Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 – 06:31 am GMT

PDB ID	:	2C8A
Title	:	Structure of the wild-type C3bot1 Exoenzyme (Nicotinamide-bound state, crystal form I)
Authors	:	Stura, E.A.; Menetrey, J.; Flatau, G.; Boquet, P.; Menez, A.
Deposited on	:	2005-12-03
Resolution	:	1.70 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 (i)) were used in the production of this report:

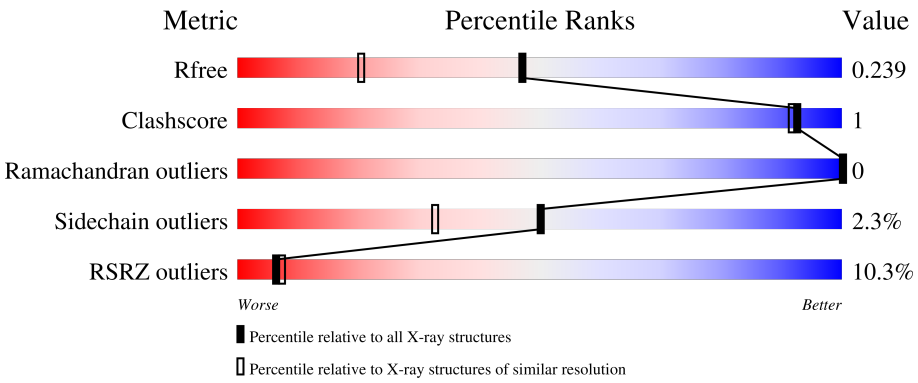
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	211	11% 92% 6% •
1	B	211	10% 88% 7% • •
1	C	211	9% 94% • •
1	D	211	10% 89% 7% •

2 Entry composition (i)

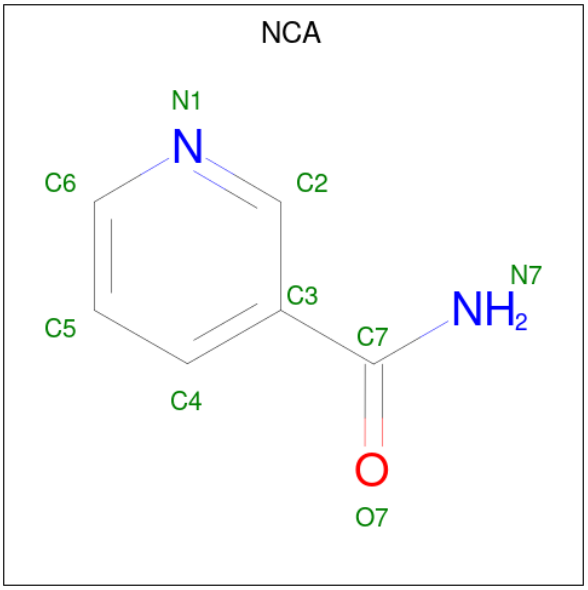
There are 4 unique types of molecules in this entry. The entry contains 7268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MONO-ADP-RIBOSYLTRANSFERASE C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1630	1037	278	308	7	0	0	0
1	B	202	1587	1009	270	301	7	0	0	0
1	C	207	1625	1034	277	307	7	0	0	0
1	D	202	1588	1010	270	301	7	0	0	0

- Molecule 2 is NICOTINAMIDE (three-letter code: NCA) (formula: $C_6H_6N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	6	2	1	0	0
2	B	1	9	6	2	1	0	0

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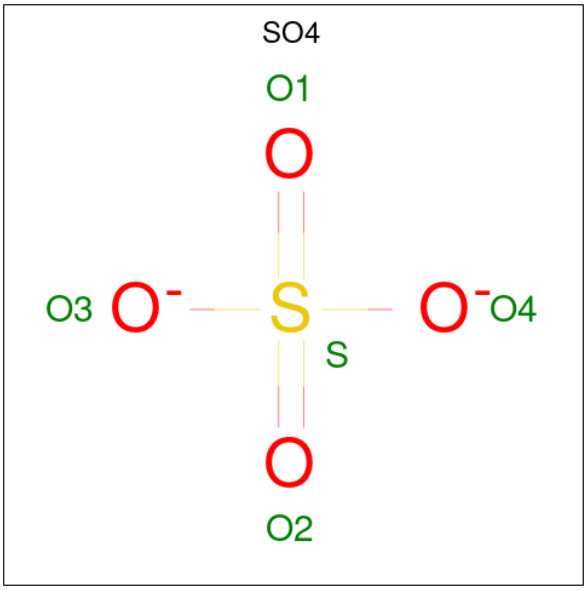
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	9	6	2	1	0	0
			Total	C	N	O		
2	D	1	9	6	2	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	218	218	218	0	0
			Total	O		
4	B	187	187	187	0	0
			Total	O		
4	C	204	204	204	0	0

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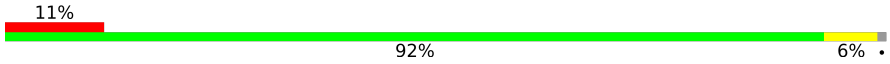
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	173	173	173	0	0

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.

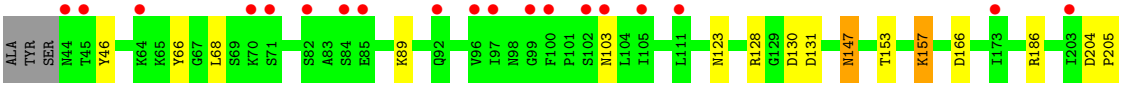
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

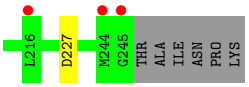
Chain A:



• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

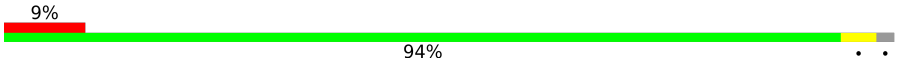
Chain B:

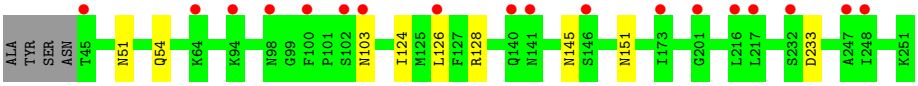




• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

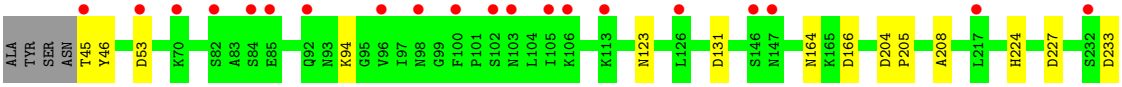
Chain C:

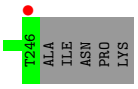




• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.74Å 74.64Å 118.96Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	24.33 – 1.70 24.36 – 1.69	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.33-1.70) 98.9 (24.36-1.69)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.235 0.212 , 0.239	Depositor DCC
R_{free} test set	4994 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7268	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NCA

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	0.33	0/1659	0.63	2/2229 (0.1%)
1	B	0.31	0/1615	0.64	4/2168 (0.2%)
1	C	0.31	0/1654	0.63	1/2222 (0.0%)
1	D	0.32	0/1616	0.62	4/2170 (0.2%)
All	All	0.32	0/6544	0.63	11/8789 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	ASP	CB-CG-OD2	7.40	124.96	118.30
1	C	233	ASP	CB-CG-OD2	7.04	124.63	118.30
1	D	233	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	131	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	227	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	131	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	227	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	227	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	131	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	130	ASP	CB-CG-OD2	5.11	122.89	118.30
1	D	53	ASP	CB-CG-OD2	5.10	122.89	118.30

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	1630	0	1654	4	0
1	B	1587	0	1605	7	0
1	C	1625	0	1652	3	0
1	D	1588	0	1610	7	0
2	A	9	0	6	0	0
2	B	9	0	6	0	0
2	C	9	0	6	0	0
2	D	9	0	6	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	218	0	0	1	0
4	B	187	0	0	0	0
4	C	204	0	0	0	0
4	D	173	0	0	0	0
All	All	7268	0	6545	19	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 1.

All (19) 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:145:ASN:HD21	1:C:151:ASN:HD22	1.33	0.76
1:B:157:LYS:HE3	1:D:208:ALA:HB1	1.82	0.61
1:A:54:GLN:HE22	1:D:45:THR:HG23	1.70	0.57
1:C:51:ASN:HD21	1:C:54:GLN:NE2	2.07	0.52
1:B:153:THR:HG22	1:B:157:LYS:HZ3	1.75	0.49
1:D:164:ASN:OD1	1:D:224:HIS:HE1	1.95	0.48
1:B:153:THR:O	1:B:157:LYS:HE2	2.13	0.48
1:C:124:ILE:HD12	1:C:126:LEU:HD21	1.96	0.47
1:B:46:TYR:CD2	1:B:123:ASN:HB3	2.51	0.46
1:B:66:TYR:HB3	1:B:68:LEU:HD13	1.98	0.46
1:A:212:GLN:NE2	4:A:2193:HOH:O	2.49	0.45
1:D:46:TYR:CD2	1:D:123:ASN:HB3	2.52	0.45
1:B:147:ASN:C	1:B:147:ASN:HD22	2.20	0.45
1:D:204:ASP:N	1:D:205:PRO:CD	2.82	0.43
1:A:46:TYR:CD2	1:A:123:ASN:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASP:N	1:B:205:PRO:CD	2.83	0.41
1:D:166:ASP:OD1	1:D:224:HIS:HD2	2.03	0.41
1:D:164:ASN:OD1	1:D:224:HIS:CE1	2.74	0.41
1:A:122:GLU:HG3	1:A:124:ILE:HG23	2.02	0.41

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	206/211 (98%)	205 (100%)	1 (0%)	0	100	100
1	B	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
1	C	205/211 (97%)	204 (100%)	1 (0%)	0	100	100
1	D	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
All	All	811/844 (96%)	805 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	176/179 (98%)	169 (96%)	7 (4%)	31	13
1	B	171/179 (96%)	165 (96%)	6 (4%)	36	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	176/179 (98%)	174 (99%)	2 (1%)	73	63
1	D	172/179 (96%)	171 (99%)	1 (1%)	86	80
All	All	695/716 (97%)	679 (98%)	16 (2%)	50	33

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	102	SER
1	A	113	LYS
1	A	125	MET
1	A	152	LYS
1	A	220	HIS
1	A	232	SER
1	B	89	LYS
1	B	103	ASN
1	B	128	ARG
1	B	147	ASN
1	B	157	LYS
1	B	186	ARG
1	C	103	ASN
1	C	128	ARG
1	D	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	54	GLN
1	A	62	GLN
1	A	116	ASN
1	A	140	GLN
1	A	182	GLN
1	A	212	GLN
1	B	60	ASN
1	B	103	ASN
1	B	107	GLN
1	B	140	GLN
1	B	147	ASN
1	C	54	GLN

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Mol	Chain	Res	Type
1	C	93	ASN
1	C	145	ASN
1	D	60	ASN
1	D	116	ASN
1	D	140	GLN
1	D	182	GLN
1	D	224	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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1253	-	4,4,4	0.16	0	6,6,6	0.13	0
2	NCA	C	1252	-	9,9,9	0.49	0	11,11,11	1.42	2 (18%)
2	NCA	B	1246	-	9,9,9	0.40	0	11,11,11	1.37	2 (18%)
3	SO4	B	1247	-	4,4,4	0.17	0	6,6,6	0.09	0
3	SO4	D	1248	-	4,4,4	0.15	0	6,6,6	0.15	0
2	NCA	A	1252	-	9,9,9	0.50	0	11,11,11	1.58	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NCA	D	1247	-	9,9,9	0.52	0	11,11,11	1.46	2 (18%)
3	SO4	C	1253	-	4,4,4	0.13	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NCA	D	1247	-	-	0/4/4/4	0/1/1/1
2	NCA	C	1252	-	-	0/4/4/4	0/1/1/1
2	NCA	B	1246	-	-	0/4/4/4	0/1/1/1
2	NCA	A	1252	-	-	0/4/4/4	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1252	NCA	C3-C7-N7	3.09	121.46	117.75
2	C	1252	NCA	C6-N1-C2	2.85	121.77	116.85
2	D	1247	NCA	C3-C7-N7	2.75	121.05	117.75
2	A	1252	NCA	C6-N1-C2	2.67	121.46	116.85
2	D	1247	NCA	C6-N1-C2	2.58	121.31	116.85
2	C	1252	NCA	C3-C7-N7	2.36	120.58	117.75
2	B	1246	NCA	C6-N1-C2	2.28	120.79	116.85
2	B	1246	NCA	C3-C7-N7	2.21	120.40	117.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	208/211 (98%)	0.58	23 (11%)	5	6	17, 27, 39, 55	0
1	B	202/211 (95%)	0.75	22 (10%)	5	6	20, 29, 51, 76	0
1	C	207/211 (98%)	0.47	18 (8%)	10	11	18, 26, 46, 59	0
1	D	202/211 (95%)	0.61	21 (10%)	6	7	19, 29, 49, 62	0
All	All	819/844 (97%)	0.60	84 (10%)	6	7	17, 27, 48, 76	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	LYS	7.8
1	B	44	ASN	5.0
1	A	44	ASN	5.0
1	A	247	ALA	4.8
1	B	100	PHE	4.8
1	B	45	THR	4.3
1	B	97	ILE	4.1
1	A	248	ILE	4.1
1	C	45	THR	4.0
1	B	102	SER	4.0
1	C	216	LEU	3.8
1	B	99	GLY	3.8
1	D	70	LYS	3.7
1	C	98	ASN	3.7
1	A	246	THR	3.6
1	B	82	SER	3.6
1	B	244	MET	3.6
1	C	103	ASN	3.6
1	D	113	LYS	3.5
1	D	85	GLU	3.5
1	D	84	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	45	THR	3.4
1	B	203	ILE	3.4
1	B	96	VAL	3.4
1	A	249	ASN	3.4
1	A	216	LEU	3.3
1	B	85	GLU	3.3
1	D	96	VAL	3.2
1	B	92	GLN	3.2
1	B	103	ASN	3.1
1	A	217	LEU	3.1
1	D	53	ASP	3.1
1	C	126	LEU	3.0
1	B	216	LEU	3.0
1	B	245	GLY	2.9
1	C	146	SER	2.9
1	D	232	SER	2.8
1	D	92	GLN	2.8
1	A	126	LEU	2.8
1	A	232	SER	2.8
1	D	100	PHE	2.8
1	A	250	PRO	2.8
1	C	140	GLN	2.7
1	B	84	SER	2.7
1	D	45	THR	2.6
1	C	232	SER	2.6
1	D	217	LEU	2.6
1	A	229	ARG	2.6
1	D	82	SER	2.6
1	D	98	ASN	2.5
1	B	173	ILE	2.5
1	A	158	ALA	2.5
1	C	100	PHE	2.4
1	D	105	ILE	2.4
1	B	71	SER	2.4
1	B	64	LYS	2.4
1	D	106	LYS	2.4
1	D	146	SER	2.4
1	A	173	ILE	2.4
1	C	248	ILE	2.4
1	B	70	LYS	2.3
1	D	103	ASN	2.3
1	C	247	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	146	SER	2.3
1	C	173	ILE	2.3
1	D	102	SER	2.3
1	C	141	ASN	2.2
1	D	147	ASN	2.2
1	A	92	GLN	2.2
1	A	79	TYR	2.2
1	A	83	ALA	2.2
1	A	103	ASN	2.2
1	D	246	THR	2.2
1	D	126	LEU	2.2
1	B	105	ILE	2.2
1	A	245	GLY	2.2
1	A	233	ASP	2.2
1	C	64	LYS	2.1
1	C	102	SER	2.1
1	A	192	PHE	2.1
1	C	217	LEU	2.1
1	C	94	LYS	2.1
1	C	201	GLY	2.0
1	B	111	LEU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	1247	5/5	0.79	0.18	60,61,61,61	0
3	SO4	C	1253	5/5	0.88	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	1248	5/5	0.88	0.13	62,62,63,63	0
2	NCA	D	1247	9/9	0.92	0.10	22,22,23,23	0
3	SO4	A	1253	5/5	0.95	0.15	49,49,50,50	0
2	NCA	B	1246	9/9	0.96	0.08	20,23,24,24	0
2	NCA	C	1252	9/9	0.97	0.07	20,21,22,22	0
2	NCA	A	1252	9/9	0.98	0.10	20,21,21,22	0

6.5 Other polymers (i)

There are no such residues in this entry.