



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 AM GMT

PDB ID : 2OUU
Title : crystal structure of PDE10A2 mutant D674A in complex with cGMP
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Deposited on : 2007-02-12
Resolution : 1.52 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 ⓘ](#)) 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

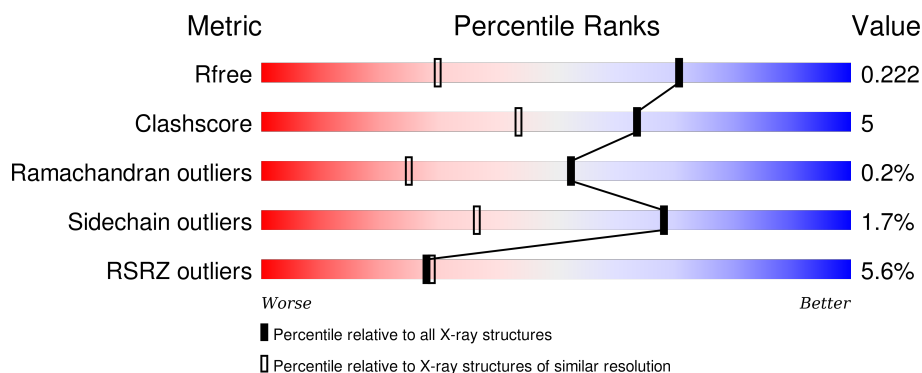
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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 $\leq 5\%$. 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	331	
1	B	331	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5624 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 cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2665	1702	453	485	25			
1	B	312	Total	C	N	O	S	0	0	0
			2522	1608	431	458	25			

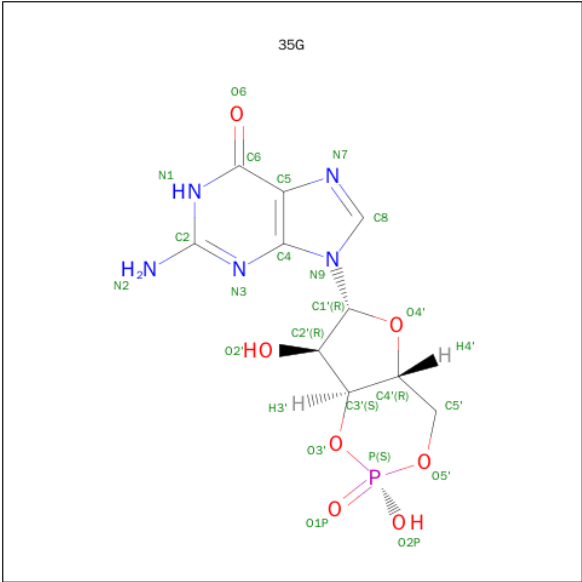
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	-	CLONING ARTIFACT	UNP Q9Y233
A	447	HIS	-	CLONING ARTIFACT	UNP Q9Y233
A	448	MET	-	CLONING ARTIFACT	UNP Q9Y233
A	674	ALA	ASP	ENGINEERED	UNP Q9Y233
B	446	SER	-	CLONING ARTIFACT	UNP Q9Y233
B	447	HIS	-	CLONING ARTIFACT	UNP Q9Y233
B	448	MET	-	CLONING ARTIFACT	UNP Q9Y233
B	674	ALA	ASP	ENGINEERED	UNP Q9Y233

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-3',5'-MONOPHOSPHATE (three-letter code: 35G) (formula: C₁₀H₁₂N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

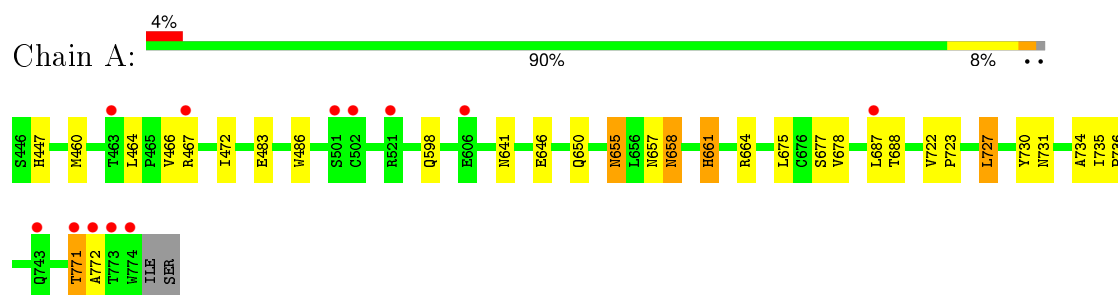
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		
4	B	146	Total	O	0	0
			146	146		

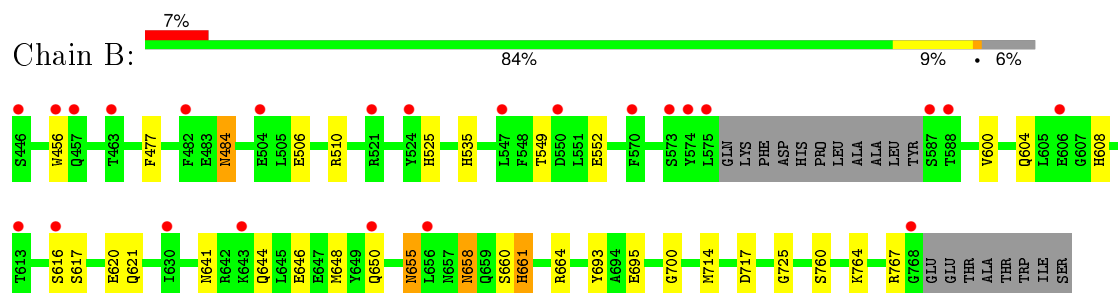
3 Residue-property plots [i](#)

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: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.72Å 81.99Å 153.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.52 29.05 – 1.52	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.52) 96.0 (29.05-1.52)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 1.52Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.222 0.204 , 0.222	Depositor DCC
R_{free} test set	9187 reflections (9.98%)	DCC
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 95579 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5624	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 35G, MG

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	0.35	0/2732	0.60	0/3701
1	B	0.34	0/2582	0.57	0/3493
All	All	0.35	0/5314	0.58	0/7194

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	2665	0	2623	29	0
1	B	2522	0	2492	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	69	0	33	3	0
4	A	220	0	0	3	0
4	B	146	0	0	1	0
All	All	5624	0	5148	54	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 (54) 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:655:ASN:H	1:B:661:HIS:HD2	1.27	0.79
1:A:646:GLU:HG3	1:A:650:GLN:HE21	1.47	0.78
1:A:641:ASN:HD22	1:A:664:ARG:HH11	1.31	0.78
1:A:655:ASN:H	1:A:661:HIS:HD2	1.33	0.74
3:A:778:35G:H3'	3:A:778:35G:N3	2.02	0.73
1:B:641:ASN:HD22	1:B:664:ARG:HH11	1.37	0.73
1:A:447:HIS:HE1	1:A:598:GLN:HE22	1.42	0.68
1:A:646:GLU:HG3	1:A:650:GLN:NE2	2.09	0.67
1:A:771:THR:HG22	1:A:772:ALA:H	1.60	0.67
1:B:456:TRP:CZ3	1:B:506:GLU:HG3	2.33	0.63
1:B:646:GLU:HG3	1:B:650:GLN:HE21	1.63	0.63
1:B:760:SER:O	1:B:764:LYS:HG2	2.00	0.62
1:B:658:ASN:C	1:B:658:ASN:HD22	2.02	0.62
1:B:655:ASN:H	1:B:661:HIS:CD2	2.16	0.60
1:A:771:THR:HG22	1:A:772:ALA:N	2.16	0.60
1:A:658:ASN:HD22	1:A:658:ASN:C	2.04	0.60
1:B:600:VAL:O	1:B:604:GLN:HG3	2.02	0.58
1:A:655:ASN:H	1:A:661:HIS:CD2	2.19	0.58
1:B:616:SER:O	1:B:620:GLU:HG2	2.04	0.57
1:A:447:HIS:CE1	1:A:598:GLN:HE22	2.23	0.57
1:A:675:LEU:HD23	3:A:778:35G:O2'	2.05	0.56
1:B:484:ASN:HD22	1:B:484:ASN:N	2.04	0.56
1:B:477:PHE:HB3	1:B:535:HIS:CE1	2.43	0.53
1:A:727:LEU:HD22	1:A:731:ASN:ND2	2.23	0.53
1:B:525:HIS:NE2	1:B:695:GLU:OE2	2.41	0.52
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.45	0.52
1:A:687:LEU:HD22	4:A:102:HOH:O	2.11	0.49
1:B:484:ASN:HD22	1:B:484:ASN:H	1.59	0.48
1:B:700:GLY:HA3	1:B:714:MET:O	2.14	0.48
1:A:687:LEU:C	1:A:687:LEU:HD23	2.34	0.47
1:A:646:GLU:CG	1:A:650:GLN:HE21	2.23	0.46
1:A:466:VAL:HG23	1:A:467:ARG:N	2.30	0.46
1:B:617:SER:O	1:B:621:GLN:HG3	2.15	0.46
1:A:655:ASN:ND2	1:A:657:ASN:H	2.14	0.45
1:A:677:SER:HB2	1:A:688:THR:HG21	1.98	0.44
1:A:771:THR:CG2	1:A:772:ALA:H	2.23	0.44
1:A:722:VAL:HB	1:A:723:PRO:HD3	2.00	0.44
1:A:771:THR:CG2	1:A:772:ALA:N	2.80	0.43
1:A:464:LEU:HD21	1:A:472:ILE:CD1	2.48	0.43
1:B:510:ARG:HG2	1:B:608:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ASN:ND2	1:B:660:SER:H	2.18	0.42
1:B:549:THR:OG1	1:B:552:GLU:HG3	2.20	0.42
1:A:730:TYR:HA	1:A:734:ALA:HB3	2.01	0.41
1:B:644:GLN:O	1:B:648:MET:HE2	2.20	0.41
3:A:778:35G:H4'	4:A:9:HOH:O	2.20	0.41
1:A:447:HIS:HE1	1:A:598:GLN:NE2	2.13	0.41
1:B:655:ASN:N	1:B:661:HIS:HD2	2.06	0.41
1:A:675:LEU:O	1:A:678:VAL:HG22	2.20	0.41
1:B:641:ASN:ND2	1:B:664:ARG:HH11	2.13	0.41
1:A:598:GLN:NE2	4:A:243:HOH:O	2.53	0.41
1:A:771:THR:HG22	4:B:140:HOH:O	2.20	0.41
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.03	0.41
1:B:693:TYR:OH	1:B:725:GLY:HA3	2.21	0.40
1:B:767:ARG:HH11	1:B:767:ARG:HG2	1.86	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	327/331 (99%)	320 (98%)	6 (2%)	1 (0%)	46	19
1	B	308/331 (93%)	304 (99%)	4 (1%)	0	100	100
All	All	635/662 (96%)	624 (98%)	10 (2%)	1 (0%)	52	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	771	THR

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	296/298 (99%)	291 (98%)	5 (2%)	68	36
1	B	282/298 (95%)	277 (98%)	5 (2%)	66	34
All	All	578/596 (97%)	568 (98%)	10 (2%)	68	36

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	MET
1	A	655	ASN
1	A	658	ASN
1	A	661	HIS
1	A	727	LEU
1	B	484	ASN
1	B	655	ASN
1	B	658	ASN
1	B	661	HIS
1	B	717	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	HIS
1	A	457	GLN
1	A	593	GLN
1	A	598	GLN
1	A	604	GLN
1	A	641	ASN
1	A	650	GLN
1	A	655	ASN
1	A	658	ASN
1	A	661	HIS
1	A	724	GLN
1	A	761	GLN

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Mol	Chain	Res	Type
1	B	484	ASN
1	B	593	GLN
1	B	641	ASN
1	B	650	GLN
1	B	655	ASN
1	B	658	ASN
1	B	661	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 ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
3	35G	A	778	-	20,26,26	1.38	2 (10%)	21,41,41	2.78	4 (19%)
3	35G	A	779	-	20,26,26	1.28	2 (10%)	21,41,41	2.91	4 (19%)
3	35G	A	780	-	20,26,26	1.33	1 (5%)	21,41,41	3.03	5 (23%)

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
3	35G	A	778	-	-	0/0/31/31	0/4/4/4
3	35G	A	779	-	-	0/0/31/31	0/4/4/4
3	35G	A	780	-	-	0/0/31/31	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	779	35G	O3'-C3'	-2.07	1.41	1.44
3	A	778	35G	P-O3'	2.21	1.61	1.58
3	A	780	35G	C6-N1	3.55	1.39	1.33
3	A	779	35G	C6-N1	3.58	1.39	1.33
3	A	778	35G	C6-N1	3.74	1.40	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	779	35G	C5-C6-N1	-8.86	111.47	123.59
3	A	780	35G	C5-C6-N1	-8.83	111.52	123.59
3	A	778	35G	C5-C6-N1	-8.77	111.59	123.59
3	A	780	35G	O3'-C3'-C4'	-6.65	105.41	110.72
3	A	779	35G	O3'-C3'-C4'	-5.70	106.17	110.72
3	A	778	35G	O3'-C3'-C4'	-4.97	106.75	110.72
3	A	778	35G	N3-C2-N1	-2.43	123.75	127.44
3	A	780	35G	N3-C2-N1	-2.42	123.77	127.44
3	A	779	35G	N3-C2-N1	-2.35	123.86	127.44
3	A	780	35G	C6-C5-C4	-2.14	118.34	120.90
3	A	778	35G	C6-N1-C2	6.52	124.99	115.94
3	A	779	35G	C6-N1-C2	6.68	125.21	115.94
3	A	780	35G	C6-N1-C2	6.72	125.26	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	778	35G	3	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(Å ²)	Q<0.9
1	A	329/331 (99%)	0.22	12 (3%) 46 49	11, 17, 26, 40	0
1	B	312/331 (94%)	0.50	24 (7%) 16 16	13, 20, 30, 37	0
All	All	641/662 (96%)	0.36	36 (5%) 28 29	11, 18, 30, 40	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	SER	9.8
1	A	773	THR	8.6
1	A	771	THR	7.8
1	B	574	TYR	5.3
1	A	774	TRP	4.7
1	B	456	TRP	4.7
1	B	575	LEU	4.6
1	B	524	TYR	4.3
1	B	457	GLN	4.3
1	A	467	ARG	4.3
1	B	521	ARG	4.1
1	B	768	GLY	4.0
1	B	573	SER	4.0
1	B	616	SER	3.6
1	B	482	PHE	3.3
1	B	650	GLN	3.3
1	B	656	LEU	3.0
1	B	570	PHE	3.0
1	A	606	GLU	3.0
1	B	587	SER	2.8
1	B	550	ASP	2.8
1	A	772	ALA	2.8
1	B	613	THR	2.7
1	B	547	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	687	LEU	2.6
1	A	521	ARG	2.4
1	A	501	SER	2.4
1	B	630	ILE	2.4
1	A	463	THR	2.3
1	B	588	THR	2.3
1	B	504	GLU	2.3
1	B	643	LYS	2.2
1	B	606	GLU	2.2
1	A	502	CYS	2.1
1	B	463	THR	2.0
1	A	743	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	35G	A	778	23/23	0.83	0.15	1.92	28,29,30,30	0
3	35G	A	780	23/23	0.92	0.11	0.40	17,19,21,22	0
2	MG	A	777	1/1	1.00	0.09	0.38	12,12,12,12	0
2	MG	B	777	1/1	0.99	0.09	-0.27	17,17,17,17	0
3	35G	A	779	23/23	0.95	0.07	-0.40	14,16,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.