



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 PM UTC

PDB ID : 6AF0 / pdb_00006af0
Title : Structure of Ctr9, Paf1 and Cdc73 ternary complex from *Myceliophthora thermophila*
Authors : Wang, Z.; Deng, P.; Zhou, Y.
Deposited on : 2018-08-07
Resolution : 2.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

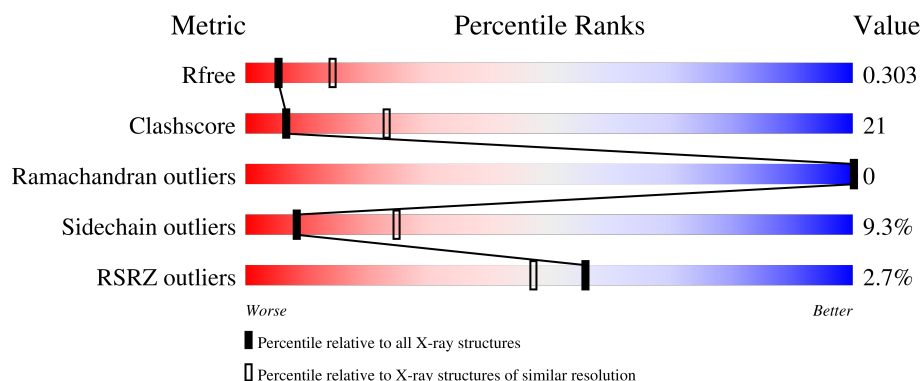
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	939	 3% 60% 32% 2% 3%
2	P	121	 2% 58% 24% 6% 12%
3	C	74	 3% 31% 24% 43%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8372 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	905	Total	C	N	O	S	0	0	0
			7228	4562	1276	1362	28			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP G2QC65

- Molecule 2 is a protein called Paf1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	107	Total	C	N	O	S	0	0	0
			810	517	141	149	3			

There is a discrepancy between the modelled and reference sequences:

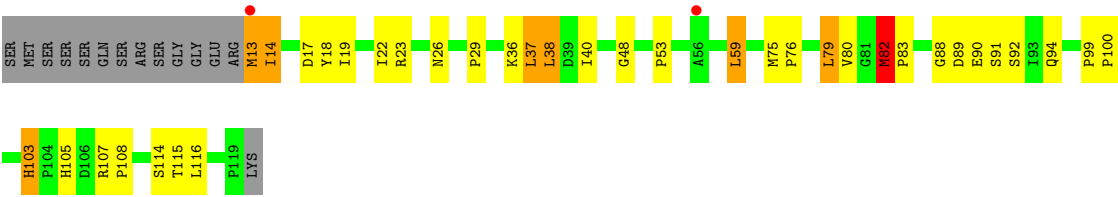
Chain	Residue	Modelled	Actual	Comment	Reference
P	0	SER	-	expression tag	UNP G2QDK9

- Molecule 3 is a protein called Cdc73 protein.

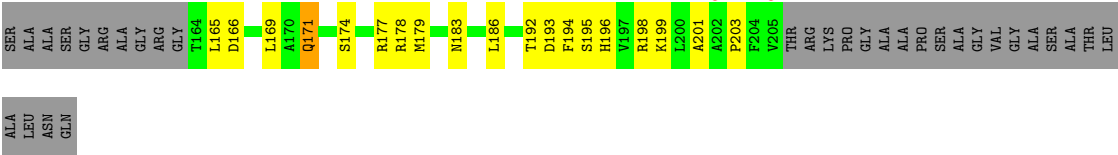
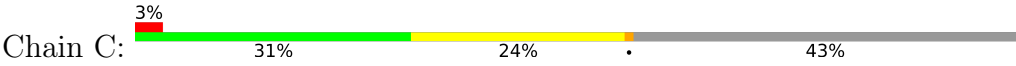
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	42	Total	C	N	O	S	0	0	0
			334	209	66	58	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	154	SER	-	expression tag	UNP G2Q3X1



● Molecule 3: Cdc73 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.87Å 237.79Å 62.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.89 – 2.88 118.89 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.3 (118.89-2.88) 99.3 (118.89-2.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.245 , 0.309 0.244 , 0.303	Depositor DCC
R_{free} test set	1729 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	90.3	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.0	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	0.94	EDS
Total number of atoms	8372	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	3/7365 (0.0%)	1.01	10/9941 (0.1%)
2	P	0.76	0/836	1.03	5/1148 (0.4%)
3	C	0.60	0/340	0.91	0/457
All	All	0.73	3/8541 (0.0%)	1.01	15/11546 (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
2	P	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLU	CD-OE2	9.08	1.42	1.25
1	A	49	GLU	CD-OE1	7.99	1.40	1.25
1	A	964	GLU	CD-OE1	6.04	1.36	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLN	N-CA-C	-9.97	97.37	110.53
1	A	832	GLY	N-CA-C	-9.68	96.38	112.83
1	A	165	PRO	N-CA-C	-7.80	99.24	111.34
1	A	410	ARG	N-CA-C	-7.41	98.46	108.24
2	P	88	GLY	N-CA-C	7.18	121.34	112.73
2	P	48	GLY	N-CA-C	6.04	121.11	114.40
2	P	103	HIS	CA-C-N	5.80	125.93	119.32
2	P	103	HIS	C-N-CA	5.80	125.93	119.32
1	A	141	SER	N-CA-C	-5.78	102.90	110.53
1	A	46	ASP	N-CA-C	-5.71	100.89	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	40	ILE	N-CA-C	5.54	112.60	107.56
1	A	558	PRO	CA-C-N	5.28	124.91	119.05
1	A	558	PRO	C-N-CA	5.28	124.91	119.05
1	A	324	THR	CB-CA-C	-5.15	102.76	110.90
1	A	792	ILE	CB-CA-C	-5.15	105.11	112.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	82	MET	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7228	0	7201	335	0
2	P	810	0	811	41	0
3	C	334	0	343	14	0
All	All	8372	0	8355	359	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 21.

All (359) 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:A:49:GLU:HG3	1:A:50:VAL:HG23	1.39	1.01
1:A:44:MET:CE	1:A:49:GLU:HG2	1.91	1.01
1:A:431:GLU:HA	1:A:434:LEU:HG	1.44	0.97
1:A:44:MET:HE2	1:A:49:GLU:HG2	1.44	0.96
1:A:44:MET:HG2	1:A:49:GLU:CD	1.93	0.94
2:P:13:MET:SD	2:P:13:MET:C	2.51	0.94
1:A:84:ALA:O	1:A:88:GLN:NE2	2.01	0.94
1:A:895:LEU:O	1:A:955:ARG:NH2	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:MET:CE	1:A:50:VAL:HG23	1.99	0.92
1:A:316:ILE:O	1:A:320:LYS:HG3	1.67	0.92
1:A:166:ALA:HA	1:A:171:PHE:CZ	2.06	0.89
1:A:121:TRP:CE2	2:P:79:LEU:CD1	2.56	0.89
1:A:44:MET:CE	1:A:49:GLU:CG	2.51	0.89
1:A:49:GLU:HG3	1:A:50:VAL:H	1.39	0.87
1:A:368:THR:HG22	1:A:370:VAL:H	1.41	0.85
1:A:269:GLN:O	1:A:270:LEU:HB2	1.77	0.84
1:A:49:GLU:HG3	1:A:50:VAL:N	1.92	0.84
1:A:200:GLU:OE2	1:A:203:ARG:NH1	2.09	0.84
1:A:44:MET:HB2	1:A:49:GLU:HG2	1.61	0.83
1:A:916:GLU:O	1:A:919:ILE:HG13	1.79	0.83
1:A:624:LYS:O	1:A:628:THR:HG23	1.79	0.82
1:A:44:MET:HB2	1:A:49:GLU:CG	2.10	0.82
1:A:121:TRP:CE2	2:P:79:LEU:HD11	2.15	0.81
1:A:44:MET:HB2	1:A:49:GLU:CB	2.10	0.81
1:A:46:ASP:C	1:A:47:ASP:OD1	2.24	0.81
1:A:44:MET:HE2	1:A:49:GLU:CG	2.11	0.80
1:A:935:ARG:NH1	1:A:939:GLU:OE2	2.15	0.80
1:A:44:MET:HE3	1:A:50:VAL:HG23	1.64	0.78
1:A:622:ILE:HD11	1:A:649:ILE:HG23	1.63	0.78
1:A:733:GLU:HG2	2:P:23:ARG:HH12	1.48	0.78
1:A:44:MET:SD	1:A:71:GLU:OE2	2.42	0.78
1:A:784:TYR:CE1	1:A:813:GLU:HG2	2.19	0.78
1:A:781:ARG:O	1:A:783:ASP:N	2.17	0.78
2:P:14:ILE:HG23	2:P:14:ILE:O	1.84	0.77
1:A:368:THR:HG21	1:A:373:ILE:HB	1.67	0.76
1:A:121:TRP:CZ2	2:P:79:LEU:HD11	2.21	0.76
1:A:789:GLN:HA	1:A:792:ILE:HD12	1.68	0.75
1:A:121:TRP:CE2	2:P:79:LEU:HD12	2.21	0.74
1:A:135:PRO:O	1:A:138:VAL:HG13	1.87	0.74
1:A:49:GLU:HG3	1:A:50:VAL:CG2	2.18	0.74
1:A:943:ASN:O	1:A:946:ARG:HG2	1.88	0.74
1:A:49:GLU:CG	1:A:50:VAL:HG23	2.18	0.74
1:A:44:MET:HE3	1:A:50:VAL:CG2	2.18	0.74
1:A:44:MET:CE	1:A:50:VAL:CG2	2.66	0.74
1:A:157:LEU:HD21	1:A:174:ARG:HD2	1.71	0.73
1:A:141:SER:HB3	1:A:142:GLU:OE2	1.88	0.73
1:A:879:HIS:CE1	1:A:880:PHE:CE1	2.77	0.73
1:A:121:TRP:CD2	2:P:79:LEU:HD12	2.23	0.73
1:A:134:ALA:HB3	1:A:138:VAL:HG12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:GLU:CG	2:P:23:ARG:HH12	2.01	0.72
1:A:229:ARG:NH1	1:A:233:SER:OG	2.24	0.71
1:A:324:THR:O	1:A:328:GLN:HB3	1.91	0.71
1:A:837:ALA:HB1	1:A:880:PHE:HE2	1.56	0.71
1:A:136:ASP:OD2	1:A:136:ASP:N	2.24	0.70
1:A:154:THR:HG22	1:A:177:LEU:HD21	1.73	0.70
1:A:638:ASP:OD1	1:A:638:ASP:N	2.25	0.69
1:A:408:ALA:O	1:A:409:GLU:HB2	1.91	0.69
1:A:44:MET:HE3	1:A:49:GLU:CG	2.22	0.69
1:A:134:ALA:HB1	1:A:135:PRO:HD2	1.73	0.69
1:A:138:VAL:HB	1:A:139:PRO:C	2.17	0.69
1:A:47:ASP:C	1:A:48:VAL:HG23	2.19	0.68
1:A:933:TYR:HB2	1:A:938:ILE:HD11	1.75	0.68
1:A:321:LYS:HE3	1:A:325:GLU:OE1	1.94	0.67
1:A:75:ARG:HD2	1:A:111:GLU:HB3	1.75	0.67
1:A:44:MET:HA	1:A:71:GLU:OE2	1.94	0.67
1:A:879:HIS:ND1	1:A:880:PHE:CE1	2.62	0.67
2:P:79:LEU:O	2:P:82:MET:HB2	1.95	0.67
1:A:898:MET:O	1:A:955:ARG:NH1	2.26	0.66
1:A:157:LEU:HD21	1:A:174:ARG:CD	2.26	0.66
1:A:765:LYS:HA	3:C:192:THR:O	1.95	0.66
1:A:492:ASP:O	1:A:497:LEU:HD11	1.96	0.65
1:A:44:MET:CB	1:A:49:GLU:HG2	2.26	0.65
1:A:963:TYR:HD2	1:A:963:TYR:O	1.79	0.65
1:A:483:LEU:HB2	1:A:507:LEU:HD13	1.79	0.65
1:A:362:HIS:O	1:A:366:GLN:HG3	1.96	0.65
1:A:556:LEU:O	1:A:591:ARG:NH2	2.30	0.64
1:A:555:LYS:C	1:A:556:LEU:HD23	2.22	0.64
1:A:44:MET:C	1:A:46:ASP:O	2.41	0.64
1:A:308:VAL:HG22	1:A:309:PRO:HD2	1.79	0.64
2:P:13:MET:SD	2:P:14:ILE:N	2.71	0.63
2:P:13:MET:CG	2:P:14:ILE:N	2.60	0.62
1:A:44:MET:HB2	1:A:49:GLU:HB2	1.81	0.62
1:A:139:PRO:O	1:A:141:SER:O	2.18	0.62
1:A:354:PHE:HB3	1:A:384:LYS:HD2	1.81	0.62
1:A:44:MET:HE2	1:A:50:VAL:HG23	1.82	0.62
1:A:44:MET:HE3	1:A:49:GLU:OE2	2.00	0.62
1:A:484:GLU:OE1	1:A:507:LEU:HD21	1.99	0.62
1:A:879:HIS:CE1	1:A:880:PHE:HE1	2.17	0.61
1:A:417:PHE:HA	1:A:439:MET:HE1	1.81	0.61
1:A:760:LEU:HD11	3:C:194:PHE:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:HIS:ND1	1:A:880:PHE:CD1	2.69	0.61
1:A:903:ARG:NH1	1:A:955:ARG:CZ	2.63	0.61
1:A:140:ALA:O	1:A:143:ALA:HB2	2.00	0.61
2:P:22:ILE:O	2:P:23:ARG:HG2	2.01	0.61
1:A:71:GLU:HA	1:A:71:GLU:OE1	1.99	0.61
1:A:767:ALA:HB1	1:A:794:VAL:HG23	1.81	0.60
1:A:677:ARG:HB3	1:A:709:LEU:HD12	1.84	0.60
1:A:904:ASN:OD1	1:A:905:SER:N	2.34	0.60
1:A:141:SER:C	1:A:142:GLU:CD	2.69	0.60
1:A:771:GLN:OE1	2:P:26:ASN:ND2	2.34	0.60
3:C:171:GLN:O	3:C:174:SER:OG	2.15	0.60
1:A:885:ALA:HB1	1:A:922:LEU:CD1	2.30	0.59
1:A:556:LEU:CB	1:A:591:ARG:HH21	2.14	0.59
1:A:703:ARG:HB3	1:A:726:LEU:HD13	1.83	0.59
1:A:723:MET:HE2	1:A:723:MET:HA	1.83	0.59
2:P:103:HIS:HD2	2:P:105:HIS:H	1.50	0.59
1:A:644:THR:HA	1:A:666:LEU:HD11	1.84	0.59
1:A:964:GLU:O	1:A:964:GLU:HG2	2.03	0.59
1:A:44:MET:CG	1:A:49:GLU:HG2	2.33	0.58
1:A:142:GLU:CD	1:A:142:GLU:N	2.61	0.58
1:A:32:ARG:HD3	2:P:80:VAL:O	2.02	0.58
1:A:46:ASP:N	1:A:46:ASP:OD1	2.32	0.58
1:A:700:PRO:HB3	1:A:703:ARG:CZ	2.34	0.58
1:A:822:GLU:HA	1:A:825:GLU:HB2	1.84	0.58
1:A:44:MET:O	1:A:46:ASP:O	2.21	0.57
1:A:735:ARG:HD3	1:A:737:GLU:HG3	1.86	0.57
1:A:788:LEU:HD11	1:A:811:TYR:HE2	1.68	0.57
1:A:210:GLU:HA	1:A:213:ILE:HD12	1.86	0.57
1:A:637:SER:OG	1:A:643:ARG:NH2	2.37	0.57
3:C:166:ASP:HB3	3:C:169:LEU:HD13	1.87	0.57
1:A:737:GLU:HB2	1:A:741:ASP:HB3	1.86	0.57
1:A:117:THR:HG22	1:A:170:LEU:HD21	1.86	0.57
1:A:707:HIS:HA	1:A:710:GLN:CB	2.35	0.57
1:A:268:TRP:CD1	1:A:268:TRP:C	2.83	0.56
2:P:22:ILE:C	2:P:23:ARG:HG2	2.29	0.56
1:A:405:ARG:HD2	1:A:412:TYR:HB2	1.87	0.56
1:A:141:SER:HB3	1:A:142:GLU:CD	2.29	0.56
1:A:638:ASP:OD2	3:C:169:LEU:HD11	2.06	0.56
1:A:75:ARG:HD2	1:A:111:GLU:CB	2.35	0.56
1:A:165:PRO:CD	1:A:165:PRO:O	2.51	0.56
1:A:71:GLU:HB3	1:A:73:SER:OG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:CD	1:A:100:ARG:HD3	2.30	0.56
1:A:809:HIS:CG	2:P:22:ILE:HD11	2.40	0.56
1:A:828:LEU:O	1:A:834:ALA:HA	2.05	0.56
1:A:936:HIS:HA	1:A:939:GLU:CG	2.36	0.55
1:A:65:CYS:HB3	1:A:100:ARG:HD2	1.87	0.55
1:A:622:ILE:O	1:A:626:ILE:HG13	2.05	0.55
1:A:879:HIS:H	1:A:879:HIS:CD2	2.23	0.55
1:A:44:MET:CG	1:A:49:GLU:CD	2.76	0.55
1:A:295:ILE:HD11	1:A:340:THR:HG23	1.87	0.55
1:A:709:LEU:C	1:A:709:LEU:HD23	2.32	0.55
1:A:172:LEU:HD12	2:P:79:LEU:HD21	1.87	0.55
1:A:386:HIS:CG	2:P:53:PRO:HG3	2.41	0.55
1:A:266:CYS:O	1:A:269:GLN:O	2.25	0.55
1:A:409:GLU:OE2	1:A:409:GLU:CA	2.54	0.54
1:A:837:ALA:HB1	1:A:880:PHE:CE2	2.41	0.54
1:A:811:TYR:CD1	1:A:819:LYS:HB3	2.43	0.54
2:P:83:PRO:HD2	2:P:92:SER:HB3	1.89	0.54
1:A:945:ALA:HA	1:A:948:THR:OG1	2.08	0.54
1:A:673:ASP:O	1:A:677:ARG:HG2	2.07	0.54
1:A:937:ASP:OD2	2:P:13:MET:HA	2.08	0.54
1:A:963:TYR:O	1:A:963:TYR:CD2	2.61	0.54
1:A:707:HIS:HA	1:A:710:GLN:HB2	1.90	0.53
1:A:715:HIS:HB3	1:A:762:LEU:HD13	1.90	0.53
1:A:724:GLY:O	1:A:728:LEU:HB2	2.08	0.53
1:A:75:ARG:CD	1:A:111:GLU:HB3	2.39	0.53
1:A:267:PHE:O	1:A:269:GLN:O	2.26	0.53
1:A:531:ILE:HG22	1:A:557:LEU:HD11	1.90	0.53
1:A:49:GLU:CG	1:A:50:VAL:H	2.08	0.53
1:A:659:GLY:O	1:A:663:VAL:HG23	2.09	0.53
1:A:710:GLN:NE2	1:A:714:LYS:O	2.40	0.53
1:A:804:TYR:CE1	1:A:826:ILE:HG21	2.44	0.53
1:A:354:PHE:CD1	1:A:384:LYS:HG3	2.44	0.53
1:A:713:ASP:OD2	1:A:715:HIS:N	2.42	0.53
1:A:364:ALA:O	1:A:368:THR:OG1	2.27	0.53
1:A:384:LYS:NZ	1:A:385:GLU:OE1	2.32	0.53
1:A:557:LEU:HB3	1:A:558:PRO:CD	2.39	0.53
1:A:703:ARG:CB	1:A:723:MET:HE1	2.39	0.53
1:A:576:ARG:O	1:A:580:GLU:HG3	2.09	0.53
1:A:703:ARG:HB2	1:A:723:MET:HE1	1.90	0.53
1:A:935:ARG:O	1:A:939:GLU:HG2	2.09	0.52
1:A:713:ASP:OD2	1:A:713:ASP:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:TYR:CE1	1:A:819:LYS:HB3	2.44	0.52
1:A:961:ARG:O	1:A:964:GLU:HB3	2.09	0.52
1:A:44:MET:CB	1:A:49:GLU:CG	2.84	0.52
1:A:555:LYS:O	1:A:556:LEU:HD23	2.09	0.52
1:A:667:TYR:OH	1:A:677:ARG:NH1	2.43	0.52
1:A:742:ARG:HH22	1:A:743:GLN:HG3	1.75	0.51
1:A:302:LEU:HD13	1:A:323:MET:HE2	1.93	0.51
1:A:782:LYS:HB3	1:A:784:TYR:CE2	2.45	0.51
1:A:786:ASN:OD1	1:A:786:ASN:N	2.42	0.51
1:A:868:LYS:O	1:A:871:VAL:HG12	2.10	0.51
1:A:398:TYR:CZ	1:A:418:GLY:HA3	2.46	0.51
1:A:138:VAL:HG23	1:A:139:PRO:HA	1.92	0.51
1:A:790:ILE:O	1:A:794:VAL:HG12	2.10	0.51
1:A:121:TRP:NE1	2:P:79:LEU:CD1	2.73	0.50
1:A:963:TYR:O	1:A:964:GLU:C	2.53	0.50
1:A:294:ASN:HB2	1:A:330:SER:HB2	1.93	0.50
1:A:658:GLU:OE1	1:A:658:GLU:N	2.35	0.50
1:A:109:GLN:HB3	1:A:163:ILE:HD13	1.92	0.50
1:A:557:LEU:CD1	1:A:557:LEU:N	2.75	0.50
1:A:811:TYR:CB	1:A:820:ALA:HB2	2.40	0.50
1:A:124:LEU:O	1:A:127:SER:HB3	2.12	0.50
1:A:164:ASN:OD1	1:A:165:PRO:O	2.30	0.50
1:A:788:LEU:O	1:A:792:ILE:HG13	2.12	0.50
1:A:221:MET:HA	1:A:224:VAL:HG12	1.94	0.50
1:A:273:LYS:HE3	1:A:303:ASP:OD2	2.12	0.50
1:A:690:LYS:HD2	1:A:690:LYS:O	2.12	0.50
1:A:44:MET:CG	1:A:49:GLU:CG	2.90	0.50
1:A:654:ASN:HB3	1:A:658:GLU:OE1	2.12	0.50
3:C:193:ASP:OD1	3:C:195:SER:OG	2.23	0.49
1:A:33:PHE:HB3	1:A:87:LYS:HD2	1.93	0.49
1:A:557:LEU:N	1:A:557:LEU:HD13	2.27	0.49
1:A:767:ALA:HB3	1:A:798:ILE:HD11	1.93	0.49
1:A:164:ASN:C	1:A:165:PRO:O	2.48	0.49
1:A:44:MET:SD	1:A:49:GLU:HG2	2.52	0.49
1:A:620:GLY:O	1:A:622:ILE:N	2.45	0.49
1:A:735:ARG:HG2	1:A:741:ASP:OD2	2.12	0.49
1:A:860:TYR:HB3	1:A:891:ILE:HG12	1.95	0.48
1:A:375:SER:OG	1:A:405:ARG:NE	2.44	0.48
1:A:398:TYR:CE1	1:A:418:GLY:HA3	2.48	0.48
1:A:417:PHE:CE1	1:A:421:GLN:OE1	2.66	0.48
1:A:413:LEU:HB3	1:A:414:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:TYR:HE2	1:A:779:GLU:HB2	1.78	0.48
1:A:45:GLN:N	1:A:71:GLU:OE2	2.47	0.48
1:A:470:GLU:OE1	1:A:472:LYS:NZ	2.46	0.48
1:A:714:LYS:HG2	1:A:715:HIS:CD2	2.49	0.48
1:A:718:TYR:OH	2:P:29:PRO:O	2.30	0.47
1:A:811:TYR:HB3	1:A:820:ALA:HB2	1.95	0.47
1:A:407:GLY:O	1:A:410:ARG:O	2.32	0.47
1:A:417:PHE:CA	1:A:439:MET:HE1	2.43	0.47
1:A:668:GLN:O	1:A:671:PRO:HG3	2.14	0.47
1:A:602:ASP:O	1:A:606:THR:HG23	2.15	0.47
3:C:183:ASN:HA	3:C:186:LEU:HD12	1.95	0.47
1:A:616:TYR:CE2	1:A:628:THR:HG21	2.50	0.47
1:A:887:VAL:O	1:A:891:ILE:HG13	2.15	0.47
1:A:379:TYR:CE2	1:A:383:ARG:HD2	2.50	0.47
1:A:440:ILE:HD12	1:A:441:GLN:N	2.29	0.47
1:A:243:ALA:O	1:A:247:VAL:HG23	2.15	0.47
1:A:477:LYS:HD2	1:A:477:LYS:O	2.15	0.47
1:A:65:CYS:SG	1:A:97:MET:HG2	2.55	0.47
1:A:791:PHE:HA	1:A:794:VAL:HG12	1.96	0.46
3:C:195:SER:O	3:C:198:ARG:HB3	2.15	0.46
1:A:714:LYS:HG2	1:A:715:HIS:HD2	1.80	0.46
1:A:880:PHE:N	1:A:880:PHE:HD1	2.14	0.46
1:A:798:ILE:HG22	1:A:800:ASP:H	1.80	0.46
1:A:817:PHE:O	1:A:821:ILE:HG12	2.16	0.46
1:A:157:LEU:HD12	1:A:170:LEU:HD22	1.98	0.46
1:A:125:TRP:CD1	1:A:125:TRP:C	2.94	0.46
1:A:47:ASP:C	1:A:48:VAL:CG2	2.89	0.46
1:A:301:TYR:CB	1:A:322:ALA:HB2	2.46	0.45
1:A:308:VAL:HG22	1:A:309:PRO:CD	2.43	0.45
1:A:791:PHE:HA	1:A:794:VAL:CG1	2.46	0.45
1:A:788:LEU:CD1	1:A:811:TYR:HE2	2.29	0.45
1:A:879:HIS:ND1	1:A:880:PHE:HE1	2.07	0.45
1:A:885:ALA:HB1	1:A:922:LEU:HD11	1.97	0.45
1:A:109:GLN:HA	1:A:112:LYS:HB2	1.97	0.45
1:A:409:GLU:OE2	1:A:409:GLU:N	2.49	0.45
1:A:880:PHE:CD1	1:A:880:PHE:N	2.84	0.45
1:A:876:ASP:OD1	1:A:876:ASP:N	2.44	0.45
1:A:903:ARG:HG2	1:A:904:ASN:N	2.31	0.45
1:A:947:ASN:C	1:A:947:ASN:OD1	2.60	0.45
1:A:267:PHE:C	1:A:269:GLN:O	2.60	0.45
1:A:150:LEU:O	1:A:154:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:OE2	1:A:409:GLU:HA	2.15	0.45
1:A:557:LEU:HB3	1:A:558:PRO:HD2	1.98	0.45
1:A:707:HIS:HA	1:A:710:GLN:HB3	1.98	0.45
1:A:43:PRO:HD3	1:A:77:TYR:CZ	2.51	0.45
1:A:425:LEU:O	1:A:426:LYS:HB2	2.16	0.45
1:A:44:MET:HE3	1:A:49:GLU:CD	2.42	0.45
1:A:165:PRO:O	1:A:166:ALA:HB3	2.17	0.45
1:A:244:TYR:CZ	2:P:75:MET:HE1	2.52	0.45
1:A:47:ASP:OD1	1:A:47:ASP:N	2.48	0.45
2:P:38:LEU:HD12	2:P:38:LEU:HA	1.84	0.45
1:A:742:ARG:HH12	1:A:743:GLN:HG3	1.82	0.44
1:A:933:TYR:CE2	2:P:19:ILE:HD11	2.52	0.44
1:A:64:LEU:CD2	1:A:81:VAL:HG11	2.47	0.44
1:A:556:LEU:HB3	1:A:591:ARG:HH21	1.80	0.44
1:A:725:ASN:ND2	2:P:26:ASN:O	2.50	0.44
1:A:946:ARG:CG	1:A:947:ASN:N	2.80	0.44
1:A:878:LEU:HD23	1:A:932:PRO:HD3	2.00	0.44
1:A:903:ARG:HH11	1:A:955:ARG:CZ	2.30	0.44
1:A:116:ILE:HG22	1:A:160:ALA:HB2	1.98	0.44
1:A:274:ASP:O	1:A:277:LYS:HB3	2.16	0.44
2:P:13:MET:HG3	2:P:14:ILE:N	2.31	0.44
1:A:610:PHE:CE2	2:P:36:LYS:HE2	2.53	0.44
1:A:32:ARG:HB2	2:P:82:MET:SD	2.58	0.44
1:A:348:PHE:O	1:A:349:LEU:C	2.59	0.44
1:A:735:ARG:HD2	1:A:741:ASP:OD2	2.18	0.44
2:P:37:LEU:HD23	3:C:179:MET:HB3	2.00	0.44
1:A:833:LYS:H	1:A:833:LYS:HG2	1.44	0.44
1:A:735:ARG:CD	1:A:741:ASP:OD2	2.66	0.43
1:A:773:ILE:HD13	3:C:201:ALA:HB2	2.00	0.43
1:A:429:LEU:O	1:A:433:LYS:HG3	2.18	0.43
1:A:690:LYS:O	1:A:691:LYS:C	2.60	0.43
1:A:219:ARG:O	2:P:94:GLN:HA	2.18	0.43
1:A:403:ASP:O	1:A:406:GLY:N	2.41	0.43
1:A:325:GLU:O	1:A:329:LYS:HB2	2.19	0.43
2:P:90:GLU:O	2:P:91:SER:C	2.61	0.43
1:A:277:LYS:NZ	1:A:281:GLU:OE2	2.51	0.43
3:C:199:LYS:O	3:C:203:PRO:HD3	2.18	0.43
1:A:295:ILE:HD11	1:A:340:THR:CG2	2.48	0.43
1:A:509:ARG:O	1:A:512:GLU:HB3	2.18	0.43
1:A:463:ASN:HD21	1:A:470:GLU:H	1.66	0.43
1:A:903:ARG:HH11	1:A:955:ARG:NH2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ASP:HB3	1:A:676:VAL:HB	2.02	0.42
1:A:899:ARG:O	1:A:902:GLU:HG2	2.19	0.42
1:A:301:TYR:HB2	1:A:322:ALA:HB2	2.01	0.42
1:A:783:ASP:OD2	1:A:786:ASN:ND2	2.52	0.42
1:A:934:PRO:O	1:A:938:ILE:HD13	2.18	0.42
2:P:17:ASP:OD1	2:P:18:TYR:N	2.52	0.42
1:A:57:LEU:HD11	1:A:88:GLN:NE2	2.34	0.42
1:A:174:ARG:HD2	1:A:174:ARG:HA	1.86	0.42
1:A:403:ASP:HA	1:A:407:GLY:CA	2.49	0.42
1:A:756:PHE:CZ	1:A:772:GLY:HA3	2.55	0.42
1:A:44:MET:HG2	1:A:49:GLU:CG	2.50	0.42
1:A:431:GLU:O	1:A:435:ARG:HG2	2.19	0.42
1:A:524:GLN:O	1:A:527:GLU:HB3	2.19	0.42
1:A:793:LYS:HD2	1:A:796:GLU:CD	2.45	0.42
1:A:57:LEU:N	1:A:57:LEU:HD12	2.35	0.42
1:A:75:ARG:HB2	1:A:111:GLU:HG2	2.01	0.42
2:P:107:ARG:N	2:P:108:PRO:CD	2.82	0.42
1:A:747:ALA:O	1:A:750:ASN:HB2	2.19	0.42
1:A:47:ASP:O	1:A:49:GLU:N	2.53	0.42
1:A:165:PRO:O	1:A:165:PRO:HD2	2.19	0.42
1:A:573:GLY:O	1:A:575:HIS:N	2.52	0.42
1:A:174:ARG:O	1:A:178:ILE:HG13	2.19	0.42
1:A:778:VAL:HG13	1:A:779:GLU:HG3	2.01	0.42
1:A:269:GLN:O	1:A:270:LEU:CB	2.52	0.41
1:A:878:LEU:CD2	1:A:931:PRO:HA	2.50	0.41
1:A:244:TYR:OH	2:P:75:MET:HE1	2.20	0.41
1:A:666:LEU:HD23	1:A:666:LEU:O	2.20	0.41
1:A:794:VAL:HA	1:A:797:THR:HG22	2.01	0.41
3:C:196:HIS:O	3:C:199:LYS:HB2	2.20	0.41
1:A:69:GLU:OE2	1:A:100:ARG:HD3	2.19	0.41
1:A:113:LEU:O	1:A:117:THR:HG23	2.19	0.41
1:A:150:LEU:HD23	1:A:181:LYS:HG3	2.02	0.41
1:A:375:SER:HB2	1:A:401:ALA:O	2.20	0.41
1:A:640:THR:HG21	1:A:670:ASN:ND2	2.35	0.41
1:A:677:ARG:HH21	1:A:709:LEU:HA	1.85	0.41
1:A:953:LEU:O	1:A:957:LEU:HD13	2.20	0.41
1:A:69:GLU:HG2	1:A:104:VAL:HG21	2.01	0.41
1:A:908:LEU:HD13	1:A:956:ALA:HA	2.02	0.41
1:A:145:THR:O	1:A:148:TYR:HB3	2.20	0.41
1:A:644:THR:HA	1:A:666:LEU:CD1	2.49	0.41
1:A:257:PRO:HG3	2:P:76:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:O	1:A:104:VAL:HG23	2.21	0.41
1:A:273:LYS:HE3	1:A:303:ASP:CG	2.46	0.41
1:A:677:ARG:HH21	1:A:709:LEU:CA	2.33	0.41
1:A:886:PHE:CZ	2:P:17:ASP:HA	2.56	0.41
1:A:323:MET:O	1:A:327:THR:HB	2.21	0.41
2:P:99:PRO:HA	2:P:100:PRO:HD3	1.92	0.41
1:A:115:ILE:HD12	1:A:116:ILE:N	2.36	0.40
1:A:512:GLU:CD	3:C:177:ARG:HH12	2.29	0.40
1:A:32:ARG:HH11	1:A:256:ASP:CG	2.29	0.40
1:A:688:ASN:O	1:A:691:LYS:HB3	2.20	0.40
3:C:195:SER:HB3	3:C:198:ARG:HH12	1.86	0.40
1:A:313:PRO:O	1:A:316:ILE:HG12	2.21	0.40
1:A:413:LEU:CD2	2:P:59:LEU:HD11	2.51	0.40
1:A:885:ALA:HB1	1:A:922:LEU:HD12	2.03	0.40
1:A:554:ARG:HG2	1:A:554:ARG:HH11	1.86	0.40
1:A:686:LYS:HB3	1:A:686:LYS:HE2	1.91	0.40
1:A:737:GLU:HB2	1:A:741:ASP:CB	2.50	0.40
1:A:939:GLU:HG2	1:A:939:GLU:H	1.66	0.40
1:A:433:LYS:HE3	1:A:456:TYR:HE1	1.87	0.40
1:A:498:SER:HA	1:A:499:PRO:HD3	1.91	0.40
1:A:782:LYS:HB3	1:A:784:TYR:HE2	1.86	0.40
1:A:935:ARG:HG3	1:A:936:HIS:N	2.35	0.40
1:A:942:ALA:O	1:A:945:ALA:HB3	2.22	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	897/939 (96%)	842 (94%)	55 (6%)	0	100	100
2	P	105/121 (87%)	100 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	40/74 (54%)	39 (98%)	1 (2%)	0	100	100
All	All	1042/1134 (92%)	981 (94%)	61 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	759/782 (97%)	691 (91%)	68 (9%)	9	26
2	P	89/101 (88%)	78 (88%)	11 (12%)	4	13
3	C	35/52 (67%)	32 (91%)	3 (9%)	10	28
All	All	883/935 (94%)	801 (91%)	82 (9%)	8	25

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	32	ARG
1	A	46	ASP
1	A	47	ASP
1	A	48	VAL
1	A	50	VAL
1	A	51	GLU
1	A	88	GLN
1	A	89	ASN
1	A	96	GLU
1	A	99	LEU
1	A	103	ASN
1	A	105	LEU
1	A	136	ASP
1	A	138	VAL
1	A	141	SER
1	A	142	GLU

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Mol	Chain	Res	Type
1	A	144	LYS
1	A	188	SER
1	A	189	LYS
1	A	273	LYS
1	A	308	VAL
1	A	321	LYS
1	A	344	PHE
1	A	393	ARG
1	A	409	GLU
1	A	438	LYS
1	A	475	GLU
1	A	488	SER
1	A	494	LYS
1	A	497	LEU
1	A	555	LYS
1	A	557	LEU
1	A	576	ARG
1	A	599	LEU
1	A	621	ASP
1	A	638	ASP
1	A	653	ARG
1	A	663	VAL
1	A	690	LYS
1	A	691	LYS
1	A	707	HIS
1	A	723	MET
1	A	737	GLU
1	A	738	THR
1	A	740	GLN
1	A	741	ASP
1	A	744	LYS
1	A	754	GLU
1	A	757	ASP
1	A	761	GLN
1	A	777	LEU
1	A	781	ARG
1	A	785	LYS
1	A	786	ASN
1	A	814	LEU
1	A	831	GLU
1	A	833	LYS
1	A	861	LYS

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Mol	Chain	Res	Type
1	A	876	ASP
1	A	879	HIS
1	A	909	GLU
1	A	935	ARG
1	A	936	HIS
1	A	939	GLU
1	A	944	MET
1	A	955	ARG
1	A	964	GLU
2	P	13	MET
2	P	14	ILE
2	P	37	LEU
2	P	38	LEU
2	P	59	LEU
2	P	79	LEU
2	P	82	MET
2	P	89	ASP
2	P	114	SER
2	P	115	THR
2	P	116	LEU
3	C	165	LEU
3	C	171	GLN
3	C	178	ARG

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

Mol	Chain	Res	Type
1	A	45	GLN
1	A	88	GLN
1	A	151	GLN
1	A	421	GLN
1	A	441	GLN
1	A	463	ASN
1	A	571	GLN
1	A	654	ASN
1	A	668	GLN
1	A	670	ASN
1	A	688	ASN
1	A	715	HIS
1	A	802	HIS
1	A	896	HIS
1	A	907	GLN

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Mol	Chain	Res	Type
1	A	943	ASN
2	P	98	GLN
2	P	103	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	905/939 (96%)	0.21	24 (2%) 56 47	51, 92, 132, 172	0
2	P	107/121 (88%)	0.08	2 (1%) 66 58	57, 78, 116, 128	0
3	C	42/74 (56%)	0.54	2 (4%) 35 28	71, 105, 127, 144	0
All	All	1054/1134 (92%)	0.21	28 (2%) 56 47	51, 91, 131, 172	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	13	MET	4.1
1	A	952	GLN	3.8
1	A	49	GLU	3.5
3	C	205	VAL	3.4
3	C	202	ALA	3.1
1	A	958	ALA	2.8
1	A	706	LYS	2.7
1	A	707	HIS	2.6
1	A	957	LEU	2.6
1	A	490	TRP	2.6
1	A	50	VAL	2.5
1	A	709	LEU	2.5
1	A	143	ALA	2.4
1	A	710	GLN	2.4
2	P	56	ALA	2.3
1	A	190	ALA	2.3
1	A	195	ASP	2.3
1	A	948	THR	2.2
1	A	944	MET	2.2
1	A	344	PHE	2.2
1	A	705	TYR	2.2
1	A	96	GLU	2.1
1	A	649	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	703	ARG	2.1
1	A	634	SER	2.0
1	A	960	GLN	2.0
1	A	556	LEU	2.0
1	A	48	VAL	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.