Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:01 PM GMT

PDB ID	:	1DOS
Title	:	STRUCTURE OF FRUCTOSE-BISPHOSPHATE ALDOLASE
Authors	:	Blom, N.; Tetreault, S.; Coulombe, R.; Sygusch, J.
Deposited on	:	1996-06-24
Resolution	:	1.67 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 (i) symbol.

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

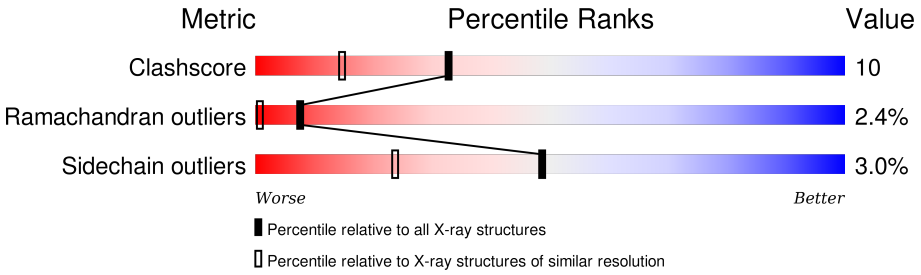
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.67 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))
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	358	79% 18%
1	B	358	79% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8513 atoms, of which 1232 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 ALDOLASE CLASS II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	358	Total	C	H	N	O	S	0	15	0
			3482	1815	616	485	554	12			
1	B	358	Total	C	H	N	O	S	0	15	0
			3482	1815	616	485	554	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	ALA	PRO	CONFLICT	UNP P0AB71
B	231	ALA	PRO	CONFLICT	UNP P0AB71

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

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

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 1 1	0	0
3	B	1	Total N 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	626	Total O 626 626	0	0
4	B	917	Total O 917 917	0	0

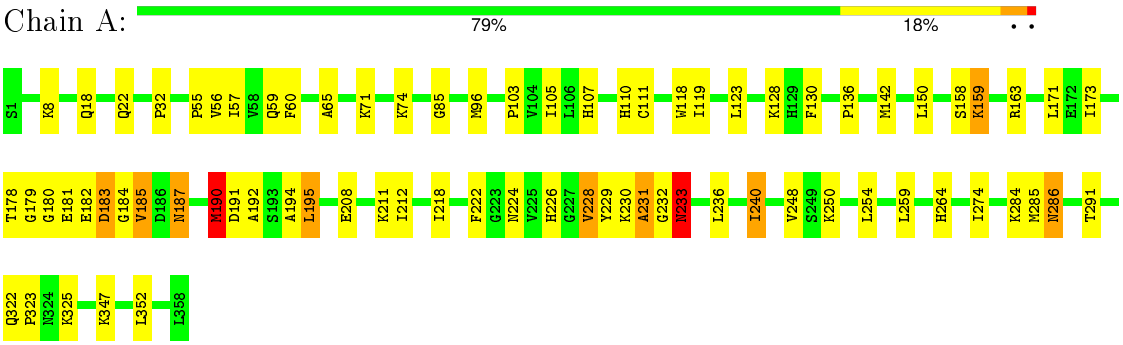
3 Residue-property plots (i)

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.

Note EDS was not executed.

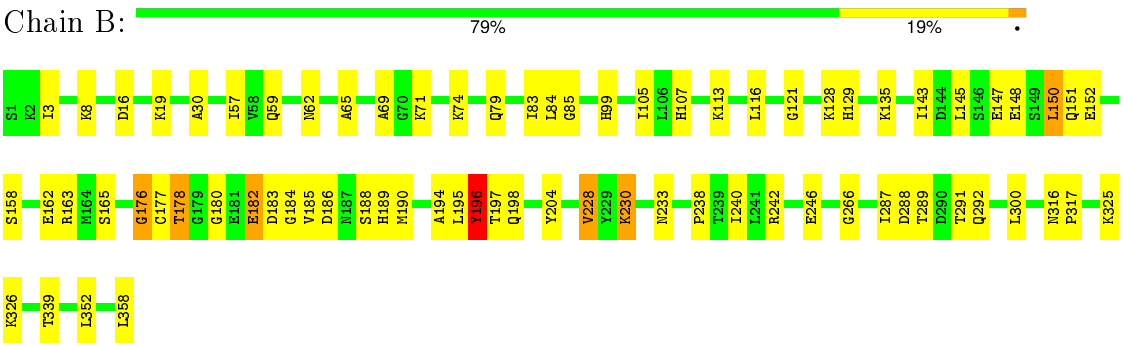
- Molecule 1: ALDOLASE CLASS II

Chain A:



- Molecule 1: ALDOLASE CLASS II

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.53Å 73.38Å 57.80Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	10.00 – 1.67	Depositor
% Data completeness (in resolution range)	87.4 (10.00-1.67)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , 0.204	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8513	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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: NH4, 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	0.36	0/2679	0.67	2/3623 (0.1%)
1	B	0.34	0/2679	0.60	1/3623 (0.0%)
All	All	0.35	0/5358	0.64	3/7246 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	ASN	N-CA-C	6.95	129.76	111.00
1	A	190	MET	CG-SD-CE	6.75	111.00	100.20
1	B	176	GLY	N-CA-C	5.33	126.43	113.10

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	2866	616	2793	60	0
1	B	2866	616	2793	60	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	626	0	0	18	0
4	B	917	0	0	30	0
All	All	7281	1232	5586	118	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 10.

All (118) 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:A:190:MET:SD	4:A:1387:HOH:O	2.37	0.83
1:B:300:LEU:HA	4:B:1457:HOH:O	1.85	0.77
1:A:228:VAL:HG12	1:A:229:TYR:H	1.53	0.73
1:A:118:TRP:HZ2	4:A:1008:HOH:O	1.71	0.73
1:B:113:LYS:HD3	4:B:1502:HOH:O	1.89	0.72
1:A:190:MET:HE3	1:A:191:ASP:H	1.54	0.72
1:B:339:THR:HG21	4:B:2141:HOH:O	1.88	0.72
1:A:173[2]:ILE:HD11	1:A:218:ILE:HG12	1.75	0.68
1:B:195:LEU:HB2	4:B:1399:HOH:O	1.95	0.67
1:B:163:ARG:HD2	4:B:2126:HOH:O	1.96	0.66
1:A:192:ALA:HA	4:A:1535:HOH:O	1.96	0.66
1:B:182:GLU:HA	4:B:1498:HOH:O	1.94	0.66
4:A:1606:HOH:O	1:B:325:LYS:HG2	1.96	0.65
1:B:242:ARG:O	1:B:246:GLU:HG2	1.97	0.64
1:A:130:PHE:HB2	4:A:1564:HOH:O	1.97	0.64
1:A:110[2]:HIS:NE2	1:A:264[2]:HIS:CE1	2.66	0.62
1:A:190:MET:HA	4:A:1402:HOH:O	1.99	0.62
1:A:18:GLN:O	1:A:22:GLN:HG3	1.99	0.61
1:A:228:VAL:HG12	1:A:229:TYR:N	2.15	0.61
1:A:96:MET:SD	4:B:2112:HOH:O	2.55	0.61
1:B:158:SER:O	1:B:162:GLU:HG3	2.01	0.61
1:A:222:PHE:HB3	1:A:240:ILE:HG12	1.83	0.60
1:A:228:VAL:CG1	1:A:229:TYR:H	2.15	0.60
1:A:173[1]:ILE:HD11	1:A:218:ILE:HG12	1.83	0.60
1:B:69:ALA:HA	4:B:2112:HOH:O	2.01	0.60
1:A:190:MET:CE	1:A:191:ASP:H	2.14	0.60
1:B:62:ASN:HD21	1:B:79:GLN:NE2	1.99	0.60
1:A:284:LYS:HZ2	1:A:286:ASN:HD21	1.50	0.59
4:A:1599:HOH:O	1:B:71:LYS:HG2	2.03	0.59
1:A:136:PRO:HA	4:A:1564:HOH:O	2.03	0.59
1:A:74:LYS:HB3	1:B:99:HIS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:HD3	4:B:1891:HOH:O	2.04	0.58
1:B:182:GLU:HG3	4:B:2040:HOH:O	2.03	0.58
1:A:57:ILE:HG12	1:A:105:ILE:HB	1.86	0.57
1:A:65:ALA:HB2	4:A:1008:HOH:O	2.05	0.57
1:B:194:ALA:HA	4:B:1958:HOH:O	2.03	0.57
1:B:16:ASP:HA	1:B:19:LYS:HD2	1.86	0.57
1:A:180:GLY:HA3	1:A:231:ALA:HB3	1.86	0.57
1:B:228:VAL:HG21	4:B:2129:HOH:O	2.05	0.57
1:A:250:LYS:HD3	4:A:1192:HOH:O	2.05	0.56
1:B:30:ALA:HB3	1:B:352:LEU:HD22	1.86	0.56
1:A:110[2]:HIS:CE1	1:A:264[2]:HIS:CE1	2.94	0.56
1:A:284:LYS:NZ	1:A:286:ASN:HD21	2.03	0.55
1:B:128:LYS:HE2	1:B:128:LYS:HA	1.88	0.55
1:A:274:ILE:HG12	1:A:285:MET:HE1	1.89	0.55
1:A:194:ALA:H	1:A:195:LEU:HD23	1.72	0.54
1:B:147:GLU:HA	1:B:178:THR:HA	1.88	0.54
1:A:224:ASN:O	1:A:226[2]:HIS:HD2	1.90	0.54
1:B:152:GLU:HG3	4:B:2099:HOH:O	2.06	0.54
1:B:113:LYS:HA	1:B:116:LEU:HG	1.89	0.54
1:B:189:HIS:HB2	4:B:1480:HOH:O	2.07	0.53
1:A:60:PHE:HZ	4:A:1474:HOH:O	1.91	0.53
1:B:240:ILE:HG23	4:B:2225:HOH:O	2.08	0.52
1:B:184:GLY:O	1:B:186:ASP:N	2.42	0.51
1:B:287:ILE:HG21	4:B:1437:HOH:O	2.10	0.51
1:A:111[2]:CYS:SG	1:A:119:ILE:HG12	2.49	0.51
1:B:182:GLU:HG2	1:B:183:ASP:N	2.26	0.51
1:B:182:GLU:HG2	1:B:183:ASP:H	1.76	0.51
1:A:231:ALA:HA	4:A:1437:HOH:O	2.11	0.51
1:B:230:LYS:HD2	4:B:1832:HOH:O	2.11	0.51
1:B:238:PRO:HD3	4:B:1377:HOH:O	2.11	0.51
1:B:182:GLU:CG	1:B:183:ASP:H	2.23	0.51
1:B:57:ILE:HG12	1:B:105:ILE:HB	1.93	0.51
1:B:246:GLU:HG3	4:B:1805:HOH:O	2.10	0.50
1:B:107:HIS:NE2	3:B:1324:NH4:N	2.61	0.49
1:B:151:GLN:HB3	4:B:1888:HOH:O	2.12	0.49
1:A:178:THR:HA	1:A:195:LEU:HB2	1.95	0.49
1:B:196:TYR:HB3	1:B:197:THR:H	1.54	0.48
1:B:326:LYS:HG2	4:B:1603:HOH:O	2.13	0.48
1:A:182:GLU:H	1:A:231:ALA:HB1	1.79	0.48
1:A:71:LYS:HG2	4:B:1326:HOH:O	2.14	0.48
1:B:143[1]:ILE:HG22	1:B:145[1]:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143[2]:ILE:HG22	1:B:145[2]:LEU:HG	1.96	0.47
1:A:230:LYS:HD2	1:A:233:ASN:HA	1.96	0.47
1:A:208:GLU:HA	1:A:211:LYS:HE2	1.95	0.47
1:B:188:SER:O	1:B:189:HIS:HB2	2.15	0.47
1:B:150:LEU:HD11	1:B:204:TYR:CD2	2.50	0.47
1:A:159:LYS:HA	1:A:159:LYS:CE	2.44	0.47
1:A:56:VAL:HG22	1:A:57:ILE:N	2.30	0.47
1:A:230:LYS:HD3	4:A:1456:HOH:O	2.14	0.47
1:A:325:LYS:HE3	4:A:1619:HOH:O	2.14	0.47
1:B:65:ALA:O	1:B:85:GLY:HA3	2.15	0.46
1:B:195:LEU:HA	4:B:1551:HOH:O	2.15	0.46
1:B:184:GLY:HA2	4:B:1404:HOH:O	2.15	0.46
1:A:325:LYS:HD3	1:B:289:THR:HG23	1.98	0.46
1:A:142:MET:CE	1:A:264[2]:HIS:HE1	2.29	0.45
1:A:142:MET:HE1	1:A:264[2]:HIS:HE1	1.81	0.45
4:A:1588:HOH:O	1:B:84:LEU:HD21	2.14	0.45
1:A:158:SER:HB2	1:A:212:ILE:CD1	2.46	0.45
1:A:181:GLU:HG3	1:A:183:ASP:HB2	1.99	0.45
1:B:190:MET:HB3	4:B:2039:HOH:O	2.17	0.45
1:A:123:LEU:HD13	1:A:163:ARG:HD3	1.99	0.45
1:A:128:LYS:HE2	4:A:1439:HOH:O	2.17	0.45
1:B:198:GLN:HG2	4:B:1845:HOH:O	2.17	0.44
1:A:230:LYS:HB3	1:A:230:LYS:HE3	1.79	0.43
1:A:222:PHE:CB	1:A:240:ILE:HG12	2.47	0.43
1:A:228:VAL:CG1	1:A:229:TYR:N	2.79	0.43
1:B:165:SER:HA	4:B:1618:HOH:O	2.18	0.43
1:B:266:GLY:N	4:B:1926:HOH:O	2.51	0.43
1:B:3:ILE:HB	1:B:358:LEU:HA	2.00	0.43
1:B:59:GLN:HA	1:B:107:HIS:O	2.19	0.43
1:A:248:VAL:HG12	1:A:254:LEU:HD12	2.01	0.42
1:B:288:ASP:O	1:B:292:GLN:HG3	2.19	0.42
1:A:65:ALA:O	1:A:85:GLY:HA3	2.19	0.42
1:B:316:ASN:HB2	1:B:317:PRO:CD	2.50	0.42
1:B:129:HIS:HD2	1:B:135:LYS:O	2.03	0.42
1:A:178:THR:HG23	4:A:1452:HOH:O	2.20	0.42
1:B:83:ILE:HD13	1:B:121:GLY:HA3	2.01	0.41
1:A:8:LYS:HE3	1:A:8:LYS:HB2	1.73	0.41
1:A:55:PRO:HB3	1:A:103:PRO:HG2	2.02	0.41
1:A:32:PRO:HG3	1:A:352:LEU:HD12	2.02	0.41
1:A:59:GLN:HA	1:A:107:HIS:O	2.21	0.41
1:B:230:LYS:NZ	1:B:233:ASN:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LYS:HD3	4:B:1789:HOH:O	2.21	0.41
1:A:322:GLN:HA	1:A:323:PRO:HD3	1.88	0.40
1:B:8:LYS:HE2	4:B:1496:HOH:O	2.21	0.40
1:A:347:LYS:HE2	4:A:1332:HOH:O	2.21	0.40
1:A:286:ASN:N	1:A:286:ASN:HD22	2.18	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	371/358 (104%)	348 (94%)	15 (4%)	8 (2%)	8 1
1	B	371/358 (104%)	343 (92%)	19 (5%)	9 (2%)	7 1
All	All	742/716 (104%)	691 (93%)	34 (5%)	17 (2%)	7 1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	VAL
1	B	178	THR
1	B	185	VAL
1	B	177	CYS
1	B	182	GLU
1	B	230	LYS
1	A	185	VAL
1	A	179	GLY
1	A	184	GLY
1	A	187	ASN
1	A	231	ALA
1	B	196	TYR
1	A	233	ASN

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Mol	Chain	Res	Type
1	B	176	GLY
1	A	232	GLY
1	B	228	VAL
1	B	180	GLY

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	282/295 (96%)	269 (95%)	13 (5%)	33 11
1	B	282/295 (96%)	278 (99%)	4 (1%)	74 57
All	All	564/590 (96%)	547 (97%)	17 (3%)	48 24

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	LEU
1	A	159	LYS
1	A	171	LEU
1	A	183	ASP
1	A	185	VAL
1	A	190	MET
1	A	195	LEU
1	A	233	ASN
1	A	236	LEU
1	A	240	ILE
1	A	259	LEU
1	A	286	ASN
1	A	291	THR
1	B	148	GLU
1	B	150	LEU
1	B	196	TYR
1	B	291	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	28	ASN
1	A	99	HIS
1	A	256	HIS
1	A	286	ASN
1	A	292	GLN
1	A	301	ASN
1	B	18	GLN
1	B	79	GLN
1	B	91	HIS
1	B	129	HIS
1	B	313	GLN

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 6 ligands modelled in this entry, 2 are modelled with single atom and 4 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.

No monomer is involved in short contacts.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.