Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 12:02 pm BST

PDB ID	:	8CR7
Title	:	Crystal structure of recombinant LasB from Pseudomonas aeruginosa PA7
Authors	:	Kolling, D.; Koehnke, J.
Deposited on	:	2023-03-07
Resolution	:	1.50 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:

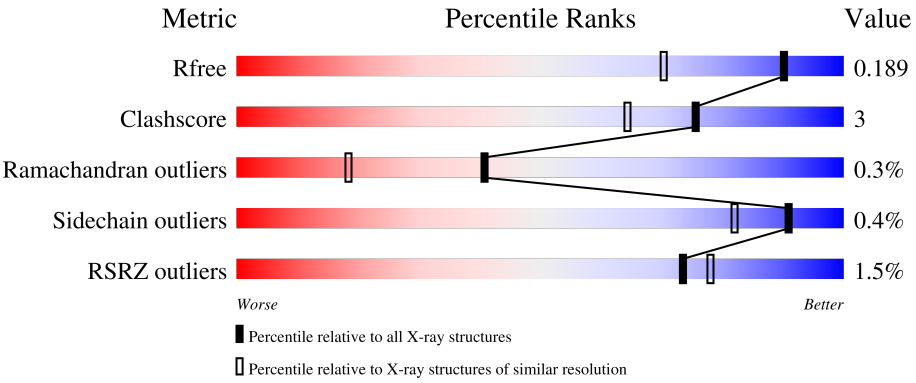
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	514	55% . 42%
1	B	514	% 53% 5% 42%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9556 atoms, of which 4284 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 Pro-elastase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	H	N	O	S	0	0	0
			4453	1454	2142	398	446	13			
1	B	298	Total	C	H	N	O	S	0	0	0
			4453	1454	2142	398	446	13			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-197	MET	-	initiating methionine	UNP P14756
A	-196	LYS	-	expression tag	UNP P14756
A	-195	TYR	-	expression tag	UNP P14756
A	-194	LEU	-	expression tag	UNP P14756
A	-193	LEU	-	expression tag	UNP P14756
A	-192	PRO	-	expression tag	UNP P14756
A	-191	THR	-	expression tag	UNP P14756
A	-190	ALA	-	expression tag	UNP P14756
A	-189	ALA	-	expression tag	UNP P14756
A	-188	ALA	-	expression tag	UNP P14756
A	-187	GLY	-	expression tag	UNP P14756
A	-186	LEU	-	expression tag	UNP P14756
A	-185	LEU	-	expression tag	UNP P14756
A	-184	LEU	-	expression tag	UNP P14756
A	-183	LEU	-	expression tag	UNP P14756
A	-182	ALA	-	expression tag	UNP P14756
A	-181	ALA	-	expression tag	UNP P14756
A	-180	GLN	-	expression tag	UNP P14756
A	-179	PRO	-	expression tag	UNP P14756
A	-178	ALA	-	expression tag	UNP P14756
A	-177	MET	-	expression tag	UNP P14756
A	-176	ALA	-	expression tag	UNP P14756
A	-175	MET	-	expression tag	UNP P14756
A	-174	GLY	-	expression tag	UNP P14756
A	2	GLN	GLU	conflict	UNP P14756

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASN	THR	conflict	UNP P14756
A	19	THR	SER	conflict	UNP P14756
A	51	SER	THR	conflict	UNP P14756
A	66	ILE	VAL	conflict	UNP P14756
A	88	LYS	ARG	conflict	UNP P14756
A	93	ALA	THR	conflict	UNP P14756
A	154	VAL	ILE	conflict	UNP P14756
A	214	GLY	SER	conflict	UNP P14756
A	264	THR	ASN	conflict	UNP P14756
A	265	PHE	TYR	conflict	UNP P14756
A	282	PRO	SER	conflict	UNP P14756
A	302	GLU	-	expression tag	UNP P14756
A	303	ASN	-	expression tag	UNP P14756
A	304	LEU	-	expression tag	UNP P14756
A	305	TYR	-	expression tag	UNP P14756
A	306	PHE	-	expression tag	UNP P14756
A	307	GLN	-	expression tag	UNP P14756
A	308	GLY	-	expression tag	UNP P14756
A	309	LEU	-	expression tag	UNP P14756
A	310	GLU	-	expression tag	UNP P14756
A	311	HIS	-	expression tag	UNP P14756
A	312	HIS	-	expression tag	UNP P14756
A	313	HIS	-	expression tag	UNP P14756
A	314	HIS	-	expression tag	UNP P14756
A	315	HIS	-	expression tag	UNP P14756
A	316	HIS	-	expression tag	UNP P14756
B	-197	MET	-	initiating methionine	UNP P14756
B	-196	LYS	-	expression tag	UNP P14756
B	-195	TYR	-	expression tag	UNP P14756
B	-194	LEU	-	expression tag	UNP P14756
B	-193	LEU	-	expression tag	UNP P14756
B	-192	PRO	-	expression tag	UNP P14756
B	-191	THR	-	expression tag	UNP P14756
B	-190	ALA	-	expression tag	UNP P14756
B	-189	ALA	-	expression tag	UNP P14756
B	-188	ALA	-	expression tag	UNP P14756
B	-187	GLY	-	expression tag	UNP P14756
B	-186	LEU	-	expression tag	UNP P14756
B	-185	LEU	-	expression tag	UNP P14756
B	-184	LEU	-	expression tag	UNP P14756
B	-183	LEU	-	expression tag	UNP P14756
B	-182	ALA	-	expression tag	UNP P14756

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-181	ALA	-	expression tag	UNP P14756
B	-180	GLN	-	expression tag	UNP P14756
B	-179	PRO	-	expression tag	UNP P14756
B	-178	ALA	-	expression tag	UNP P14756
B	-177	MET	-	expression tag	UNP P14756
B	-176	ALA	-	expression tag	UNP P14756
B	-175	MET	-	expression tag	UNP P14756
B	-174	GLY	-	expression tag	UNP P14756
B	2	GLN	GLU	conflict	UNP P14756
B	16	ASN	THR	conflict	UNP P14756
B	19	THR	SER	conflict	UNP P14756
B	51	SER	THR	conflict	UNP P14756
B	66	ILE	VAL	conflict	UNP P14756
B	88	LYS	ARG	conflict	UNP P14756
B	93	ALA	THR	conflict	UNP P14756
B	154	VAL	ILE	conflict	UNP P14756
B	214	GLY	SER	conflict	UNP P14756
B	264	THR	ASN	conflict	UNP P14756
B	265	PHE	TYR	conflict	UNP P14756
B	282	PRO	SER	conflict	UNP P14756
B	302	GLU	-	expression tag	UNP P14756
B	303	ASN	-	expression tag	UNP P14756
B	304	LEU	-	expression tag	UNP P14756
B	305	TYR	-	expression tag	UNP P14756
B	306	PHE	-	expression tag	UNP P14756
B	307	GLN	-	expression tag	UNP P14756
B	308	GLY	-	expression tag	UNP P14756
B	309	LEU	-	expression tag	UNP P14756
B	310	GLU	-	expression tag	UNP P14756
B	311	HIS	-	expression tag	UNP P14756
B	312	HIS	-	expression tag	UNP P14756
B	313	HIS	-	expression tag	UNP P14756
B	314	HIS	-	expression tag	UNP P14756
B	315	HIS	-	expression tag	UNP P14756
B	316	HIS	-	expression tag	UNP P14756

- 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	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is water.

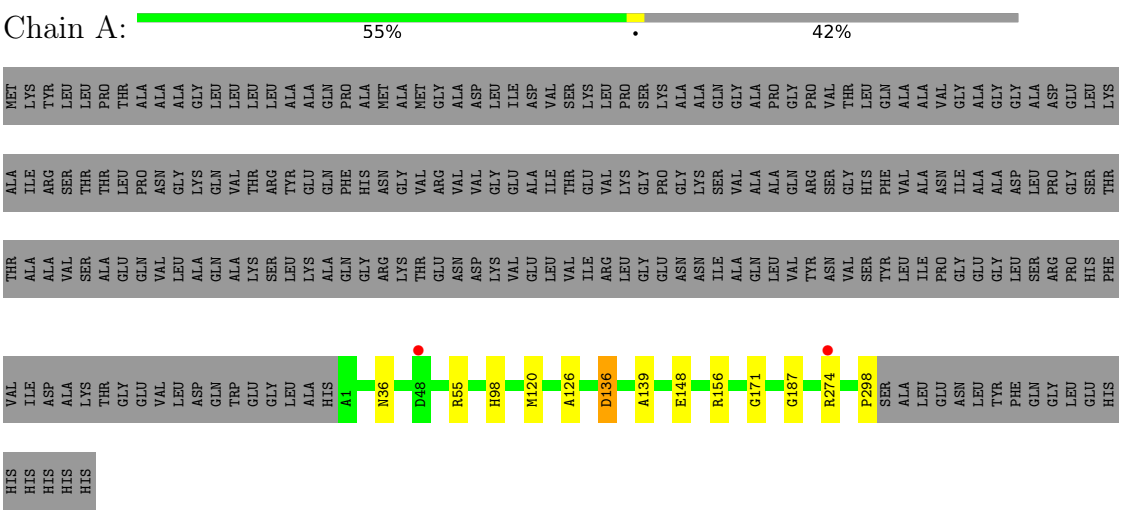
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	360	Total O 360 360	0	0
4	B	286	Total O 286 286	0	0

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.

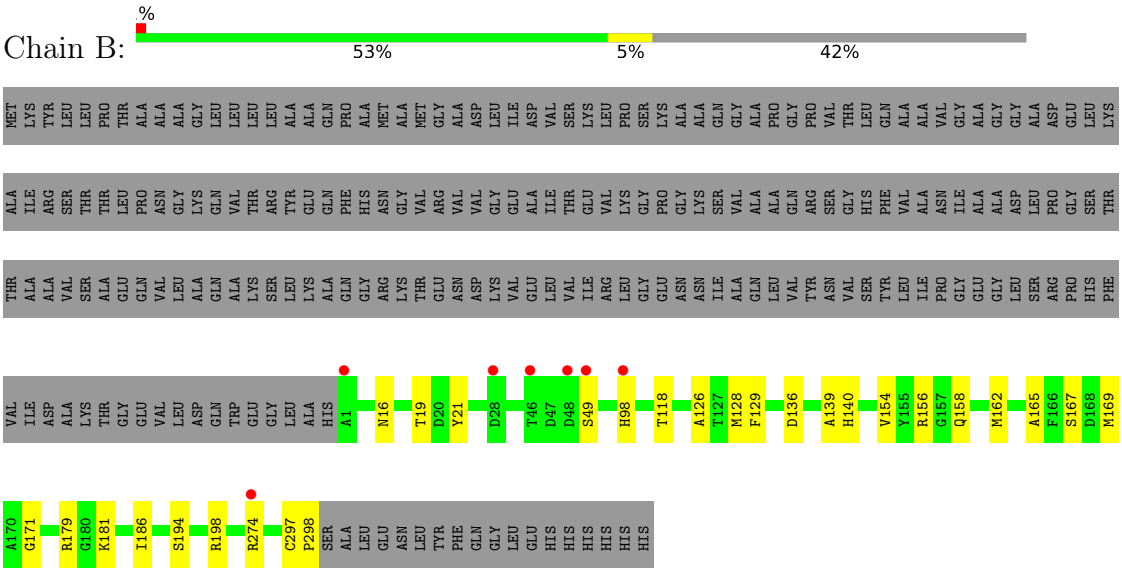
• Molecule 1: Pro-elastase

Chain A:



• Molecule 1: Pro-elastase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.16Å 64.27Å 73.40Å 90.00° 108.09° 90.00°	Depositor
Resolution (Å)	43.11 – 1.50 43.11 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.11-1.50) 99.3 (43.11-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.164 , 0.189 0.163 , 0.189	Depositor DCC
R_{free} test set	4270 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 52.2	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	0.97	EDS
Total number of atoms	9556	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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, CA

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	0.71	2/2374 (0.1%)	0.85	4/3217 (0.1%)
1	B	0.63	1/2374 (0.0%)	0.77	3/3217 (0.1%)
All	All	0.67	3/4748 (0.1%)	0.81	7/6434 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	ARG	CZ-NH2	12.82	1.49	1.33
1	A	274	ARG	CZ-NH1	7.16	1.42	1.33
1	B	181	LYS	CE-NZ	-5.38	1.35	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	B	274	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	136	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	B	274	ARG	CA-CB-CG	6.24	127.13	113.40
1	A	136	ASP	CB-CG-OD1	6.23	123.90	118.30
1	B	136	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	274	ARG	CD-NE-CZ	5.54	131.35	123.60

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	2311	2142	2144	11	0
1	B	2311	2142	2144	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	360	0	0	10	3
4	B	286	0	0	6	5
All	All	5272	4284	4288	28	5

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 3.

All (28) 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:179:ARG:HD2	4:B:713:HOH:O	1.45	1.12
1:B:179:ARG:NE	4:B:502:HOH:O	2.01	0.89
1:B:21:TYR:OH	4:B:501:HOH:O	2.00	0.80
1:A:298:PRO:O	4:A:502:HOH:O	2.09	0.71
1:A:187:GLY:HA2	4:A:503:HOH:O	1.92	0.68
1:B:16:ASN:HB2	1:B:19:THR:CG2	2.26	0.66
1:A:156:ARG:HD2	4:A:677:HOH:O	1.98	0.64
1:A:136:ASP:OD1	4:A:503:HOH:O	2.16	0.62
1:B:154:VAL:HG12	1:B:156:ARG:HG2	1.86	0.57
1:B:194:SER:O	4:B:503:HOH:O	2.17	0.56
1:A:148:GLU:OE2	4:A:504:HOH:O	2.17	0.56
1:B:179:ARG:CD	4:B:502:HOH:O	2.47	0.56
1:B:179:ARG:HD3	4:B:502:HOH:O	2.08	0.54
1:B:16:ASN:HB2	1:B:19:THR:HG23	1.91	0.52
1:A:36:ASN:OD1	4:A:505:HOH:O	2.19	0.52
1:B:165:ALA:O	1:B:169:MET:HG3	2.10	0.51
1:A:156:ARG:NE	4:A:501:HOH:O	2.01	0.51
1:B:98:HIS:HE1	1:B:118:THR:O	1.98	0.46
1:B:158:GLN:O	1:B:162:MET:HG3	2.16	0.46
1:B:186:ILE:HB	1:B:198:ARG:HB2	1.99	0.45
1:B:128:MET:HG2	1:B:129:PHE:CE2	2.53	0.44
1:A:98:HIS:HE1	4:A:536:HOH:O	2.00	0.44
1:B:139:ALA:HB3	1:B:171:GLY:HA2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:NH2	4:A:507:HOH:O	2.28	0.42
1:A:139:ALA:HB3	1:A:171:GLY:HA2	2.02	0.42
1:B:297:CYS:HA	1:B:298:PRO:HD3	1.88	0.42
1:B:140:HIS:CG	1:B:167:SER:HB3	2.55	0.41
1:A:98:HIS:CE1	4:A:536:HOH:O	2.71	0.41

All (5) 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)
4:A:533:HOH:O	4:B:660:HOH:O[1_454]	1.94	0.26
4:A:838:HOH:O	4:B:684:HOH:O[2_546]	1.96	0.24
4:A:652:HOH:O	4:B:741:HOH:O[2_656]	2.04	0.16
4:B:519:HOH:O	4:B:612:HOH:O[2_546]	2.09	0.11
4:B:774:HOH:O	4:B:782:HOH:O[2_546]	2.17	0.03

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	296/514 (58%)	287 (97%)	8 (3%)	1 (0%)	41 18
1	B	296/514 (58%)	285 (96%)	10 (3%)	1 (0%)	41 18
All	All	592/1028 (58%)	572 (97%)	18 (3%)	2 (0%)	41 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	ALA
1	A	126	ALA

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	237/400 (59%)	236 (100%)	1 (0%)	91 82
1	B	237/400 (59%)	236 (100%)	1 (0%)	91 82
All	All	474/800 (59%)	472 (100%)	2 (0%)	91 82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	MET
1	B	49	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	B	98	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

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

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	298/514 (57%)	-0.37	2 (0%)	87	90	12, 17, 27, 41	0
1	B	298/514 (57%)	-0.15	7 (2%)	60	65	13, 22, 37, 51	0
All	All	596/1028 (57%)	-0.26	9 (1%)	73	78	12, 19, 34, 51	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	HIS	4.3
1	B	49	SER	3.8
1	B	274	ARG	3.6
1	B	48	ASP	3.4
1	A	48	ASP	2.6
1	B	28	ASP	2.4
1	B	1	ALA	2.4
1	A	274	ARG	2.1
1	B	46	THR	2.1

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 monosaccharides 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. 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
2	ZN	B	401	1/1	0.99	0.04	16,16,16,16	0
2	ZN	A	401	1/1	1.00	0.08	15,15,15,15	0
3	CA	A	402	1/1	1.00	0.07	17,17,17,17	0
3	CA	B	402	1/1	1.00	0.04	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.