



Full wwPDB X-ray Structure Validation Report

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PDB ID : 4OF8
Title : Crystal Structure of Rst D1-D2
Authors : Ozkan, E.; Garcia, K.C.
Deposited on : 2014-01-14
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

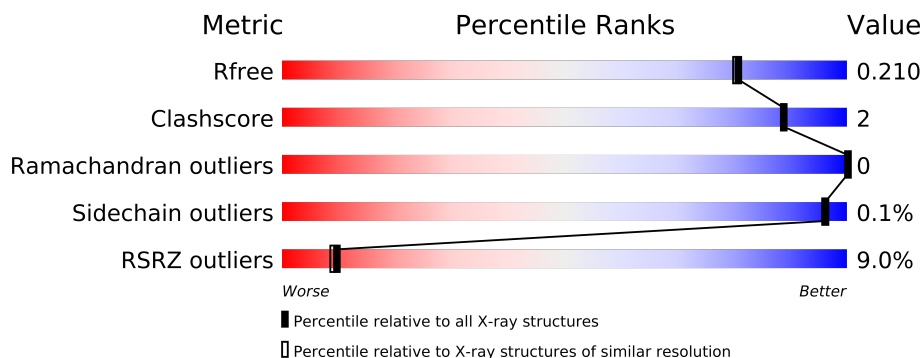
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **FAILED**
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	228	
1	B	228	
1	C	228	
1	D	228	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	A	302	-	X
3	GOL	B	302	-	X
3	GOL	D	302	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7448 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Irregular chiasm C-roughest protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1647	1027	289	324	7			
1	B	209	Total	C	N	O	S	0	1	0
			1639	1021	290	321	7			
1	C	210	Total	C	N	O	S	0	1	0
			1640	1021	288	324	7			
1	D	209	Total	C	N	O	S	0	1	0
			1639	1021	290	321	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	-	EXPRESSION TAG	UNP Q08180
A	18	ASP	-	EXPRESSION TAG	UNP Q08180
A	19	PRO	-	EXPRESSION TAG	UNP Q08180
A	238	HIS	-	EXPRESSION TAG	UNP Q08180
A	239	HIS	-	EXPRESSION TAG	UNP Q08180
A	240	HIS	-	EXPRESSION TAG	UNP Q08180
A	241	HIS	-	EXPRESSION TAG	UNP Q08180
A	242	HIS	-	EXPRESSION TAG	UNP Q08180
A	243	HIS	-	EXPRESSION TAG	UNP Q08180
A	244	HIS	-	EXPRESSION TAG	UNP Q08180
B	17	ALA	-	EXPRESSION TAG	UNP Q08180
B	18	ASP	-	EXPRESSION TAG	UNP Q08180
B	19	PRO	-	EXPRESSION TAG	UNP Q08180
B	238	HIS	-	EXPRESSION TAG	UNP Q08180
B	239	HIS	-	EXPRESSION TAG	UNP Q08180
B	240	HIS	-	EXPRESSION TAG	UNP Q08180
B	241	HIS	-	EXPRESSION TAG	UNP Q08180
B	242	HIS	-	EXPRESSION TAG	UNP Q08180
B	243	HIS	-	EXPRESSION TAG	UNP Q08180
B	244	HIS	-	EXPRESSION TAG	UNP Q08180
C	17	ALA	-	EXPRESSION TAG	UNP Q08180

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	ASP	-	EXPRESSION TAG	UNP Q08180
C	19	PRO	-	EXPRESSION TAG	UNP Q08180
C	238	HIS	-	EXPRESSION TAG	UNP Q08180
C	239	HIS	-	EXPRESSION TAG	UNP Q08180
C	240	HIS	-	EXPRESSION TAG	UNP Q08180
C	241	HIS	-	EXPRESSION TAG	UNP Q08180
C	242	HIS	-	EXPRESSION TAG	UNP Q08180
C	243	HIS	-	EXPRESSION TAG	UNP Q08180
C	244	HIS	-	EXPRESSION TAG	UNP Q08180
D	17	ALA	-	EXPRESSION TAG	UNP Q08180
D	18	ASP	-	EXPRESSION TAG	UNP Q08180
D	19	PRO	-	EXPRESSION TAG	UNP Q08180
D	238	HIS	-	EXPRESSION TAG	UNP Q08180
D	239	HIS	-	EXPRESSION TAG	UNP Q08180
D	240	HIS	-	EXPRESSION TAG	UNP Q08180
D	241	HIS	-	EXPRESSION TAG	UNP Q08180
D	242	HIS	-	EXPRESSION TAG	UNP Q08180
D	243	HIS	-	EXPRESSION TAG	UNP Q08180
D	244	HIS	-	EXPRESSION TAG	UNP Q08180

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	188	Total	O	0	0
			188	188		
4	C	229	Total	O	0	0
			229	229		
4	D	201	Total	O	0	0
			201	201		

4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.94Å 77.94Å 121.10Å 90.00° 95.44° 90.00°	Depositor
Resolution (Å)	44.57 – 1.90 44.57 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.5 (44.57-1.90) 88.5 (44.57-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, R_{free}	0.173 , 0.208 0.175 , 0.210	Depositor DCC
R_{free} test set	3889 reflections (5.04%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7448	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.38	0/1679	0.51	0/2281
1	B	0.35	0/1673	0.51	0/2272
1	C	0.37	0/1674	0.51	0/2274
1	D	0.34	0/1673	0.51	0/2272
All	All	0.36	0/6699	0.51	0/9099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1647	0	0	1	0
1	B	1639	0	0	7	0
1	C	1640	0	0	2	0
1	D	1639	0	0	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	0	0
3	B	12	0	16	0	0
3	D	12	0	16	0	0
4	A	225	0	0	0	0
4	B	188	0	0	4	0
4	C	229	0	0	1	0
4	D	201	0	0	5	0
All	All	7448	0	48	15	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (15) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:26:GLN:NE2	4:D:564:HOH:O	2.25	0.69
1:D:26:GLN:N	4:D:560:HOH:O	2.28	0.65
1:D:104[B]:ARG:NH1	4:D:584:HOH:O	2.33	0.61
1:B:53:ASN:OD1	1:B:55:GLN:NE2	2.34	0.61
1:C:225:ARG:NH2	4:C:560:HOH:O	2.37	0.57
1:D:104[B]:ARG:NH2	4:D:569:HOH:O	2.37	0.57
1:B:77:GLU:OE2	4:B:529:HOH:O	2.18	0.53
1:D:215:GLN:NE2	4:D:567:HOH:O	2.43	0.52
1:B:196:LYS:NZ	4:B:561:HOH:O	2.43	0.52
1:A:35:GLN:N	1:A:35:GLN:OE1	2.48	0.47
1:B:116:GLN:OE1	1:B:116:GLN:N	2.50	0.45
1:B:148:ASP:N	1:B:203:PRO:O	2.52	0.43
1:B:191:ARG:NH2	4:B:531:HOH:O	2.53	0.41
1:B:191:ARG:NH2	4:B:551:HOH:O	2.54	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	209/228 (92%)	205 (98%)	4 (2%)	0	100	100
1	B	208/228 (91%)	201 (97%)	7 (3%)	0	100	100
1	C	209/228 (92%)	208 (100%)	1 (0%)	0	100	100
1	D	208/228 (91%)	201 (97%)	7 (3%)	0	100	100
All	All	834/912 (91%)	815 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	180/196 (92%)	180 (100%)	0	100	100
1	B	180/196 (92%)	180 (100%)	0	100	100
1	C	180/196 (92%)	179 (99%)	1 (1%)	92	92
1	D	180/196 (92%)	180 (100%)	0	100	100
All	All	720/784 (92%)	719 (100%)	1 (0%)	96	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	231	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	GOL	A	302	-	5,5,5	0.34	0	5,5,5	0.22	0
3	GOL	A	303	-	5,5,5	0.25	0	5,5,5	0.44	0
3	GOL	B	302	-	5,5,5	0.24	0	5,5,5	0.38	0
3	GOL	B	303	-	5,5,5	0.33	0	5,5,5	0.31	0
3	GOL	D	302	-	5,5,5	0.18	0	5,5,5	0.76	0
3	GOL	D	303	-	5,5,5	0.34	0	5,5,5	0.38	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
3	GOL	A	302	-	-	0/4/4/4	0/0/0/0
3	GOL	A	303	-	-	0/4/4/4	0/0/0/0
3	GOL	B	302	-	-	0/4/4/4	0/0/0/0
3	GOL	B	303	-	-	0/4/4/4	0/0/0/0
3	GOL	D	302	-	-	0/4/4/4	0/0/0/0
3	GOL	D	303	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	211/228 (92%)	0.13	7 (3%) 44 45	12, 26, 74, 112	0
1	B	209/228 (91%)	0.23	16 (7%) 13 13	15, 30, 82, 109	0
1	C	210/228 (92%)	0.42	17 (8%) 12 11	16, 28, 93, 129	0
1	D	209/228 (91%)	0.62	36 (17%) 2 2	14, 31, 101, 129	0
All	All	839/912 (91%)	0.35	76 (9%) 10 9	12, 28, 90, 129	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	HIS	6.9
1	D	204	LYS	5.9
1	B	233	VAL	5.9
1	B	204	LYS	5.7
1	B	234	LYS	5.6
1	D	143	ILE	5.5
1	D	206	GLU	5.3
1	D	201	LEU	5.2
1	D	172	LEU	5.1
1	D	147	GLU	5.0
1	C	207	HIS	4.8
1	C	205	LYS	4.8
1	D	202	THR	4.8
1	D	203	PRO	4.7
1	C	234	LYS	4.7
1	D	233	VAL	4.6
1	B	207	HIS	4.6
1	D	205	LYS	4.5
1	C	143	ILE	4.0
1	C	206	GLU	3.9
1	D	148	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	208	HIS	3.9
1	C	172	LEU	3.9
1	B	171	GLY	3.9
1	A	172	LEU	3.6
1	D	146	THR	3.6
1	A	204	LYS	3.5
1	D	153	ILE	3.5
1	D	188	PRO	3.4
1	C	144	TYR	3.4
1	A	205	LYS	3.4
1	A	207	HIS	3.4
1	C	233	VAL	3.3
1	B	206	GLU	3.3
1	C	209	ASN	3.3
1	C	149	ARG	3.3
1	D	151	VAL	3.3
1	D	144	TYR	3.2
1	B	172	LEU	3.2
1	B	188	PRO	3.1
1	C	201	LEU	3.1
1	D	149	ARG	3.0
1	C	204	LYS	3.0
1	B	148	ASP	3.0
1	B	208	HIS	2.9
1	B	145	ALA	2.9
1	D	176	LEU	2.9
1	C	208	HIS	2.9
1	D	200	ARG	2.8
1	D	234	LYS	2.8
1	B	144	TYR	2.7
1	C	25	TYR	2.6
1	D	199	LEU	2.6
1	B	143	ILE	2.6
1	A	235	TYR	2.6
1	C	171	GLY	2.6
1	C	210	THR	2.5
1	A	206	GLU	2.5
1	D	232	GLU	2.5
1	C	148	ASP	2.5
1	D	231	VAL	2.4
1	D	210	THR	2.4
1	B	26	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	212	PHE	2.3
1	A	177	THR	2.2
1	D	150	LYS	2.2
1	B	205	LYS	2.2
1	D	170	ASP	2.1
1	D	198	VAL	2.1
1	B	146	THR	2.1
1	D	179	ASN	2.1
1	D	145	ALA	2.1
1	D	177	THR	2.1
1	D	142	VAL	2.1
1	D	209	ASN	2.1
1	D	187	LEU	2.0

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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	302	6/6	0.20	6.33	44,50,51,57	0
3	GOL	D	302	6/6	0.21	5.03	34,40,43,44	0
3	GOL	A	302	6/6	0.17	2.32	50,51,53,54	0
3	GOL	B	303	6/6	0.20	1.39	81,82,85,87	0
3	GOL	D	303	6/6	0.14	0.66	58,61,62,64	0
3	GOL	A	303	6/6	0.12	0.20	33,38,42,43	0
2	NA	B	301	1/1	0.05	-2.60	19,19,19,19	0
2	NA	C	301	1/1	0.04	-3.54	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NA	A	301	1/1	0.05	-3.80	20,20,20,20	0
2	NA	D	301	1/1	0.04	-3.93	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.