Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:25 PM GMT

PDB ID	:	1TKL
Title	:	Yeast Oxygen-Dependent Coproporphyrinogen Oxidase
Authors	:	Phillips, J.D.; Whitby, F.G.; Warby, C.A.; Labbe, P.; Yang, C.; Pflugrath, J.W.; Ferrara, J.D.; Robinson, H.; Kushner, J.P.; Hill, C.P.
Deposited on	:	2004-06-08
Resolution	:	2.00 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 (i) symbol.

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

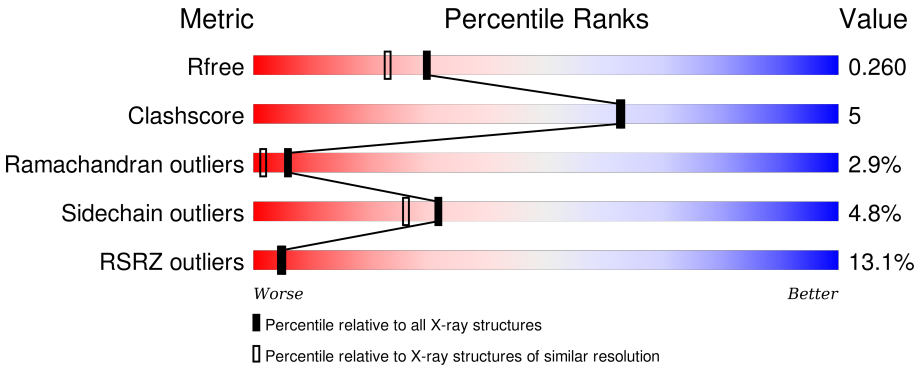
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	326	10% 80% 17%
1	B	326	14% 79% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5709 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 Coproporphyrinogen III oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	99	0	0
			2643	1680	464	489	10			
1	B	325	Total	C	N	O	S	149	1	0
			2648	1683	465	490	10			

- Molecule 2 is water.

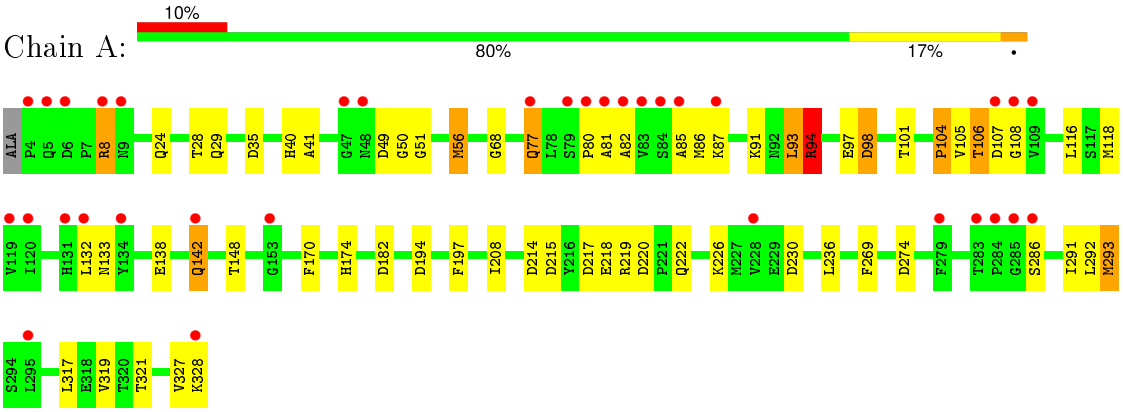
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	249	Total	O	0	0
			249	249		
2	B	169	Total	O	0	0
			169	169		

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.

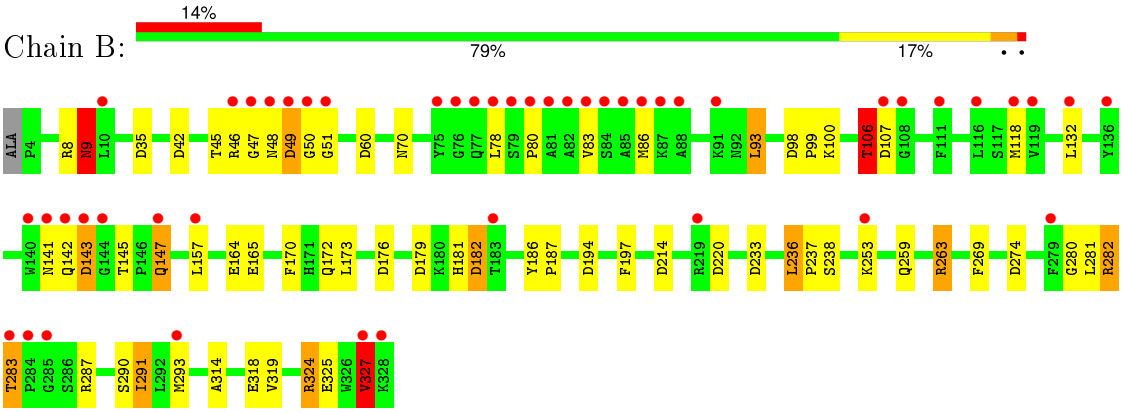
- Molecule 1: Coproporphyrinogen III oxidase

Chain A:



- Molecule 1: Coproporphyrinogen III oxidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.82Å 86.82Å 207.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.06 – 2.00 29.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (79.06-2.00) 98.4 (29.44-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.32 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.208 , 0.258 0.214 , 0.260	Depositor DCC
R_{free} test set	2731 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 53796 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5709	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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	1.33	6/2720 (0.2%)	1.54	25/3689 (0.7%)
1	B	0.84	3/2727 (0.1%)	0.95	14/3699 (0.4%)
All	All	1.11	9/5447 (0.2%)	1.28	39/7388 (0.5%)

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	A	1	8
1	B	0	6
All	All	1	14

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	LEU	C-N	-27.20	0.71	1.34
1	A	106	THR	C-N	-26.47	0.73	1.34
1	A	94	ARG	CB-CG	-23.53	0.89	1.52
1	A	94	ARG	CG-CD	-21.78	0.97	1.51
1	A	94	ARG	C-N	-21.70	0.84	1.34
1	B	106	THR	C-N	13.58	1.65	1.34
1	B	93	LEU	C-N	-11.09	1.08	1.34
1	B	9	ASN	C-N	10.07	1.57	1.34
1	A	94	ARG	N-CA	8.47	1.63	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ARG	O-C-N	-35.04	66.64	122.70
1	A	106	THR	O-C-N	-33.49	69.11	122.70
1	A	93	LEU	O-C-N	-28.38	77.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ARG	N-CA-CB	24.16	154.09	110.60
1	A	106	THR	CA-C-N	18.78	158.52	117.20
1	A	93	LEU	CA-C-N	17.18	154.99	117.20
1	A	94	ARG	C-N-CA	16.79	163.68	121.70
1	A	94	ARG	CG-CD-NE	16.72	146.91	111.80
1	A	94	ARG	CA-C-N	16.35	153.16	117.20
1	A	94	ARG	CB-CG-CD	14.09	148.22	111.60
1	A	94	ARG	CA-CB-CG	10.86	137.29	113.40
1	B	263	ARG	NE-CZ-NH2	-9.61	115.49	120.30
1	A	94	ARG	CB-CA-C	-9.04	92.32	110.40
1	B	106	THR	C-N-CA	-8.44	100.61	121.70
1	B	263	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	9	ASN	C-N-CA	-7.86	102.06	121.70
1	A	194	ASP	CB-CG-OD2	7.65	125.19	118.30
1	B	194	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	93	LEU	C-N-CA	7.08	139.41	121.70
1	A	217	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	51	GLY	N-CA-C	-6.72	96.29	113.10
1	B	60	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	274	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	214	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	182	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	215	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	35	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	220	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	233	ASP	CB-CG-OD2	6.12	123.80	118.30
1	B	35	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	176	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	49	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	179	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	98	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	214	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	230	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	220	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	49	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	274	ASP	CB-CG-OD2	5.02	122.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	94	ARG	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	PRO	Peptide
1	A	106	THR	Mainchain,Peptide
1	A	93	LEU	Mainchain,Peptide
1	A	94	ARG	Mainchain,Peptide
1	A	97	GLU	Peptide
1	B	106	THR	Mainchain,Peptide
1	B	327	VAL	Peptide
1	B	45	THR	Peptide
1	B	9	ASN	Mainchain
1	B	93	LEU	Mainchain

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	2643	0	2545	23	0
1	B	2648	0	2555	29	0
2	A	249	0	0	4	0
2	B	169	0	0	3	0
All	All	5709	0	5100	52	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 5.

All (52) 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:324:ARG:NH1	1:B:325:GLU:O	2.03	0.92
1:A:41:ALA:HB2	1:A:56:MET:HE1	1.71	0.73
1:A:41:ALA:HB2	1:A:56:MET:CE	2.22	0.69
1:B:47:GLY:O	1:B:49:ASP:N	2.27	0.68
1:B:42:ASP:HB2	2:B:663:HOH:O	1.94	0.68
1:B:290:SER:HA	1:B:293:MET:HE2	1.75	0.67
1:A:286:SER:HB2	1:A:291:ILE:HD11	1.82	0.61
1:B:86:MET:HA	2:B:909:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ARG:NE	2:B:910:HOH:O	2.34	0.59
1:B:259:GLN:O	1:B:263:ARG:HG2	2.02	0.58
1:B:280:GLY:O	1:B:282:ARG:O	2.20	0.58
1:B:287:ARG:O	1:B:291:ILE:HG23	2.02	0.58
1:A:82:ALA:HA	1:A:85:ALA:HB3	1.91	0.53
1:A:68:GLY:HA3	1:A:293:MET:SD	2.50	0.52
1:B:143:ASP:CG	1:B:143:ASP:O	2.49	0.52
1:B:70:ASN:HD21	1:B:293:MET:HE3	1.75	0.51
1:A:24:GLN:O	1:A:28:THR:HG23	2.10	0.51
1:A:118:MET:HE3	1:A:132:LEU:HB3	1.93	0.51
1:A:142:GLN:HE21	1:A:142:GLN:HA	1.76	0.51
1:A:174:HIS:HE1	2:A:505:HOH:O	1.93	0.50
1:B:141:ASN:HD22	1:B:147:GLN:HG2	1.77	0.49
1:A:77:GLN:OE1	1:A:108:GLY:HA3	2.14	0.47
1:B:324:ARG:HB2	1:B:324:ARG:HH11	1.80	0.47
1:B:319:VAL:HG13	1:B:324:ARG:HG2	1.97	0.47
1:A:138:GLU:HA	1:A:148:THR:O	2.15	0.46
1:B:281:LEU:C	1:B:282:ARG:O	2.52	0.46
1:B:70:ASN:HD21	1:B:293:MET:CE	2.29	0.45
1:A:170:PHE:O	1:A:174:HIS:HD2	2.00	0.45
1:B:80:PRO:HA	1:B:83:VAL:HB	1.97	0.45
1:B:236:LEU:N	1:B:237:PRO:HD2	2.31	0.45
1:B:282:ARG:O	1:B:283:THR:HB	2.16	0.45
1:B:172:GLN:HB2	1:B:327:VAL:HG21	1.99	0.44
1:A:317:LEU:O	1:A:321:THR:HG23	2.17	0.44
1:A:41:ALA:HB2	1:A:56:MET:HE3	1.99	0.44
1:B:157:LEU:HD13	1:B:170:PHE:CD1	2.52	0.44
1:A:197:PHE:HA	1:A:269:PHE:CE1	2.52	0.44
1:B:186:TYR:N	1:B:187:PRO:HD2	2.33	0.44
1:A:29:GLN:HG3	2:A:660:HOH:O	2.17	0.44
1:B:118:MET:HE3	1:B:132:LEU:HB3	2.00	0.43
1:B:173:LEU:HD12	1:B:238:SER:HB3	1.99	0.43
1:B:197:PHE:HA	1:B:269:PHE:CE1	2.54	0.43
1:A:218:GLU:OE1	2:A:514:HOH:O	2.21	0.43
1:A:208:ILE:HG22	1:A:319:VAL:CG1	2.49	0.42
1:A:8:ARG:HG2	1:A:222:GLN:NE2	2.35	0.41
1:A:116:LEU:O	1:A:133:ASN:HA	2.20	0.41
1:A:82:ALA:O	1:A:86:MET:N	2.50	0.41
1:A:219:ARG:NH2	2:A:738:HOH:O	2.54	0.41
1:B:181:HIS:O	1:B:182:ASP:HB2	2.21	0.40
1:B:46:ARG:O	1:B:51:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:VAL:HG22	1:B:324:ARG:HD3	2.03	0.40
1:A:77:GLN:HB3	1:A:77:GLN:HE21	1.70	0.40
1:B:314:ALA:O	1:B:318:GLU:HG3	2.21	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	323/326 (99%)	305 (94%)	11 (3%)	7 (2%)	8	3
1	B	324/326 (99%)	297 (92%)	15 (5%)	12 (4%)	4	1
All	All	647/652 (99%)	602 (93%)	26 (4%)	19 (3%)	6	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
1	A	94	ARG
1	A	107	ASP
1	B	48	ASN
1	B	142	GLN
1	B	143	ASP
1	A	80	PRO
1	A	105	VAL
1	B	182	ASP
1	A	104	PRO
1	B	8	ARG
1	B	99	PRO
1	B	100	LYS
1	B	107	ASP
1	A	50	GLY

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Mol	Chain	Res	Type
1	B	9	ASN
1	B	50	GLY
1	B	147	GLN
1	B	283	THR

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	282/282 (100%)	267 (95%)	15 (5%)	28 22
1	B	283/282 (100%)	271 (96%)	12 (4%)	36 31
All	All	565/564 (100%)	538 (95%)	27 (5%)	31 26

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	40	HIS
1	A	56	MET
1	A	77	GLN
1	A	87	LYS
1	A	91	LYS
1	A	98	ASP
1	A	101	THR
1	A	142	GLN
1	A	226	LYS
1	A	236	LEU
1	A	292	LEU
1	A	293	MET
1	A	327	VAL
1	A	328	LYS
1	B	78	LEU
1	B	98	ASP
1	B	106	THR
1	B	145	THR

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Mol	Chain	Res	Type
1	B	164	GLU
1	B	165	GLU
1	B	236	LEU
1	B	253	LYS
1	B	282	ARG
1	B	291	ILE
1	B	324	ARG
1	B	327	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	142	GLN
1	A	174	HIS
1	B	70	ASN

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	312/326 (95%)	0.47	34 (10%)	7	8	20, 33, 56, 69	0
1	B	306/326 (93%)	0.94	47 (15%)	3	3	24, 40, 79, 94	0
All	All	618/652 (94%)	0.70	81 (13%)	5	5	20, 36, 69, 94	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	LEU	9.2
1	B	50	GLY	8.2
1	A	4	PRO	7.8
1	B	107	ASP	7.6
1	B	108	GLY	7.5
1	B	85	ALA	7.5
1	B	88	ALA	7.0
1	A	84	SER	6.6
1	A	107	ASP	6.2
1	B	47	GLY	5.7
1	B	49	ASP	5.7
1	B	82	ALA	5.4
1	B	142	GLN	5.2
1	B	48	ASN	5.2
1	B	84	SER	4.9
1	B	51	GLY	4.8
1	B	46	ARG	4.7
1	B	80	PRO	4.7
1	B	144	GLY	4.6
1	A	79	SER	4.6
1	B	86	MET	4.6
1	A	83	VAL	4.5
1	B	83	VAL	4.3
1	B	327	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	4.2
1	A	279	PHE	4.0
1	A	5	GLN	4.0
1	A	81	ALA	3.9
1	B	81	ALA	3.9
1	B	141	ASN	3.8
1	B	143	ASP	3.8
1	A	285	GLY	3.7
1	B	285	GLY	3.7
1	B	147	GLN	3.7
1	B	284	PRO	3.6
1	A	284	PRO	3.3
1	B	10	LEU	3.3
1	B	79	SER	3.2
1	A	108	GLY	3.2
1	A	132	LEU	3.1
1	B	119	VAL	3.0
1	B	140	TRP	2.9
1	A	47	GLY	2.8
1	A	131	HIS	2.8
1	A	119	VAL	2.7
1	B	293	MET	2.7
1	B	279	PHE	2.7
1	B	111	PHE	2.7
1	B	328	LYS	2.7
1	B	219	ARG	2.7
1	B	132	LEU	2.6
1	A	120	ILE	2.6
1	A	142	GLN	2.6
1	A	80	PRO	2.6
1	B	118	MET	2.6
1	A	283	THR	2.5
1	A	85	ALA	2.5
1	A	328	LYS	2.3
1	B	75	TYR	2.3
1	A	87	LYS	2.3
1	B	77	GLN	2.3
1	A	286	SER	2.3
1	B	283	THR	2.3
1	B	87	LYS	2.3
1	B	91	LYS	2.2
1	A	228	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	157	LEU	2.2
1	A	153	GLY	2.2
1	A	134	TYR	2.1
1	A	82	ALA	2.1
1	A	295	LEU	2.1
1	B	116	LEU	2.1
1	A	48	ASN	2.1
1	B	76	GLY	2.1
1	A	9	ASN	2.1
1	B	136	TYR	2.1
1	B	253	LYS	2.1
1	A	77	GLN	2.0
1	A	109	VAL	2.0
1	B	183	THR	2.0
1	A	8	ARG	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.