wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:46 PM GMT

PDB ID	:	3UVA
Title	:	Crystal structure of L-rhamnose isomerase mutant W38F from Bacillus halodurans in complex with Mn
Authors	:	Doan, T.T.N.; Prabhu, P.; Jeya, M.; Kim, J.K.; Kang, L.W.; Lee, J.K.
Deposited on	:	2011-11-29
Resolution	:	2.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

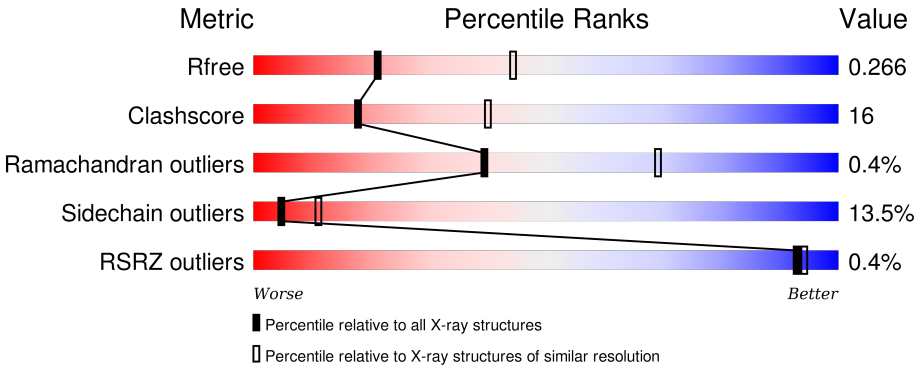
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.69 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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. 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	424	67% 22% 5% 5%
1	B	424	58% 30% 7% • 5%
1	C	424	% 67% 23% 6% •
1	D	424	61% 29% 5% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13649 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 L-Rhamnose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3289	2108	565	607	9			
1	B	404	Total	C	N	O	S	0	0	0
			3301	2115	567	609	10			
1	C	405	Total	C	N	O	S	0	0	0
			3307	2118	568	611	10			
1	D	403	Total	C	N	O	S	0	0	0
			3291	2110	564	608	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	38	PHE	TRP	ENGINEERED MUTATION	UNP Q9KCL9
B	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	38	PHE	TRP	ENGINEERED MUTATION	UNP Q9KCL9
C	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	38	PHE	TRP	ENGINEERED MUTATION	UNP Q9KCL9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	38	PHE	TRP	ENGINEERED MUTATION	UNP Q9KCL9

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

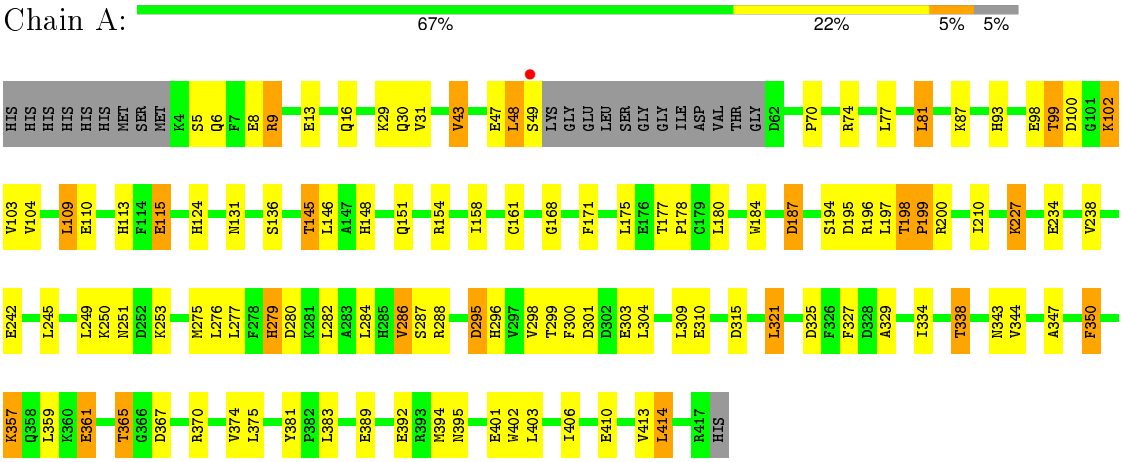
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	133	Total O 133 133	0	0
3	B	103	Total O 103 103	0	0
3	C	131	Total O 131 131	0	0
3	D	86	Total O 86 86	0	0

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.

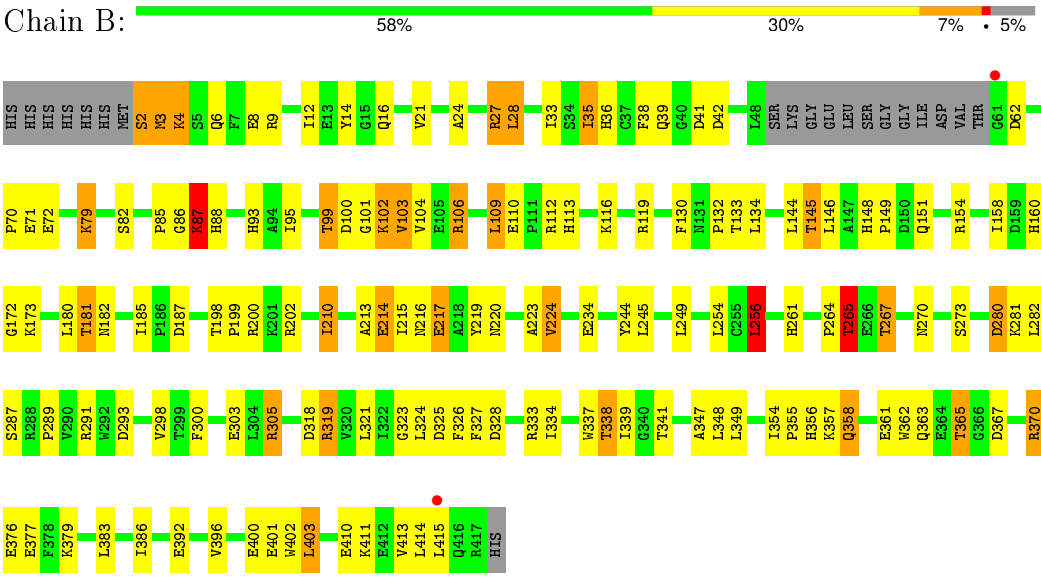
- Molecule 1: L-Rhamnose isomerase

Chain A:



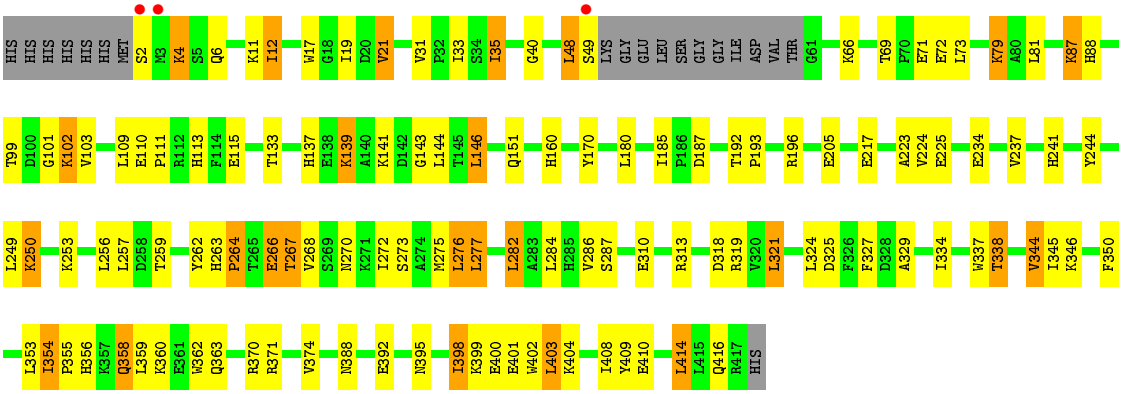
- Molecule 1: L-Rhamnose isomerase

Chain B:



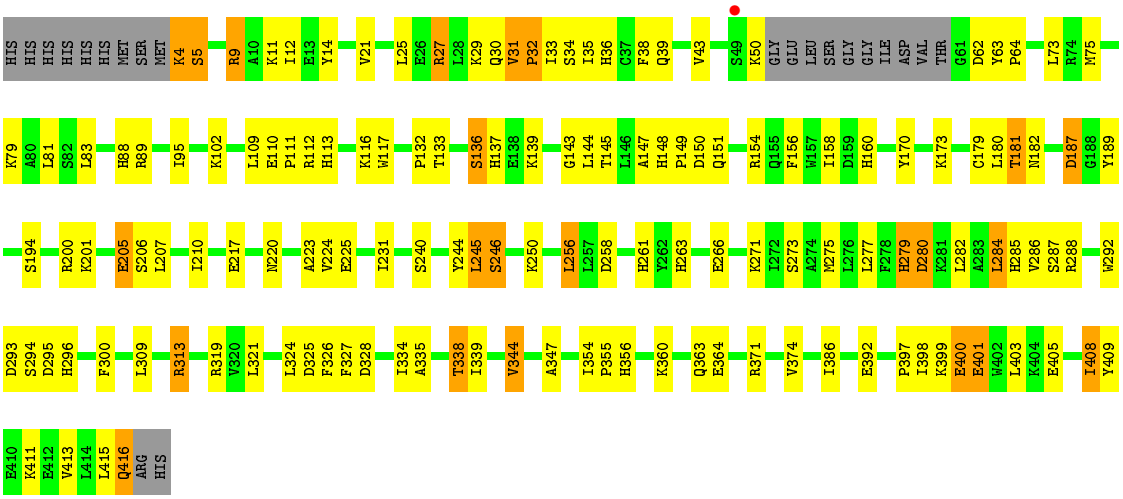
- Molecule 1: L-Rhamnose isomerase

Chain C:



- Molecule 1: L-Rhamnose isomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.37Å 164.78Å 92.82Å 90.00° 117.01° 90.00°	Depositor
Resolution (Å)	45.87 – 2.69 45.87 – 2.69	Depositor EDS
% Data completeness (in resolution range)	88.0 (45.87-2.69) 88.0 (45.87-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.266 0.189 , 0.266	Depositor DCC
R_{free} test set	2778 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.1	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 54306 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13649	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.82	0/3369	0.85	5/4560 (0.1%)
1	B	0.76	1/3381 (0.0%)	0.84	3/4575 (0.1%)
1	C	0.80	5/3387 (0.1%)	0.84	0/4583
1	D	0.82	0/3371	0.82	1/4562 (0.0%)
All	All	0.80	6/13508 (0.0%)	0.84	9/18280 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	GLU	CD-OE2	-5.56	1.19	1.25
1	C	266	GLU	CD-OE1	-5.55	1.19	1.25
1	C	262	TYR	CE1-CZ	-5.44	1.31	1.38
1	C	205	GLU	CB-CG	5.31	1.62	1.52
1	C	392	GLU	CG-CD	5.22	1.59	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	87	LYS	N-CA-C	-5.69	95.65	111.00
1	D	415	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	415	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	301	ASP	CB-CG-OD1	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ASP	CB-CG-OD1	5.26	123.04	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	GLU	Peptide

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	3289	0	3245	92	1
1	B	3301	0	3257	153	0
1	C	3307	0	3262	81	0
1	D	3291	0	3248	105	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	133	0	0	5	0
3	B	103	0	0	4	0
3	C	131	0	0	6	0
3	D	86	0	0	4	0
All	All	13649	0	13012	415	1

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 16.

The worst 5 of 415 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:B:102:LYS:HA	1:B:103:VAL:CG2	1.14	1.53
1:B:102:LYS:CA	1:B:103:VAL:HG23	1.49	1.40
1:B:102:LYS:CA	1:B:103:VAL:CG2	2.06	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ARG:O	1:D:30:GLN:HG2	1.30	1.27
1:A:48:LEU:HD13	1:A:48:LEU:C	1.54	1.22

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:OH	1:D:400:GLU:OE2[1_655]	2.15	0.05

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	398/424 (94%)	365 (92%)	32 (8%)	1 (0%)	46	75
1	B	400/424 (94%)	371 (93%)	27 (7%)	2 (0%)	34	63
1	C	401/424 (95%)	374 (93%)	26 (6%)	1 (0%)	52	80
1	D	399/424 (94%)	372 (93%)	24 (6%)	3 (1%)	24	51
All	All	1598/1696 (94%)	1482 (93%)	109 (7%)	7 (0%)	39	69

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	THR
1	D	136	SER
1	C	259	THR
1	D	32	PRO
1	D	293	ASP

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	352/370 (95%)	311 (88%)	41 (12%)	7 16
1	B	353/370 (95%)	297 (84%)	56 (16%)	3 8
1	C	354/370 (96%)	308 (87%)	46 (13%)	5 12
1	D	352/370 (95%)	304 (86%)	48 (14%)	5 11
All	All	1411/1480 (95%)	1220 (86%)	191 (14%)	5 11

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	338	THR
1	C	81	LEU
1	D	284	LEU
1	B	357	LYS
1	B	411	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	131	ASN
1	C	241	HIS
1	D	356	HIS
1	C	137	HIS
1	C	160	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

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, 95^{th} 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	402/424 (94%)	-0.56	1 (0%)	95	96	17, 29, 48, 68	0
1	B	404/424 (95%)	-0.50	2 (0%)	91	93	19, 32, 53, 77	0
1	C	405/424 (95%)	-0.55	3 (0%)	89	90	18, 31, 46, 84	0
1	D	403/424 (95%)	-0.48	1 (0%)	95	96	19, 31, 51, 72	0
All	All	1614/1696 (95%)	-0.52	7 (0%)	93	94	17, 31, 50, 84	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	MET	5.1
1	C	2	SER	4.3
1	B	415	LEU	2.6
1	A	49	SER	2.4
1	C	49	SER	2.2

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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MN	A	420	1/1	0.94	0.20	2.00	81,81,81,81	0
2	MN	D	420	1/1	0.93	0.17	1.49	75,75,75,75	0
2	MN	B	420	1/1	0.93	0.14	0.13	74,74,74,74	0
2	MN	C	420	1/1	0.97	0.13	-0.48	67,67,67,67	0
2	MN	D	419	1/1	0.98	0.06	-3.15	71,71,71,71	0
2	MN	A	419	1/1	0.96	0.07	-3.28	69,69,69,69	0
2	MN	C	419	1/1	0.95	0.13	-	81,81,81,81	0
2	MN	B	419	1/1	0.94	0.10	-	82,82,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.