W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 12, 2024 – 08:57 PM EST

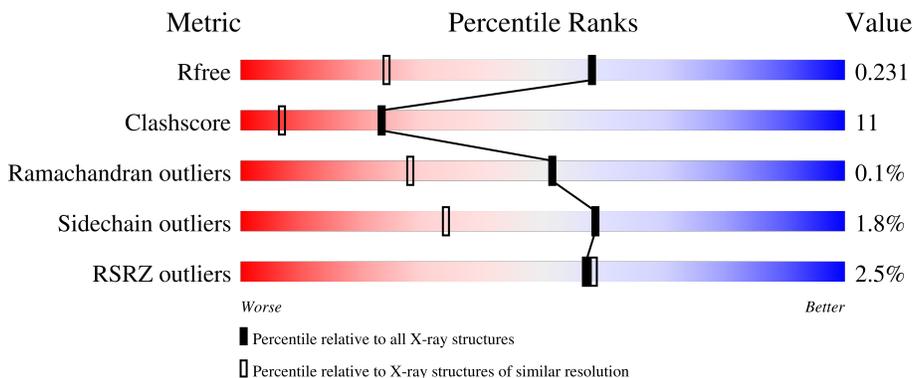|		
PDB ID	:	3ITU
Title	:	hPDE2A catalytic domain complexed with IBMX
Authors	:	Pandit, J.
Deposited on	:	2009-08-28
Resolution	:	1.58 Å(reported)

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 1.58 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		11
Ramachandran outliers		0.1%
Sidechain outliers		1.8%
RSRZ outliers		2.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

⬚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	345	2% / 82% / 14% ··
1	B	345	2% / 75% / 18% ··
1	C	345	3% / 73% / 19% · 5%
1	D	345	3% / 78% / 15% · 5%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 12700 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2767	1763	474	505	25			
1	B	333	Total	C	N	O	S	0	0	0
			2732	1743	469	495	25			
1	C	327	Total	C	N	O	S	0	0	0
			2676	1707	460	484	25			
1	D	327	Total	C	N	O	S	0	0	0
			2676	1707	460	484	25			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	expression tag	UNP O00408
A	576	SER	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
A	578	MET	-	expression tag	UNP O00408
B	575	GLY	-	expression tag	UNP O00408
B	576	SER	-	expression tag	UNP O00408
B	577	ALA	-	expression tag	UNP O00408
B	578	MET	-	expression tag	UNP O00408
C	575	GLY	-	expression tag	UNP O00408
C	576	SER	-	expression tag	UNP O00408
C	577	ALA	-	expression tag	UNP O00408
C	578	MET	-	expression tag	UNP O00408
D	575	GLY	-	expression tag	UNP O00408
D	576	SER	-	expression tag	UNP O00408
D	577	ALA	-	expression tag	UNP O00408
D	578	MET	-	expression tag	UNP O00408

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

- Molecule 4 is 3-ISOBUTYL-1-METHYLXANTHINE (three-letter code: IBM) (formula: $C_{10}H_{14}N_4O_2$).
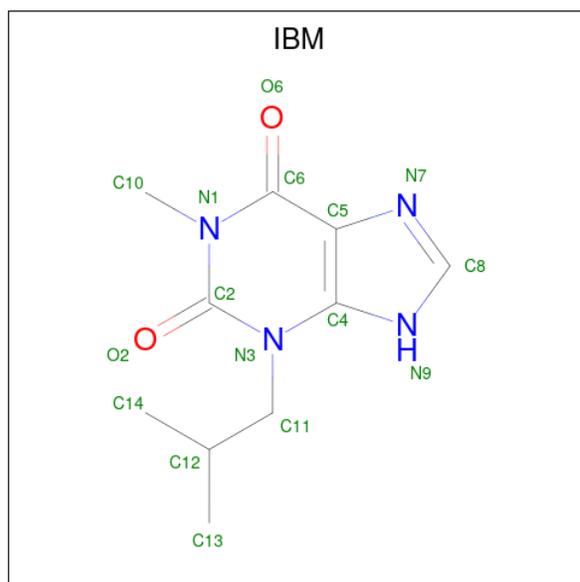
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 16	C 10	N 4	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 16	C 10	N 4	O 2	0	0
4	C	1	Total 16	C 10	N 4	O 2	0	0
4	D	1	Total 16	C 10	N 4	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	514	Total 514	O 514	0	0
5	B	447	Total 447	O 447	0	0
5	C	397	Total 397	O 397	0	0
5	D	419	Total 419	O 419	0	0

3 Residue-property plots ⓘ

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.
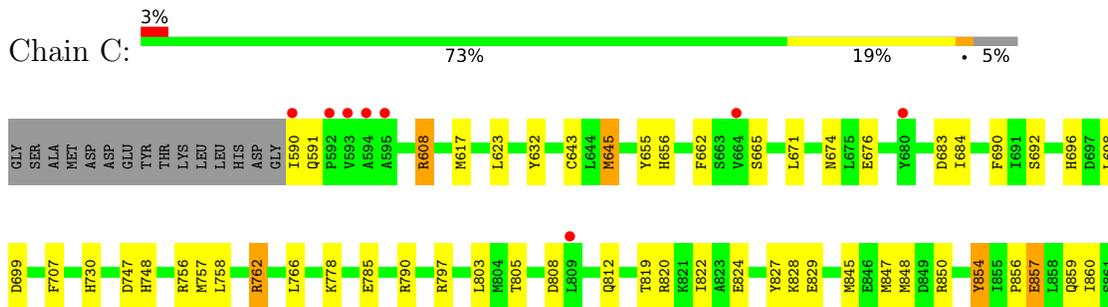
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase
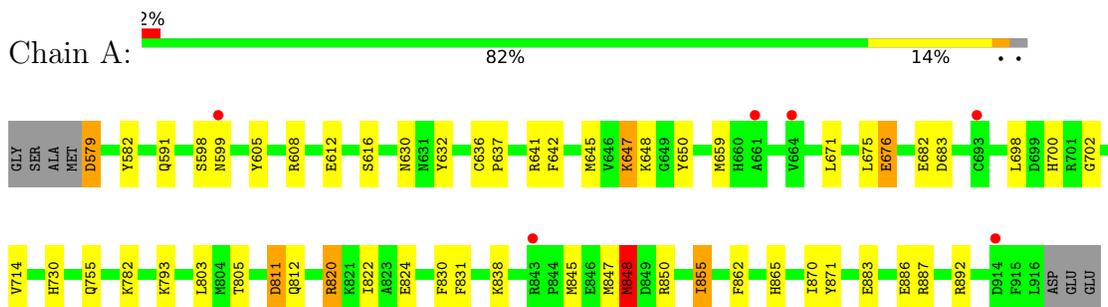
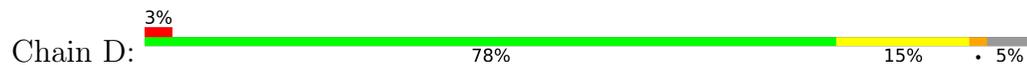- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

• Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain D:
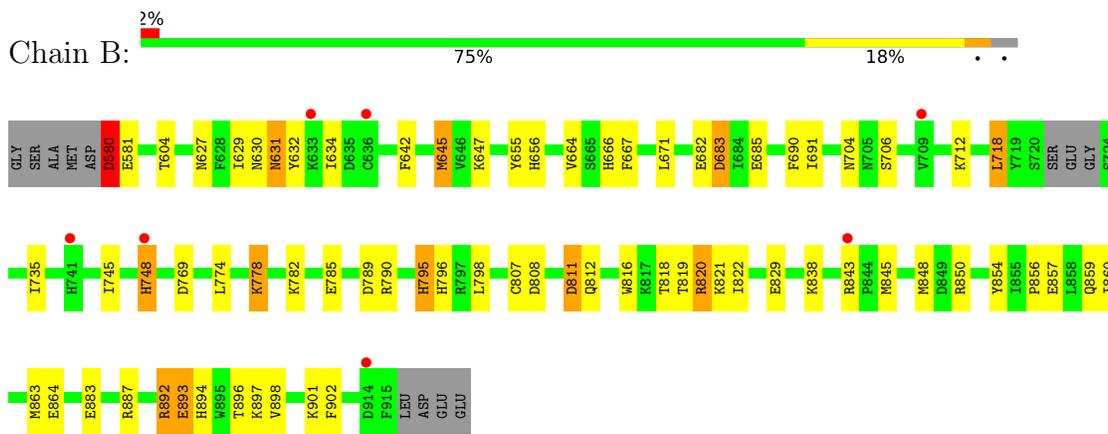
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.81Å 73.29Å 91.53Å 109.30° 88.80° 89.00°	Depositor
Resolution (Å)	50.00 – 1.58 30.35 – 1.58	Depositor EDS
% Data completeness (in resolution range)	83.8 (50.00-1.58) 83.7 (30.35-1.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.233 0.172 , 0.231	Depositor DCC
R_{free} test set	7854 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.6	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12700	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IBM, ZN

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	1.41	13/2834 (0.5%)	1.20	8/3824 (0.2%)
1	B	1.36	9/2798 (0.3%)	1.17	13/3774 (0.3%)
1	C	1.30	8/2741 (0.3%)	1.22	18/3698 (0.5%)
1	D	1.37	12/2741 (0.4%)	1.15	10/3698 (0.3%)
All	All	1.36	42/11114 (0.4%)	1.19	49/14994 (0.3%)

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	682	GLU	CB-CG	8.42	1.68	1.52
1	B	682	GLU	CG-CD	7.93	1.63	1.51
1	D	857	GLU	CG-CD	7.40	1.63	1.51
1	B	848	MET	CB-CG	7.20	1.74	1.51
1	A	650	TYR	CE2-CZ	6.69	1.47	1.38

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	608	ARG	NE-CZ-NH2	-14.63	112.99	120.30
1	C	808	ASP	CB-CG-OD2	-11.42	108.02	118.30
1	C	608	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	C	808	ASP	CB-CG-OD1	9.83	127.14	118.30
1	B	808	ASP	CB-CG-OD1	8.59	126.03	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	2767	0	2709	59	0
1	B	2732	0	2679	74	0
1	C	2676	0	2630	74	0
1	D	2676	0	2630	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	14	3	0
4	B	16	0	14	3	0
4	C	16	0	14	1	0
4	D	16	0	14	1	0
5	A	514	0	0	36	0
5	B	447	0	0	21	2
5	C	397	0	0	30	2
5	D	419	0	0	12	0
All	All	12700	0	10704	244	2

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 11.

The worst 5 of 244 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:643:CYS:HB3	5:C:1708:HOH:O	1.27	1.29
1:B:892:ARG:HH12	1:B:896:THR:CG2	1.57	1.18
1:D:892:ARG:HH12	1:D:896:THR:HG21	1.14	1.10
1:B:745:ILE:O	1:B:748:HIS:CE1	2.05	1.09
1:B:745:ILE:O	1:B:748:HIS:HE1	1.33	1.09

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:311:HOH:O	5:C:924:HOH:O[1_545]	2.00	0.20
5:B:311:HOH:O	5:C:1618:HOH:O[1_545]	2.19	0.01

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	336/345 (97%)	332 (99%)	4 (1%)	0	100	100
1	B	329/345 (95%)	318 (97%)	10 (3%)	1 (0%)	41	21
1	C	325/345 (94%)	320 (98%)	5 (2%)	0	100	100
1	D	325/345 (94%)	320 (98%)	5 (2%)	0	100	100
All	All	1315/1380 (95%)	1290 (98%)	24 (2%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	631	ASN

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	305/310 (98%)	300 (98%)	5 (2%)	62	39
1	B	301/310 (97%)	293 (97%)	8 (3%)	44	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	295/310 (95%)	292 (99%)	3 (1%)	76	59
1	D	295/310 (95%)	290 (98%)	5 (2%)	60	36
All	All	1196/1240 (96%)	1175 (98%)	21 (2%)	59	34

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	857	GLU
1	D	684	ILE
1	D	896	THR
1	D	820	ARG
1	D	599	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	911	ASN
1	D	627	ASN
1	C	730	HIS
1	D	791	ASN
1	B	666	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	#$|Z| > 2$
4	IBM	A	999	-	8,17,17	1.09	0	10,25,25	2.67	3 (30%)
4	IBM	C	999	-	8,17,17	2.19	1 (12%)	10,25,25	1.60	2 (20%)
4	IBM	B	999	-	8,17,17	1.07	0	10,25,25	1.43	2 (20%)
4	IBM	D	999	-	8,17,17	1.36	2 (25%)	10,25,25	1.99	3 (30%)

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
4	IBM	A	999	-	-	0/4/4/4	0/2/2/2
4	IBM	C	999	-	-	0/4/4/4	0/2/2/2
4	IBM	B	999	-	-	0/4/4/4	0/2/2/2
4	IBM	D	999	-	-	0/4/4/4	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	999	IBM	C11-N3	-5.63	1.42	1.48
4	D	999	IBM	C6-N1	2.39	1.41	1.38
4	D	999	IBM	O6-C6	2.27	1.30	1.24

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	IBM	C4-C5-C6	-6.99	115.47	119.96
4	C	999	IBM	C11-N3-C4	4.02	122.00	118.41
4	D	999	IBM	C4-C5-N7	-3.71	105.53	109.40
4	A	999	IBM	C11-N3-C4	3.33	121.39	118.41
4	B	999	IBM	C11-N3-C4	3.03	121.12	118.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	IBM	3	0
4	C	999	IBM	1	0
4	B	999	IBM	3	0
4	D	999	IBM	1	0

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, 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(Å²)	Q<0.9
1	A	338/345 (97%)	-0.01	6 (1%)	68	70	8, 17, 31, 43	0
1	B	333/345 (96%)	0.06	7 (2%)	63	65	10, 20, 32, 44	0
1	C	327/345 (94%)	0.14	9 (2%)	53	54	11, 21, 36, 44	0
1	D	327/345 (94%)	0.17	11 (3%)	45	46	9, 20, 35, 47	0
All	All	1325/1380 (96%)	0.09	33 (2%)	57	58	8, 19, 34, 47	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	593	VAL	4.9
1	D	599	ASN	3.9
1	D	590	ILE	3.7
1	D	594	ALA	3.6
1	D	914	ASP	3.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
4	IBM	B	999	16/16	0.91	0.12	23,25,28,30	0
4	IBM	C	999	16/16	0.93	0.16	25,28,30,31	0
4	IBM	A	999	16/16	0.94	0.11	17,21,22,24	0
4	IBM	D	999	16/16	0.95	0.14	18,22,25,29	0
3	MG	A	920	1/1	1.00	0.08	10,10,10,10	0
3	MG	B	920	1/1	1.00	0.05	10,10,10,10	0
3	MG	C	920	1/1	1.00	0.11	12,12,12,12	0
3	MG	D	920	1/1	1.00	0.14	12,12,12,12	0
2	ZN	A	1	1/1	1.00	0.06	13,13,13,13	0
2	ZN	B	2	1/1	1.00	0.06	13,13,13,13	0
2	ZN	C	3	1/1	1.00	0.06	14,14,14,14	0
2	ZN	D	4	1/1	1.00	0.07	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.