



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 AM UTC

PDB ID : 4YU6 / pdb_00004yu6
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

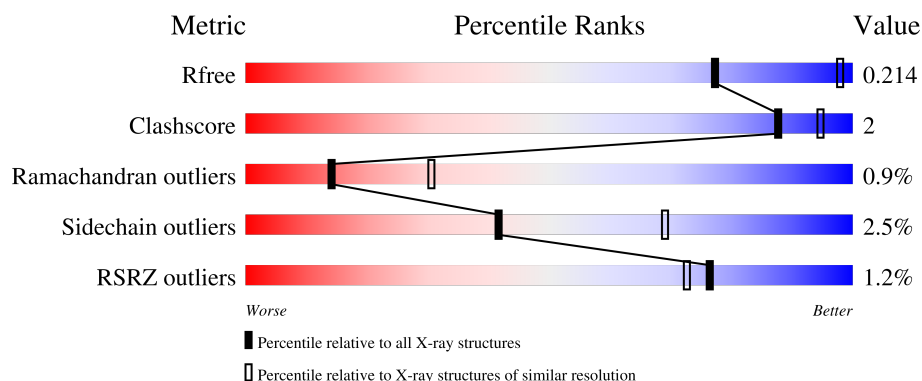
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

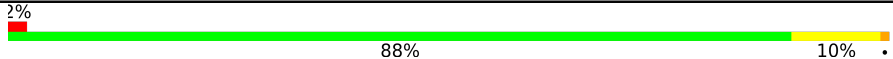
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	756	 2% 88% 10%
1	B	756	 1% 86% 7% 6%

2 Entry composition

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 (CCD ID: ZN) (formula: Zn).

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

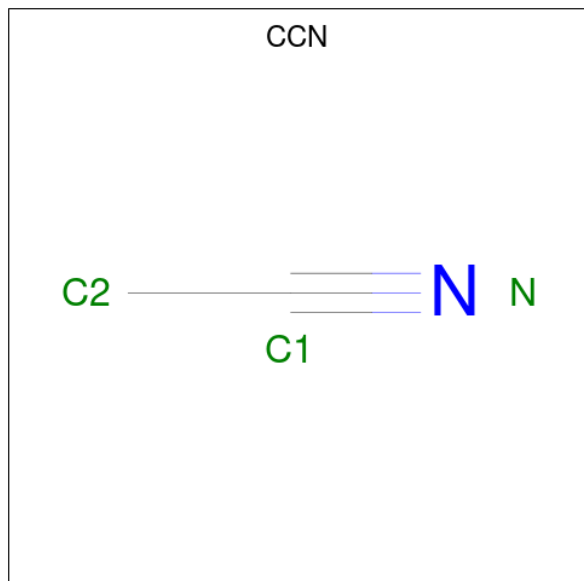
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is ACETONITRILE (CCD ID: CCN) (formula: C₂H₃N).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 7 is water.

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

4 Data and refinement statistics

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 47.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.67-2.60) 99.7 (47.67-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (1.42%)	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)	0.33 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.019 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	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.*

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

5.1 Standard geometry

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

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	0.85	1/6022 (0.0%)	1.30	36/8139 (0.4%)
1	B	0.84	0/5648	1.25	20/7640 (0.3%)
All	All	0.85	1/11670 (0.0%)	1.27	56/15779 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	605	MET	SD-CE	-6.01	1.64	1.79

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	ASN	CA-C-N	7.04	130.87	120.87
1	B	50	ASN	C-N-CA	7.04	130.87	120.87
1	A	291	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	99	ALA	CA-C-N	6.94	134.79	121.54
1	A	99	ALA	C-N-CA	6.94	134.79	121.54
1	A	50	ASN	CA-C-N	6.83	130.58	120.87
1	A	50	ASN	C-N-CA	6.83	130.58	120.87
1	B	699	ASP	CA-CB-CG	6.67	119.28	112.60
1	A	144	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	85	GLU	CB-CG-CD	6.30	123.31	112.60
1	A	145	GLY	CA-C-N	6.14	129.56	120.90
1	A	145	GLY	C-N-CA	6.14	129.56	120.90
1	A	699	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	678	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	678	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	305	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	595	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	450	ASP	CA-CB-CG	5.86	118.46	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	606	ASP	CA-CB-CG	5.86	118.45	112.60
1	A	595	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	758	ASP	CA-CB-CG	5.75	118.34	112.60
1	B	627	LYS	N-CA-C	-5.71	105.98	113.17
1	A	606	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	287	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	429	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	294	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	384	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	175	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	195	ARG	CA-C-N	5.35	127.71	120.38
1	A	195	ARG	C-N-CA	5.35	127.71	120.38
1	B	384	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	347	GLU	N-CA-C	5.34	117.52	111.11
1	A	175	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	339	LEU	CA-C-N	5.29	130.88	122.10
1	A	339	LEU	C-N-CA	5.29	130.88	122.10
1	A	101	THR	CA-C-N	5.25	131.57	121.54
1	A	101	THR	C-N-CA	5.25	131.57	121.54
1	A	761	VAL	N-CA-CB	5.23	116.42	110.72
1	B	758	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	564	LYS	N-CA-C	5.17	118.03	109.85
1	A	473	GLY	CA-C-N	5.16	130.11	122.94
1	A	473	GLY	C-N-CA	5.16	130.11	122.94
1	B	768	ALA	CA-C-N	5.15	127.70	120.28
1	B	768	ALA	C-N-CA	5.15	127.70	120.28
1	B	473	GLY	CA-C-N	5.14	130.13	122.99
1	B	473	GLY	C-N-CA	5.14	130.13	122.99
1	B	392	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	429	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	757	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	392	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	210	LEU	CA-C-N	5.01	127.50	120.28
1	B	210	LEU	C-N-CA	5.01	127.50	120.28
1	A	369	PRO	CA-C-N	5.01	127.00	120.28
1	A	369	PRO	C-N-CA	5.01	127.00	120.28
1	B	59	GLU	CB-CG-CD	5.01	121.12	112.60
1	A	298	ASP	CA-CB-CG	5.00	117.60	112.60

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	25	0
1	B	5516	0	5265	19	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
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	44	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 (44) 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:A:603:PHE:HE2	1:A:605:MET:HE2	1.59	0.67
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:VAL:HG22	1:A:549:LYS:HG2	1.89	0.52
1:A:144:ASN:C	1:A:146:GLN:H	2.20	0.50
1:A:117:MET:HE3	1:A:504:MET:HG3	1.92	0.50
1:A:433:LEU:HD22	1:A:437:MET:HE3	1.94	0.49
1:B:175:ASP:HB2	1:B:246:LYS:HA	1.95	0.49
1:A:590:PHE:CG	1:A:605:MET:HE1	2.47	0.48
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: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:B:171:VAL:HG11	1:B:273:ALA:CB	2.47	0.44
1:A:143:LEU:C	1:A:145:GLY:H	2.26	0.43
1:A:508:LEU:HD13	1:A:605:MET:HE3	2.01	0.43
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:703:GLU:H	1:A:703:GLU:CD	2.28	0.41
1:A:366:THR:HG21	1:A:380:ALA:HB1	2.02	0.41
1:B:703:GLU:H	1:B:703:GLU:CD	2.27	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

5.3.1 Protein backbone

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%)	9	21
1	B	704/756 (93%)	676 (96%)	25 (4%)	3 (0%)	30	51
All	All	1456/1512 (96%)	1387 (95%)	56 (4%)	13 (1%)	14	30

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
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 ⓘ

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%)	608 (97%)	17 (3%)	39	67
1	B	584/627 (93%)	571 (98%)	13 (2%)	45	72
All	All	1209/1254 (96%)	1179 (98%)	30 (2%)	42	69

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

Mol	Chain	Res	Type
1	A	88	GLN
1	A	94	LYS
1	A	96	ILE
1	A	101	THR
1	A	111	LYS
1	A	137	GLU
1	A	140	LYS
1	A	144	ASN
1	A	153	LYS
1	A	312	MET
1	A	341	ILE
1	A	450	ASP
1	A	482	LYS
1	A	483	SER
1	A	615	GLN
1	A	706	VAL
1	A	761	VAL
1	B	63	GLU
1	B	74	GLU
1	B	133	GLU
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	609	ASN
1	B	615	GLN
1	B	706	VAL
1	B	761	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	68	ASN
1	A	88	GLN
1	A	129	ASN
1	A	301	GLN
1	A	363	HIS
1	A	541	HIS
1	A	766	GLN
1	A	901	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	903	HIS
1	B	68	ASN
1	B	88	GLN
1	B	144	ASN
1	B	199	GLN
1	B	301	GLN
1	B	428	GLN
1	B	766	GLN
1	B	782	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 oligosaccharides 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	B	1007	-	2,2,2	0.32	0	1,1,1	0.61	0
5	CCN	B	1008	-	2,2,2	0.35	0	1,1,1	0.59	0
5	CCN	A	1008	2	2,2,2	0.37	0	1,1,1	0.62	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 [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	754/756 (99%)	-0.22	14 (1%) 66 61	36, 56, 105, 134	0
1	B	708/756 (93%)	-0.29	4 (0%) 85 83	37, 56, 92, 137	0
All	All	1462/1512 (96%)	-0.25	18 (1%) 76 73	36, 56, 99, 137	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ILE	4.3
1	A	102	ALA	3.2
1	A	143	LEU	3.1
1	A	132	PRO	3.0
1	A	94	LYS	2.9
1	A	97	LEU	2.8
1	B	143	LEU	2.8
1	A	103	LYS	2.7
1	B	297	SER	2.5
1	A	93	ASN	2.4
1	A	130	VAL	2.3
1	A	664	LYS	2.2
1	A	101	THR	2.2
1	B	312	MET	2.2
1	A	128	LYS	2.2
1	A	92	ALA	2.1
1	A	99	ALA	2.0
1	B	141	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	CCN	B	1007	3/3	0.65	0.24	71,71,72,72	0
5	CCN	B	1008	3/3	0.83	0.23	56,56,57,58	0
5	CCN	A	1008	3/3	0.91	0.17	73,73,74,76	0
4	NA	A	1010	1/1	0.92	0.08	64,64,64,64	0
4	NA	A	1007	1/1	0.92	0.10	69,69,69,69	0
6	K	B	1006	1/1	0.92	0.09	80,80,80,80	0
6	K	A	1009	1/1	0.94	0.13	85,85,85,85	0
3	CA	A	1005	1/1	0.98	0.05	54,54,54,54	0
3	CA	A	1006	1/1	0.98	0.07	78,78,78,78	0
3	CA	A	1004	1/1	0.98	0.05	64,64,64,64	0
3	CA	A	1003	1/1	0.99	0.07	63,63,63,63	0
2	ZN	A	1001	1/1	0.99	0.06	56,56,56,56	0
2	ZN	B	1001	1/1	0.99	0.03	54,54,54,54	0
3	CA	A	1002	1/1	0.99	0.02	50,50,50,50	0
3	CA	B	1002	1/1	0.99	0.04	50,50,50,50	0
3	CA	B	1004	1/1	0.99	0.03	52,52,52,52	0
3	CA	B	1005	1/1	0.99	0.02	70,70,70,70	0
3	CA	B	1003	1/1	1.00	0.02	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.