Full wwPDB X-ray Structure Validation Report (i)

May 15, 2023 – 06:10 PM JST

PDB ID	:	8J8Q
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 (i) 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 (1)) were used in the production of this report:

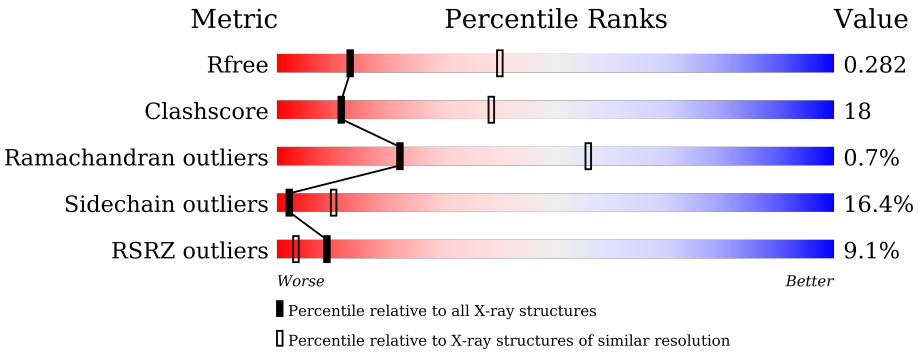
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (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 <=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	9% 60% 28% 8% 5%
2	P	111	2% 52% 29% 6% • 12%
3	R	77	8% 60% 21% 9% 10%
4	A	81	7% 36% 12% 6% 46%

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
			Total	C	N	O	S	Se			
1	C	866	7031	4489	1184	1338	6	14	0	0	0

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

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

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
			Total	C	N	O	Se			
3	R	69	594	373	107	112	2	0	0	0

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

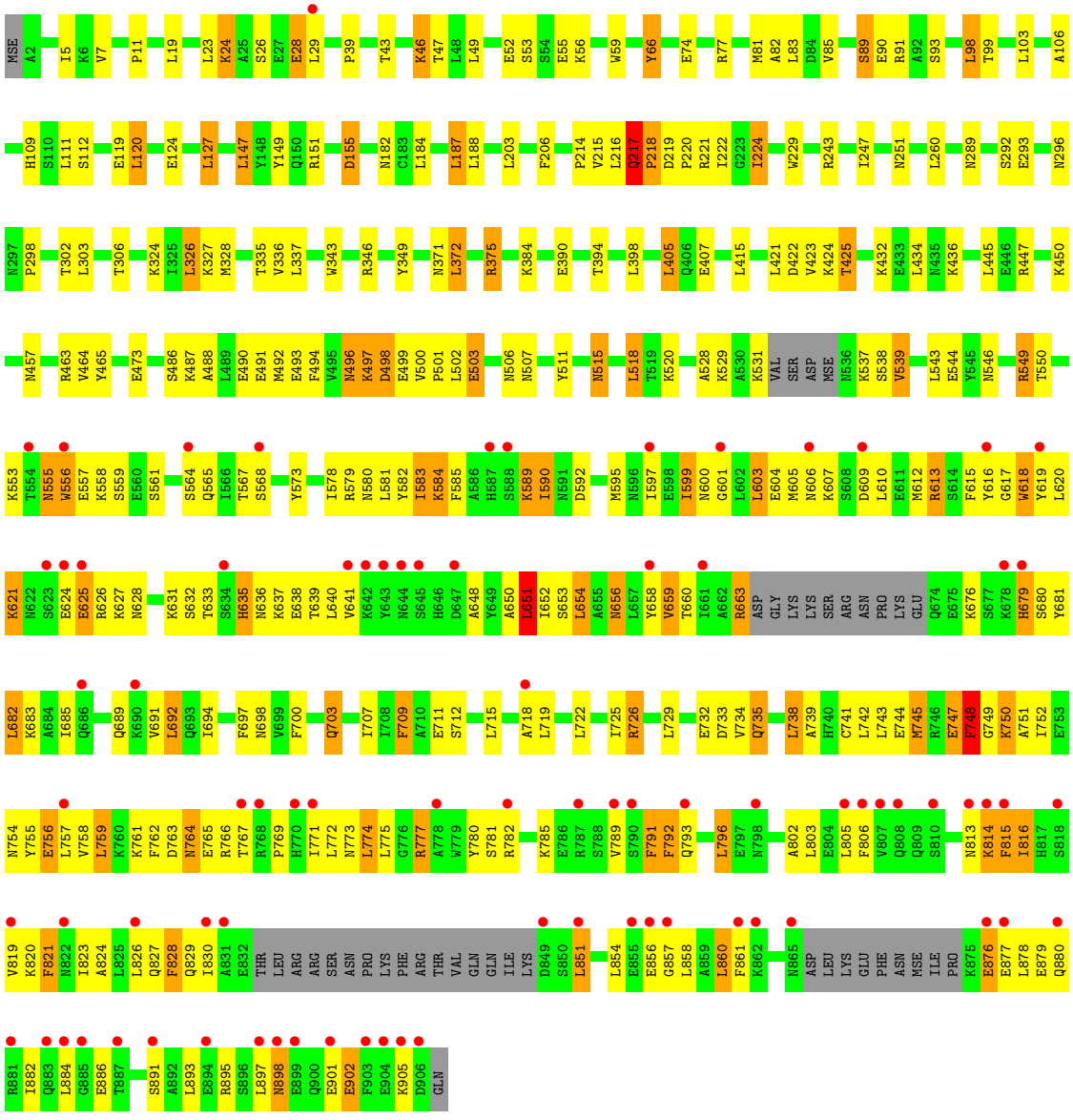
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
4	A	44	347	218	63	65	1	0	0	0

3 Residue-property plots (i)

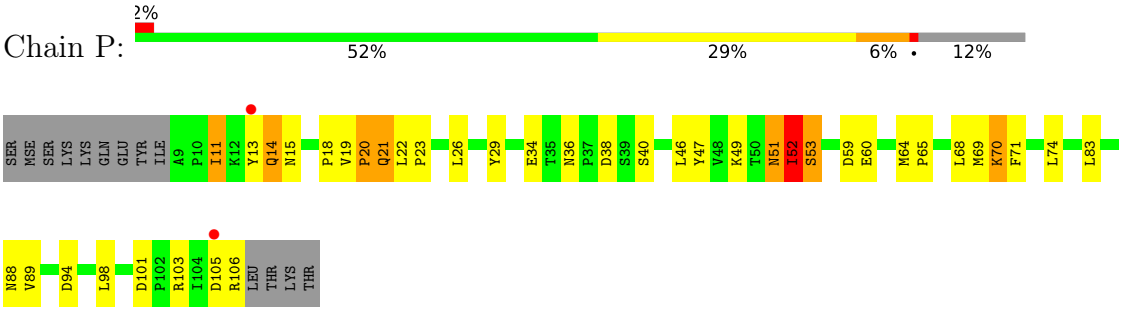
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

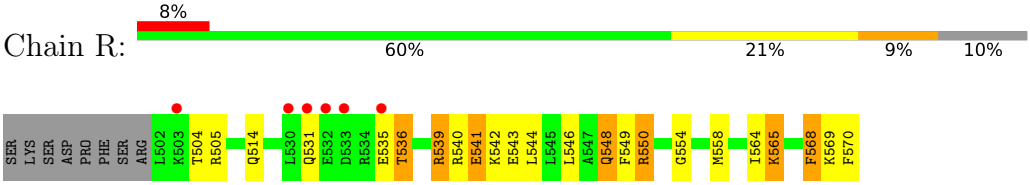
Chain C:



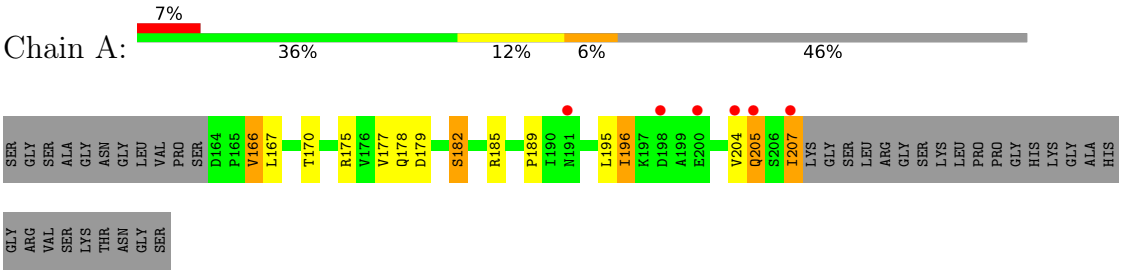
• Molecule 2: PAF1-like protein



• Molecule 3: RTF1-like protein



• Molecule 4: CDC73-like protein



4 Data and refinement statistics (i)

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) 98.7 (27.07-3.11)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.98%)	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 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	2/7144 (0.0%)	0.61	10/9608 (0.1%)
2	P	0.76	1/798 (0.1%)	0.61	1/1082 (0.1%)
3	R	0.25	0/597	0.47	0/783
4	A	0.25	0/350	0.40	0/470
All	All	0.52	3/8889 (0.0%)	0.60	11/11943 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	618	TRP	CB-CG	-8.97	1.34	1.50
1	C	219	ASP	CB-CG	-5.99	1.39	1.51
2	P	52	ILE	C-O	-5.45	1.12	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	217	GLN	C-N-CD	-13.56	90.77	120.60
1	C	26	SER	N-CA-C	8.31	133.44	111.00
1	C	217	GLN	C-N-CA	7.65	154.13	122.00
2	P	51	ASN	N-CA-C	7.18	130.40	111.00
1	C	748	PHE	N-CA-C	6.70	129.09	111.00
1	C	651	LEU	CA-CB-CG	5.91	128.90	115.30
1	C	796	LEU	CA-CB-CG	5.49	127.94	115.30
1	C	498	ASP	C-N-CA	-5.44	108.09	121.70
1	C	89	SER	N-CA-CB	5.38	118.56	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	625	GLU	N-CA-C	5.11	124.80	111.00
1	C	85	VAL	CB-CA-C	-5.06	101.78	111.40

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	285	0
2	P	784	0	805	43	0
3	R	594	0	610	11	0
4	A	347	0	356	10	0
All	All	8756	0	8846	310	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 (310) 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: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
1:C:626:ARG:HD3	1:C:631:LYS:CG	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:733:ASP:OD1	2:P:14:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:103:LEU:HD21	1:C:147:LEU:HD22	1.91	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:546:ASN:O	1:C:550:THR:OG1	2.20	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:349:TYR:OH	2:P:38:ASP:O	2.20	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:561:SER:O	1:C:565:GLN:HG2	2.12	0.49
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:28:GLU:H	1:C:28:GLU:CD	2.16	0.49
1:C:120:LEU:O	1:C:124:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:627:LYS:O	1:C:628:ASN:C	2.52	0.48
1:C:633:THR:HB	1:C:637:LYS:HZ1	1.79	0.48
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: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:23:LEU:HD23	1:C:52:GLU:CD	2.35	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:793:GLN:HG3	1:C:830:ILE:HD13	1.98	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: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:633:THR:HB	1:C:637:LYS:HZ2	1.80	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:ASP:CG	1:C:624:GLU:HB3	2.38	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
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:621:LYS:HZ1	1:C:632:SER:HA	1.85	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:496:ASN:ND2	1:C:496:ASN:C	2.72	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: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:620:LEU:HD12	1:C:621:LYS:HZ1	1.85	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:529:LYS:NZ	1:C:544:GLU:OE2	2.38	0.41
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:877:GLU:HG3	1:C:878:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:749:GLY:O	1:C:750:LYS:C	2.59	0.40
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:24:LYS:HZ3	1:C:24:LYS:HG2	1.77	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%)	25 59
2	P	96/111 (86%)	89 (93%)	6 (6%)	1 (1%)	15 48
3	R	67/77 (87%)	62 (92%)	5 (8%)	0	100 100
4	A	42/81 (52%)	39 (93%)	2 (5%)	1 (2%)	6 26
All	All	1061/1176 (90%)	995 (94%)	59 (6%)	7 (1%)	22 56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	625	GLU

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Mol	Chain	Res	Type
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%)	658 (84%)	122 (16%)	2 11
2	P	92/102 (90%)	77 (84%)	15 (16%)	2 10
3	R	62/68 (91%)	48 (77%)	14 (23%)	1 3
4	A	38/63 (60%)	30 (79%)	8 (21%)	1 5
All	All	972/1036 (94%)	813 (84%)	159 (16%)	2 10

All (159) 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	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
1	C	147	LEU
1	C	155	ASP
1	C	187	LEU

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Mol	Chain	Res	Type
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	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	424	LYS
1	C	425	THR
1	C	434	LEU
1	C	491	GLU
1	C	496	ASN
1	C	497	LYS
1	C	498	ASP
1	C	503	GLU
1	C	515	ASN
1	C	518	LEU
1	C	520	LYS
1	C	537	LYS
1	C	539	VAL
1	C	549	ARG
1	C	553	LYS
1	C	555	ASN
1	C	556	TRP
1	C	557	GLU
1	C	559	SER
1	C	567	THR
1	C	573	TYR
1	C	579	ARG
1	C	583	ILE
1	C	584	LYS
1	C	589	LYS

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Mol	Chain	Res	Type
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	635	HIS
1	C	640	LEU
1	C	651	LEU
1	C	654	LEU
1	C	656	ASN
1	C	658	TYR
1	C	659	VAL
1	C	663	ARG
1	C	679	HIS
1	C	682	LEU
1	C	692	LEU
1	C	694	ILE
1	C	703	GLN
1	C	709	PHE
1	C	712	SER
1	C	715	LEU
1	C	725	ILE
1	C	726	ARG
1	C	729	LEU
1	C	732	GLU
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	762	PHE
1	C	763	ASP
1	C	764	ASN
1	C	771	ILE
1	C	774	LEU
1	C	775	LEU

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Mol	Chain	Res	Type
1	C	777	ARG
1	C	781	SER
1	C	789	VAL
1	C	791	PHE
1	C	792	PHE
1	C	796	LEU
1	C	805	LEU
1	C	814	LYS
1	C	815	PHE
1	C	816	ILE
1	C	821	PHE
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	69	MSE
2	P	70	LYS
2	P	89	VAL
2	P	105	ASP
3	R	504	THR
3	R	531	GLN
3	R	535	GLU
3	R	536	THR

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Mol	Chain	Res	Type
3	R	539	ARG
3	R	541	GLU
3	R	546	LEU
3	R	548	GLN
3	R	550	ARG
3	R	564	ILE
3	R	565	LYS
3	R	568	PHE
3	R	569	LYS
3	R	570	PHE
4	A	166	VAL
4	A	167	LEU
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	104	ASN
1	C	182	ASN
1	C	251	ASN
1	C	295	GLN
1	C	371	ASN
1	C	406	GLN
1	C	435	ASN
1	C	438	ASN
1	C	458	GLN
1	C	475	GLN
1	C	496	ASN
1	C	506	ASN
1	C	515	ASN
1	C	555	ASN
1	C	606	ASN
1	C	636	ASN
1	C	703	GLN
1	C	740	HIS
1	C	764	ASN
1	C	798	ASN

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Mol	Chain	Res	Type
1	C	900	GLN
4	A	178	GLN
4	A	180	HIS
4	A	181	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 monosaccharides 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, 95^{th} 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%)	0.38	82 (9%) 8 3	8, 51, 226, 310	0
2	P	96/111 (86%)	-0.20	2 (2%) 63 43	8, 27, 123, 151	0
3	R	67/77 (87%)	0.24	6 (8%) 9 3	18, 39, 84, 97	0
4	A	43/81 (53%)	0.85	6 (13%) 2 1	53, 83, 120, 133	0
All	All	1058/1176 (89%)	0.34	96 (9%) 9 3	8, 48, 211, 310	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	883	GLN	5.6
4	A	205	GLN	5.3
1	C	822	ASN	5.0
1	C	855	GLU	4.6
1	C	818	SER	4.6
1	C	757	LEU	4.5
1	C	831	ALA	4.5
1	C	641	VAL	4.5
1	C	790	SER	4.5
1	C	767	THR	4.4
1	C	619	TYR	4.3
1	C	815	PHE	4.3
1	C	851	LEU	4.3
1	C	897	LEU	4.1
1	C	588	SER	4.1
1	C	661	ILE	4.0
1	C	813	ASN	4.0
1	C	587	HIS	3.8
1	C	771	ILE	3.8
3	R	531	GLN	3.7
1	C	568	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	887	THR	3.7
1	C	597	ILE	3.7
1	C	880	GLN	3.6
1	C	826	LEU	3.6
1	C	856	GLU	3.6
1	C	807	VAL	3.6
1	C	678	LYS	3.6
1	C	778	ALA	3.5
1	C	644	ASN	3.5
1	C	885	GLY	3.5
1	C	904	GLU	3.4
1	C	884	LEU	3.4
1	C	624	GLU	3.4
1	C	625	GLU	3.4
1	C	861	PHE	3.4
1	C	894	GLU	3.3
1	C	891	SER	3.3
2	P	105	ASP	3.3
1	C	642	LYS	3.3
3	R	503	LYS	3.2
1	C	623	SER	3.1
1	C	798	ASN	3.0
1	C	806	PHE	3.0
3	R	535	GLU	3.0
4	A	191	ASN	3.0
1	C	814	LYS	3.0
1	C	903	PHE	3.0
1	C	808	GLN	3.0
1	C	865	ASN	2.9
3	R	532	GLU	2.9
1	C	810	SER	2.8
1	C	782	ARG	2.8
1	C	819	VAL	2.7
3	R	533	ASP	2.7
1	C	690	LYS	2.7
1	C	29	LEU	2.6
1	C	906	ASP	2.6
2	P	13	TYR	2.6
1	C	658	TYR	2.6
1	C	770	HIS	2.5
1	C	554	THR	2.5
1	C	805	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	A	207	ILE	2.5
1	C	793	GLN	2.5
1	C	601	GLY	2.4
1	C	606	ASN	2.4
1	C	857	GLY	2.4
1	C	898	ASN	2.4
1	C	634	SER	2.4
1	C	877	GLU	2.4
1	C	862	LYS	2.4
1	C	789	VAL	2.3
1	C	876	GLU	2.3
1	C	556	TRP	2.2
3	R	530	LEU	2.2
1	C	787	ARG	2.2
4	A	200	GLU	2.2
1	C	645	SER	2.2
1	C	609	ASP	2.2
1	C	647	ASP	2.2
1	C	905	LYS	2.2
1	C	718	ALA	2.2
1	C	849	ASP	2.1
1	C	899	GLU	2.1
1	C	616	TYR	2.1
4	A	204	VAL	2.1
4	A	198	ASP	2.1
1	C	881	ARG	2.1
1	C	768	ARG	2.1
1	C	679	HIS	2.1
1	C	643	TYR	2.1
1	C	564	SER	2.0
1	C	901	GLU	2.0
1	C	830	ILE	2.0
1	C	686	GLN	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.