Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:54 AM EDT

PDB ID	:	4KIR
Title	:	Crystal Structure of D-Hydantoinase from Bacillus sp. AR9 in C2221 space group
Authors	:	Kumar, V.; Kishan, K.V.R.
Deposited on	:	2013-05-02
Resolution	:	2.80 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 (1)) were used in the production of this report:

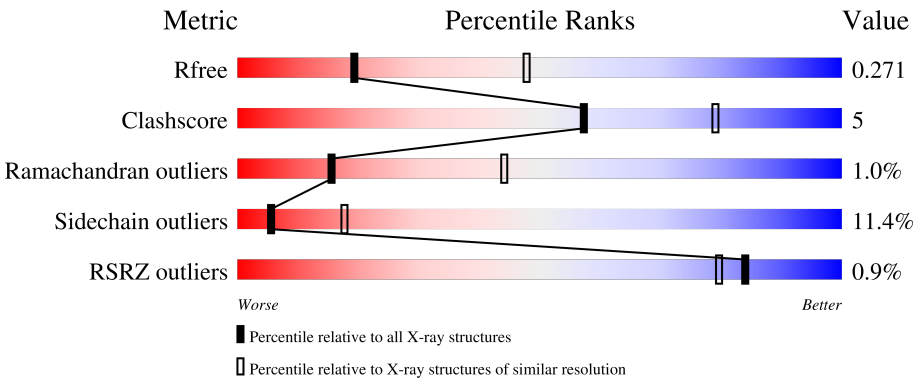
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	460	% 81% 15%
1	B	460	% 80% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7088 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 D-hydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3537	2244	603	678	12	0	0	0
1	B	456	3531	2240	601	678	12	0	2	0

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

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

- Molecule 3 is water.

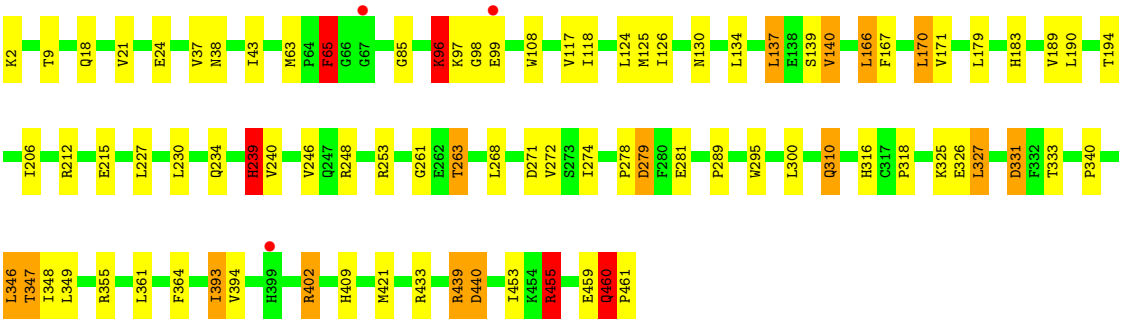
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	4	4	4	0	0
3	B	12	12	12	0	0

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.

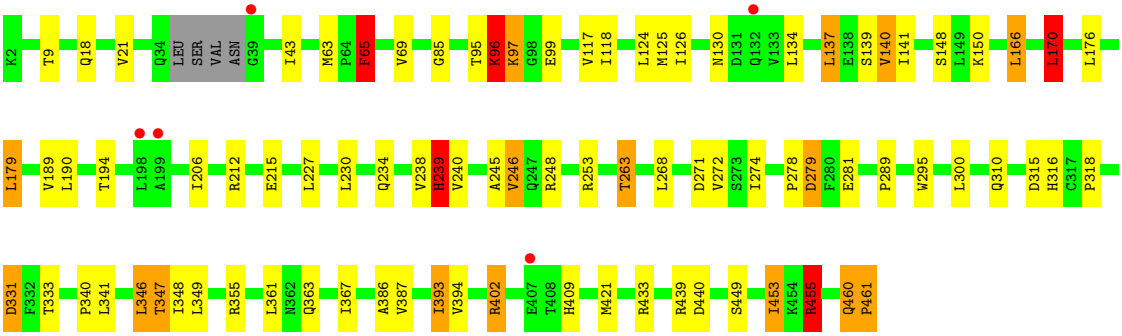
• Molecule 1: D-hydantoinase

Chain A:



• Molecule 1: D-hydantoinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	90.88Å 185.24Å 113.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.41 – 2.80 25.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.6 (25.41-2.80) 87.8 (25.41-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.271 0.192 , 0.271	Depositor DCC
R_{free} test set	1079 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7088	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

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	0.69	0/3612	0.93	14/4897 (0.3%)
1	B	0.69	0/3605	0.97	16/4885 (0.3%)
All	All	0.69	0/7217	0.95	30/9782 (0.3%)

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	LYS	CB-CA-C	13.52	137.43	110.40
1	A	327	LEU	N-CA-C	-10.73	82.02	111.00
1	B	460	GLN	N-CA-C	9.93	137.80	111.00
1	B	96	LYS	N-CA-C	-8.93	86.89	111.00
1	B	150	LYS	CD-CE-NZ	7.95	129.98	111.70
1	B	97	LYS	CB-CA-C	7.35	125.10	110.40
1	A	460	GLN	N-CA-C	-7.25	91.41	111.00
1	A	239	HIS	N-CA-C	6.97	129.81	111.00
1	B	239	HIS	N-CA-C	6.84	129.48	111.00
1	B	279	ASP	N-CA-C	-6.83	92.56	111.00
1	B	461	PRO	N-CA-CB	6.78	111.43	103.30
1	B	315	ASP	CB-CG-OD1	6.76	124.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	ASP	N-CA-C	-6.45	93.58	111.00
1	B	460	GLN	CB-CA-C	-6.41	97.58	110.40
1	A	460	GLN	C-N-CA	6.27	148.34	122.00
1	A	461	PRO	N-CA-CB	6.22	110.77	103.30
1	A	253	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	96	LYS	CB-CA-C	6.15	122.70	110.40
1	A	325	LYS	CB-CA-C	-5.91	98.58	110.40
1	B	253	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	433	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	253	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	455	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	433	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	402	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	253	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	402	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	96	LYS	N-CA-C	-5.19	96.99	111.00
1	B	455	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	170	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	GLN	Peptide
1	A	65	PHE	Peptide
1	A	98	GLY	Peptide
1	B	65	PHE	Peptide

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	3537	0	3463	33	0
1	B	3531	0	3460	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	0	3	0
All	All	7088	0	6923	68	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 5.

All (68) 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:96:LYS:O	1:A:99:GLU:HB3	1.38	1.20
1:B:96:LYS:O	1:B:99:GLU:HB3	1.48	1.12
1:B:460:GLN:O	1:B:461:PRO:CB	2.18	0.89
1:B:453[B]:ILE:HD13	1:B:453[B]:ILE:C	2.01	0.80
1:B:96:LYS:O	1:B:99:GLU:CB	2.28	0.79
1:A:326:GLU:O	1:A:327:LEU:C	2.32	0.68
1:A:230:LEU:HD21	1:B:215[B]:GLU:HB2	1.77	0.67
1:A:459:GLU:O	1:A:460:GLN:O	2.13	0.67
1:B:95:THR:HB	1:B:99:GLU:OE1	1.98	0.64
1:B:117:VAL:HG23	1:B:118:ILE:HG23	1.79	0.64
1:B:240:VAL:O	1:B:263:THR:HG23	1.99	0.62
1:A:459:GLU:C	1:A:460:GLN:O	2.29	0.61
1:A:240:VAL:O	1:A:263:THR:HG23	2.01	0.60
1:B:316:HIS:CE1	1:B:318:PRO:HG3	2.37	0.58
1:A:117:VAL:HG23	1:A:118:ILE:HG23	1.86	0.57
1:B:279:ASP:O	1:B:281:GLU:N	2.37	0.56
1:B:453[B]:ILE:C	1:B:453[B]:ILE:CD1	2.71	0.56
1:B:271:ASP:O	1:B:274:ILE:HG22	2.08	0.54
1:B:166:LEU:HD22	1:B:170:LEU:CD2	2.38	0.54
1:A:215:GLU:HB2	1:B:230:LEU:HD21	1.91	0.53
1:B:63:MET:HE3	1:B:65:PHE:HB2	1.92	0.52
1:A:166:LEU:HD22	1:A:170:LEU:CD2	2.39	0.52
1:A:137:LEU:HA	1:A:140:VAL:CG1	2.41	0.51
1:A:326:GLU:C	1:A:327:LEU:O	2.35	0.50
1:A:271:ASP:O	1:A:274:ILE:HG22	2.12	0.50
1:A:85:GLY:HA3	1:A:346:LEU:HD12	1.94	0.50
1:B:316:HIS:NE2	1:B:318:PRO:HG3	2.27	0.50
1:B:279:ASP:C	1:B:281:GLU:H	2.14	0.49
1:B:137:LEU:HA	1:B:140:VAL:CG1	2.42	0.49
1:A:183:HIS:CE1	1:A:239:HIS:CE1	3.00	0.49
1:A:227:LEU:HD22	1:B:189:VAL:HG11	1.95	0.49
1:A:316:HIS:CE1	1:A:318:PRO:HG3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:HG2	1:B:126:ILE:N	2.27	0.48
1:B:341:LEU:HA	3:B:602:HOH:O	2.14	0.48
1:B:455:ARG:HG2	1:B:455:ARG:HH11	1.80	0.47
1:A:230:LEU:HD21	1:B:215[A]:GLU:HB2	1.96	0.47
1:B:85:GLY:HA3	1:B:346:LEU:HD12	1.96	0.47
1:A:190:LEU:HD22	1:A:212:ARG:HA	1.97	0.47
1:B:190:LEU:HD22	1:B:212:ARG:HA	1.96	0.46
1:A:331:ASP:OD2	1:A:333:THR:OG1	2.19	0.46
1:A:63:MET:HE3	1:A:65:PHE:HB2	1.98	0.45
1:A:393:ILE:CG2	1:A:394:VAL:N	2.79	0.45
1:A:261:GLY:N	1:A:310:GLN:OE1	2.42	0.44
1:A:2:LYS:HG2	1:A:24:GLU:HG3	2.00	0.44
1:B:347:THR:HG21	1:B:402:ARG:HH22	1.83	0.44
1:A:239:HIS:CE1	1:A:289:PRO:HD3	2.52	0.44
1:A:125:MET:HG2	1:A:126:ILE:N	2.32	0.43
1:B:245:ALA:O	1:B:246:VAL:C	2.55	0.43
1:A:347:THR:HG21	1:A:402:ARG:HH22	1.83	0.43
1:A:189:VAL:HG11	1:B:227:LEU:HD22	2.00	0.42
1:B:386:ALA:HA	3:B:607:HOH:O	2.17	0.42
1:B:363:GLN:O	1:B:367:ILE:HB	2.18	0.42
1:A:439:ARG:O	1:A:440:ASP:C	2.58	0.42
1:A:279:ASP:C	1:A:281:GLU:H	2.22	0.42
1:A:455:ARG:HG2	1:A:455:ARG:HH11	1.85	0.41
1:B:238:VAL:HG23	1:B:239:HIS:CE1	2.54	0.41
1:A:215:GLU:OE2	1:A:215:GLU:HA	2.20	0.41
1:B:453[B]:ILE:HD13	1:B:453[B]:ILE:O	2.18	0.41
1:B:96:LYS:HE3	1:B:96:LYS:HA	2.00	0.41
1:B:148:SER:HA	1:B:179:LEU:O	2.20	0.41
1:B:455:ARG:HH11	1:B:455:ARG:CG	2.33	0.41
1:B:393:ILE:CG2	1:B:394:VAL:N	2.83	0.41
1:B:239:HIS:CE1	1:B:289:PRO:HD3	2.56	0.41
1:B:331:ASP:OD2	1:B:333:THR:OG1	2.26	0.40
1:B:387:VAL:HG23	3:B:607:HOH:O	2.21	0.40
1:B:141:ILE:HD12	1:B:176:LEU:HD13	2.02	0.40
1:A:37:VAL:O	1:A:38:ASN:C	2.58	0.40
1:A:167:PHE:O	1:A:171:VAL:HG13	2.20	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	458/460 (100%)	418 (91%)	35 (8%)	5 (1%)	14	41
1	B	454/460 (99%)	412 (91%)	38 (8%)	4 (1%)	17	46
All	All	912/920 (99%)	830 (91%)	73 (8%)	9 (1%)	15	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	440	ASP
1	B	239	HIS
1	B	340	PRO
1	A	340	PRO
1	B	440	ASP
1	A	278	PRO
1	A	460	GLN
1	B	278	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	370/374 (99%)	328 (89%)	42 (11%)	5	18
1	B	371/374 (99%)	328 (88%)	43 (12%)	5	17
All	All	741/748 (99%)	656 (88%)	85 (12%)	5	17

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	18	GLN
1	A	21	VAL
1	A	43	ILE
1	A	65	PHE
1	A	96	LYS
1	A	97	LYS
1	A	108	TRP
1	A	124	LEU
1	A	130	ASN
1	A	134	LEU
1	A	137	LEU
1	A	139	SER
1	A	140	VAL
1	A	166	LEU
1	A	170	LEU
1	A	179	LEU
1	A	194	THR
1	A	206	ILE
1	A	234	GLN
1	A	246	VAL
1	A	248	ARG
1	A	263	THR
1	A	268	LEU
1	A	272	VAL
1	A	295	TRP
1	A	300	LEU
1	A	310	GLN
1	A	331	ASP
1	A	346	LEU
1	A	347	THR
1	A	348	ILE
1	A	349	LEU
1	A	355	ARG
1	A	361	LEU
1	A	364	PHE
1	A	393	ILE
1	A	409	HIS
1	A	421	MET
1	A	439	ARG
1	A	453	ILE
1	A	455	ARG

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Mol	Chain	Res	Type
1	B	9	THR
1	B	18	GLN
1	B	21	VAL
1	B	43	ILE
1	B	65	PHE
1	B	69	VAL
1	B	96	LYS
1	B	97	LYS
1	B	124	LEU
1	B	130	ASN
1	B	134	LEU
1	B	137	LEU
1	B	139	SER
1	B	140	VAL
1	B	166	LEU
1	B	170	LEU
1	B	179	LEU
1	B	194	THR
1	B	206	ILE
1	B	234	GLN
1	B	246	VAL
1	B	248	ARG
1	B	263	THR
1	B	268	LEU
1	B	272	VAL
1	B	295	TRP
1	B	300	LEU
1	B	310	GLN
1	B	331	ASP
1	B	346	LEU
1	B	347	THR
1	B	348	ILE
1	B	349	LEU
1	B	355	ARG
1	B	361	LEU
1	B	393	ILE
1	B	409	HIS
1	B	421	MET
1	B	439	ARG
1	B	449	SER
1	B	453[A]	ILE
1	B	453[B]	ILE

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Mol	Chain	Res	Type
1	B	455	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	306	ASN
1	A	412	ASN
1	B	202	ASN
1	B	306	ASN

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 4 ligands modelled in this entry, 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 (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	460/460 (100%)	-0.43	3 (0%)	87	84	20, 43, 72, 130	0
1	B	456/460 (99%)	-0.41	5 (1%)	80	75	22, 44, 72, 100	0
All	All	916/920 (99%)	-0.42	8 (0%)	84	80	20, 44, 72, 130	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	GLY	3.6
1	A	67	GLY	3.5
1	B	132	GLN	2.9
1	A	99	GLU	2.2
1	A	399	HIS	2.2
1	B	199	ALA	2.1
1	B	198	LEU	2.1
1	B	407	GLU	2.1

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	MN	B	501	1/1	0.90	0.10	58,58,58,58	0
2	MN	A	501	1/1	0.98	0.09	62,62,62,62	0
2	MN	B	502	1/1	0.98	0.07	47,47,47,47	0
2	MN	A	502	1/1	0.99	0.06	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.