Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 02:07 pm BST

PDB ID	:	4YU6
Title	:	Crystal structure of Bacillus anthracis immune inhibitor A2 peptidase zymogen
Authors	:	Arolas, J.L.; Goulas, T.; Gomis-Ruth, F.X.
Deposited on	:	2015-03-18
Resolution	:	2.60 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:

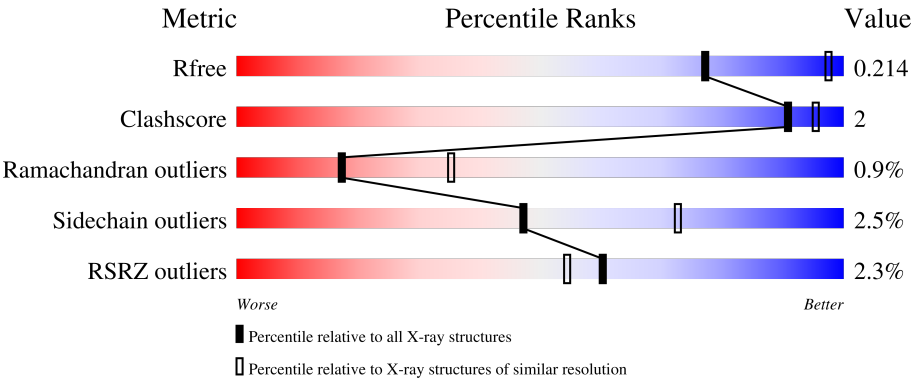
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	756	3% 92% 7%
1	B	756	2% 88% 6% 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11591 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 Immune inhibitor A, metalloprotease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	0	0	0
			5883	3705	998	1169	11			
1	B	708	Total	C	N	O	S	0	0	0
			5516	3476	933	1097	10			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	HIS	TYR	conflict	UNP D8H130
A	380	ALA	GLU	engineered mutation	UNP D8H130
A	630	LEU	VAL	conflict	UNP D8H130
A	746	ASN	LYS	conflict	UNP D8H130
A	776	LYS	ASN	conflict	UNP D8H130
A	901	HIS	-	expression tag	UNP D8H130
A	902	HIS	-	expression tag	UNP D8H130
A	903	HIS	-	expression tag	UNP D8H130
A	904	HIS	-	expression tag	UNP D8H130
A	905	HIS	-	expression tag	UNP D8H130
A	906	HIS	-	expression tag	UNP D8H130
B	275	HIS	TYR	conflict	UNP D8H130
B	380	ALA	GLU	engineered mutation	UNP D8H130
B	630	LEU	VAL	conflict	UNP D8H130
B	746	ASN	LYS	conflict	UNP D8H130
B	776	LYS	ASN	conflict	UNP D8H130
B	901	HIS	-	expression tag	UNP D8H130
B	902	HIS	-	expression tag	UNP D8H130
B	903	HIS	-	expression tag	UNP D8H130
B	904	HIS	-	expression tag	UNP D8H130
B	905	HIS	-	expression tag	UNP D8H130
B	906	HIS	-	expression tag	UNP D8H130

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

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

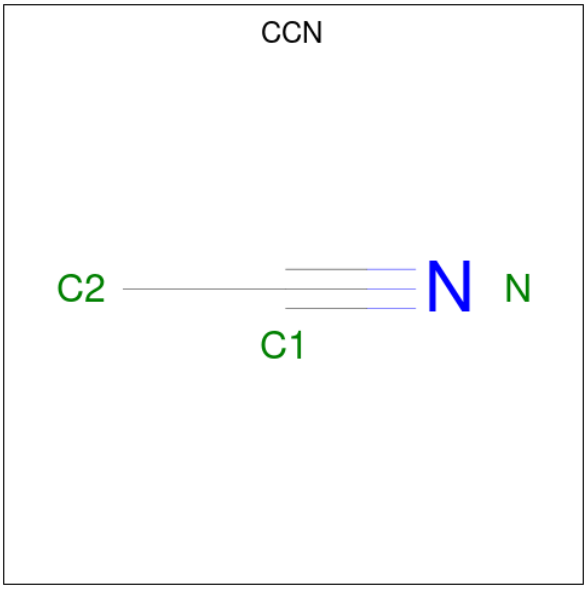
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Ca 5 5	0	0
3	B	4	Total Ca 4 4	0	0

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

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

- Molecule 5 is ACETONITRILE (three-letter code: CCN) (formula: C_2H_3N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 3 2 1	0	0
5	B	1	Total C N 3 2 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N 3 2 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0

- Molecule 7 is water.

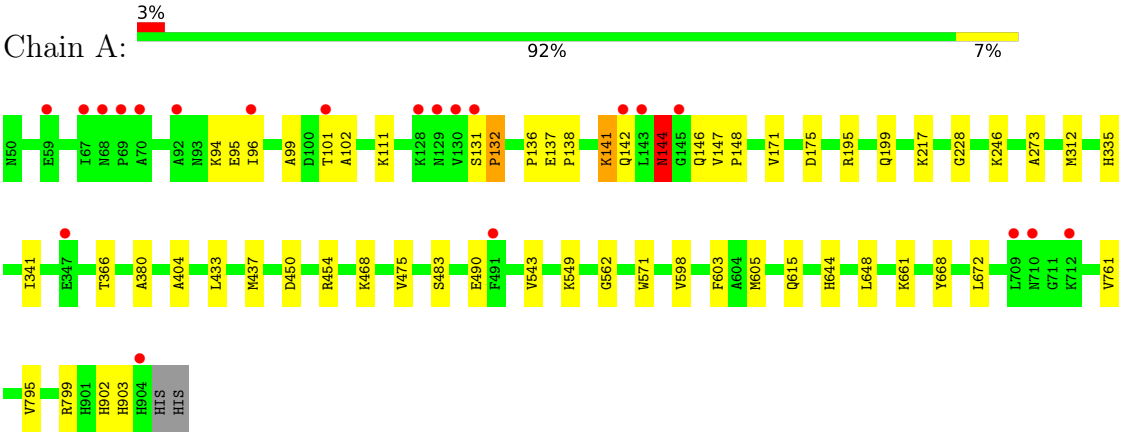
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	87	Total O 87 87	0	0
7	B	81	Total O 81 81	0	0

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.

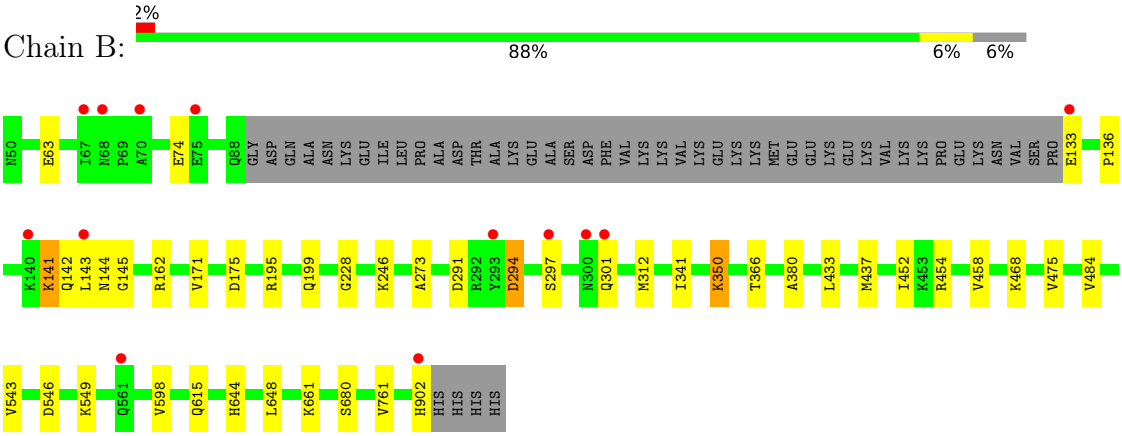
• Molecule 1: Immune inhibitor A, metalloprotease

Chain A:



• Molecule 1: Immune inhibitor A, metalloprotease

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	176.98Å 108.87Å 100.41Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	47.67 – 2.60 47.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.67-2.60) 99.7 (47.66-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.171 , 0.211 0.174 , 0.214	Depositor DCC
R_{free} test set	729 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.019 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11591	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, CCN, CA, NA

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	0.51	0/6022	0.71	1/8139 (0.0%)
1	B	0.50	0/5648	0.69	0/7640
All	All	0.50	0/11670	0.70	1/15779 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ALA	C-N-CA	5.24	134.79	121.70

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	5883	0	5647	20	0
1	B	5516	0	5265	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
4	A	2	0	0	0	0
5	A	3	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	6	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	87	0	0	0	0
7	B	81	0	0	0	0
All	All	11591	0	10921	38	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 (38) 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:162:ARG:NH1	1:B:297:SER:HA	1.86	0.90
1:B:162:ARG:HH12	1:B:297:SER:HA	1.52	0.73
1:B:291:ASP:HB3	1:B:294:ASP:O	1.97	0.63
1:A:131:SER:HB2	1:A:132:PRO:HA	1.81	0.61
1:B:341:ILE:HD12	1:B:341:ILE:H	1.68	0.59
1:B:171:VAL:HG11	1:B:273:ALA:HB2	1.85	0.57
1:A:171:VAL:HG11	1:A:273:ALA:HB2	1.85	0.56
1:B:543:VAL:HG22	1:B:549:LYS:HG2	1.88	0.56
1:B:195:ARG:O	1:B:199:GLN:HG3	2.06	0.55
1:A:141:LYS:HB3	1:A:146:GLN:O	2.07	0.55
1:B:475:VAL:HB	1:B:648:LEU:HB2	1.89	0.54
1:A:475:VAL:HB	1:A:648:LEU:HB2	1.89	0.54
1:A:195:ARG:O	1:A:199:GLN:HG3	2.07	0.53
1:A:543:VAL:HG22	1:A:549:LYS:HG2	1.89	0.52
1:A:603:PHE:HE2	1:A:605:MET:HE2	1.77	0.50
1:B:175:ASP:HB2	1:B:246:LYS:HA	1.95	0.49
1:B:433:LEU:HD22	1:B:437:MET:HE3	1.95	0.48
1:A:175:ASP:HB2	1:A:246:LYS:HA	1.95	0.48
1:A:228:GLY:HA3	1:A:468:LYS:HG3	1.95	0.47
1:B:350:LYS:O	1:B:350:LYS:HG2	2.13	0.47
1:B:228:GLY:HA3	1:B:468:LYS:HG3	1.96	0.46
1:A:433:LEU:HD22	1:A:437:MET:HE3	1.96	0.46
1:B:484:VAL:HG11	1:B:680:SER:HB2	1.97	0.46
1:A:141:LYS:HB2	1:A:148:PRO:HD3	1.98	0.46
1:A:136:PRO:HB3	1:A:147:VAL:HG11	1.98	0.45
1:B:452:ILE:HG23	1:B:458:VAL:HG23	1.98	0.45
1:B:454:ARG:HG2	1:B:902:HIS:CD2	2.51	0.45
1:A:144:ASN:C	1:A:146:GLN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:HG11	1:B:273:ALA:CB	2.47	0.44
1:A:490:GLU:HB2	1:A:571:TRP:CD1	2.55	0.42
1:B:366:THR:HG21	1:B:380:ALA:HB1	2.02	0.42
1:A:672:LEU:HD13	1:A:795:VAL:HG21	2.01	0.42
1:A:366:THR:HG21	1:A:380:ALA:HB1	2.02	0.41
1:A:454:ARG:HB3	1:A:902:HIS:ND1	2.35	0.41
1:A:171:VAL:HG11	1:A:273:ALA:CB	2.48	0.41
1:B:141:LYS:HG2	1:B:145:GLY:HA2	2.02	0.41
1:A:95:GLU:HG3	1:A:335:HIS:CD2	2.56	0.40
1:A:404:ALA:HB3	1:A:668:TYR:CZ	2.57	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	752/756 (100%)	711 (94%)	31 (4%)	10 (1%)	12	24
1	B	704/756 (93%)	676 (96%)	25 (4%)	3 (0%)	34	57
All	All	1456/1512 (96%)	1387 (95%)	56 (4%)	13 (1%)	17	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	A	132	PRO
1	A	562	GLY
1	B	141	LYS
1	A	96	ILE
1	A	141	LYS
1	A	903	HIS
1	B	142	GLN

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	144	ASN
1	A	598	VAL
1	B	598	VAL
1	A	138	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	625/627 (100%)	610 (98%)	15 (2%)	49	74
1	B	584/627 (93%)	569 (97%)	15 (3%)	46	72
All	All	1209/1254 (96%)	1179 (98%)	30 (2%)	47	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LYS
1	A	101	THR
1	A	111	LYS
1	A	137	GLU
1	A	144	ASN
1	A	217	LYS
1	A	312	MET
1	A	341	ILE
1	A	450	ASP
1	A	483	SER
1	A	615	GLN
1	A	644	HIS
1	A	661	LYS
1	A	761	VAL
1	A	799	ARG
1	B	63	GLU
1	B	74	GLU
1	B	133	GLU

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Mol	Chain	Res	Type
1	B	136	PRO
1	B	143	LEU
1	B	144	ASN
1	B	294	ASP
1	B	301	GLN
1	B	312	MET
1	B	350	LYS
1	B	546	ASP
1	B	615	GLN
1	B	644	HIS
1	B	661	LYS
1	B	761	VAL

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	301	GLN
1	A	363	HIS
1	B	199	GLN
1	B	301	GLN
1	B	902	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	CCN	A	1008	2	2,2,2	0.35	0	1,1,1	0.62	0
5	CCN	B	1008	-	2,2,2	0.34	0	1,1,1	0.59	0
5	CCN	B	1007	-	2,2,2	0.31	0	1,1,1	0.61	0

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

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	754/756 (99%)	0.02	21 (2%)	53	46	36, 56, 105, 134	0
1	B	708/756 (93%)	-0.16	13 (1%)	68	64	37, 56, 92, 137	0
All	All	1462/1512 (96%)	-0.07	34 (2%)	60	54	36, 56, 99, 137	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	VAL	6.4
1	B	297	SER	6.2
1	A	70	ALA	4.8
1	A	131	SER	4.8
1	A	142	GLN	4.2
1	A	67	ILE	3.7
1	B	301	GLN	3.6
1	B	561	GLN	3.3
1	A	712	LYS	3.2
1	A	709	LEU	3.2
1	A	129	ASN	3.1
1	B	300	ASN	2.9
1	A	143	LEU	2.8
1	B	293	TYR	2.8
1	B	75	GLU	2.7
1	A	710	ASN	2.7
1	A	347	GLU	2.6
1	A	491	PHE	2.6
1	A	69	PRO	2.6
1	A	145	GLY	2.6
1	B	902	HIS	2.5
1	A	59	GLU	2.5
1	B	133	GLU	2.5
1	B	143	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	140	LYS	2.4
1	A	68	ASN	2.3
1	A	92	ALA	2.2
1	A	128	LYS	2.2
1	B	68	ASN	2.2
1	A	904	HIS	2.2
1	B	70	ALA	2.2
1	A	101	THR	2.1
1	A	96	ILE	2.1
1	B	67	ILE	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, 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	B-factors(Å^2)	Q<0.9
4	NA	A	1010	1/1	0.84	0.32	64,64,64,64	0
5	CCN	B	1007	3/3	0.86	0.13	71,71,72,72	0
4	NA	A	1007	1/1	0.89	0.34	69,69,69,69	0
6	K	B	1006	1/1	0.90	0.11	80,80,80,80	0
6	K	A	1009	1/1	0.91	0.28	85,85,85,85	0
5	CCN	B	1008	3/3	0.95	0.21	56,56,57,58	0
3	CA	B	1005	1/1	0.95	0.05	70,70,70,70	0
3	CA	A	1004	1/1	0.95	0.09	64,64,64,64	0
3	CA	A	1005	1/1	0.96	0.15	54,54,54,54	0
3	CA	A	1006	1/1	0.97	0.07	78,78,78,78	0
2	ZN	A	1001	1/1	0.98	0.22	56,56,56,56	0
3	CA	B	1004	1/1	0.98	0.09	52,52,52,52	0
3	CA	A	1003	1/1	0.98	0.04	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CCN	A	1008	3/3	0.99	0.31	73,73,74,76	0
2	ZN	B	1001	1/1	0.99	0.16	54,54,54,54	0
3	CA	A	1002	1/1	0.99	0.13	50,50,50,50	0
3	CA	B	1002	1/1	0.99	0.17	50,50,50,50	0
3	CA	B	1003	1/1	0.99	0.05	66,66,66,66	0

6.5 Other polymers

There are no such residues in this entry.