



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 10:02 PM GMT

PDB ID : 3SPU
Title : apo NDM-1 Crystal Structure
Authors : Strynadka, N.C.J.; King, D.T.
Deposited on : 2011-07-03
Resolution : 2.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

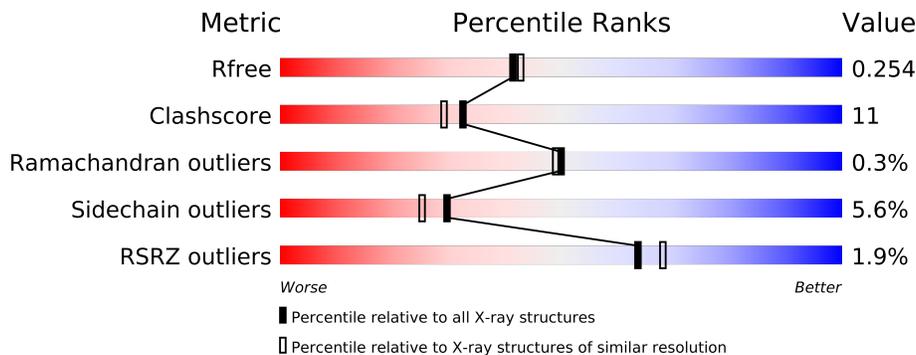
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	
1	B	265	
1	C	265	
1	D	265	
1	E	265	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9130 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Beta-lactamase NDM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	Total 1728	C 1089	N 307	O 324	S 8	0	4	0
1	B	238	Total 1769	C 1110	N 314	O 336	S 9	0	0	0
1	C	232	Total 1728	C 1089	N 307	O 324	S 8	0	4	0
1	D	231	Total 1721	C 1084	N 306	O 323	S 8	0	3	0
1	E	227	Total 1686	C 1061	N 298	O 319	S 8	0	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LYS	-	EXPRESSION TAG	UNP C7C422
A	272	LEU	-	EXPRESSION TAG	UNP C7C422
A	273	VAL	-	EXPRESSION TAG	UNP C7C422
A	274	PRO	-	EXPRESSION TAG	UNP C7C422
A	275	ARG	-	EXPRESSION TAG	UNP C7C422
A	276	GLY	-	EXPRESSION TAG	UNP C7C422
A	277	SER	-	EXPRESSION TAG	UNP C7C422
A	278	ALA	-	EXPRESSION TAG	UNP C7C422
A	279	ALA	-	EXPRESSION TAG	UNP C7C422
A	280	ALA	-	EXPRESSION TAG	UNP C7C422
A	281	ALA	-	EXPRESSION TAG	UNP C7C422
A	282	LEU	-	EXPRESSION TAG	UNP C7C422
A	283	GLU	-	EXPRESSION TAG	UNP C7C422
A	284	HIS	-	EXPRESSION TAG	UNP C7C422
A	285	HIS	-	EXPRESSION TAG	UNP C7C422
A	286	HIS	-	EXPRESSION TAG	UNP C7C422
A	287	HIS	-	EXPRESSION TAG	UNP C7C422
A	288	HIS	-	EXPRESSION TAG	UNP C7C422
A	289	HIS	-	EXPRESSION TAG	UNP C7C422

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Chain	Residue	Modelled	Actual	Comment	Reference
A	290	HIS	-	EXPRESSION TAG	UNP C7C422
A	291	HIS	-	EXPRESSION TAG	UNP C7C422
B	271	LYS	-	EXPRESSION TAG	UNP C7C422
B	272	LEU	-	EXPRESSION TAG	UNP C7C422
B	273	VAL	-	EXPRESSION TAG	UNP C7C422
B	274	PRO	-	EXPRESSION TAG	UNP C7C422
B	275	ARG	-	EXPRESSION TAG	UNP C7C422
B	276	GLY	-	EXPRESSION TAG	UNP C7C422
B	277	SER	-	EXPRESSION TAG	UNP C7C422
B	278	ALA	-	EXPRESSION TAG	UNP C7C422
B	279	ALA	-	EXPRESSION TAG	UNP C7C422
B	280	ALA	-	EXPRESSION TAG	UNP C7C422
B	281	ALA	-	EXPRESSION TAG	UNP C7C422
B	282	LEU	-	EXPRESSION TAG	UNP C7C422
B	283	GLU	-	EXPRESSION TAG	UNP C7C422
B	284	HIS	-	EXPRESSION TAG	UNP C7C422
B	285	HIS	-	EXPRESSION TAG	UNP C7C422
B	286	HIS	-	EXPRESSION TAG	UNP C7C422
B	287	HIS	-	EXPRESSION TAG	UNP C7C422
B	288	HIS	-	EXPRESSION TAG	UNP C7C422
B	289	HIS	-	EXPRESSION TAG	UNP C7C422
B	290	HIS	-	EXPRESSION TAG	UNP C7C422
B	291	HIS	-	EXPRESSION TAG	UNP C7C422
C	271	LYS	-	EXPRESSION TAG	UNP C7C422
C	272	LEU	-	EXPRESSION TAG	UNP C7C422
C	273	VAL	-	EXPRESSION TAG	UNP C7C422
C	274	PRO	-	EXPRESSION TAG	UNP C7C422
C	275	ARG	-	EXPRESSION TAG	UNP C7C422
C	276	GLY	-	EXPRESSION TAG	UNP C7C422
C	277	SER	-	EXPRESSION TAG	UNP C7C422
C	278	ALA	-	EXPRESSION TAG	UNP C7C422
C	279	ALA	-	EXPRESSION TAG	UNP C7C422
C	280	ALA	-	EXPRESSION TAG	UNP C7C422
C	281	ALA	-	EXPRESSION TAG	UNP C7C422
C	282	LEU	-	EXPRESSION TAG	UNP C7C422
C	283	GLU	-	EXPRESSION TAG	UNP C7C422
C	284	HIS	-	EXPRESSION TAG	UNP C7C422
C	285	HIS	-	EXPRESSION TAG	UNP C7C422
C	286	HIS	-	EXPRESSION TAG	UNP C7C422
C	287	HIS	-	EXPRESSION TAG	UNP C7C422
C	288	HIS	-	EXPRESSION TAG	UNP C7C422
C	289	HIS	-	EXPRESSION TAG	UNP C7C422

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Chain	Residue	Modelled	Actual	Comment	Reference
C	290	HIS	-	EXPRESSION TAG	UNP C7C422
C	291	HIS	-	EXPRESSION TAG	UNP C7C422
D	271	LYS	-	EXPRESSION TAG	UNP C7C422
D	272	LEU	-	EXPRESSION TAG	UNP C7C422
D	273	VAL	-	EXPRESSION TAG	UNP C7C422
D	274	PRO	-	EXPRESSION TAG	UNP C7C422
D	275	ARG	-	EXPRESSION TAG	UNP C7C422
D	276	GLY	-	EXPRESSION TAG	UNP C7C422
D	277	SER	-	EXPRESSION TAG	UNP C7C422
D	278	ALA	-	EXPRESSION TAG	UNP C7C422
D	279	ALA	-	EXPRESSION TAG	UNP C7C422
D	280	ALA	-	EXPRESSION TAG	UNP C7C422
D	281	ALA	-	EXPRESSION TAG	UNP C7C422
D	282	LEU	-	EXPRESSION TAG	UNP C7C422
D	283	GLU	-	EXPRESSION TAG	UNP C7C422
D	284	HIS	-	EXPRESSION TAG	UNP C7C422
D	285	HIS	-	EXPRESSION TAG	UNP C7C422
D	286	HIS	-	EXPRESSION TAG	UNP C7C422
D	287	HIS	-	EXPRESSION TAG	UNP C7C422
D	288	HIS	-	EXPRESSION TAG	UNP C7C422
D	289	HIS	-	EXPRESSION TAG	UNP C7C422
D	290	HIS	-	EXPRESSION TAG	UNP C7C422
D	291	HIS	-	EXPRESSION TAG	UNP C7C422
E	271	LYS	-	EXPRESSION TAG	UNP C7C422
E	272	LEU	-	EXPRESSION TAG	UNP C7C422
E	273	VAL	-	EXPRESSION TAG	UNP C7C422
E	274	PRO	-	EXPRESSION TAG	UNP C7C422
E	275	ARG	-	EXPRESSION TAG	UNP C7C422
E	276	GLY	-	EXPRESSION TAG	UNP C7C422
E	277	SER	-	EXPRESSION TAG	UNP C7C422
E	278	ALA	-	EXPRESSION TAG	UNP C7C422
E	279	ALA	-	EXPRESSION TAG	UNP C7C422
E	280	ALA	-	EXPRESSION TAG	UNP C7C422
E	281	ALA	-	EXPRESSION TAG	UNP C7C422
E	282	LEU	-	EXPRESSION TAG	UNP C7C422
E	283	GLU	-	EXPRESSION TAG	UNP C7C422
E	284	HIS	-	EXPRESSION TAG	UNP C7C422
E	285	HIS	-	EXPRESSION TAG	UNP C7C422
E	286	HIS	-	EXPRESSION TAG	UNP C7C422
E	287	HIS	-	EXPRESSION TAG	UNP C7C422
E	288	HIS	-	EXPRESSION TAG	UNP C7C422
E	289	HIS	-	EXPRESSION TAG	UNP C7C422

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Chain	Residue	Modelled	Actual	Comment	Reference
E	290	HIS	-	EXPRESSION TAG	UNP C7C422
E	291	HIS	-	EXPRESSION TAG	UNP C7C422

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

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

- Molecule 3 is water.

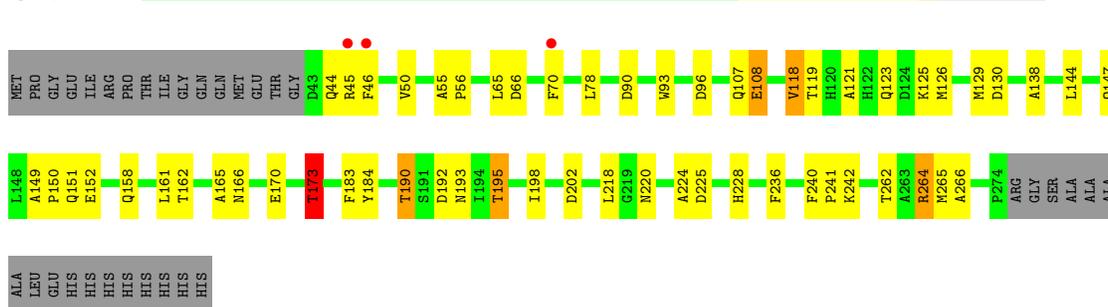
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	W	488	Total 488	O 488	0	0

3 Residue-property plots

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.

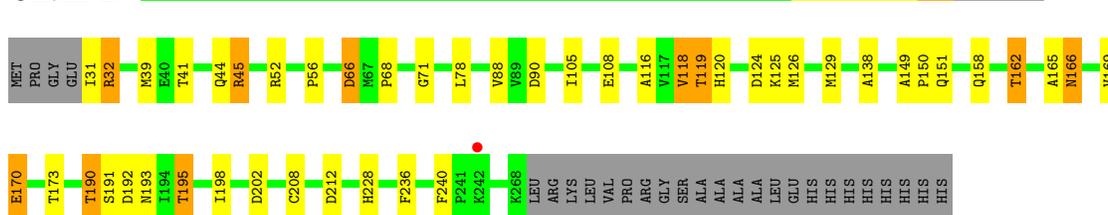
- Molecule 1: Beta-lactamase NDM-1

Chain A:



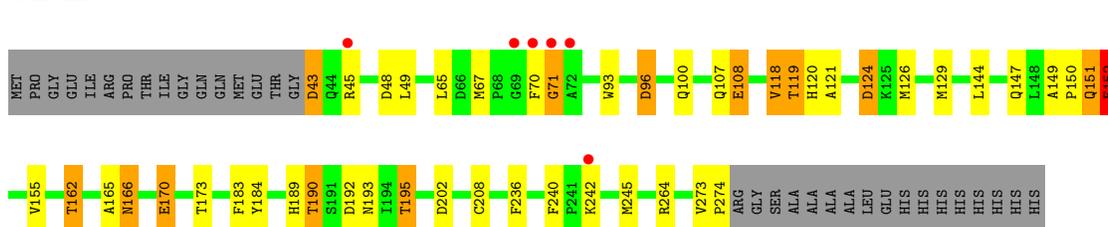
- Molecule 1: Beta-lactamase NDM-1

Chain B:



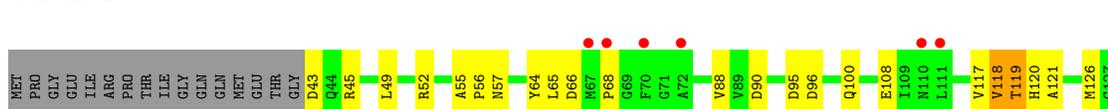
- Molecule 1: Beta-lactamase NDM-1

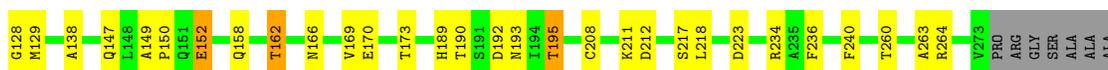
Chain C:



- Molecule 1: Beta-lactamase NDM-1

Chain D:





ALA
LEU
GLU
GLU
HIS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Beta-lactamase NDM-1

Chain E:



HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.54Å 73.90Å 77.41Å 70.32° 75.86° 65.30°	Depositor
Resolution (Å)	43.67 – 2.10 43.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.67-2.10) 96.0 (43.66-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.216 , 0.253 0.218 , 0.254	Depositor DCC
R_{free} test set	3563 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 32.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 70203 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9130	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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:
ZN

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	1.13	9/1737 (0.5%)	0.87	2/2366 (0.1%)
1	B	1.26	11/1810 (0.6%)	0.89	6/2465 (0.2%)
1	C	1.22	10/1737 (0.6%)	0.90	6/2366 (0.3%)
1	D	1.12	9/1737 (0.5%)	0.83	1/2366 (0.0%)
1	E	1.15	9/1726 (0.5%)	0.91	5/2352 (0.2%)
All	All	1.18	48/8747 (0.5%)	0.88	20/11915 (0.2%)

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	GLU	CD-OE1	16.75	1.44	1.25
1	B	118	VAL	CB-CG2	-14.18	1.23	1.52
1	B	118	VAL	CB-CG1	-13.45	1.24	1.52
1	E	118	VAL	CB-CG2	-12.79	1.25	1.52
1	B	56	PRO	C-O	-11.47	1.00	1.23

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	ASP	CB-CG-OD2	5.93	123.63	118.30
1	E	152	GLU	O-C-N	-5.91	113.15	123.20
1	B	118	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	B	56	PRO	O-C-N	-5.87	113.31	122.70
1	C	124	ASP	CB-CG-OD2	5.81	123.53	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1728	0	1687	56	0
1	B	1769	0	1715	30	0
1	C	1728	0	1687	47	0
1	D	1721	0	1680	31	0
1	E	1686	0	1633	48	0
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
2	E	2	0	0	0	0
3	W	488	0	0	13	0
All	All	9130	0	8402	193	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 193 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:VAL:HG11	1:A:126:MET:HG2	1.40	0.99
1:E:176:ASN:N	1:E:176:ASN:OD1	1.99	0.93
1:B:162:THR:HG22	1:B:170:GLU:HG3	1.48	0.93
1:E:162:THR:HG22	1:E:170:GLU:HG3	1.51	0.91
1:D:162:THR:HG22	1:D:170:GLU:HG3	1.52	0.91

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	230/265 (87%)	224 (97%)	6 (3%)	0	100	100
1	B	236/265 (89%)	231 (98%)	5 (2%)	0	100	100
1	C	230/265 (87%)	223 (97%)	6 (3%)	1 (0%)	43	39
1	D	229/265 (86%)	225 (98%)	4 (2%)	0	100	100
1	E	225/265 (85%)	212 (94%)	11 (5%)	2 (1%)	25	17
All	All	1150/1325 (87%)	1115 (97%)	32 (3%)	3 (0%)	50	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	GLY
1	E	213	SER
1	E	90	ASP

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	171/200 (86%)	162 (95%)	9 (5%)	32	28
1	B	179/200 (90%)	167 (93%)	12 (7%)	23	18
1	C	171/200 (86%)	160 (94%)	11 (6%)	25	20
1	D	171/200 (86%)	163 (95%)	8 (5%)	36	33
1	E	170/200 (85%)	162 (95%)	8 (5%)	36	33
All	All	862/1000 (86%)	814 (94%)	48 (6%)	30	25

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	43	ASP
1	C	152	GLU
1	E	162	THR
1	C	45	ARG
1	C	107	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	123	GLN
1	C	158	GLN
1	E	193	ASN
1	C	151	GLN
1	C	166	ASN

5.3.3 RNA [i](#)

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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.

5.7 Other polymers [i](#)

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, 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	232/265 (87%)	0.21	3 (1%) 74 78	16, 25, 43, 61	0
1	B	238/265 (89%)	-0.06	1 (0%) 90 92	16, 25, 44, 61	0
1	C	232/265 (87%)	0.20	6 (2%) 53 58	16, 25, 46, 61	0
1	D	231/265 (87%)	0.10	6 (2%) 53 58	16, 25, 44, 61	0
1	E	227/265 (85%)	0.16	6 (2%) 53 58	17, 25, 49, 61	0
All	All	1160/1325 (87%)	0.12	22 (1%) 64 68	16, 25, 46, 61	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	PRO	5.7
1	C	69	GLY	5.4
1	D	70	PHE	5.2
1	C	70	PHE	4.9
1	C	72	ALA	4.4

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	B	1005	1/1	0.11	0.15	25,25,25,25	0
2	ZN	A	1007	1/1	0.10	-0.89	24,24,24,24	0
2	ZN	E	1001	1/1	0.07	-1.15	33,33,33,33	0
2	ZN	B	1006	1/1	0.08	-1.26	34,34,34,34	0
2	ZN	D	1003	1/1	0.07	-1.54	24,24,24,24	0
2	ZN	C	1009	1/1	0.08	-1.82	25,25,25,25	0
2	ZN	D	1004	1/1	0.06	-2.04	33,33,33,33	0
2	ZN	A	1008	1/1	0.03	-2.28	32,32,32,32	0
2	ZN	E	1002	1/1	0.03	-2.28	37,37,37,37	0
2	ZN	C	1010	1/1	0.04	-4.04	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.