



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:21 PM GMT

PDB ID : 3QZ2
Title : The structure of cysteine-free human insulin degrading enzyme
Authors : Guo, Q.; Tang, W.J.
Deposited on : 2011-03-04
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

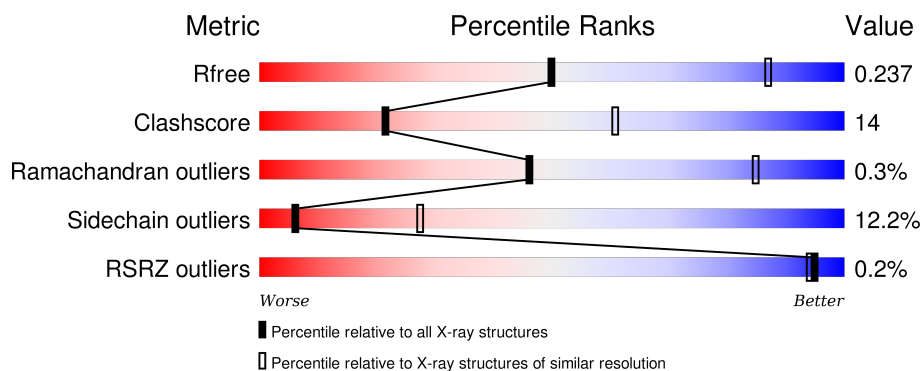
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	990	
1	B	990	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15748 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	0
			7790	5019	1308	1441	22			
1	B	952	Total	C	N	O	S	0	0	0
			7780	5013	1305	1440	22			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P14735
A	31	HIS	-	EXPRESSION TAG	UNP P14735
A	32	HIS	-	EXPRESSION TAG	UNP P14735
A	33	HIS	-	EXPRESSION TAG	UNP P14735
A	34	HIS	-	EXPRESSION TAG	UNP P14735
A	35	HIS	-	EXPRESSION TAG	UNP P14735
A	36	HIS	-	EXPRESSION TAG	UNP P14735
A	37	ALA	-	EXPRESSION TAG	UNP P14735
A	38	ALA	-	EXPRESSION TAG	UNP P14735
A	39	GLY	-	EXPRESSION TAG	UNP P14735
A	40	ILE	-	EXPRESSION TAG	UNP P14735
A	41	PRO	-	EXPRESSION TAG	UNP P14735
A	110	LEU	CYS	ENGINEERED MUTATION	UNP P14735
A	171	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	178	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	257	VAL	CYS	ENGINEERED MUTATION	UNP P14735
A	414	LEU	CYS	ENGINEERED MUTATION	UNP P14735
A	573	ASN	CYS	ENGINEERED MUTATION	UNP P14735
A	590	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	789	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	812	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	819	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	904	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	966	ASN	CYS	ENGINEERED MUTATION	UNP P14735
A	974	ALA	CYS	ENGINEERED MUTATION	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	EXPRESSION TAG	UNP P14735
B	31	HIS	-	EXPRESSION TAG	UNP P14735
B	32	HIS	-	EXPRESSION TAG	UNP P14735
B	33	HIS	-	EXPRESSION TAG	UNP P14735
B	34	HIS	-	EXPRESSION TAG	UNP P14735
B	35	HIS	-	EXPRESSION TAG	UNP P14735
B	36	HIS	-	EXPRESSION TAG	UNP P14735
B	37	ALA	-	EXPRESSION TAG	UNP P14735
B	38	ALA	-	EXPRESSION TAG	UNP P14735
B	39	GLY	-	EXPRESSION TAG	UNP P14735
B	40	ILE	-	EXPRESSION TAG	UNP P14735
B	41	PRO	-	EXPRESSION TAG	UNP P14735
B	110	LEU	CYS	ENGINEERED MUTATION	UNP P14735
B	171	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	178	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	257	VAL	CYS	ENGINEERED MUTATION	UNP P14735
B	414	LEU	CYS	ENGINEERED MUTATION	UNP P14735
B	573	ASN	CYS	ENGINEERED MUTATION	UNP P14735
B	590	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	789	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	812	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	819	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	904	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	966	ASN	CYS	ENGINEERED MUTATION	UNP P14735
B	974	ALA	CYS	ENGINEERED MUTATION	UNP P14735

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

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

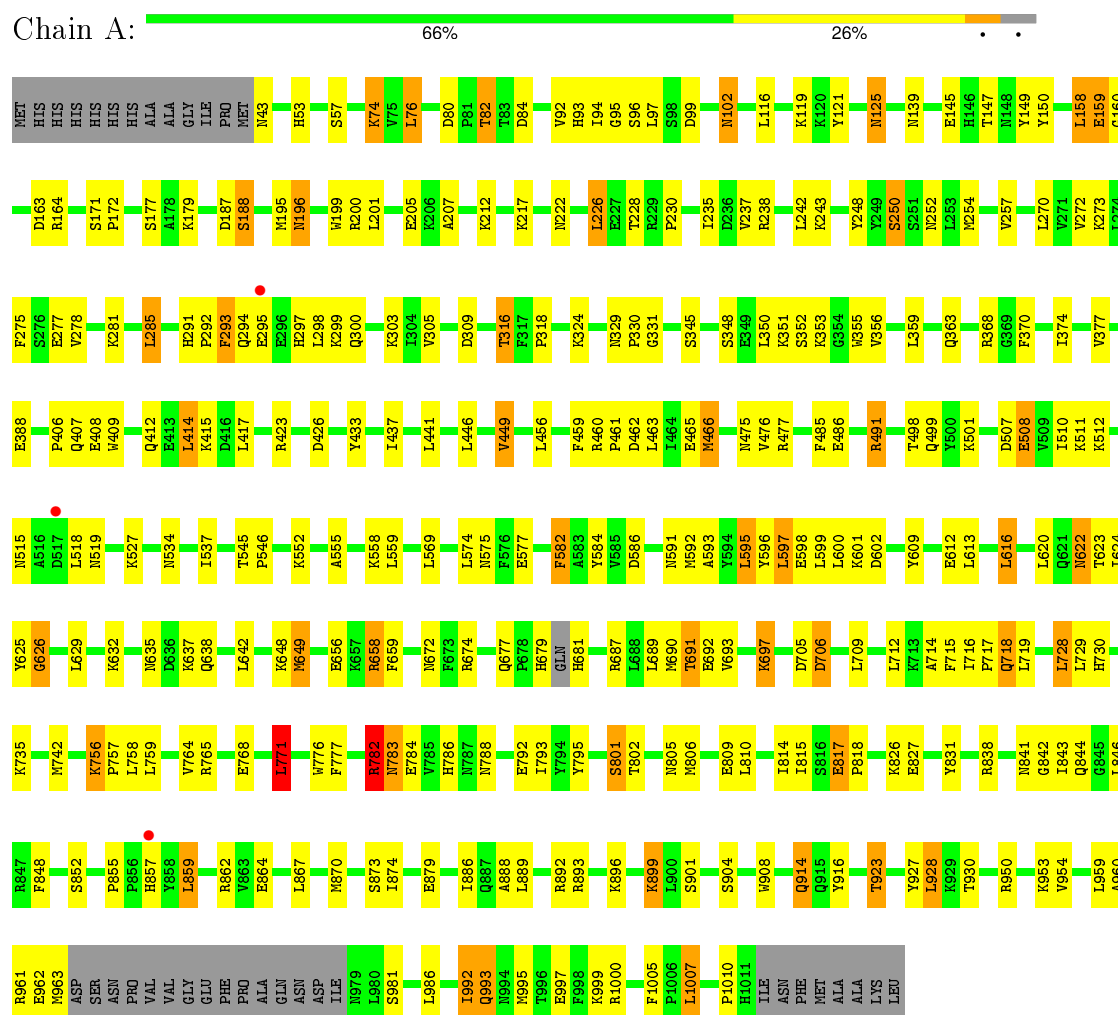
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	94	Total O 94 94	0	0
3	B	82	Total O 82 82	0	0

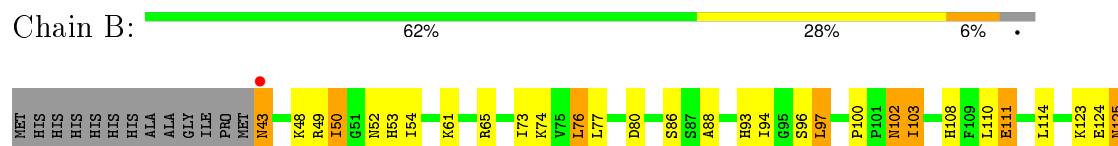
3 Residue-property plots

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: Insulin-degrading enzyme



- Molecule 1: Insulin-degrading enzyme



R950	R951	R952	K953	A960	R961	E962	N963	ASP	SER	ASN	PRO	VAL	VAL	GLY	GLU	PHE	PRO	ALA	GLN	ASN	ASP	ILE	N979	L980	Q993	T996	R1000	L1007	V1008	K1009	P1010	H1011	ILE	ASN	PHE	MET	ALA	ALA	LYS	LEU												
V863	E864	A865	F866	L867	I868	T869	M870	S873	I874	E875	D876	M877	E880	A881	K884	Q887	A888	L889	A890	E891	K898	K899	L900	S901	K906	Y907	W908	I912	S913	Q914	T923	Y927	L928	K929	T930	L931	T932	K933	E934	I937	K938	E942	M943	V946	D947	A948	F949					
Q770	R774	G775	L776	Q781	R782	N783	H786	N787	N788	I791	Y795	D798	Y799	Q800	S801	T802	S803	E804	N805	L810	E817	P818	L823	E827	Y831	R838	N841	Q844	L846	R847	F848	I849	I850	Q851	S852	P855	P856	HIS	Y858	L859	S860	E861	R862									
M672	F673	R674	A675	E676	Q677	P678	H679	GLN	H681	Y685	L686	R687	L688	T691	E692	V693	A694	W695	K701	E702	D706	L712	I716	I725	L728	A737	I741	P742	Q743	M744	D747	I750	E751	T755	L758	L759	P760	Q762	L763	Y766	R767	L770	V769									
L595	Y596	L597	E598	L599	L600	I601	D602	S603	E612	L616	S617	Y618	D619	L620	Q621	W622	T623	W625	G626	W627	W628	L629	W634	N635	D636	W637	T640	L641	L642	W643	W644	T645	I646	E647	W648	B653	T654	D655	E656	W657	R658	T659	T662	R663	B664	A665	W666	W667	R668	S669	L670	N671
R460	P461	D462	I463	I464	E465	W466	K470	L471	A472	R473	W474	W475	V481	D490	R491	T498	Q502	G505	P506	I510	K511	W512	Q514	D517	F522	K523	L524	K527	I531	P532	T533	N534	L540	D565	K566	L574	N575	F576	E577	F578	A583	P587	N591	E458	F459							
K351	Y356	L359	Q363	K364	S365	L379	T391	L392	F395	Q396	G405	P406	W409	V410	E413	L414	L417	F522	K523	L524	K527	I531	P532	T533	N534	L540	D565	K566	L574	N575	F576	E577	F578	A583	P587	N591	E458	F459														
M254	A255	V257	V258	L259	Q260	R261	L264	T268	L270	V271	V272	N282	L285	P286	E287	F288	P289	E290	H291	Q294	E295	E296	H297	L298	I304	D309	I310	R311	N312	L313	Y314	V315	T316	F317	P318	Y326	K327	S328	N329	Y333	L337	E341	L346	L347	K243							
E126	L131	A135	S138	N139	G144	N148	Y149	Y150	F151	H155	E156	H157	L158	L162	D163	R164	L173	E176	S177	A178	K179	S188	E189	N196	D197	A198	W199	L200	L201	L204	T208	K212	K223	L226	R229	V237	W238	Q239	L243													

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.07Å 262.07Å 90.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 49.53 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.20) 99.6 (49.53-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.172 , 0.241 0.173 , 0.237	Depositor DCC
R_{free} test set	2967 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58587 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15748	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.84	4/7984 (0.1%)	0.90	13/10800 (0.1%)
1	B	0.81	5/7972 (0.1%)	0.88	8/10782 (0.1%)
All	All	0.82	9/15956 (0.1%)	0.89	21/21582 (0.1%)

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	2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	GLU	CG-CD	8.82	1.65	1.51
1	B	453	GLU	CB-CG	6.97	1.65	1.52
1	B	577	GLU	CG-CD	6.67	1.61	1.51
1	B	50	ILE	CG1-CD1	6.24	1.93	1.50
1	A	577	GLU	CB-CG	5.81	1.63	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	GLU	CB-CA-C	-8.45	93.50	110.40
1	A	992	ILE	O-C-N	-8.15	109.66	122.70
1	A	285	LEU	CA-CB-CG	7.45	132.43	115.30
1	A	993	GLN	N-CA-CB	7.26	123.68	110.60
1	A	626	GLY	N-CA-C	-6.86	95.94	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	992	ILE	Mainchain,Peptide

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	7790	0	7724	208	0
1	B	7780	0	7717	231	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	94	0	0	38	0
3	B	82	0	0	20	0
All	All	15748	0	15441	436	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 14.

The worst 5 of 436 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:50:ILE:CG1	1:B:50:ILE:CD1	1.93	1.44
1:B:782:ARG:HD2	3:B:1059:HOH:O	1.46	1.12
1:B:679:HIS:O	1:B:681:HIS:N	1.86	1.09
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.12	1.08
1:B:856:PRO:O	1:B:858:TYR:N	1.88	1.07

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	947/990 (96%)	881 (93%)	65 (7%)	1 (0%)	56	91
1	B	944/990 (95%)	876 (93%)	63 (7%)	5 (0%)	34	78
All	All	1891/1980 (96%)	1757 (93%)	128 (7%)	6 (0%)	46	85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	946	VAL
1	A	228	THR
1	B	406	PRO
1	B	405	GLY
1	B	587	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	847/879 (96%)	761 (90%)	86 (10%)	9	36
1	B	846/879 (96%)	725 (86%)	121 (14%)	4	19
All	All	1693/1758 (96%)	1486 (88%)	207 (12%)	6	27

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	LEU

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	898	LYS
1	B	111	GLU
1	B	201	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	828	GLN
1	B	102	ASN
1	B	821	ASN
1	A	841	ASN
1	A	988	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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	953/990 (96%)	-0.32	3 (0%) 94 93	11, 25, 40, 60	0
1	B	952/990 (96%)	-0.29	1 (0%) 95 95	14, 27, 41, 61	0
All	All	1905/1980 (96%)	-0.30	4 (0%) 95 94	11, 26, 41, 61	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	857	HIS	2.7
1	B	43	ASN	2.5
1	A	295	GLU	2.3
1	A	517	ASP	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	2	1/1	0.97	0.11	-	28,28,28,28	0
2	ZN	A	1	1/1	0.98	0.10	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.