



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 04:03 am BST

PDB ID : 4C93
Title : Crystal structure of the carboxy-terminal domain of yeast Ctf4 bound to Pol alpha.
Authors : Simon, A.C.; Pellegrini, L.
Deposited on : 2013-10-02
Resolution : 2.69 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

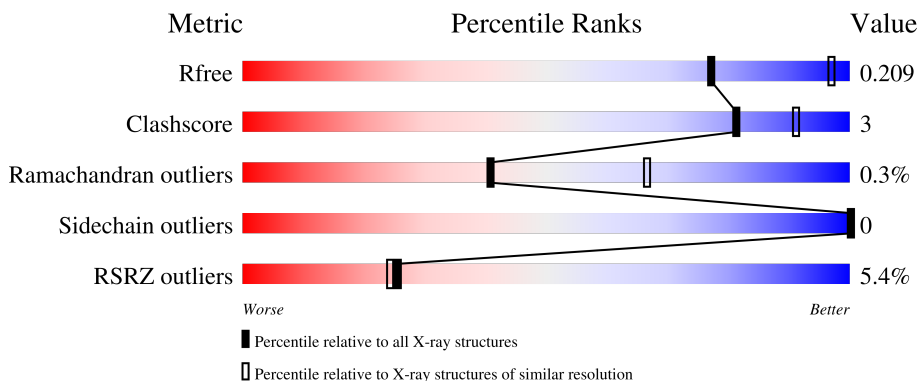
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	478	
1	B	478	
1	C	478	
2	D	13	
2	E	13	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9617 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 DNA POLYMERASE ALPHA-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	Total 3416	C 2193	N 566	O 642	S 15	0	1	0
1	B	431	Total 3472	C 2227	N 576	O 653	S 16	0	1	0
1	C	296	Total 2405	C 1562	N 392	O 440	S 11	0	1	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	MET	-	expression tag	UNP Q01454
A	451	GLY	-	expression tag	UNP Q01454
A	452	SER	-	expression tag	UNP Q01454
A	453	SER	-	expression tag	UNP Q01454
A	454	HIS	-	expression tag	UNP Q01454
A	455	HIS	-	expression tag	UNP Q01454
A	456	HIS	-	expression tag	UNP Q01454
A	457	HIS	-	expression tag	UNP Q01454
A	458	HIS	-	expression tag	UNP Q01454
A	459	HIS	-	expression tag	UNP Q01454
A	460	SER	-	expression tag	UNP Q01454
A	461	GLN	-	expression tag	UNP Q01454
A	462	ASP	-	expression tag	UNP Q01454
A	463	PRO	-	expression tag	UNP Q01454
A	464	GLU	-	expression tag	UNP Q01454
A	465	ASN	-	expression tag	UNP Q01454
A	466	LEU	-	expression tag	UNP Q01454
A	467	TYR	-	expression tag	UNP Q01454
A	468	PHE	-	expression tag	UNP Q01454
A	469	GLN	-	expression tag	UNP Q01454
A	470	GLY	-	expression tag	UNP Q01454
B	450	MET	-	expression tag	UNP Q01454
B	451	GLY	-	expression tag	UNP Q01454

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	SER	-	expression tag	UNP Q01454
B	453	SER	-	expression tag	UNP Q01454
B	454	HIS	-	expression tag	UNP Q01454
B	455	HIS	-	expression tag	UNP Q01454
B	456	HIS	-	expression tag	UNP Q01454
B	457	HIS	-	expression tag	UNP Q01454
B	458	HIS	-	expression tag	UNP Q01454
B	459	HIS	-	expression tag	UNP Q01454
B	460	SER	-	expression tag	UNP Q01454
B	461	GLN	-	expression tag	UNP Q01454
B	462	ASP	-	expression tag	UNP Q01454
B	463	PRO	-	expression tag	UNP Q01454
B	464	GLU	-	expression tag	UNP Q01454
B	465	ASN	-	expression tag	UNP Q01454
B	466	LEU	-	expression tag	UNP Q01454
B	467	TYR	-	expression tag	UNP Q01454
B	468	PHE	-	expression tag	UNP Q01454
B	469	GLN	-	expression tag	UNP Q01454
B	470	GLY	-	expression tag	UNP Q01454
C	450	MET	-	expression tag	UNP Q01454
C	451	GLY	-	expression tag	UNP Q01454
C	452	SER	-	expression tag	UNP Q01454
C	453	SER	-	expression tag	UNP Q01454
C	454	HIS	-	expression tag	UNP Q01454
C	455	HIS	-	expression tag	UNP Q01454
C	456	HIS	-	expression tag	UNP Q01454
C	457	HIS	-	expression tag	UNP Q01454
C	458	HIS	-	expression tag	UNP Q01454
C	459	HIS	-	expression tag	UNP Q01454
C	460	SER	-	expression tag	UNP Q01454
C	461	GLN	-	expression tag	UNP Q01454
C	462	ASP	-	expression tag	UNP Q01454
C	463	PRO	-	expression tag	UNP Q01454
C	464	GLU	-	expression tag	UNP Q01454
C	465	ASN	-	expression tag	UNP Q01454
C	466	LEU	-	expression tag	UNP Q01454
C	467	TYR	-	expression tag	UNP Q01454
C	468	PHE	-	expression tag	UNP Q01454
C	469	GLN	-	expression tag	UNP Q01454
C	470	GLY	-	expression tag	UNP Q01454

- Molecule 2 is a protein called DNA POLYMERASE ALPHA CATALYTIC SUBUNIT A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	0	0	0
			82	53	10	19			
2	E	10	Total	C	N	O	0	0	0
			82	53	10	19			

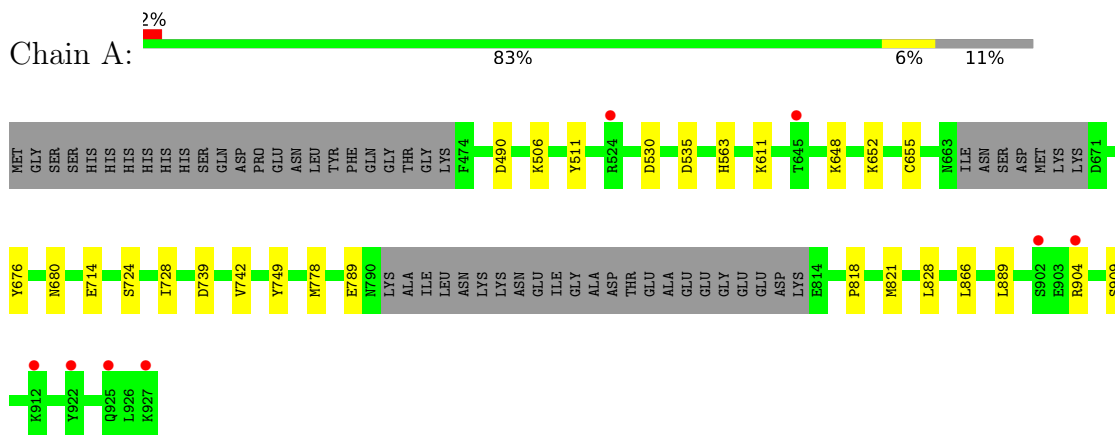
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	64	Total	O	0	0
			64	64		
3	C	28	Total	O	0	0
			28	28		

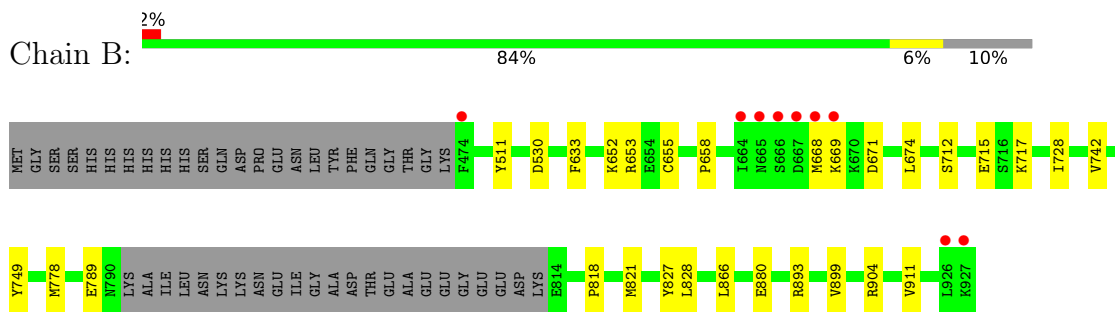
3 Residue-property plots [i](#)

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.

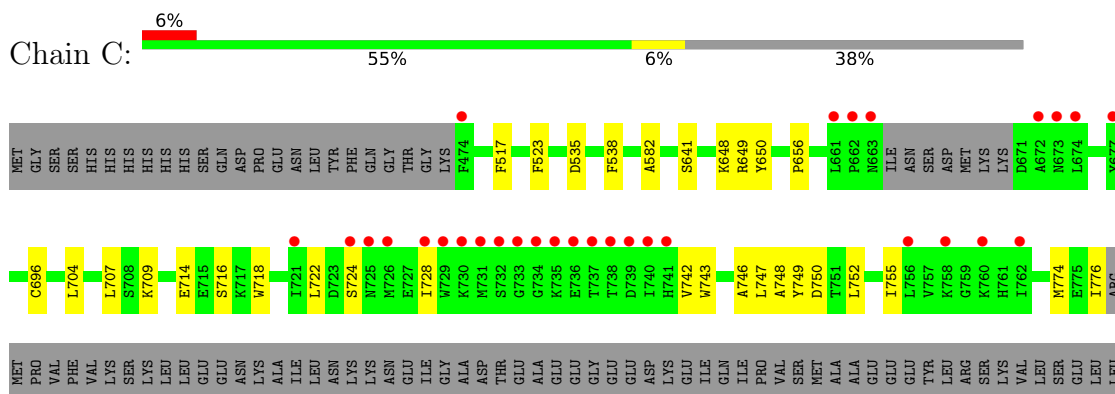
- Molecule 1: DNA POLYMERASE ALPHA-BINDING PROTEIN



- Molecule 1: DNA POLYMERASE ALPHA-BINDING PROTEIN



- Molecule 1: DNA POLYMERASE ALPHA-BINDING PROTEIN



THR ASP THR THR LEU LEU ASN ASP ASP GLY GLU MET TYR GLY ASN GLU ASN ASN VAL VAL LEU ALA ALA LEU ASN GLY ALA TYR ASP ASP LYS LYS LEU LEU ARG LEU PHE ALA SER ALA CYS SER ASP GLN ASN VAL VAL LYS LYS ALA ALA SER SER LEU LEU HIS GLU LEU LYS GLN ASP ARG ALA THR THR ALA

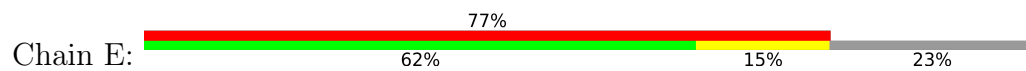
ALA VAL LYS ILE SER GLU ARG ALA GLU LEU PRO SER LEU VAL LYS LYS ILE ASN ASN ILE ARG GLU ALA ARG TYR GLU LYS LYS

- Molecule 2: DNA POLYMERASE ALPHA CATALYTIC SUBUNIT A



ILE ASP ASN F140 D141 D142 I143 L144 G145 E146 S149

- Molecule 2: DNA POLYMERASE ALPHA CATALYTIC SUBUNIT A



ILE ASP ASN F140 D141 D142 I143 L144 G145 E146 F147 E148 S149

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.98Å 100.00Å 219.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.69 49.20 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.20-2.69) 99.5 (49.20-2.69)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.172 , 0.210 0.172 , 0.209	Depositor DCC
R_{free} test set	2761 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtrriage
Anisotropy	0.221	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9617	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/3501	0.40	0/4741
1	B	0.24	0/3558	0.40	0/4817
1	C	0.23	0/2481	0.39	0/3370
2	D	0.24	0/83	0.30	0/110
2	E	0.25	0/83	0.32	0/110
All	All	0.23	0/9706	0.40	0/13148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3356	18	0
1	B	3472	0	3418	18	0
1	C	2405	0	2326	19	0
2	D	82	0	67	1	0
2	E	82	0	67	2	0
3	A	68	0	0	1	0
3	B	64	0	0	0	0
3	C	28	0	0	0	0
All	All	9617	0	9234	49	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 3.

All (49) 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:B:789:GLU:HG3	1:B:818:PRO:HG3	1.79	0.64
1:A:904:ARG:NH1	2:D:142:ASP:OD1	2.37	0.58
1:A:648:LYS:HB3	1:B:717:LYS:HD3	1.86	0.57
1:A:778:MET:HG3	1:A:828:LEU:HB3	1.88	0.56
1:A:511:TYR:HB2	1:A:530:ASP:HB3	1.88	0.56
1:A:652:LYS:NZ	1:A:655:CYS:SG	2.64	0.55
1:B:904:ARG:NH1	2:E:142:ASP:OD1	2.40	0.55
1:A:789:GLU:HG3	1:A:818:PRO:HG3	1.90	0.53
1:B:653:ARG:HD2	1:C:714:GLU:HG2	1.89	0.53
1:B:893:ARG:NH2	2:E:147:PHE:O	2.41	0.53
1:A:490:ASP:HB3	1:A:506:LYS:HB2	1.90	0.53
1:B:778:MET:HG3	1:B:828:LEU:HB3	1.91	0.52
1:C:747:LEU:HD11	1:C:776:ILE:HD11	1.91	0.52
1:B:669:LYS:HA	1:B:674:LEU:HD22	1.92	0.52
1:A:563:HIS:ND1	1:B:880:GLU:OE1	2.33	0.51
1:B:818:PRO:HG2	1:B:821:MET:HB3	1.92	0.51
1:C:535:ASP:N	1:C:535:ASP:OD1	2.44	0.51
1:C:728:ILE:HD11	1:C:742:VAL:HG23	1.93	0.51
1:C:722:LEU:HD21	1:C:774:MET:HE2	1.92	0.50
1:B:899:VAL:HG13	1:B:911:VAL:HG13	1.94	0.50
1:A:611:LYS:NZ	1:B:658:PRO:O	2.39	0.49
1:C:704:LEU:HD22	1:C:752:LEU:HD13	1.95	0.48
1:C:724:SER:HB2	1:C:742:VAL:HG21	1.97	0.47
1:A:724:SER:HB2	1:A:742:VAL:HG21	1.96	0.47
1:B:712:SER:HB2	1:B:715:GLU:HB2	1.97	0.46
1:C:743:TRP:HB3	1:C:755:ILE:HB	1.98	0.46
1:C:648:LYS:HE2	1:C:650:TYR:CZ	2.51	0.46
1:A:739:ASP:OD1	1:A:739:ASP:N	2.47	0.45
1:B:652:LYS:NZ	1:B:655:CYS:SG	2.70	0.45
1:A:714:GLU:OE1	1:C:649:ARG:NE	2.45	0.45
1:C:538:PHE:CG	1:C:582:ALA:HA	2.51	0.45
1:A:866:LEU:HD23	1:A:889:LEU:HD23	2.00	0.44
1:A:728:ILE:HD11	1:A:742:VAL:HG23	2.01	0.43
1:A:818:PRO:HG2	1:A:821:MET:HB3	2.00	0.43
1:A:535:ASP:OD1	1:A:535:ASP:N	2.49	0.43
1:B:728:ILE:HD11	1:B:742:VAL:HG23	2.00	0.43
1:A:909:SER:OG	3:A:2067:HOH:O	2.21	0.42
1:B:668:MET:HA	1:B:671:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:PHE:CG	1:C:523:PHE:HB2	2.55	0.42
1:C:746:ALA:O	1:C:752:LEU:HD12	2.20	0.42
1:A:676:TYR:O	1:A:680:ASN:N	2.53	0.41
1:B:633:PHE:CD1	1:C:656:PRO:HG3	2.55	0.41
1:C:696:CYS:HB3	1:C:704:LEU:HD11	2.01	0.41
1:C:707:LEU:HD13	1:C:718:TRP:CE2	2.56	0.41
1:C:748:ALA:O	1:C:750:ASP:N	2.53	0.41
1:B:511:TYR:HB2	1:B:530:ASP:HB3	2.02	0.41
1:B:827:TYR:CD1	1:B:866:LEU:HD13	2.57	0.40
1:C:641:SER:OG	1:C:648:LYS:HE3	2.21	0.40
1:C:709:LYS:O	1:C:716:SER:OG	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/478 (88%)	404 (96%)	14 (3%)	1 (0%)	47	73
1	B	428/478 (90%)	414 (97%)	13 (3%)	1 (0%)	47	73
1	C	293/478 (61%)	275 (94%)	17 (6%)	1 (0%)	41	66
2	D	8/13 (62%)	8 (100%)	0	0	100	100
2	E	8/13 (62%)	8 (100%)	0	0	100	100
All	All	1156/1460 (79%)	1109 (96%)	44 (4%)	3 (0%)	41	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	TYR
1	B	749	TYR
1	C	749	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/422 (89%)	377 (100%)	0	100	100
1	B	384/422 (91%)	384 (100%)	0	100	100
1	C	267/422 (63%)	267 (100%)	0	100	100
2	D	9/12 (75%)	9 (100%)	0	100	100
2	E	9/12 (75%)	9 (100%)	0	100	100
All	All	1046/1290 (81%)	1046 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	GLN
1	A	634	HIS
1	B	559	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 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, 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	424/478 (88%)	-0.01	8 (1%) 66 69	29, 48, 93, 123	0
1	B	431/478 (90%)	-0.04	9 (2%) 63 65	29, 50, 97, 142	0
1	C	296/478 (61%)	0.30	30 (10%) 7 5	34, 59, 115, 157	0
2	D	10/13 (76%)	2.15	6 (60%) 0 0	81, 100, 116, 117	0
2	E	10/13 (76%)	4.01	10 (100%) 0 0	105, 118, 134, 139	0
All	All	1171/1460 (80%)	0.11	63 (5%) 25 24	29, 52, 105, 157	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	729	TRP	5.0
1	C	733	GLY	5.0
1	C	736	GLU	4.9
2	E	148	GLU	4.7
2	E	143	ILE	4.7
2	E	149	SER	4.7
1	B	927	LYS	4.6
1	C	731	MET	4.6
2	E	146	GLU	4.6
1	C	732	SER	4.5
2	E	144	LEU	4.5
1	C	734	GLY	4.4
1	C	738	THR	4.4
1	B	666	SER	4.2
2	E	147	PHE	4.1
2	E	140	PHE	4.1
1	C	760	LYS	4.0
1	C	728	ILE	3.9
1	C	740	ILE	3.9
1	B	668	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	474	PHE	3.5
1	B	926	LEU	3.5
1	C	737	THR	3.4
1	C	735	LYS	3.3
1	C	724	SER	3.3
1	C	662	PRO	3.3
1	B	665	ASN	3.3
2	E	142	ASP	3.2
1	C	739	ASP	3.1
2	D	142	ASP	3.1
2	D	146	GLU	3.1
1	C	725	ASN	3.1
2	E	145	GLY	3.1
1	C	672	ALA	2.9
2	D	140	PHE	2.8
1	A	524	ARG	2.8
1	C	474	PHE	2.8
1	C	673	ASN	2.8
1	A	645	THR	2.8
1	B	667	ASP	2.7
1	C	721	ILE	2.7
1	C	756	LEU	2.6
2	D	141	ASP	2.6
2	D	149	SER	2.6
1	C	674	LEU	2.6
1	B	669	LYS	2.6
1	A	904	ARG	2.5
2	E	141	ASP	2.5
1	C	726	MET	2.5
1	C	663	ASN	2.4
1	C	730	LYS	2.4
1	C	758	LYS	2.4
2	D	144	LEU	2.3
1	A	927	LYS	2.3
1	C	677	TYR	2.3
1	A	902	SER	2.2
1	A	922	TYR	2.2
1	A	925	GLN	2.2
1	C	762	ILE	2.1
1	C	741	HIS	2.1
1	B	664	ILE	2.0
1	C	661	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	912	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 monosaccharides 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.