	5.21	121.89	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	GLN	Peptide
1	C	609	ASP	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	C	7031	0	7075	289	0
2	P	784	0	805	45	0
3	R	594	0	610	11	0
4	A	347	0	356	10	0
All	All	8756	0	8846	316	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 18.

All (316) 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:C:747:GLU:HG3	1:C:782:ARG:NH2	1.41	1.32
1:C:747:GLU:HG3	1:C:782:ARG:CZ	1.58	1.32
1:C:747:GLU:CG	1:C:782:ARG:NH2	2.06	1.19
1:C:747:GLU:CG	1:C:782:ARG:CZ	2.28	1.10
1:C:626:ARG:HD3	1:C:631:LYS:HG3	1.45	0.99
1:C:742:LEU:HD23	1:C:745:MSE:SE	2.12	0.98
1:C:813:ASN:O	1:C:816:ILE:CD1	2.11	0.98
1:C:773:ASN:HD22	1:C:815:PHE:HE1	1.04	0.95
1:C:813:ASN:O	1:C:816:ILE:HD11	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:TRP:CE3	1:C:82:ALA:HB2	2.07	0.88
1:C:229:TRP:HE1	2:P:53:SER:HB3	1.39	0.87
1:C:496:ASN:ND2	1:C:496:ASN:O	2.07	0.86
1:C:556:TRP:H	1:C:556:TRP:CD1	1.87	0.86
1:C:748:PHE:HD1	1:C:782:ARG:NH2	1.75	0.83
1:C:747:GLU:HG3	1:C:782:ARG:HH21	1.42	0.83
1:C:816:ILE:H	1:C:816:ILE:HD12	1.43	0.83
1:C:747:GLU:HG3	1:C:782:ARG:NE	1.95	0.82
1:C:747:GLU:CB	1:C:782:ARG:NH2	2.43	0.81
1:C:492:MSE:HE2	1:C:501:PRO:HD3	1.64	0.80
1:C:744:GLU:OE2	2:P:11:ILE:HG12	1.80	0.80
1:C:206:PHE:HB3	1:C:224:ILE:HG22	1.63	0.79
1:C:813:ASN:O	1:C:816:ILE:HD12	1.83	0.79
1:C:773:ASN:ND2	1:C:815:PHE:HE1	1.81	0.79
1:C:806:PHE:HD2	1:C:819:VAL:HG11	1.48	0.78
1:C:769:PRO:HA	1:C:806:PHE:HE1	1.49	0.77
1:C:722:LEU:HB3	1:C:738:LEU:HG	1.67	0.77
1:C:748:PHE:CD1	1:C:782:ARG:NH2	2.53	0.77
1:C:782:ARG:HE	1:C:785:LYS:HE2	1.49	0.75
1:C:806:PHE:CE2	1:C:819:VAL:HG21	2.21	0.75
1:C:496:ASN:ND2	1:C:499:GLU:H	1.85	0.75
1:C:626:ARG:CZ	1:C:631:LYS:HD2	2.18	0.73
1:C:747:GLU:HB3	1:C:782:ARG:NH2	2.03	0.73
1:C:697:PHE:HB2	4:A:185:ARG:HD3	1.71	0.72
1:C:538:SER:HA	4:A:170:THR:HG22	1.70	0.72
1:C:806:PHE:CD2	1:C:819:VAL:HG11	2.24	0.72
1:C:621:LYS:H	1:C:621:LYS:HD2	1.53	0.72
1:C:496:ASN:ND2	1:C:499:GLU:N	2.38	0.71
1:C:748:PHE:CD2	1:C:752:ILE:HD12	2.25	0.71
1:C:633:THR:HB	1:C:637:LYS:NZ	2.06	0.71
1:C:595:MSE:HG3	1:C:619:TYR:CE2	2.25	0.70
1:C:604:GLU:HB3	1:C:607:LYS:HE2	1.73	0.70
1:C:816:ILE:HD12	1:C:816:ILE:N	2.07	0.70
1:C:879:GLU:HA	1:C:882:ILE:HD12	1.72	0.70
1:C:592:ASP:OD2	1:C:624:GLU:HB3	1.91	0.69
1:C:621:LYS:HD2	1:C:621:LYS:N	2.07	0.69
1:C:748:PHE:CG	1:C:782:ARG:HG3	2.26	0.69
1:C:747:GLU:HG2	1:C:782:ARG:CZ	2.19	0.69
1:C:748:PHE:HD2	1:C:752:ILE:HD12	1.56	0.69
1:C:620:LEU:CD2	1:C:626:ARG:HD2	2.22	0.68
1:C:603:LEU:HD21	1:C:616:TYR:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:ARG:HD3	1:C:631:LYS:CG	2.23	0.67
1:C:902:GLU:HA	1:C:905:LYS:HD2	1.77	0.66
1:C:620:LEU:HD22	1:C:626:ARG:HD2	1.78	0.66
1:C:663:ARG:NH1	1:C:711:GLU:OE1	2.29	0.66
1:C:803:LEU:HD13	1:C:819:VAL:HG13	1.78	0.65
1:C:742:LEU:HD13	1:C:750:LYS:HB3	1.77	0.64
1:C:748:PHE:H	1:C:782:ARG:HH21	1.43	0.64
1:C:792:PHE:HB3	1:C:830:ILE:HG12	1.79	0.64
1:C:827:GLN:HE22	1:C:860:LEU:HD13	1.63	0.64
1:C:703:GLN:NE2	2:P:15:ASN:OD1	2.31	0.64
1:C:782:ARG:NE	1:C:785:LYS:HE2	2.12	0.63
1:C:506:ASN:HD21	1:C:546:ASN:HD22	1.47	0.63
1:C:496:ASN:HD21	1:C:499:GLU:N	1.97	0.63
1:C:556:TRP:CD1	1:C:556:TRP:N	2.65	0.63
2:P:74:LEU:HD22	2:P:83:LEU:HD21	1.81	0.63
1:C:303:LEU:HD21	2:P:52:ILE:HD11	1.80	0.63
1:C:747:GLU:HG3	1:C:782:ARG:CD	2.29	0.63
1:C:260:LEU:HD22	2:P:52:ILE:HG12	1.79	0.63
1:C:496:ASN:HD22	1:C:499:GLU:H	1.47	0.62
1:C:709:PHE:HB3	1:C:718:ALA:HB2	1.79	0.62
1:C:492:MSE:HE2	1:C:501:PRO:CD	2.28	0.62
1:C:595:MSE:HG3	1:C:619:TYR:HE2	1.65	0.62
3:R:539:ARG:HA	3:R:542:LYS:HG3	1.82	0.62
1:C:556:TRP:H	1:C:556:TRP:HD1	1.43	0.61
1:C:854:LEU:HG	1:C:893:LEU:HD12	1.81	0.61
1:C:806:PHE:HD2	1:C:819:VAL:CG1	2.14	0.60
1:C:772:LEU:HB3	1:C:802:ALA:HB2	1.83	0.60
1:C:445:LEU:HD22	1:C:464:VAL:HG23	1.84	0.60
1:C:59:TRP:CZ3	1:C:82:ALA:HB2	2.36	0.60
1:C:83:LEU:O	1:C:91:ARG:NH2	2.33	0.60
1:C:488:ALA:O	1:C:492:MSE:HB2	2.01	0.60
1:C:739:ALA:HB2	1:C:754:ASN:HB2	1.84	0.60
1:C:124:GLU:OE2	1:C:151:ARG:NH2	2.35	0.60
1:C:590:ILE:HD11	1:C:595:MSE:HB2	1.84	0.59
1:C:806:PHE:CE2	1:C:819:VAL:CG2	2.85	0.59
1:C:858:LEU:HD22	1:C:886:GLU:HG2	1.84	0.59
1:C:24:LYS:N	1:C:52:GLU:OE1	2.30	0.59
1:C:375:ARG:HB3	1:C:398:LEU:HD11	1.85	0.59
2:P:52:ILE:HG23	2:P:52:ILE:O	2.03	0.59
1:C:616:TYR:CZ	1:C:620:LEU:HD11	2.37	0.58
1:C:620:LEU:HD22	1:C:626:ARG:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:ASP:OD1	2:P:14:GLN:NE2	2.36	0.58
1:C:43:THR:HG23	1:C:81:MSE:HE1	1.84	0.58
1:C:302:THR:O	1:C:306:THR:HG23	2.03	0.58
1:C:492:MSE:HG2	1:C:500:VAL:HG22	1.85	0.58
1:C:621:LYS:HE3	1:C:632:SER:OG	2.04	0.58
1:C:636:ASN:ND2	1:C:653:SER:OG	2.36	0.58
4:A:166:VAL:O	4:A:170:THR:HG23	2.03	0.58
1:C:372:LEU:HD11	1:C:405:LEU:HD21	1.86	0.57
1:C:680:SER:HA	1:C:683:LYS:HD2	1.85	0.57
1:C:349:TYR:OH	2:P:38:ASP:O	2.20	0.57
1:C:306:THR:HG22	1:C:343:TRP:CE2	2.40	0.57
1:C:447:ARG:HA	1:C:450:LYS:HE3	1.86	0.57
1:C:821:PHE:HD1	1:C:821:PHE:O	1.86	0.57
1:C:851:LEU:HD22	1:C:893:LEU:HB3	1.87	0.56
1:C:582:TYR:HE2	1:C:618:TRP:CH2	2.23	0.56
1:C:503:GLU:HG3	2:P:29:TYR:HA	1.87	0.56
1:C:610:LEU:HD23	1:C:610:LEU:H	1.70	0.56
2:P:47:TYR:O	2:P:51:ASN:HB3	2.05	0.56
1:C:493:GLU:O	1:C:497:LYS:HG3	2.05	0.56
1:C:465:TYR:HB2	1:C:488:ALA:HB2	1.88	0.56
1:C:432:LYS:O	1:C:436:LYS:HG2	2.05	0.56
1:C:581:LEU:HD13	1:C:595:MSE:SE	2.56	0.56
1:C:621:LYS:O	1:C:627:LYS:HD3	2.06	0.56
1:C:511:TYR:O	1:C:515:ASN:ND2	2.38	0.56
1:C:564:SER:O	1:C:568:SER:N	2.38	0.56
1:C:681:TYR:OH	1:C:711:GLU:OE2	2.23	0.55
1:C:747:GLU:HG3	1:C:782:ARG:HD3	1.88	0.55
1:C:748:PHE:HD2	1:C:752:ILE:CD1	2.19	0.55
1:C:539:VAL:O	1:C:543:LEU:HG	2.05	0.55
1:C:621:LYS:CE	1:C:632:SER:OG	2.54	0.55
2:P:26:LEU:HD13	4:A:177:VAL:HB	1.89	0.55
1:C:89:SER:O	1:C:89:SER:OG	2.23	0.55
1:C:486:SER:O	1:C:490:GLU:HG3	2.06	0.55
1:C:638:GLU:HA	1:C:641:VAL:HG22	1.89	0.54
1:C:748:PHE:HD1	1:C:782:ARG:HH21	1.52	0.54
2:P:103:ARG:HB3	2:P:106:ARG:HH21	1.72	0.54
1:C:854:LEU:O	1:C:858:LEU:HG	2.07	0.54
1:C:901:GLU:O	1:C:905:LYS:HG3	2.08	0.54
2:P:103:ARG:O	2:P:106:ARG:NE	2.41	0.54
1:C:726:ARG:HH22	1:C:757:LEU:HD21	1.73	0.54
1:C:28:GLU:CD	1:C:28:GLU:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:PRO:O	1:C:221:ARG:NH2	2.41	0.53
1:C:791:PHE:CD1	1:C:791:PHE:N	2.76	0.53
1:C:549:ARG:HH12	2:P:21:GLN:HG2	1.73	0.53
1:C:549:ARG:NH1	2:P:21:GLN:HG2	2.24	0.53
1:C:375:ARG:NH2	1:C:394:THR:O	2.42	0.53
1:C:891:SER:O	1:C:895:ARG:HG2	2.08	0.53
1:C:627:LYS:O	1:C:628:ASN:C	2.52	0.52
1:C:747:GLU:HB3	1:C:782:ARG:HH22	1.70	0.52
1:C:735:GLN:NE2	1:C:754:ASN:O	2.42	0.52
1:C:791:PHE:N	1:C:791:PHE:HD1	2.07	0.52
1:C:277:LYS:O	1:C:281:SER:OG	2.23	0.52
1:C:503:GLU:O	1:C:507:ASN:ND2	2.42	0.52
4:A:178:GLN:HG2	4:A:182:SER:HB2	1.90	0.52
1:C:23:LEU:HD23	1:C:52:GLU:CD	2.35	0.52
1:C:103:LEU:HD21	1:C:147:LEU:HD22	1.91	0.52
1:C:621:LYS:HZ1	1:C:632:SER:HA	1.75	0.52
1:C:346:ARG:HH21	2:P:40:SER:HB2	1.75	0.52
1:C:735:GLN:HE21	1:C:758:VAL:HG23	1.75	0.52
1:C:296:ASN:HB3	1:C:328:MSE:HE1	1.92	0.51
1:C:620:LEU:HD22	1:C:626:ARG:CB	2.41	0.51
1:C:289:ASN:O	1:C:292:SER:OG	2.29	0.51
1:C:473:GLU:OE2	4:A:175:ARG:NH1	2.44	0.51
1:C:726:ARG:NH1	1:C:735:GLN:OE1	2.43	0.51
1:C:595:MSE:CG	1:C:619:TYR:HE2	2.24	0.51
1:C:626:ARG:NE	1:C:631:LYS:HD2	2.25	0.51
2:P:103:ARG:HB3	2:P:106:ARG:HE	1.74	0.51
3:R:536:THR:HG22	3:R:539:ARG:HD2	1.92	0.51
1:C:748:PHE:N	1:C:782:ARG:HH21	2.07	0.50
1:C:806:PHE:HE2	1:C:819:VAL:CG2	2.23	0.50
1:C:77:ARG:O	1:C:81:MSE:HG3	2.11	0.50
1:C:184:LEU:HD21	2:P:71:PHE:CZ	2.45	0.50
1:C:748:PHE:HB3	1:C:782:ARG:HG3	1.94	0.50
1:C:515:ASN:H	1:C:515:ASN:HD22	1.58	0.50
1:C:538:SER:HB3	4:A:170:THR:HA	1.93	0.50
1:C:769:PRO:HA	1:C:806:PHE:CE1	2.38	0.50
1:C:56:LYS:NZ	1:C:93:SER:OG	2.37	0.50
1:C:764:ASN:HB3	1:C:767:THR:OG1	2.12	0.50
1:C:599:ILE:O	1:C:603:LEU:N	2.46	0.49
1:C:741:CYS:O	1:C:745:MSE:HB3	2.12	0.49
1:C:546:ASN:O	1:C:550:THR:OG1	2.20	0.49
1:C:561:SER:O	1:C:565:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:GLU:O	1:C:769:PRO:HD2	2.13	0.49
1:C:585:PHE:HA	1:C:590:ILE:HG21	1.94	0.49
1:C:106:ALA:HB2	1:C:119:GLU:HB2	1.95	0.49
1:C:656:ASN:O	1:C:660:THR:HG23	2.13	0.49
1:C:120:LEU:O	1:C:124:GLU:HG2	2.13	0.49
1:C:55:GLU:O	1:C:59:TRP:HD1	1.95	0.49
1:C:650:ALA:O	1:C:653:SER:OG	2.27	0.49
1:C:613:ARG:O	1:C:616:TYR:HB3	2.13	0.48
1:C:827:GLN:OE1	1:C:857:GLY:HA2	2.13	0.48
1:C:600:ASN:HA	1:C:603:LEU:HB2	1.94	0.48
1:C:685:ILE:HG22	1:C:689:GLN:NE2	2.28	0.48
1:C:506:ASN:HD21	1:C:546:ASN:ND2	2.12	0.48
1:C:217:GLN:HG2	2:P:70:LYS:HD3	1.96	0.48
1:C:243:ARG:CZ	1:C:247:ILE:HD11	2.44	0.48
1:C:592:ASP:CG	1:C:624:GLU:HB3	2.38	0.47
1:C:651:LEU:HD11	1:C:691:VAL:HB	1.95	0.47
1:C:773:ASN:HB2	1:C:815:PHE:CE1	2.49	0.47
1:C:656:ASN:O	1:C:659:VAL:HG12	2.14	0.47
1:C:821:PHE:CD1	1:C:824:ALA:HB3	2.49	0.47
1:C:496:ASN:ND2	1:C:496:ASN:C	2.72	0.47
1:C:555:ASN:HB3	1:C:558:LYS:HE2	1.97	0.47
1:C:754:ASN:O	1:C:758:VAL:HG23	2.14	0.47
1:C:39:PRO:O	1:C:66:TYR:OH	2.22	0.47
1:C:222:ILE:HD11	1:C:251:ASN:HD21	1.80	0.47
2:P:19:VAL:O	2:P:21:GLN:N	2.47	0.47
1:C:590:ILE:HD12	1:C:595:MSE:HE2	1.97	0.47
1:C:502:LEU:HD11	1:C:528:ALA:O	2.14	0.47
1:C:184:LEU:HD23	2:P:83:LEU:HD22	1.96	0.46
1:C:601:GLY:O	1:C:605:MSE:HB2	2.15	0.46
1:C:303:LEU:CD2	2:P:52:ILE:HD11	2.46	0.46
3:R:536:THR:O	3:R:540:ARG:NH1	2.48	0.46
1:C:494:PHE:O	1:C:494:PHE:CD1	2.67	0.46
1:C:703:GLN:HG3	1:C:734:VAL:HG22	1.97	0.46
1:C:769:PRO:CA	1:C:806:PHE:HE1	2.24	0.46
1:C:777:ARG:O	1:C:780:TYR:HB3	2.15	0.46
1:C:24:LYS:HE3	1:C:53:SER:HB3	1.98	0.46
1:C:821:PHE:HD1	1:C:824:ALA:HB3	1.80	0.46
1:C:821:PHE:CD1	1:C:821:PHE:C	2.93	0.46
3:R:565:LYS:HE3	3:R:568:PHE:HZ	1.79	0.46
2:P:21:GLN:NE2	2:P:23:PRO:HD3	2.30	0.46
1:C:422:ASP:HB3	1:C:425:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:TYR:CE1	1:C:774:LEU:HD21	2.51	0.46
1:C:155:ASP:N	1:C:155:ASP:OD1	2.48	0.45
1:C:529:LYS:NZ	1:C:544:GLU:OE2	2.38	0.45
1:C:618:TRP:CZ2	2:P:19:VAL:HG22	2.51	0.45
1:C:218:PRO:HG3	2:P:65:PRO:O	2.16	0.45
1:C:492:MSE:CE	1:C:501:PRO:CD	2.94	0.45
1:C:621:LYS:NZ	1:C:632:SER:HA	2.31	0.45
1:C:637:LYS:O	1:C:641:VAL:HG13	2.15	0.45
1:C:749:GLY:O	1:C:750:LYS:C	2.59	0.45
1:C:793:GLN:HG3	1:C:830:ILE:HD13	1.98	0.45
1:C:633:THR:HB	1:C:637:LYS:HZ2	1.79	0.45
1:C:828:PHE:HD1	1:C:828:PHE:HA	1.65	0.45
1:C:824:ALA:HA	1:C:827:GLN:OE1	2.16	0.45
1:C:599:ILE:HG23	1:C:603:LEU:HD23	1.97	0.45
1:C:821:PHE:O	1:C:821:PHE:CD1	2.69	0.45
1:C:595:MSE:CG	1:C:619:TYR:CE2	2.96	0.45
1:C:676:LYS:HA	1:C:679:HIS:HB2	1.99	0.45
3:R:549:PHE:HB3	3:R:558:MSE:HG3	1.99	0.45
1:C:682:LEU:HA	1:C:685:ILE:HD12	1.97	0.45
1:C:633:THR:O	1:C:637:LYS:HD2	2.17	0.45
1:C:703:GLN:HE22	2:P:15:ASN:HA	1.82	0.45
1:C:120:LEU:HD23	1:C:151:ARG:CZ	2.47	0.45
1:C:224:ILE:CD1	2:P:98:LEU:HB3	2.48	0.44
1:C:648:ALA:O	1:C:652:ILE:HB	2.17	0.44
1:C:457:ASN:O	3:R:550:ARG:NH1	2.45	0.44
1:C:502:LEU:HD23	1:C:539:VAL:HG21	1.99	0.44
1:C:803:LEU:HD13	1:C:820:LYS:HG3	1.98	0.44
3:R:540:ARG:O	3:R:543:GLU:HB3	2.18	0.44
1:C:756:GLU:H	1:C:756:GLU:HG2	1.37	0.44
1:C:816:ILE:CD1	1:C:816:ILE:H	2.06	0.44
2:P:101:ASP:OD1	3:R:514:GLN:NE2	2.48	0.44
1:C:617:GLY:O	1:C:621:LYS:HD2	2.18	0.44
1:C:182:ASN:ND2	2:P:83:LEU:HB3	2.32	0.44
2:P:34:GLU:H	2:P:34:GLU:CD	2.25	0.44
2:P:88:ASN:HA	3:R:505:ARG:CZ	2.48	0.44
3:R:541:GLU:HG3	3:R:544:LEU:HD23	1.99	0.44
1:C:719:LEU:HD22	1:C:745:MSE:HE1	1.98	0.44
1:C:390:GLU:OE1	1:C:390:GLU:N	2.48	0.44
1:C:502:LEU:HD13	1:C:531:LYS:HB3	1.99	0.44
1:C:578:ILE:HD11	1:C:612:MSE:HA	1.99	0.44
1:C:898:ASN:O	1:C:901:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:LYS:HE2	1:C:632:SER:HB3	2.00	0.43
1:C:654:LEU:HD22	1:C:654:LEU:HA	1.87	0.43
1:C:747:GLU:OE2	1:C:747:GLU:HA	2.18	0.43
1:C:590:ILE:CD1	1:C:595:MSE:HB2	2.47	0.43
1:C:742:LEU:HD22	1:C:750:LYS:HB3	2.00	0.43
1:C:149:TYR:OH	2:P:60:GLU:O	2.26	0.43
1:C:7:VAL:HG22	1:C:247:ILE:HD12	2.01	0.43
1:C:111:LEU:HG	1:C:112:SER:H	1.84	0.43
1:C:692:LEU:HB3	4:A:196:ILE:HG23	2.00	0.43
1:C:719:LEU:HD22	1:C:745:MSE:CE	2.49	0.43
1:C:893:LEU:HD23	1:C:893:LEU:HA	1.81	0.43
2:P:67:ASP:C	2:P:69:MSE:H	2.27	0.43
1:C:220:PRO:O	1:C:224:ILE:HG23	2.19	0.42
1:C:487:LYS:HE3	1:C:487:LYS:HB2	1.79	0.42
1:C:633:THR:HB	1:C:637:LYS:HZ1	1.80	0.42
1:C:744:GLU:OE2	2:P:11:ILE:CG1	2.59	0.42
1:C:814:LYS:H	1:C:814:LYS:HG2	1.45	0.42
1:C:620:LEU:HD22	1:C:626:ARG:CD	2.48	0.42
1:C:748:PHE:CB	1:C:782:ARG:HG3	2.48	0.42
1:C:463:ARG:HH12	2:P:36:ASN:ND2	2.17	0.42
1:C:580:ASN:HA	1:C:583:ILE:HG22	2.01	0.42
1:C:615:PHE:HA	2:P:20:PRO:HG2	2.01	0.42
1:C:803:LEU:HA	1:C:819:VAL:HG11	2.00	0.42
4:A:205:GLN:HE21	4:A:205:GLN:HB3	1.59	0.42
1:C:99:THR:HG21	1:C:127:LEU:HG	2.02	0.42
1:C:298:PRO:HB2	1:C:336:VAL:HG11	2.00	0.42
1:C:700:PHE:CZ	2:P:18:PRO:HG3	2.55	0.42
1:C:764:ASN:HD22	1:C:766:ARG:H	1.66	0.42
1:C:813:ASN:C	1:C:815:PHE:N	2.74	0.42
1:C:803:LEU:HB2	1:C:823:ILE:HD11	2.01	0.42
1:C:43:THR:HA	1:C:46:LYS:HB3	2.02	0.42
1:C:224:ILE:HD11	2:P:98:LEU:HB3	2.01	0.42
1:C:707:ILE:HG12	2:P:13:TYR:HB3	2.01	0.42
1:C:187:LEU:HD21	2:P:64:MSE:HE2	2.02	0.42
1:C:518:LEU:H	1:C:518:LEU:HG	1.61	0.42
1:C:384:LYS:HE2	2:P:38:ASP:HB2	2.02	0.41
1:C:46:LYS:HG3	1:C:47:THR:N	2.34	0.41
1:C:327:LYS:HA	1:C:327:LYS:HD3	1.72	0.41
1:C:876:GLU:O	1:C:880:GLN:HG2	2.19	0.41
2:P:103:ARG:O	2:P:106:ARG:HG3	2.21	0.41
1:C:24:LYS:HZ3	1:C:24:LYS:HG2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.82	0.41
3:R:548:GLN:O	3:R:554:GLY:HA3	2.20	0.41
1:C:398:LEU:HD23	1:C:398:LEU:HA	1.95	0.41
1:C:184:LEU:HD13	1:C:184:LEU:HA	1.95	0.41
1:C:224:ILE:HD11	2:P:98:LEU:HD13	2.03	0.41
1:C:584:LYS:HG2	1:C:589:LYS:HB3	2.02	0.41
1:C:813:ASN:C	1:C:815:PHE:H	2.29	0.41
1:C:877:GLU:HG3	1:C:878:LEU:HD12	2.03	0.41
2:P:94:ASP:O	2:P:98:LEU:HG	2.21	0.41
1:C:5:ILE:HG21	1:C:215:VAL:HA	2.02	0.41
1:C:613:ARG:HD2	1:C:639:THR:HG22	2.02	0.41
1:C:581:LEU:HD23	1:C:581:LEU:HA	1.85	0.40
1:C:759:LEU:HA	1:C:759:LEU:HD13	1.75	0.40
1:C:806:PHE:N	1:C:806:PHE:CD1	2.88	0.40
4:A:204:VAL:HA	4:A:207:ILE:HB	2.03	0.40
1:C:98:LEU:HD12	1:C:98:LEU:HA	1.88	0.40
1:C:74:GLU:OE1	1:C:74:GLU:N	2.54	0.40
1:C:494:PHE:O	1:C:494:PHE:CG	2.75	0.40
1:C:635:HIS:O	1:C:639:THR:HG23	2.21	0.40
1:C:748:PHE:O	1:C:751:ALA:N	2.55	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	C	856/907 (94%)	805 (94%)	46 (5%)	5 (1%)	21	50
2	P	96/111 (86%)	89 (93%)	6 (6%)	1 (1%)	12	39
3	R	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
4	A	42/81 (52%)	39 (93%)	2 (5%)	1 (2%)	4	21
All	All	1061/1176 (90%)	995 (94%)	59 (6%)	7 (1%)	18	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	625	GLU
1	C	597	ILE
1	C	698	ASN
2	P	20	PRO
1	C	11	PRO
4	A	189	PRO
1	C	218	PRO

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	C	780/803 (97%)	666 (85%)	114 (15%)	3	13
2	P	92/102 (90%)	75 (82%)	17 (18%)	1	7
3	R	62/68 (91%)	49 (79%)	13 (21%)	1	5
4	A	38/63 (60%)	29 (76%)	9 (24%)	1	3
All	All	972/1036 (94%)	819 (84%)	153 (16%)	2	11

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	19	LEU
1	C	24	LYS
1	C	28	GLU
1	C	29	LEU
1	C	30	VAL
1	C	46	LYS
1	C	49	LEU
1	C	66	TYR
1	C	90	GLU
1	C	98	LEU
1	C	109	HIS
1	C	120	LEU
1	C	127	LEU

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Mol	Chain	Res	Type
1	C	147	LEU
1	C	155	ASP
1	C	187	LEU
1	C	188	LEU
1	C	203	LEU
1	C	216	LEU
1	C	224	ILE
1	C	293	GLU
1	C	324	LYS
1	C	325	ILE
1	C	326	LEU
1	C	335	THR
1	C	337	LEU
1	C	371	ASN
1	C	372	LEU
1	C	375	ARG
1	C	405	LEU
1	C	407	GLU
1	C	415	LEU
1	C	421	LEU
1	C	423	VAL
1	C	425	THR
1	C	434	LEU
1	C	491	GLU
1	C	495	VAL
1	C	496	ASN
1	C	497	LYS
1	C	503	GLU
1	C	515	ASN
1	C	518	LEU
1	C	520	LYS
1	C	536	ASN
1	C	537	LYS
1	C	539	VAL
1	C	549	ARG
1	C	556	TRP
1	C	557	GLU
1	C	559	SER
1	C	565	GLN
1	C	567	THR
1	C	583	ILE
1	C	584	LYS

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Mol	Chain	Res	Type
1	C	589	LYS
1	C	590	ILE
1	C	599	ILE
1	C	603	LEU
1	C	606	ASN
1	C	613	ARG
1	C	621	LYS
1	C	627	LYS
1	C	635	HIS
1	C	640	LEU
1	C	651	LEU
1	C	652	ILE
1	C	654	LEU
1	C	656	ASN
1	C	659	VAL
1	C	682	LEU
1	C	692	LEU
1	C	694	ILE
1	C	699	VAL
1	C	709	PHE
1	C	712	SER
1	C	715	LEU
1	C	725	ILE
1	C	735	GLN
1	C	738	LEU
1	C	743	LEU
1	C	745	MSE
1	C	747	GLU
1	C	748	PHE
1	C	750	LYS
1	C	756	GLU
1	C	759	LEU
1	C	761	LYS
1	C	764	ASN
1	C	771	ILE
1	C	774	LEU
1	C	775	LEU
1	C	777	ARG
1	C	781	SER
1	C	789	VAL
1	C	791	PHE
1	C	792	PHE

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Mol	Chain	Res	Type
1	C	796	LEU
1	C	805	LEU
1	C	814	LYS
1	C	815	PHE
1	C	816	ILE
1	C	826	LEU
1	C	828	PHE
1	C	829	GLN
1	C	851	LEU
1	C	856	GLU
1	C	860	LEU
1	C	861	PHE
1	C	876	GLU
1	C	884	LEU
1	C	897	LEU
1	C	898	ASN
1	C	902	GLU
2	P	11	ILE
2	P	14	GLN
2	P	21	GLN
2	P	22	LEU
2	P	34	GLU
2	P	46	LEU
2	P	49	LYS
2	P	52	ILE
2	P	53	SER
2	P	59	ASP
2	P	68	LEU
2	P	70	LYS
2	P	78	LEU
2	P	81	LYS
2	P	89	VAL
2	P	99	LEU
2	P	105	ASP
3	R	504	THR
3	R	531	GLN
3	R	535	GLU
3	R	536	THR
3	R	541	GLU
3	R	544	LEU
3	R	546	LEU
3	R	548	GLN

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Mol	Chain	Res	Type
3	R	550	ARG
3	R	564	ILE
3	R	565	LYS
3	R	569	LYS
3	R	570	PHE
4	A	166	VAL
4	A	167	LEU
4	A	172	LYS
4	A	179	ASP
4	A	182	SER
4	A	195	LEU
4	A	196	ILE
4	A	205	GLN
4	A	207	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	104	ASN
1	C	182	ASN
1	C	251	ASN
1	C	294	ASN
1	C	371	ASN
1	C	435	ASN
1	C	438	ASN
1	C	443	GLN
1	C	458	GLN
1	C	475	GLN
1	C	496	ASN
1	C	506	ASN
1	C	515	ASN
1	C	540	ASN
1	C	636	ASN
1	C	703	GLN
1	C	740	HIS
1	C	764	ASN
1	C	829	GLN
1	C	865	ASN
1	C	900	GLN
4	A	173	ASN
4	A	205	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

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	C	852/907 (93%)	1.33	244 (28%) 1 1	8, 51, 226, 310	0
2	P	96/111 (86%)	0.54	6 (6%) 26 14	8, 27, 123, 151	0
3	R	67/77 (87%)	0.98	11 (16%) 4 2	18, 39, 84, 97	0
4	A	43/81 (53%)	1.62	14 (32%) 1 1	53, 83, 120, 133	0
All	All	1058/1176 (89%)	1.25	275 (25%) 1 1	8, 48, 211, 310	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	826	LEU	7.5
1	C	822	ASN	6.6
1	C	778	ALA	6.6
1	C	771	ILE	6.5
1	C	818	SER	6.4
3	R	531	GLN	6.3
1	C	815	PHE	6.1
1	C	864	LEU	5.9
1	C	856	GLU	5.6
1	C	619	TYR	5.5
1	C	887	THR	5.4
1	C	831	ALA	5.3
1	C	770	HIS	5.3
1	C	890	LYS	5.3
1	C	865	ASN	5.2
1	C	825	LEU	5.2
1	C	884	LEU	5.1
1	C	641	VAL	5.1
1	C	661	ILE	5.1
1	C	767	THR	5.0
1	C	556	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	875	LYS	4.8
1	C	658	TYR	4.8
1	C	810	SER	4.8
4	A	207	ILE	4.7
1	C	897	LEU	4.7
1	C	806	PHE	4.7
1	C	805	LEU	4.6
1	C	851	LEU	4.6
1	C	894	GLU	4.6
1	C	780	TYR	4.5
1	C	828	PHE	4.4
1	C	748	PHE	4.3
1	C	860	LEU	4.3
1	C	606	ASN	4.2
1	C	906	ASP	4.2
1	C	827	GLN	4.2
1	C	587	HIS	4.2
1	C	768	ARG	4.2
1	C	654	LEU	4.1
1	C	878	LEU	4.1
1	C	811	ALA	4.1
1	C	642	LYS	4.1
1	C	830	ILE	4.1
1	C	779	TRP	4.1
1	C	789	VAL	4.0
1	C	774	LEU	4.0
1	C	609	ASP	4.0
1	C	624	GLU	4.0
1	C	625	GLU	4.0
1	C	759	LEU	4.0
1	C	787	ARG	3.9
1	C	891	SER	3.9
1	C	743	LEU	3.9
1	C	896	SER	3.9
1	C	803	LEU	3.9
3	R	530	LEU	3.9
1	C	785	LYS	3.8
1	C	829	GLN	3.8
1	C	903	PHE	3.8
1	C	738	LEU	3.8
1	C	862	LYS	3.7
1	C	750	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	832	GLU	3.7
1	C	886	GLU	3.7
1	C	678	LYS	3.7
1	C	814	LYS	3.7
1	C	855	GLU	3.7
1	C	902	GLU	3.7
1	C	777	ARG	3.7
1	C	791	PHE	3.7
1	C	781	SER	3.6
1	C	782	ARG	3.6
1	C	800	LYS	3.6
1	C	776	GLY	3.6
1	C	680	SER	3.6
1	C	819	VAL	3.5
1	C	108	GLY	3.5
1	C	568	SER	3.5
1	C	904	GLU	3.4
1	C	858	LEU	3.4
1	C	616	TYR	3.4
1	C	657	LEU	3.4
1	C	645	SER	3.4
1	C	888	THR	3.4
1	C	900	GLN	3.4
4	A	180	HIS	3.4
1	C	622	ASN	3.4
1	C	659	VAL	3.4
1	C	893	LEU	3.4
2	P	9	ALA	3.4
1	C	817	HIS	3.4
1	C	788	SER	3.3
1	C	792	PHE	3.3
3	R	532	GLU	3.3
1	C	769	PRO	3.3
1	C	554	THR	3.3
1	C	798	ASN	3.3
1	C	876	GLU	3.3
1	C	646	HIS	3.3
1	C	850	SER	3.3
1	C	715	LEU	3.2
1	C	849	ASP	3.2
1	C	821	PHE	3.2
1	C	857	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	P	12	LYS	3.2
1	C	647	ASP	3.2
1	C	636	ASN	3.2
1	C	854	LEU	3.2
1	C	585	PHE	3.2
1	C	560	GLU	3.2
1	C	863	GLU	3.2
1	C	643	TYR	3.2
1	C	718	ALA	3.2
1	C	794	LYS	3.2
1	C	632	SER	3.2
1	C	793	GLN	3.2
1	C	756	GLU	3.1
1	C	852	GLU	3.1
1	C	478	TYR	3.1
4	A	203	LEU	3.1
1	C	644	ASN	3.1
1	C	801	THR	3.1
1	C	807	VAL	3.1
1	C	752	ILE	3.1
2	P	105	ASP	3.1
3	R	541	GLU	3.1
1	C	676	LYS	3.1
1	C	899	GLU	3.1
1	C	685	ILE	3.1
1	C	691	VAL	3.0
1	C	634	SER	3.0
2	P	11	ILE	3.0
1	C	757	LEU	3.0
1	C	597	ILE	3.0
1	C	761	LYS	3.0
1	C	861	PHE	3.0
1	C	638	GLU	3.0
1	C	682	LEU	2.9
1	C	747	GLU	2.9
3	R	535	GLU	2.9
1	C	684	ALA	2.9
4	A	198	ASP	2.9
1	C	563	TYR	2.9
4	A	205	GLN	2.9
1	C	701	ALA	2.9
1	C	635	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	746	ARG	2.9
4	A	193	GLY	2.9
1	C	895	ARG	2.9
1	C	880	GLN	2.8
1	C	713	LYS	2.8
1	C	723	ARG	2.8
1	C	885	GLY	2.8
1	C	613	ARG	2.8
1	C	529	LYS	2.8
1	C	537	LYS	2.8
1	C	689	GLN	2.8
1	C	608	SER	2.8
1	C	901	GLU	2.8
1	C	564	SER	2.7
1	C	727	ASP	2.7
1	C	631	LYS	2.7
1	C	693	GLN	2.7
1	C	602	LEU	2.7
1	C	905	LYS	2.7
1	C	813	ASN	2.7
1	C	898	ASN	2.7
1	C	539	VAL	2.7
1	C	617	GLY	2.7
1	C	639	THR	2.7
1	C	679	HIS	2.7
1	C	582	TYR	2.7
1	C	796	LEU	2.7
2	P	13	TYR	2.7
1	C	717	PRO	2.6
1	C	823	ILE	2.6
1	C	783	GLY	2.6
3	R	502	LEU	2.6
1	C	681	TYR	2.6
3	R	539	ARG	2.6
1	C	623	SER	2.6
1	C	755	TYR	2.6
1	C	809	GLN	2.6
1	C	736	LEU	2.6
3	R	503	LYS	2.6
1	C	741	CYS	2.5
1	C	775	LEU	2.5
1	C	27	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	404	SER	2.5
1	C	575	SER	2.5
1	C	590	ILE	2.5
1	C	586	ALA	2.5
1	C	754	ASN	2.5
1	C	401	THR	2.5
1	C	653	SER	2.5
1	C	655	ALA	2.5
1	C	772	LEU	2.5
1	C	734	VAL	2.5
1	C	732	GLU	2.4
1	C	577	ARG	2.4
1	C	592	ASP	2.4
1	C	656	ASN	2.4
1	C	716	GLY	2.4
1	C	588	SER	2.4
1	C	600	ASN	2.4
4	A	190	ILE	2.4
1	C	690	LYS	2.4
1	C	696	PRO	2.4
1	C	688	TYR	2.4
1	C	25	ALA	2.4
1	C	674	GLN	2.4
1	C	722	LEU	2.4
1	C	742	LEU	2.4
1	C	293	GLU	2.4
1	C	802	ALA	2.3
3	R	533	ASP	2.3
1	C	650	ALA	2.3
1	C	573	TYR	2.3
1	C	620	LEU	2.3
1	C	762	PHE	2.3
4	A	200	GLU	2.3
1	C	2	ALA	2.3
1	C	712	SER	2.3
1	C	109	HIS	2.3
1	C	731	ASN	2.3
1	C	883	GLN	2.3
1	C	557	GLU	2.3
1	C	598	GLU	2.3
1	C	881	ARG	2.3
1	C	816	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	799	ALA	2.3
4	A	194	TYR	2.3
1	C	67	CYS	2.3
1	C	740	HIS	2.2
1	C	628	ASN	2.2
1	C	786	GLU	2.2
3	R	567	ASP	2.2
1	C	704	GLY	2.2
1	C	637	LYS	2.2
1	C	808	GLN	2.2
2	P	10	PRO	2.2
1	C	812	LYS	2.2
1	C	724	LYS	2.2
1	C	820	LYS	2.2
1	C	663	ARG	2.2
1	C	252	THR	2.2
4	A	170	THR	2.2
1	C	677	SER	2.2
1	C	683	LYS	2.2
4	A	181	ASN	2.2
1	C	44	ASP	2.2
1	C	853	GLY	2.1
1	C	773	ASN	2.1
1	C	795	ALA	2.1
4	A	177	VAL	2.1
3	R	536	THR	2.1
1	C	516	GLY	2.1
1	C	610	LEU	2.1
4	A	196	ILE	2.1
1	C	36	THR	2.1
1	C	660	THR	2.1
1	C	576	ALA	2.1
1	C	274	GLU	2.1
1	C	30	VAL	2.1
1	C	607	LYS	2.1
1	C	601	GLY	2.1
1	C	604	GLU	2.1
1	C	708	ILE	2.0
4	A	195	LEU	2.0
1	C	633	THR	2.0
1	C	83	LEU	2.0
1	C	882	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	558	LYS	2.0
1	C	584	LYS	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.