Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2023 – 09:51 PM EDT

PDB ID	:	1S5M
Title	:	Xylose Isomerase in Substrate and Inhibitor Michaelis States: Atomic Resolution Studies of a Metal-Mediated Hydride Shift
Authors	:	Fenn, T.D.; Ringe, D.; Petsko, G.A.
Deposited on	:	2004-01-21
Resolution	:	0.98 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 (i) 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 (i)) were used in the production of this report:

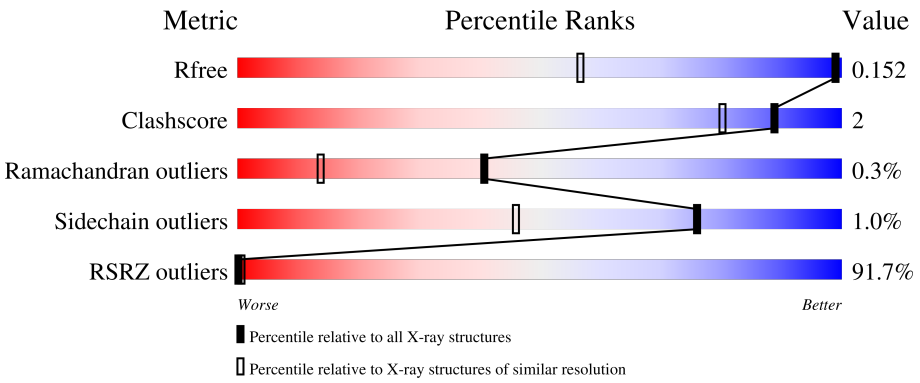
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 0.98 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	1166 (1.06-0.90)
Clashscore	141614	1241 (1.06-0.90)
Ramachandran outliers	138981	1159 (1.06-0.90)
Sidechain outliers	138945	1161 (1.06-0.90)
RSRZ outliers	127900	1132 (1.06-0.90)

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 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 <=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	386	92% 88% 11% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6830 atoms, of which 3140 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.

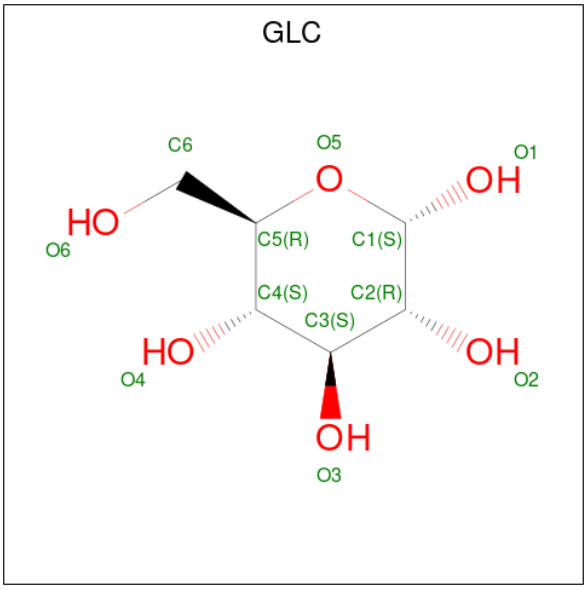
- Molecule 1 is a protein called Xylose isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	386	6378	2036	3128	589	615	10	0	45	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	ILE	THR	SEE REMARK 999	UNP P15587

- Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	24	6	12	6	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	2	2	2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0

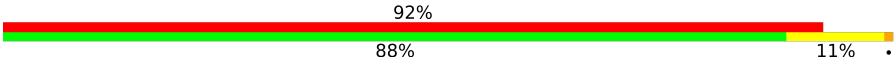
- Molecule 5 is water.

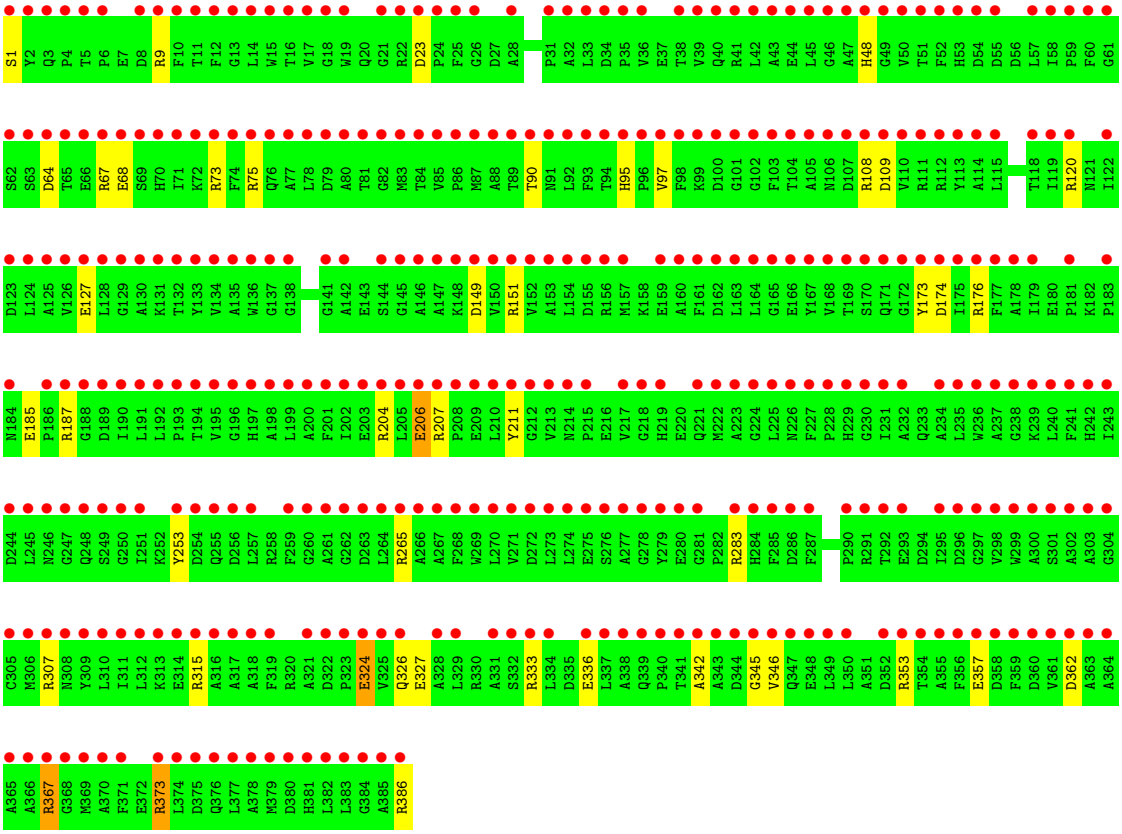
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	411	424	424	0	13

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	85.86Å 92.97Å 98.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 0.98 32.33 – 0.95	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-0.98) 88.0 (32.33-0.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 0.95Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.111 , 0.129 0.151 , 0.152	Depositor DCC
R_{free} test set	11433 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	8.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6830	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, NA, GLC

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	0.89	5/3323 (0.2%)	1.59	61/4494 (1.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	GLU	CB-CG	-9.07	1.34	1.52
1	A	73	ARG	CZ-NH2	7.58	1.43	1.33
1	A	73	ARG	CZ-NH1	7.39	1.42	1.33
1	A	315	ARG	CZ-NH2	6.21	1.41	1.33
1	A	327[A]	GLU	CD-OE2	5.99	1.32	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	ARG	CD-NE-CZ	33.46	170.44	123.60
1	A	204[A]	ARG	CD-NE-CZ	18.35	149.29	123.60
1	A	204[B]	ARG	CD-NE-CZ	18.35	149.29	123.60
1	A	386[A]	ARG	NE-CZ-NH1	16.26	128.43	120.30
1	A	386[B]	ARG	NE-CZ-NH1	16.26	128.43	120.30
1	A	386[A]	ARG	NE-CZ-NH2	-15.78	112.41	120.30
1	A	386[B]	ARG	NE-CZ-NH2	-15.78	112.41	120.30
1	A	373	ARG	NE-CZ-NH2	13.24	126.92	120.30
1	A	9[A]	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	A	9[A]	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	A	127	GLU	OE1-CD-OE2	11.31	136.87	123.30
1	A	367	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	A	211	TYR	CB-CG-CD2	11.04	127.63	121.00
1	A	120	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	315	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	315	ARG	NE-CZ-NH1	8.90	124.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207[A]	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	187	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	120	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	265[A]	ARG	CD-NE-CZ	7.59	134.23	123.60
1	A	265[B]	ARG	CD-NE-CZ	7.59	134.23	123.60
1	A	357	GLU	OE1-CD-OE2	-7.59	114.19	123.30
1	A	176[A]	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	176[B]	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	149	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	174[A]	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	A	174[B]	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	A	174[A]	ASP	O-C-N	-6.91	111.65	122.70
1	A	174[B]	ASP	O-C-N	-6.91	111.65	122.70
1	A	373	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	A	346	VAL	CA-CB-CG1	6.84	121.17	110.90
1	A	75	ARG	CD-NE-CZ	6.84	133.17	123.60
1	A	324[A]	GLU	OE1-CD-OE2	6.82	131.49	123.30
1	A	324[B]	GLU	OE1-CD-OE2	6.82	131.49	123.30
1	A	108	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	204[A]	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	204[B]	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	67	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	211	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	A	353	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	174[A]	ASP	N-CA-CB	-6.17	99.49	110.60
1	A	174[B]	ASP	N-CA-CB	-6.17	99.49	110.60
1	A	187	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	64	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	A	151[A]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	151[B]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	206[A]	GLU	OE1-CD-OE2	-5.89	116.24	123.30
1	A	206[B]	GLU	OE1-CD-OE2	-5.89	116.24	123.30
1	A	75	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	173[A]	TYR	CB-CG-CD1	5.76	124.46	121.00
1	A	173[B]	TYR	CB-CG-CD1	5.76	124.46	121.00
1	A	253	TYR	CB-CG-CD1	5.69	124.41	121.00
1	A	73	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	67	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	A	315	ARG	CD-NE-CZ	-5.60	115.76	123.60
1	A	108	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	307	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	367	ARG	NH1-CZ-NH2	5.48	125.43	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	ASP	CB-CA-C	5.45	121.29	110.40
1	A	362	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	109	ASP	CB-CG-OD1	5.04	122.83	118.30

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	3250	3128	2961	12	0
2	A	12	12	10	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	424	0	0	7	0
All	All	3690	3140	2971	12	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 (12) 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:283[B]:ARG:CZ	5:A:2413:HOH:O	1.65	1.24
1:A:283[B]:ARG:NH2	5:A:2413:HOH:O	1.58	1.12
1:A:283[B]:ARG:NE	5:A:2413:HOH:O	1.62	1.07
1:A:95:HIS:HD2	1:A:97:VAL:H	1.40	0.68
1:A:48[A]:HIS:HD2	5:A:2324:HOH:O	1.90	0.54
1:A:333:ARG:NH2	1:A:367:ARG:HD3	2.27	0.50
1:A:324[A]:GLU:OE2	1:A:373:ARG:NH2	2.47	0.48
1:A:345:GLY:N	5:A:2410:HOH:O	2.48	0.45
1:A:326[A]:GLN:NE2	5:A:2112:HOH:O	2.52	0.41
1:A:95:HIS:CD2	1:A:97:VAL:H	2.28	0.41
1:A:342:ALA:HB1	5:A:2410:HOH:O	2.20	0.41

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	408/386 (106%)	394 (97%)	13 (3%)	1 (0%)	47 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU

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	326/302 (108%)	323 (99%)	3 (1%)	78 50

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	68	GLU
1	A	90	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	308	ASN
1	A	376	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)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	GLC	A	1001	3	12,12,12	1.09	1 (8%)	17,17,17	2.03	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
2	GLC	A	1001	3	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GLC	O5-C1	3.36	1.51	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	GLC	O5-C5-C6	4.41	117.39	106.44
2	A	1001	GLC	C1-O5-C5	-4.22	105.70	113.66
2	A	1001	GLC	C6-C5-C4	-3.60	104.57	113.00
2	A	1001	GLC	O6-C6-C5	-2.66	102.17	111.29
2	A	1001	GLC	C3-C4-C5	-2.39	105.97	110.24

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	386/386 (100%)	3.57	354 (91%) 0 1	7, 10, 26, 46	0

All (354) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	10.6
1	A	78	LEU	7.9
1	A	385[A]	ALA	7.1
1	A	173[A]	TYR	7.0
1	A	174[A]	ASP	7.0
1	A	33	LEU	6.9
1	A	75	ARG	6.9
1	A	24	PRO	6.7
1	A	76	GLN	6.6
1	A	346	VAL	6.3
1	A	9[A]	ARG	6.2
1	A	163[A]	LEU	6.1
1	A	205[A]	LEU	6.1
1	A	386[A]	ARG	6.0
1	A	122	ILE	5.9
1	A	36	VAL	5.9
1	A	383	LEU	5.8
1	A	169	THR	5.6
1	A	299	TRP	5.6
1	A	356	PHE	5.6
1	A	190	ILE	5.6
1	A	126	VAL	5.6
1	A	298	VAL	5.5
1	A	6	PRO	5.5
1	A	276[A]	SER	5.5
1	A	114	ALA	5.5
1	A	208	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	125	ALA	5.5
1	A	343	ALA	5.4
1	A	382	LEU	5.4
1	A	235	LEU	5.3
1	A	65	THR	5.3
1	A	80	ALA	5.3
1	A	329	LEU	5.3
1	A	342	ALA	5.2
1	A	243	ILE	5.2
1	A	119	ILE	5.2
1	A	25	PHE	5.2
1	A	89	THR	5.2
1	A	241	PHE	5.2
1	A	61	GLY	5.2
1	A	310	LEU	5.2
1	A	15	TRP	5.1
1	A	178	ALA	5.0
1	A	98	PHE	5.0
1	A	245	LEU	5.0
1	A	370	ALA	5.0
1	A	267	ALA	4.9
1	A	269	TRP	4.9
1	A	359	PHE	4.9
1	A	157[A]	MET	4.9
1	A	113	TYR	4.9
1	A	142	ALA	4.9
1	A	347	GLN	4.8
1	A	168	VAL	4.8
1	A	266[A]	ALA	4.8
1	A	202	ILE	4.8
1	A	210	LEU	4.8
1	A	135	ALA	4.7
1	A	128	LEU	4.7
1	A	63	SER	4.7
1	A	249[A]	SER	4.7
1	A	167	TYR	4.7
1	A	204[A]	ARG	4.7
1	A	136	TRP	4.7
1	A	285	PHE	4.7
1	A	147	ALA	4.7
1	A	349[A]	LEU	4.6
1	A	28	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	217	VAL	4.6
1	A	45	LEU	4.6
1	A	152[A]	VAL	4.6
1	A	361	VAL	4.6
1	A	32	ALA	4.6
1	A	357	GLU	4.6
1	A	161	PHE	4.6
1	A	154	LEU	4.5
1	A	71	ILE	4.5
1	A	350	LEU	4.5
1	A	10[A]	PHE	4.5
1	A	283[A]	ARG	4.5
1	A	362	ASP	4.4
1	A	287[A]	PHE	4.4
1	A	41[A]	ARG	4.4
1	A	48[A]	HIS	4.4
1	A	68	GLU	4.4
1	A	193	PRO	4.4
1	A	58	ILE	4.4
1	A	133	TYR	4.4
1	A	19	TRP	4.4
1	A	250[A]	GLY	4.4
1	A	240	LEU	4.3
1	A	153	ALA	4.3
1	A	198	ALA	4.3
1	A	251	ILE	4.3
1	A	31	PRO	4.3
1	A	138	GLY	4.3
1	A	59	PRO	4.3
1	A	323	PRO	4.3
1	A	97	VAL	4.3
1	A	345	GLY	4.3
1	A	277[A]	ALA	4.3
1	A	101	GLY	4.3
1	A	192	LEU	4.3
1	A	34	ASP	4.3
1	A	177[A]	PHE	4.2
1	A	195	VAL	4.2
1	A	64	ASP	4.2
1	A	50[A]	VAL	4.2
1	A	57	LEU	4.1
1	A	199	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	325[A]	VAL	4.1
1	A	72	LYS	4.1
1	A	88	ALA	4.1
1	A	132	THR	4.1
1	A	358	ASP	4.1
1	A	124	LEU	4.1
1	A	150	VAL	4.1
1	A	227	PHE	4.1
1	A	303	ALA	4.0
1	A	115	LEU	4.0
1	A	305	CYS	4.0
1	A	12	PHE	4.0
1	A	365	ALA	4.0
1	A	90	THR	4.0
1	A	236	TRP	4.0
1	A	367	ARG	4.0
1	A	11	THR	4.0
1	A	231	ILE	4.0
1	A	295	ILE	4.0
1	A	279	TYR	4.0
1	A	265[A]	ARG	4.0
1	A	110	VAL	4.0
1	A	191	LEU	4.0
1	A	118	THR	4.0
1	A	257	LEU	3.9
1	A	271	VAL	3.9
1	A	247	GLY	3.9
1	A	206[A]	GLU	3.9
1	A	363	ALA	3.9
1	A	270	LEU	3.9
1	A	274	LEU	3.9
1	A	374	LEU	3.9
1	A	268	PHE	3.9
1	A	371	PHE	3.9
1	A	130	ALA	3.9
1	A	253	TYR	3.9
1	A	213	VAL	3.9
1	A	3[A]	GLN	3.9
1	A	16	THR	3.8
1	A	264	LEU	3.8
1	A	43	ALA	3.8
1	A	211	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	96	PRO	3.8
1	A	179	ILE	3.8
1	A	212	GLY	3.8
1	A	2	TYR	3.8
1	A	337	LEU	3.8
1	A	38	THR	3.8
1	A	104	THR	3.8
1	A	292	THR	3.8
1	A	201	PHE	3.8
1	A	223	ALA	3.8
1	A	145	GLY	3.8
1	A	194	THR	3.7
1	A	160	ALA	3.7
1	A	93	PHE	3.7
1	A	176[A]	ARG	3.7
1	A	260	GLY	3.7
1	A	47	ALA	3.7
1	A	232	ALA	3.7
1	A	35	PRO	3.7
1	A	324[A]	GLU	3.7
1	A	39	VAL	3.7
1	A	218	GLY	3.7
1	A	278	GLY	3.7
1	A	215	PRO	3.7
1	A	77	ALA	3.6
1	A	134	VAL	3.6
1	A	60	PHE	3.6
1	A	304	GLY	3.6
1	A	373	ARG	3.6
1	A	70	HIS	3.6
1	A	44	GLU	3.6
1	A	312	LEU	3.6
1	A	86	PRO	3.5
1	A	228	PRO	3.5
1	A	51[A]	THR	3.5
1	A	105	ALA	3.5
1	A	149	ASP	3.5
1	A	311	ILE	3.5
1	A	146	ALA	3.5
1	A	302	ALA	3.5
1	A	172	GLY	3.5
1	A	368	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	3.5
1	A	92	LEU	3.5
1	A	131	LYS	3.4
1	A	378	ALA	3.4
1	A	73	ARG	3.4
1	A	214	ASN	3.4
1	A	334	LEU	3.4
1	A	55	ASP	3.4
1	A	379	MET	3.4
1	A	22	ARG	3.4
1	A	314	GLU	3.4
1	A	17	VAL	3.4
1	A	377	LEU	3.4
1	A	200	ALA	3.4
1	A	261	ALA	3.4
1	A	355	ALA	3.4
1	A	181	PRO	3.4
1	A	341	THR	3.4
1	A	106	ASN	3.4
1	A	319	PHE	3.4
1	A	331	ALA	3.3
1	A	280	GLU	3.3
1	A	309	TYR	3.3
1	A	49[A]	GLY	3.3
1	A	137	GLY	3.3
1	A	171	GLN	3.3
1	A	234	ALA	3.3
1	A	286[A]	ASP	3.3
1	A	164[A]	LEU	3.3
1	A	120	ARG	3.3
1	A	144	SER	3.3
1	A	52	PHE	3.3
1	A	103	PHE	3.3
1	A	259	PHE	3.3
1	A	187	ARG	3.2
1	A	69	SER	3.2
1	A	42	LEU	3.2
1	A	225	LEU	3.2
1	A	151[A]	ARG	3.2
1	A	175[A]	ILE	3.2
1	A	364	ALA	3.2
1	A	186	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	338	ALA	3.1
1	A	102	GLY	3.1
1	A	83	MET	3.1
1	A	53	HIS	3.1
1	A	94	THR	3.1
1	A	123	ASP	3.1
1	A	381	HIS	3.0
1	A	82	GLY	3.0
1	A	224	GLY	3.0
1	A	109	ASP	3.0
1	A	318	ALA	3.0
1	A	40[A]	GLN	3.0
1	A	91	ASN	3.0
1	A	273	LEU	3.0
1	A	184	ASN	3.0
1	A	196	GLY	3.0
1	A	290	PRO	2.9
1	A	317	ALA	2.9
1	A	354	THR	2.9
1	A	230	GLY	2.9
1	A	67	ARG	2.9
1	A	242	HIS	2.9
1	A	23	ASP	2.9
1	A	244	ASP	2.9
1	A	375	ASP	2.9
1	A	306	MET	2.9
1	A	360	ASP	2.9
1	A	84	THR	2.9
1	A	300	ALA	2.9
1	A	226	ASN	2.8
1	A	353	ARG	2.8
1	A	328	ALA	2.8
1	A	340	PRO	2.8
1	A	313	LYS	2.8
1	A	111	ARG	2.8
1	A	297	GLY	2.8
1	A	197	HIS	2.8
1	A	14	LEU	2.8
1	A	308	ASN	2.8
1	A	246	ASN	2.7
1	A	79	ASP	2.7
1	A	339	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	183	PRO	2.7
1	A	141	GLY	2.7
1	A	127	GLU	2.7
1	A	229	HIS	2.6
1	A	203[A]	GLU	2.6
1	A	207[A]	ARG	2.6
1	A	256	ASP	2.6
1	A	336	GLU	2.6
1	A	4	PRO	2.6
1	A	85	VAL	2.6
1	A	5	THR	2.6
1	A	87	MET	2.6
1	A	275	GLU	2.6
1	A	384	GLY	2.6
1	A	316	ALA	2.6
1	A	326[A]	GLN	2.6
1	A	107	ASP	2.6
1	A	348[A]	GLU	2.5
1	A	81	THR	2.5
1	A	188	GLY	2.5
1	A	376	GLN	2.5
1	A	99[A]	LYS	2.5
1	A	62	SER	2.5
1	A	219	HIS	2.5
1	A	108	ARG	2.5
1	A	209	GLU	2.5
1	A	322	ASP	2.5
1	A	237	ALA	2.4
1	A	238	GLY	2.4
1	A	95	HIS	2.4
1	A	66	GLU	2.4
1	A	369	MET	2.4
1	A	162	ASP	2.4
1	A	189	ASP	2.4
1	A	296	ASP	2.4
1	A	26	GLY	2.4
1	A	291	ARG	2.4
1	A	255	GLN	2.4
1	A	239	LYS	2.4
1	A	307	ARG	2.4
1	A	221	GLN	2.4
1	A	54	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	148	LYS	2.3
1	A	165	GLY	2.3
1	A	248	GLN	2.3
1	A	366	ALA	2.3
1	A	301	SER	2.3
1	A	166	GLU	2.3
1	A	13	GLY	2.3
1	A	156	ARG	2.3
1	A	100[A]	ASP	2.3
1	A	333	ARG	2.3
1	A	263	ASP	2.3
1	A	112	ARG	2.3
1	A	155	ASP	2.3
1	A	321	ALA	2.2
1	A	8	ASP	2.2
1	A	18	GLY	2.2
1	A	293	GLU	2.2
1	A	129	GLY	2.2
1	A	170	SER	2.2
1	A	380	ASP	2.2
1	A	284[A]	HIS	2.2
1	A	344	ASP	2.2
1	A	262	GLY	2.1
1	A	352	ASP	2.1
1	A	222	MET	2.1
1	A	254	ASP	2.1
1	A	332	SER	2.1
1	A	281	GLY	2.1
1	A	315	ARG	2.0
1	A	74	PHE	2.0
1	A	46	GLY	2.0
1	A	159	GLU	2.0
1	A	272	ASP	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
2	GLC	A	1001	12/12	0.88	0.19	10,16,28,32	0
4	NA	A	2005	1/1	0.94	0.14	26,26,26,26	0
4	NA	A	2004	1/1	0.99	0.11	19,19,19,19	0
3	MN	A	2001	1/1	1.00	0.17	8,8,8,8	1
3	MN	A	2002	1/1	1.00	0.17	7,7,7,7	1

6.5 Other polymers (i)

There are no such residues in this entry.