



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:07 AM GMT

PDB ID : 1A0E
Title : XYLOSE ISOMERASE FROM THERMOTOGA NEAPOLITANA
Authors : Galloway, O.; Chopra, R.; Conti, E.; Brick, P.; Blow, D.
Deposited on : 1997-11-28
Resolution : 2.70 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>

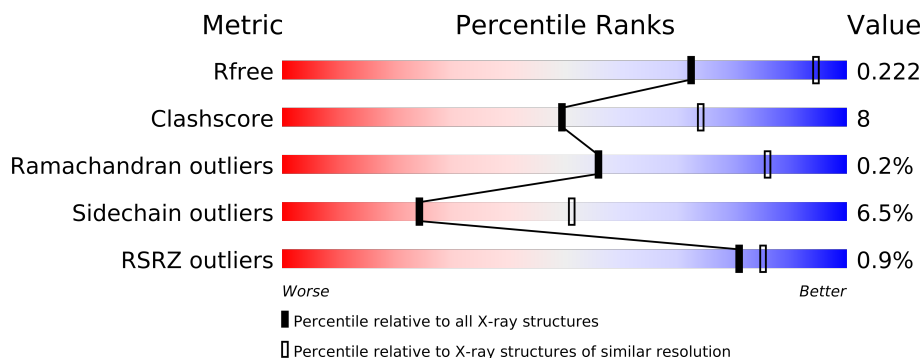
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
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 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 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	443	
1	D	443	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7274 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3506	2272	572	652	10			
1	D	443	Total	C	N	O	S	0	0	0
			3506	2272	572	652	10			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Co	0	0
			3	3		
2	D	3	Total	Co	0	0
			3	3		

- Molecule 3 is water.

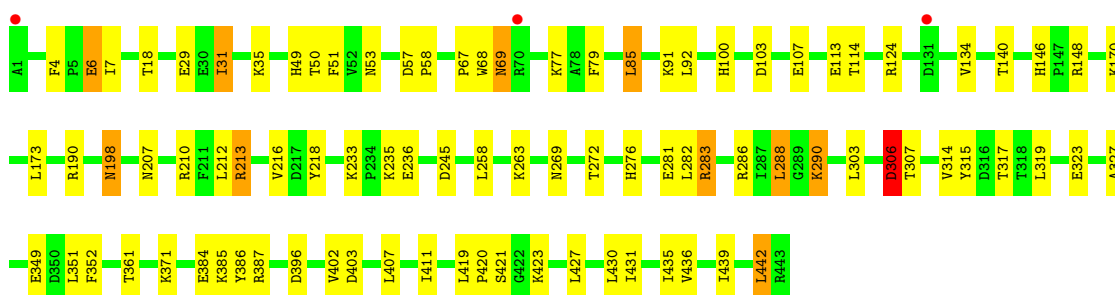
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	D	128	Total	O	0	0
			128	128		

3 Residue-property plots

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.

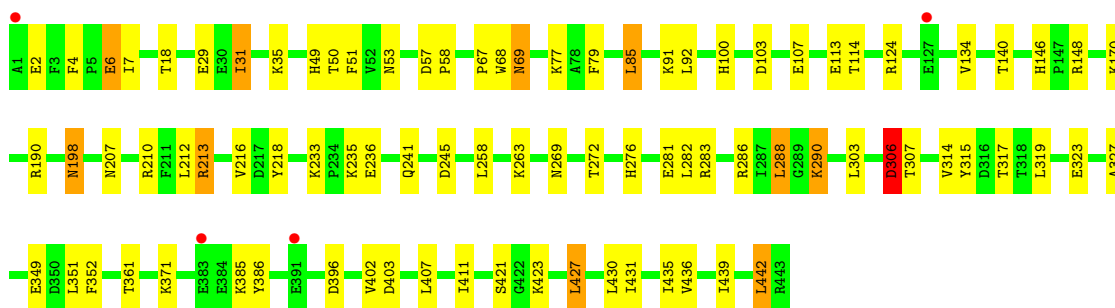
• Molecule 1: XYLOSE ISOMERASE

Chain A: 



• Molecule 1: XYLOSE ISOMERASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	161.79Å 121.87Å 98.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.50 – 2.70 12.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (12.50-2.70) 97.1 (12.49-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , 0.203 0.199 , 0.222	Depositor DCC
R_{free} test set	1265 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 26119 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7274	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	1/3596 (0.0%)	0.63	2/4865 (0.0%)
1	D	0.43	1/3596 (0.0%)	0.62	2/4865 (0.0%)
All	All	0.43	2/7192 (0.0%)	0.63	4/9730 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLU	CG-CD	5.56	1.60	1.51
1	D	349	GLU	CG-CD	5.55	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	306	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	306	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	306	ASP	CB-CG-OD1	5.82	123.53	118.30

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	3506	0	3359	57	0
1	D	3506	0	3359	51	2
2	A	3	0	0	0	1
2	D	3	0	0	0	1
3	A	128	0	0	2	0
3	D	128	0	0	3	0
All	All	7274	0	6718	104	3

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 8.

All (104) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:306:ASP:HB3	3:D:621:HOH:O	1.71	0.90
1:A:306:ASP:HB3	3:A:616:HOH:O	1.71	0.89
1:D:402:VAL:CG1	1:D:407:LEU:HG	2.08	0.84
1:A:402:VAL:CG1	1:A:407:LEU:HG	2.08	0.83
1:A:402:VAL:HG11	1:A:407:LEU:HG	1.67	0.77
1:D:402:VAL:HG11	1:D:407:LEU:HG	1.67	0.76
1:D:79:PHE:CD1	1:D:124:ARG:HD2	2.21	0.76
1:A:79:PHE:CD1	1:A:124:ARG:HD2	2.21	0.75
1:D:213:ARG:HB3	1:D:213:ARG:NH1	2.06	0.70
1:A:213:ARG:NH1	1:A:213:ARG:HB3	2.06	0.70
1:A:396:ASP:HB3	1:A:402:VAL:HG23	1.77	0.65
1:D:396:ASP:HB3	1:D:402:VAL:HG23	1.77	0.65
1:D:439:ILE:HA	1:D:442:LEU:HD22	1.80	0.63
1:A:245:ASP:HB2	1:A:281:GLU:OE2	1.99	0.63
1:D:198:ASN:C	1:D:198:ASN:HD22	2.02	0.63
1:A:439:ILE:HA	1:A:442:LEU:HD22	1.80	0.62
1:A:198:ASN:HD22	1:A:198:ASN:C	2.01	0.62
1:D:245:ASP:HB2	1:D:281:GLU:OE2	1.99	0.61
1:A:317:THR:HG21	1:A:361:THR:HG22	1.83	0.60
1:A:190:ARG:HD3	3:A:604:HOH:O	2.01	0.60
1:D:317:THR:HG21	1:D:361:THR:HG22	1.83	0.60
1:D:6:GLU:HG2	1:D:7:ILE:HD12	1.85	0.59
1:D:190:ARG:HD3	3:D:609:HOH:O	2.01	0.59
1:A:57:ASP:HB2	1:A:58:PRO:HD2	1.84	0.58
1:D:272:THR:HA	1:D:276:HIS:O	2.04	0.58
1:D:57:ASP:HB2	1:D:58:PRO:HD2	1.84	0.58
1:A:6:GLU:HG2	1:A:7:ILE:HD12	1.84	0.57
1:A:272:THR:HA	1:A:276:HIS:O	2.04	0.57
1:D:51:PHE:CZ	1:D:85:LEU:HA	2.41	0.56
1:A:51:PHE:CZ	1:A:85:LEU:HA	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:100:HIS:CD2	1:D:140:THR:HG23	2.41	0.56
1:A:233:LYS:HE2	1:A:235:LYS:O	2.06	0.56
1:A:100:HIS:CD2	1:A:140:THR:HG23	2.41	0.55
1:A:402:VAL:HG11	1:A:407:LEU:CG	2.37	0.55
1:D:402:VAL:HG11	1:D:407:LEU:CG	2.37	0.55
1:D:233:LYS:HE2	1:D:235:LYS:O	2.06	0.54
1:A:288:LEU:HB3	1:A:290:LYS:HG3	1.94	0.49
1:D:288:LEU:HB3	1:D:290:LYS:HG3	1.94	0.49
1:A:402:VAL:HG12	1:A:403:ASP:N	2.28	0.49
1:D:49:HIS:O	1:D:53:ASN:HB3	2.13	0.49
1:A:49:HIS:O	1:A:53:ASN:HB3	2.13	0.49
1:D:402:VAL:HG12	1:D:403:ASP:N	2.28	0.48
1:A:439:ILE:HG23	1:D:436:VAL:HG13	1.94	0.48
1:A:436:VAL:HG13	1:D:439:ILE:HG23	1.95	0.48
1:D:263:LYS:HA	1:D:290:LYS:HB3	1.94	0.48
1:D:67:PRO:HG2	1:D:68:TRP:CE3	2.49	0.48
1:A:263:LYS:HA	1:A:290:LYS:HB3	1.94	0.48
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.27	0.47
1:A:314:VAL:HG22	1:D:315:TYR:OH	2.14	0.47
1:D:213:ARG:HH11	1:D:213:ARG:CG	2.27	0.47
1:A:67:PRO:HG2	1:A:68:TRP:CE3	2.49	0.47
1:A:170:LYS:HG3	1:A:218:TYR:CE2	2.50	0.47
1:A:92:LEU:HD13	1:A:352:PHE:HD1	1.80	0.46
1:D:170:LYS:HG3	1:D:218:TYR:CE2	2.50	0.46
1:D:92:LEU:HD13	1:D:352:PHE:HD1	1.80	0.46
1:A:4:PHE:O	1:A:91:LYS:NZ	2.50	0.44
1:A:146:HIS:ND1	1:A:148:ARG:HB3	2.33	0.44
1:D:306:ASP:CB	3:D:621:HOH:O	2.48	0.44
1:D:4:PHE:O	1:D:91:LYS:NZ	2.50	0.44
1:D:213:ARG:HB3	1:D:213:ARG:CZ	2.48	0.44
1:A:213:ARG:CZ	1:A:213:ARG:HB3	2.48	0.44
1:D:146:HIS:ND1	1:D:148:ARG:HB3	2.33	0.44
1:A:50:THR:HG23	1:A:351:LEU:HD22	1.99	0.44
1:A:107:GLU:HG2	1:A:114:THR:OG1	2.18	0.43
1:D:50:THR:HG23	1:D:351:LEU:HD22	1.99	0.43
1:A:207:ASN:OD1	1:A:210:ARG:NH1	2.51	0.43
1:D:107:GLU:HG2	1:D:114:THR:OG1	2.18	0.43
1:A:100:HIS:HB2	1:A:103:ASP:CG	2.39	0.43
1:D:286:ARG:NH1	1:D:323:GLU:OE1	2.51	0.43
1:D:100:HIS:HB2	1:D:103:ASP:CG	2.39	0.43
1:A:303:LEU:HD12	1:A:307:THR:HG21	2.00	0.43
1:D:207:ASN:OD1	1:D:210:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:303:LEU:HD12	1:D:307:THR:HG21	2.01	0.42
1:D:439:ILE:O	1:D:442:LEU:HB2	2.19	0.42
1:A:439:ILE:O	1:A:442:LEU:HB2	2.19	0.42
1:A:213:ARG:NH1	1:A:213:ARG:CB	2.81	0.42
1:A:286:ARG:NH1	1:A:323:GLU:OE1	2.51	0.42
1:D:69:ASN:HD22	1:D:77:LYS:HE3	1.85	0.42
1:D:421:SER:HB3	1:D:423:LYS:HE2	2.01	0.42
1:A:421:SER:HB3	1:A:423:LYS:HE2	2.01	0.42
1:A:315:TYR:OH	1:D:314:VAL:HG22	2.20	0.41
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.92	0.41
1:A:286:ARG:HG3	1:A:327:ALA:HB2	2.02	0.41
1:A:69:ASN:HD22	1:A:77:LYS:HE3	1.85	0.41
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.85	0.41
1:D:385:LYS:HD3	1:D:386:TYR:CE1	2.56	0.41
1:D:286:ARG:HG3	1:D:327:ALA:HB2	2.02	0.41
1:A:385:LYS:HD3	1:A:386:TYR:CE1	2.56	0.41
1:D:213:ARG:O	1:D:216:VAL:HG22	2.21	0.41
1:A:31:ILE:HA	1:A:35:LYS:O	2.21	0.41
1:A:213:ARG:O	1:A:216:VAL:HG22	2.21	0.40
1:D:31:ILE:HA	1:D:35:LYS:O	2.22	0.40
1:D:427:LEU:O	1:D:430:LEU:HB2	2.21	0.40
1:A:384:GLU:O	1:A:387:ARG:HB2	2.22	0.40
1:D:233:LYS:O	1:D:241:GLN:HB3	2.21	0.40
1:D:402:VAL:CG1	1:D:403:ASP:N	2.84	0.40
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.77	0.40
1:A:283:ARG:HD3	1:A:323:GLU:OE1	2.22	0.40
1:A:419:LEU:HA	1:A:420:PRO:HD3	1.91	0.40
1:D:431:ILE:O	1:D:435:ILE:HG13	2.21	0.40
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.93	0.40
1:A:402:VAL:CG1	1:A:403:ASP:N	2.84	0.40
1:A:69:ASN:HD22	1:A:69:ASN:HA	1.61	0.40
1:A:431:ILE:O	1:A:435:ILE:HG13	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:493:CO:CO	2:A:493:CO:CO[3_655]	0.32	1.88
1:D:2:GLU:CG	2:D:493:CO:CO[3_555]	1.42	0.78
1:D:2:GLU:CB	1:D:2:GLU:OE2[3_555]	2.14	0.06

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	441/443 (100%)	424 (96%)	16 (4%)	1 (0%)	56	86
1	D	441/443 (100%)	424 (96%)	16 (4%)	1 (0%)	56	86
All	All	882/886 (100%)	848 (96%)	32 (4%)	2 (0%)	56	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	D	236	GLU

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	354/374 (95%)	331 (94%)	23 (6%)	24	51
1	D	354/374 (95%)	331 (94%)	23 (6%)	24	51
All	All	708/748 (95%)	662 (94%)	46 (6%)	24	51

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	18	THR
1	A	29	GLU
1	A	31	ILE
1	A	69	ASN
1	A	85	LEU
1	A	113	GLU

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Mol	Chain	Res	Type
1	A	134	VAL
1	A	198	ASN
1	A	212	LEU
1	A	213	ARG
1	A	258	LEU
1	A	269	ASN
1	A	282	LEU
1	A	283	ARG
1	A	288	LEU
1	A	290	LYS
1	A	306	ASP
1	A	319	LEU
1	A	371	LYS
1	A	411	ILE
1	A	427	LEU
1	A	442	LEU
1	D	6	GLU
1	D	18	THR
1	D	29	GLU
1	D	31	ILE
1	D	69	ASN
1	D	85	LEU
1	D	113	GLU
1	D	134	VAL
1	D	198	ASN
1	D	212	LEU
1	D	213	ARG
1	D	258	LEU
1	D	269	ASN
1	D	282	LEU
1	D	283	ARG
1	D	288	LEU
1	D	290	LYS
1	D	306	ASP
1	D	319	LEU
1	D	371	LYS
1	D	411	ILE
1	D	427	LEU
1	D	442	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	100	HIS
1	A	115	ASN
1	A	198	ASN
1	A	241	GLN
1	A	424	GLN
1	A	432	ASN
1	D	69	ASN
1	D	115	ASN
1	D	198	ASN
1	D	241	GLN
1	D	424	GLN
1	D	432	ASN

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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	443/443 (100%)	-0.69	3 (0%) 84 89	18, 36, 63, 84	0
1	D	443/443 (100%)	-0.58	4 (0%) 81 85	18, 36, 63, 84	0
All	All	886/886 (100%)	-0.63	7 (0%) 81 87	18, 36, 64, 84	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	2.9
1	D	127	GLU	2.7
1	A	70	ARG	2.4
1	A	1	ALA	2.3
1	D	391	GLU	2.3
1	A	131	ASP	2.1
1	D	383	GLU	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(\AA^2)	Q<0.9
2	CO	D	493	1/1	0.26	0.86	56,56,56,56	0
2	CO	A	492	1/1	0.07	-1.78	44,44,44,44	0
2	CO	A	491	1/1	0.04	-3.69	48,48,48,48	0
2	CO	D	492	1/1	0.05	-3.96	44,44,44,44	0
2	CO	A	493	1/1	0.08	-6.68	56,56,56,56	0
2	CO	D	491	1/1	0.04	-9.30	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.