



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 01:40 PM EDT

PDB ID : 3KX6
Title : Crystal structure of fructose-1,6-bisphosphate aldolase from Babesia bovis at 2.1Å resolution
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2009-12-02
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

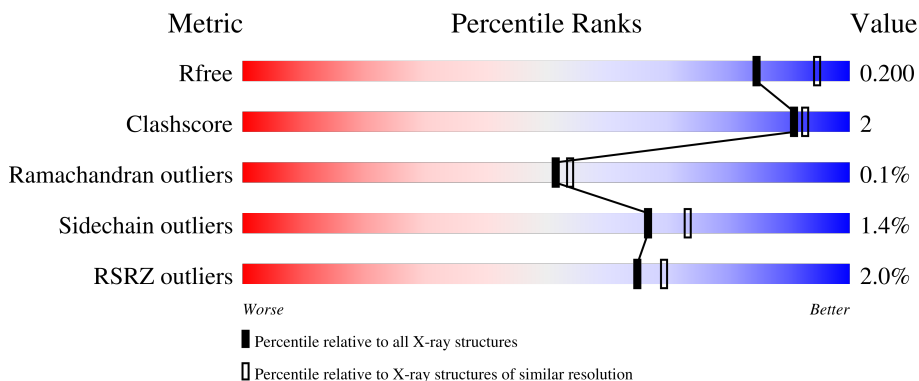
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


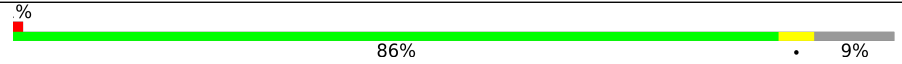
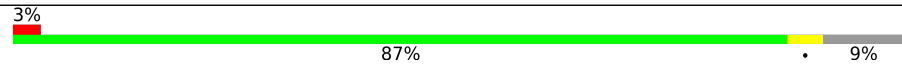

The reported resolution of this entry is 2.10 Å.

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	379	 88% 9%
1	B	379	 86% 9%
1	C	379	 87% 9%
1	D	379	 87% 9%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11265 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	2603	1634	450	507	12	0	5	0
1	B	343	2607	1634	454	507	12	0	4	0
1	C	343	2574	1614	445	503	12	0	3	0
1	D	343	2584	1622	448	502	12	0	4	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP A7AV51
A	-19	ALA	-	expression tag	UNP A7AV51
A	-18	HIS	-	expression tag	UNP A7AV51
A	-17	HIS	-	expression tag	UNP A7AV51
A	-16	HIS	-	expression tag	UNP A7AV51
A	-15	HIS	-	expression tag	UNP A7AV51
A	-14	HIS	-	expression tag	UNP A7AV51
A	-13	HIS	-	expression tag	UNP A7AV51
A	-12	MET	-	expression tag	UNP A7AV51
A	-11	GLY	-	expression tag	UNP A7AV51
A	-10	THR	-	expression tag	UNP A7AV51
A	-9	LEU	-	expression tag	UNP A7AV51
A	-8	GLU	-	expression tag	UNP A7AV51
A	-7	ALA	-	expression tag	UNP A7AV51
A	-6	GLN	-	expression tag	UNP A7AV51
A	-5	THR	-	expression tag	UNP A7AV51
A	-4	GLN	-	expression tag	UNP A7AV51
A	-3	GLY	-	expression tag	UNP A7AV51
A	-2	PRO	-	expression tag	UNP A7AV51
A	-1	GLY	-	expression tag	UNP A7AV51
A	0	SER	-	expression tag	UNP A7AV51

Continued on next page...

Continued from previous page...

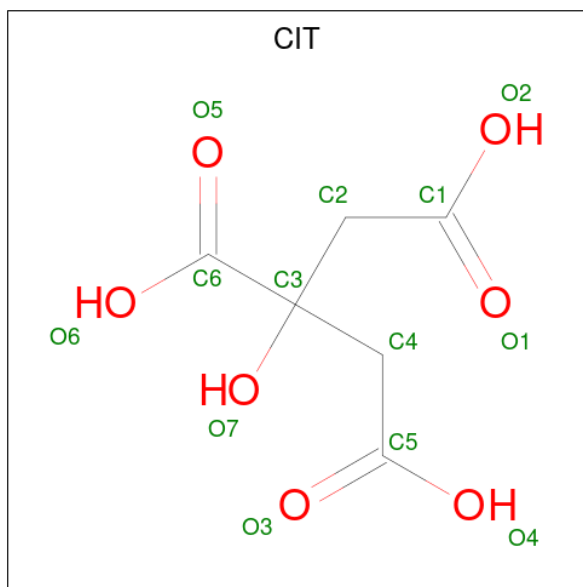
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP A7AV51
B	-19	ALA	-	expression tag	UNP A7AV51
B	-18	HIS	-	expression tag	UNP A7AV51
B	-17	HIS	-	expression tag	UNP A7AV51
B	-16	HIS	-	expression tag	UNP A7AV51
B	-15	HIS	-	expression tag	UNP A7AV51
B	-14	HIS	-	expression tag	UNP A7AV51
B	-13	HIS	-	expression tag	UNP A7AV51
B	-12	MET	-	expression tag	UNP A7AV51
B	-11	GLY	-	expression tag	UNP A7AV51
B	-10	THR	-	expression tag	UNP A7AV51
B	-9	LEU	-	expression tag	UNP A7AV51
B	-8	GLU	-	expression tag	UNP A7AV51
B	-7	ALA	-	expression tag	UNP A7AV51
B	-6	GLN	-	expression tag	UNP A7AV51
B	-5	THR	-	expression tag	UNP A7AV51
B	-4	GLN	-	expression tag	UNP A7AV51
B	-3	GLY	-	expression tag	UNP A7AV51
B	-2	PRO	-	expression tag	UNP A7AV51
B	-1	GLY	-	expression tag	UNP A7AV51
B	0	SER	-	expression tag	UNP A7AV51
C	-20	MET	-	expression tag	UNP A7AV51
C	-19	ALA	-	expression tag	UNP A7AV51
C	-18	HIS	-	expression tag	UNP A7AV51
C	-17	HIS	-	expression tag	UNP A7AV51
C	-16	HIS	-	expression tag	UNP A7AV51
C	-15	HIS	-	expression tag	UNP A7AV51
C	-14	HIS	-	expression tag	UNP A7AV51
C	-13	HIS	-	expression tag	UNP A7AV51
C	-12	MET	-	expression tag	UNP A7AV51
C	-11	GLY	-	expression tag	UNP A7AV51
C	-10	THR	-	expression tag	UNP A7AV51
C	-9	LEU	-	expression tag	UNP A7AV51
C	-8	GLU	-	expression tag	UNP A7AV51
C	-7	ALA	-	expression tag	UNP A7AV51
C	-6	GLN	-	expression tag	UNP A7AV51
C	-5	THR	-	expression tag	UNP A7AV51
C	-4	GLN	-	expression tag	UNP A7AV51
C	-3	GLY	-	expression tag	UNP A7AV51
C	-2	PRO	-	expression tag	UNP A7AV51
C	-1	GLY	-	expression tag	UNP A7AV51
C	0	SER	-	expression tag	UNP A7AV51

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP A7AV51
D	-19	ALA	-	expression tag	UNP A7AV51
D	-18	HIS	-	expression tag	UNP A7AV51
D	-17	HIS	-	expression tag	UNP A7AV51
D	-16	HIS	-	expression tag	UNP A7AV51
D	-15	HIS	-	expression tag	UNP A7AV51
D	-14	HIS	-	expression tag	UNP A7AV51
D	-13	HIS	-	expression tag	UNP A7AV51
D	-12	MET	-	expression tag	UNP A7AV51
D	-11	GLY	-	expression tag	UNP A7AV51
D	-10	THR	-	expression tag	UNP A7AV51
D	-9	LEU	-	expression tag	UNP A7AV51
D	-8	GLU	-	expression tag	UNP A7AV51
D	-7	ALA	-	expression tag	UNP A7AV51
D	-6	GLN	-	expression tag	UNP A7AV51
D	-5	THR	-	expression tag	UNP A7AV51
D	-4	GLN	-	expression tag	UNP A7AV51
D	-3	GLY	-	expression tag	UNP A7AV51
D	-2	PRO	-	expression tag	UNP A7AV51
D	-1	GLY	-	expression tag	UNP A7AV51
D	0	SER	-	expression tag	UNP A7AV51

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



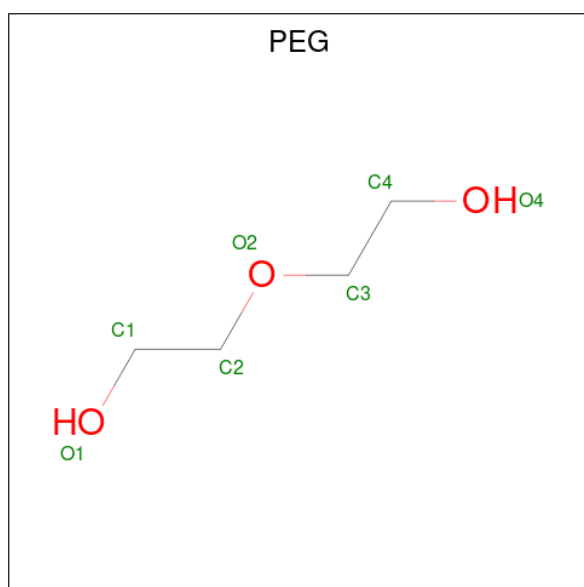
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	205	Total O 205 205	0	0
5	B	226	Total O 226 226	0	0
5	C	182	Total O 182 182	0	0
5	D	192	Total O 192 192	0	0

ASP	
LEU	
SER	
ASP	
ASP	
GLY	
GLU	
SER	
LEU	
PHE	
GLU	
A354	
I357	
Y358	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.88Å 114.16Å 174.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.10) 99.4 (19.96-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.160 , 0.193 0.166 , 0.200	Depositor DCC
R_{free} test set	4992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.644	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11265	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CIT, PEG

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	0.73	0/2659	0.70	1/3608 (0.0%)
1	B	0.76	0/2660	0.69	1/3606 (0.0%)
1	C	0.74	1/2624 (0.0%)	0.74	1/3562 (0.0%)
1	D	0.72	0/2637	0.70	2/3577 (0.1%)
All	All	0.74	1/10580 (0.0%)	0.71	5/14353 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	GLU	CG-CD	5.73	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	LEU	CA-CB-CG	9.87	138.00	115.30
1	C	163	LEU	CA-CB-CG	9.65	137.50	115.30
1	B	163	LEU	CA-CB-CG	5.87	128.80	115.30
1	D	256[A]	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	256[B]	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	2603	0	2579	10	0
1	B	2607	0	2590	14	0
1	C	2574	0	2530	8	0
1	D	2584	0	2560	6	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	1	0
3	A	7	0	10	0	0
3	B	14	0	20	0	0
3	C	14	0	20	0	0
3	D	14	0	20	0	0
4	D	4	0	6	0	0
5	A	205	0	0	5	0
5	B	226	0	0	3	0
5	C	182	0	0	4	0
5	D	192	0	0	2	0
All	All	11265	0	10350	35	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 2.

All (35) 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:D:277:MET:HE3	1:D:280:ARG:HE	1.47	0.79
1:B:277:MET:CE	1:B:280:ARG:HE	2.10	0.65
1:A:256[A]:ARG:HD3	5:A:639:HOH:O	1.98	0.64
1:B:133:LYS:NZ	5:B:647:HOH:O	2.31	0.63
1:C:44:VAL:HG21	1:C:308:LEU:HD13	1.80	0.63
1:D:277:MET:CE	1:D:280:ARG:HE	2.17	0.58
1:C:283:ASN:O	1:C:287:LYS:HG3	2.06	0.56
1:B:277:MET:HE2	1:B:280:ARG:HE	1.73	0.52
1:D:218:HIS:HD2	5:D:373:HOH:O	1.95	0.49
1:C:358:TYR:OH	5:C:899:HOH:O	2.06	0.48
1:A:104:LYS:NZ	5:A:415:HOH:O	2.45	0.48
1:D:80:LEU:HD12	1:D:91[B]:VAL:CG1	2.44	0.47
1:B:277:MET:HE1	1:B:280:ARG:HE	1.78	0.47
1:C:256[A]:ARG:HD3	5:C:612:HOH:O	2.15	0.47
1:A:156:LYS:NZ	5:A:500:HOH:O	2.36	0.46
1:A:104:LYS:HE2	5:A:395:HOH:O	2.13	0.46
1:D:273:GLN:NE2	1:D:281:HIS:ND1	2.64	0.46
1:B:277:MET:CE	1:B:280:ARG:HH11	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ALA:HB1	1:B:85:PRO:HD2	1.98	0.45
1:C:156:LYS:NZ	5:C:386:HOH:O	2.45	0.45
2:C:400:CIT:H41	5:C:836:HOH:O	2.15	0.45
1:A:31:ASP:OD2	1:A:104:LYS:HE3	2.17	0.44
1:B:63:THR:O	1:B:97:GLU:OE2	2.35	0.44
1:A:155[B]:ASN:ND2	1:C:155:ASN:OD1	2.51	0.44
1:D:256[A]:ARG:HD3	5:D:658:HOH:O	2.18	0.44
1:B:113:PRO:HA	1:C:3:VAL:HG13	2.00	0.43
1:A:104:LYS:HD3	5:A:792:HOH:O	2.18	0.43
1:B:219:LYS:NZ	5:B:814:HOH:O	2.52	0.43
1:A:38:GLN:NE2	1:A:48:ASN:HD22	2.17	0.43
1:B:3:VAL:HG21	1:C:111[A]:THR:HG21	2.01	0.42
1:B:163:LEU:HD13	5:B:535:HOH:O	2.18	0.42
1:B:266:VAL:HB	1:B:295:LEU:HD23	2.00	0.42
1:A:256[A]:ARG:HA	1:B:261:PRO:HG2	2.03	0.41
1:A:256[B]:ARG:HA	1:B:261:PRO:HG2	2.03	0.40
2:A:400:CIT:O2	2:A:400:CIT:C6	2.69	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	345/379 (91%)	340 (99%)	4 (1%)	1 (0%)	41	41
1	B	343/379 (90%)	337 (98%)	6 (2%)	0	100	100
1	C	342/379 (90%)	336 (98%)	6 (2%)	0	100	100
1	D	343/379 (90%)	338 (98%)	4 (1%)	1 (0%)	41	41
All	All	1373/1516 (91%)	1351 (98%)	20 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	PRO
1	D	187	PRO

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	276/312 (88%)	274 (99%)	2 (1%)	84 88
1	B	278/312 (89%)	275 (99%)	3 (1%)	73 79
1	C	270/312 (86%)	266 (98%)	4 (2%)	65 71
1	D	273/312 (88%)	266 (97%)	7 (3%)	46 50
All	All	1097/1248 (88%)	1081 (98%)	16 (2%)	67 71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	TYR
1	A	293	TRP
1	B	163	LEU
1	B	172	TYR
1	B	293	TRP
1	C	104	LYS
1	C	172	TYR
1	C	293	TRP
1	C	308	LEU
1	D	91[A]	VAL
1	D	91[B]	VAL
1	D	143	LYS
1	D	172	TYR
1	D	277	MET
1	D	293	TRP
1	D	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	38	GLN
1	A	82	GLN
1	A	230	ASN
1	A	312	ASN
1	A	317	ASN
1	B	230	ASN
1	C	38	GLN
1	C	155	ASN
1	C	331	GLN
1	D	218	HIS
1	D	230	ASN
1	D	273	GLN
1	D	330	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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	PEG	A	401	-	6,6,6	0.50	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	400	-	12,12,12	1.34	1 (8%)	17,17,17	1.92	3 (17%)
2	CIT	B	400	-	12,12,12	1.12	0	17,17,17	1.88	4 (23%)
3	PEG	C	401	-	6,6,6	0.37	0	5,5,5	0.32	0
3	PEG	B	401	-	6,6,6	0.49	0	5,5,5	0.70	0
3	PEG	C	402	-	6,6,6	0.53	0	5,5,5	0.42	0
3	PEG	B	402	-	6,6,6	0.58	0	5,5,5	0.45	0
3	PEG	D	401	-	6,6,6	0.35	0	5,5,5	0.51	0
3	PEG	D	402	-	6,6,6	0.51	0	5,5,5	0.35	0
4	EDO	D	400	-	3,3,3	0.69	0	2,2,2	0.11	0
2	CIT	C	400	-	12,12,12	1.39	1 (8%)	17,17,17	2.05	5 (29%)

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	PEG	A	401	-	-	1/4/4/4	-
2	CIT	A	400	-	-	2/16/16/16	-
2	CIT	B	400	-	-	2/16/16/16	-
3	PEG	C	401	-	-	2/4/4/4	-
3	PEG	B	401	-	-	4/4/4/4	-
3	PEG	C	402	-	-	2/4/4/4	-
3	PEG	B	402	-	-	0/4/4/4	-
3	PEG	D	401	-	-	3/4/4/4	-
3	PEG	D	402	-	-	4/4/4/4	-
4	EDO	D	400	-	-	0/1/1/1	-
2	CIT	C	400	-	-	2/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	CIT	O4-C5	-2.11	1.23	1.30
2	A	400	CIT	C3-C6	2.06	1.55	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	CIT	O6-C6-C3	5.39	122.42	113.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	CIT	O6-C6-C3	5.11	121.93	113.05
2	B	400	CIT	O6-C6-C3	4.46	120.79	113.05
2	C	400	CIT	O5-C6-C3	-4.13	116.41	122.25
2	A	400	CIT	O5-C6-C3	-3.30	117.58	122.25
2	B	400	CIT	O5-C6-C3	-3.13	117.82	122.25
2	C	400	CIT	O2-C1-C2	2.72	123.10	114.35
2	B	400	CIT	O2-C1-C2	2.72	123.07	114.35
2	A	400	CIT	O2-C1-C2	2.30	121.73	114.35
2	B	400	CIT	O4-C5-O3	-2.28	117.61	123.30
2	C	400	CIT	O2-C1-O1	-2.23	117.74	123.30
2	C	400	CIT	C4-C3-C6	-2.15	105.48	110.11

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	PEG	O2-C3-C4-O4
3	D	402	PEG	O1-C1-C2-O2
3	D	402	PEG	O2-C3-C4-O4
3	B	401	PEG	O2-C3-C4-O4
3	C	401	PEG	O2-C3-C4-O4
3	D	401	PEG	O2-C3-C4-O4
3	C	402	PEG	O2-C3-C4-O4
3	D	402	PEG	C4-C3-O2-C2
3	D	401	PEG	C1-C2-O2-C3
3	B	401	PEG	C1-C2-O2-C3
3	B	401	PEG	C4-C3-O2-C2
3	C	401	PEG	O1-C1-C2-O2
3	B	401	PEG	O1-C1-C2-O2
3	C	402	PEG	C1-C2-O2-C3
3	D	402	PEG	C1-C2-O2-C3
3	D	401	PEG	O1-C1-C2-O2
2	C	400	CIT	O2-C1-C2-C3
2	B	400	CIT	O1-C1-C2-C3
2	C	400	CIT	O1-C1-C2-C3
2	B	400	CIT	O2-C1-C2-C3
2	A	400	CIT	O2-C1-C2-C3
2	A	400	CIT	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	CIT	1	0
2	C	400	CIT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	344/379 (90%)	-0.34	5 (1%) 73 77	11, 19, 33, 46	0
1	B	343/379 (90%)	-0.39	3 (0%) 84 86	11, 18, 31, 38	0
1	C	343/379 (90%)	-0.32	10 (2%) 51 57	12, 19, 33, 42	0
1	D	343/379 (90%)	-0.26	10 (2%) 51 57	12, 19, 32, 47	0
All	All	1373/1516 (90%)	-0.33	28 (2%) 65 69	11, 19, 33, 47	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.1
1	C	3	VAL	5.7
1	D	358	TYR	5.6
1	D	5	LEU	4.8
1	D	354	ALA	3.7
1	C	45	GLY	3.7
1	B	341	LYS	3.2
1	C	354	ALA	3.2
1	C	316	SER	3.1
1	C	5	LEU	3.1
1	C	358	TYR	3.1
1	D	4	LYS	3.1
1	C	43	ASN	2.8
1	B	2	GLN	2.6
1	A	240	ASP	2.6
1	D	43	ASN	2.5
1	A	316	SER	2.5
1	C	8	GLU	2.5
1	D	357	ILE	2.5
1	D	6	SER	2.4
1	D	341	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	272	GLY	2.4
1	A	315	MET	2.4
1	D	194	ASP	2.4
1	B	3	VAL	2.2
1	C	42	ASP	2.2
1	C	4	LYS	2.1
1	D	282	LEU	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 monosaccharides 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. 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(Å ²)	Q<0.9
3	PEG	B	402	7/7	0.73	0.17	37,38,38,39	0
4	EDO	D	400	4/4	0.73	0.13	43,46,48,48	0
3	PEG	C	402	7/7	0.74	0.29	43,44,46,46	0
2	CIT	C	400	13/13	0.76	0.20	35,44,46,48	0
2	CIT	A	400	13/13	0.77	0.26	38,44,55,55	0
3	PEG	A	401	7/7	0.82	0.20	43,44,47,48	0
3	PEG	B	401	7/7	0.89	0.16	38,39,41,42	0
3	PEG	D	402	7/7	0.90	0.19	41,42,43,43	0
2	CIT	B	400	13/13	0.90	0.17	30,35,37,40	0
3	PEG	D	401	7/7	0.91	0.13	42,43,45,47	0
3	PEG	C	401	7/7	0.94	0.12	43,44,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.