Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:22 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

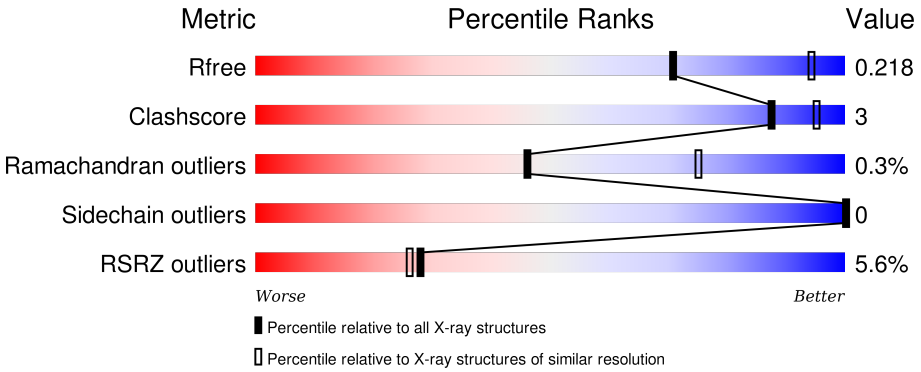
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	478	2% 83% 6% 11%
1	B	478	2% 84% 6% 10%
1	C	478	6% 55% 6% 38%
2	D	13	46% 69% 8% 23%
2	E	13	77% 62% 15% 23%

2 Entry composition

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
1	A	424	Total	C	N	O	S	0	1	0
			3416	2193	566	642	15			
1	B	431	Total	C	N	O	S	0	1	0
			3472	2227	576	653	16			
1	C	296	Total	C	N	O	S	0	1	0
			2405	1562	392	440	11			

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

Continued on next page...

Continued from previous page...

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.

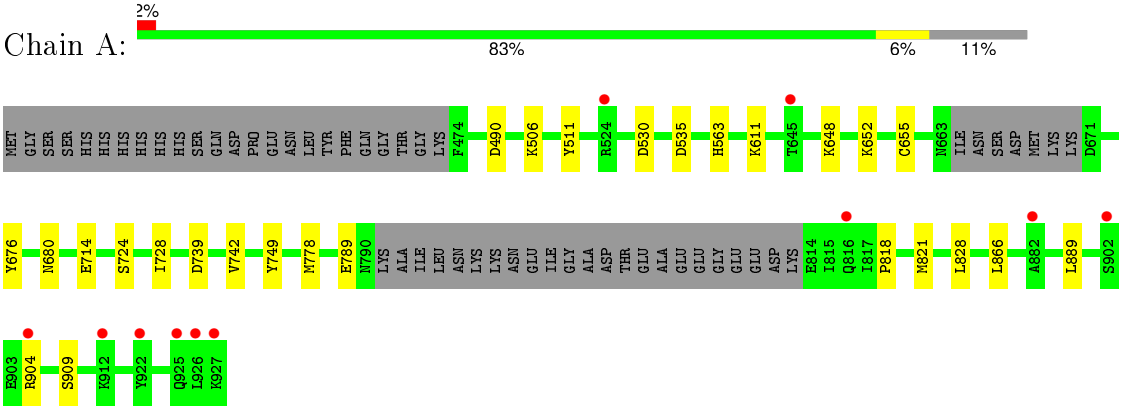
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	64	Total	O	0	0
			64	64		
3	C	28	Total	O	0	0
			28	28		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

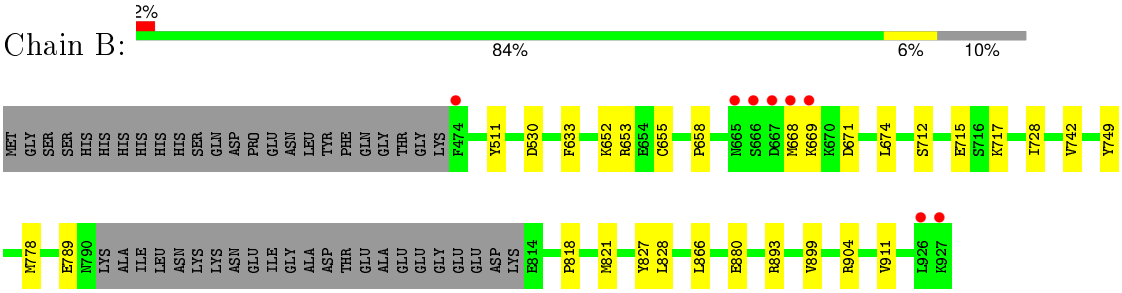
- Molecule 1: DNA POLYMERASE ALPHA-BINDING PROTEIN

Chain A:



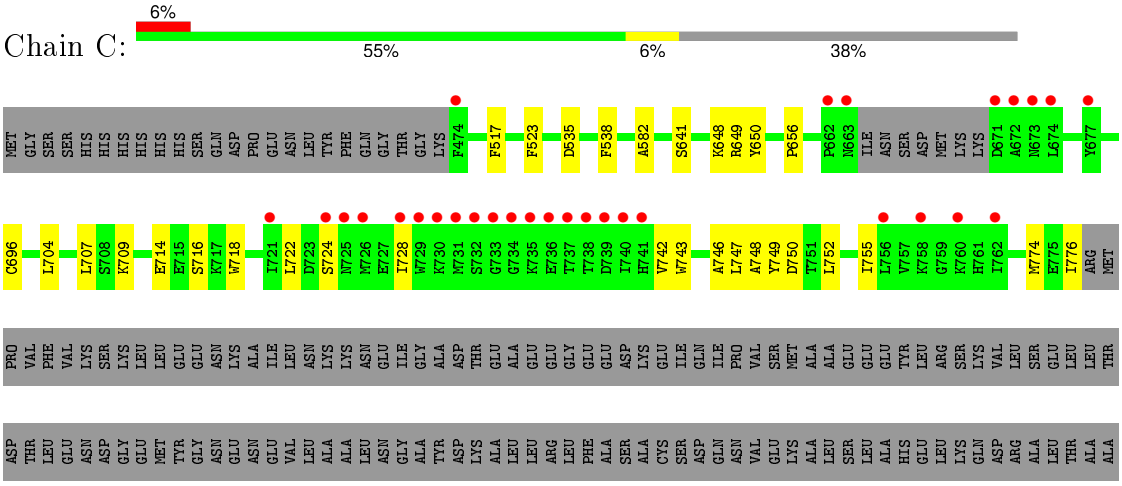
- Molecule 1: DNA POLYMERASE ALPHA-BINDING PROTEIN

Chain B:



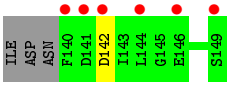
- Molecule 1: DNA POLYMERASE ALPHA-BINDING PROTEIN

Chain C:



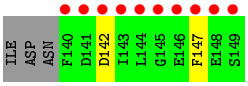
• Molecule 2: DNA POLYMERASE ALPHA CATALYTIC SUBUNIT A

Chain D:



• Molecule 2: DNA POLYMERASE ALPHA CATALYTIC SUBUNIT A

Chain E:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.23 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.172 , 0.210 0.181 , 0.218	Depositor DCC
R_{free} test set	2763 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 54707 reflections (0.002%)	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.23	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

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:B:904:ARG:NH1	2:E:142:ASP:OD1	2.40	0.55
1:A:652:LYS:NZ	1:A:655:CYS:SG	2.64	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:818:PRO:HG2	1:A:821:MET:HB3	2.00	0.43
1:A:728:ILE:HD11	1:A:742:VAL:HG23	2.01	0.43
1:B:728:ILE:HD11	1:B:742:VAL:HG23	2.00	0.43
1:A:535:ASP:OD1	1:A:535:ASP:N	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:ALA:O	1:C:752:LEU:HD12	2.20	0.42
1:C:517:PHE:CG	1:C:523:PHE:HB2	2.55	0.42
1:C:696:CYS:HB3	1:C:704:LEU:HD11	2.01	0.41
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: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: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
1:B:827:TYR:CD1	1:B:866:LEU:HD13	2.57	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%)	52	80
1	B	428/478 (90%)	414 (97%)	13 (3%)	1 (0%)	52	80
1	C	293/478 (61%)	275 (94%)	17 (6%)	1 (0%)	46	75
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%)	46	75

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

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.

Some 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	424/478 (88%)	0.03	11 (2%) 59 59	29, 48, 93, 123	0
1	B	431/478 (90%)	-0.00	8 (1%) 70 70	29, 50, 97, 142	0
1	C	296/478 (61%)	0.33	30 (10%) 9 7	34, 59, 115, 157	0
2	D	10/13 (76%)	2.21	6 (60%) 0 0	81, 100, 116, 117	0
2	E	10/13 (76%)	4.09	10 (100%) 0 0	105, 118, 134, 139	0
All	All	1171/1460 (80%)	0.15	65 (5%) 28 26	29, 52, 105, 157	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	733	GLY	5.1
1	C	729	TRP	5.0
1	C	736	GLU	5.0
1	C	731	MET	4.8
2	E	148	GLU	4.8
2	E	146	GLU	4.7
2	E	149	SER	4.7
1	B	927	LYS	4.7
2	E	143	ILE	4.7
2	E	144	LEU	4.6
1	C	732	SER	4.6
1	C	734	GLY	4.5
1	C	738	THR	4.5
1	B	666	SER	4.2
2	E	147	PHE	4.2
2	E	140	PHE	4.2
1	C	760	LYS	4.1
1	C	740	ILE	4.0
1	C	728	ILE	3.9
1	B	668	MET	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	474	PHE	3.5
1	B	926	LEU	3.5
1	C	737	THR	3.5
1	C	735	LYS	3.4
1	C	662	PRO	3.3
1	B	665	ASN	3.3
1	C	724	SER	3.3
2	E	142	ASP	3.3
2	D	142	ASP	3.2
1	C	739	ASP	3.2
2	E	145	GLY	3.2
1	C	725	ASN	3.2
2	D	146	GLU	3.1
1	C	672	ALA	2.9
1	C	474	PHE	2.9
1	C	673	ASN	2.9
2	D	140	PHE	2.9
1	A	524	ARG	2.9
1	B	667	ASP	2.9
1	A	645	THR	2.9
2	D	141	ASP	2.7
1	C	721	ILE	2.7
1	C	756	LEU	2.7
1	B	669	LYS	2.7
1	C	674	LEU	2.6
2	E	141	ASP	2.6
2	D	149	SER	2.6
1	A	904	ARG	2.6
1	C	726	MET	2.6
1	C	730	LYS	2.4
1	C	663	ASN	2.4
1	A	927	LYS	2.4
1	C	677	TYR	2.4
1	C	758	LYS	2.4
2	D	144	LEU	2.3
1	A	922	TYR	2.3
1	A	925	GLN	2.2
1	A	902	SER	2.2
1	C	741	HIS	2.2
1	C	762	ILE	2.1
1	C	671	ASP	2.1
1	A	882	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	926	LEU	2.0
1	A	912	LYS	2.0
1	A	816	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 carbohydrates 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.