



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:30 AM GMT

PDB ID : 3IOU
Title : Huntingtin amino-terminal region with 17 Gln residues - crystal C94
Authors : Kim, M.W.
Deposited on : 2009-08-14
Resolution : 3.70 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

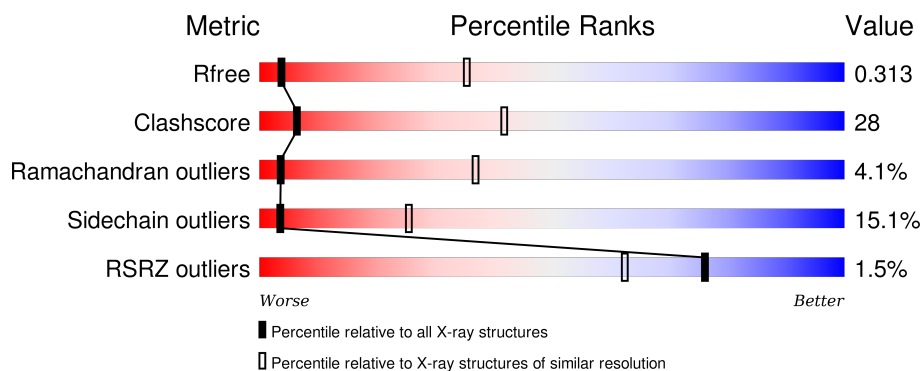
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 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	449	<div> <div>2%</div> <div>45% 35% 8% 10%</div> </div>
1	B	449	<div> <div>%</div> <div>48% 31% 8% 13%</div> </div>
1	C	449	<div> <div>%</div> <div>52% 32% 6% 11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	450	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9089 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 Maltose-binding protein, huntingtin fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3062	1974	497	583	8			
1	B	389	Total	C	N	O	S	0	1	0
			2998	1933	486	571	8			
1	C	400	Total	C	N	O	S	0	0	0
			3016	1937	494	577	8			

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	-	LINKER	? ?
A	360	ALA	-	LINKER	? ?
A	361	LEU	-	LINKER	? ?
A	362	ALA	-	LINKER	? ?
A	363	ALA	-	LINKER	? ?
A	364	ALA	-	LINKER	? ?
A	365	GLN	-	LINKER	? ?
A	366	THR	-	LINKER	? ?
A	367	ASN	-	LINKER	? ?
A	368	ALA	-	LINKER	? ?
A	369	ALA	-	LINKER	? ?
A	370	ALA	-	LINKER	? ?
A	?	-	GLN	DELETION	UNP P42858
A	?	-	GLN	DELETION	UNP P42858
A	?	-	GLN	DELETION	UNP P42858
A	?	-	GLN	DELETION	UNP P42858
A	?	-	GLN	DELETION	UNP P42858
A	?	-	GLN	DELETION	UNP P42858
A	431	GLN	-	EXPRESSION TAG	? ?
A	432	SER	-	EXPRESSION TAG	? ?
A	433	TYR	-	EXPRESSION TAG	? ?
A	434	GLN	-	EXPRESSION TAG	? ?
A	435	ILE	-	EXPRESSION TAG	? ?

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Chain	Residue	Modelled	Actual	Comment	Reference
A	436	THR	-	EXPRESSION TAG	? ?
A	437	ALA	-	EXPRESSION TAG	? ?
A	438	GLY	-	EXPRESSION TAG	? ?
A	439	LYS	-	EXPRESSION TAG	? ?
A	440	LEU	-	EXPRESSION TAG	? ?
A	441	GLY	-	EXPRESSION TAG	? ?
A	442	THR	-	EXPRESSION TAG	? ?
A	443	GLY	-	EXPRESSION TAG	? ?
A	444	ARG	-	EXPRESSION TAG	? ?
A	445	ARG	-	EXPRESSION TAG	? ?
A	446	PHE	-	EXPRESSION TAG	? ?
A	447	THR	-	EXPRESSION TAG	? ?
A	448	THR	-	EXPRESSION TAG	? ?
A	449	SER	-	EXPRESSION TAG	? ?
B	359	ALA	-	LINKER	? ?
B	360	ALA	-	LINKER	? ?
B	361	LEU	-	LINKER	? ?
B	362	ALA	-	LINKER	? ?
B	363	ALA	-	LINKER	? ?
B	364	ALA	-	LINKER	? ?
B	365	GLN	-	LINKER	? ?
B	366	THR	-	LINKER	? ?
B	367	ASN	-	LINKER	? ?
B	368	ALA	-	LINKER	? ?
B	369	ALA	-	LINKER	? ?
B	370	ALA	-	LINKER	? ?
B	?	-	GLN	DELETION	UNP P42858
B	?	-	GLN	DELETION	UNP P42858
B	?	-	GLN	DELETION	UNP P42858
B	?	-	GLN	DELETION	UNP P42858
B	?	-	GLN	DELETION	UNP P42858
B	?	-	GLN	DELETION	UNP P42858
B	431	GLN	-	EXPRESSION TAG	? ?
B	432	SER	-	EXPRESSION TAG	? ?
B	433	TYR	-	EXPRESSION TAG	? ?
B	434	GLN	-	EXPRESSION TAG	? ?
B	435	ILE	-	EXPRESSION TAG	? ?
B	436	THR	-	EXPRESSION TAG	? ?
B	437	ALA	-	EXPRESSION TAG	? ?
B	438	GLY	-	EXPRESSION TAG	? ?
B	439	LYS	-	EXPRESSION TAG	? ?
B	440	LEU	-	EXPRESSION TAG	? ?

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Chain	Residue	Modelled	Actual	Comment	Reference
B	441	GLY	-	EXPRESSION TAG	? ?
B	442	THR	-	EXPRESSION TAG	? ?
B	443	GLY	-	EXPRESSION TAG	? ?
B	444	ARG	-	EXPRESSION TAG	? ?
B	445	ARG	-	EXPRESSION TAG	? ?
B	446	PHE	-	EXPRESSION TAG	? ?
B	447	THR	-	EXPRESSION TAG	? ?
B	448	THR	-	EXPRESSION TAG	? ?
B	449	SER	-	EXPRESSION TAG	? ?
C	359	ALA	-	LINKER	? ?
C	360	ALA	-	LINKER	? ?
C	361	LEU	-	LINKER	? ?
C	362	ALA	-	LINKER	? ?
C	363	ALA	-	LINKER	? ?
C	364	ALA	-	LINKER	? ?
C	365	GLN	-	LINKER	? ?
C	366	THR	-	LINKER	? ?
C	367	ASN	-	LINKER	? ?
C	368	ALA	-	LINKER	? ?
C	369	ALA	-	LINKER	? ?
C	370	ALA	-	LINKER	? ?
C	?	-	GLN	DELETION	UNP P42858
C	?	-	GLN	DELETION	UNP P42858
C	?	-	GLN	DELETION	UNP P42858
C	?	-	GLN	DELETION	UNP P42858
C	?	-	GLN	DELETION	UNP P42858
C	?	-	GLN	DELETION	UNP P42858
C	431	GLN	-	EXPRESSION TAG	? ?
C	432	SER	-	EXPRESSION TAG	? ?
C	433	TYR	-	EXPRESSION TAG	? ?
C	434	GLN	-	EXPRESSION TAG	? ?
C	435	ILE	-	EXPRESSION TAG	? ?
C	436	THR	-	EXPRESSION TAG	? ?
C	437	ALA	-	EXPRESSION TAG	? ?
C	438	GLY	-	EXPRESSION TAG	? ?
C	439	LYS	-	EXPRESSION TAG	? ?
C	440	LEU	-	EXPRESSION TAG	? ?
C	441	GLY	-	EXPRESSION TAG	? ?
C	442	THR	-	EXPRESSION TAG	? ?
C	443	GLY	-	EXPRESSION TAG	? ?
C	444	ARG	-	EXPRESSION TAG	? ?
C	445	ARG	-	EXPRESSION TAG	? ?

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Chain	Residue	Modelled	Actual	Comment	Reference
C	446	PHE	-	EXPRESSION TAG	? ?
C	447	THR	-	EXPRESSION TAG	? ?
C	448	THR	-	EXPRESSION TAG	? ?
C	449	SER	-	EXPRESSION TAG	? ?

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Zn 3 3	0	0
2	A	4	Total Zn 4 4	0	0
2	C	1	Total Zn 1 1	0	0

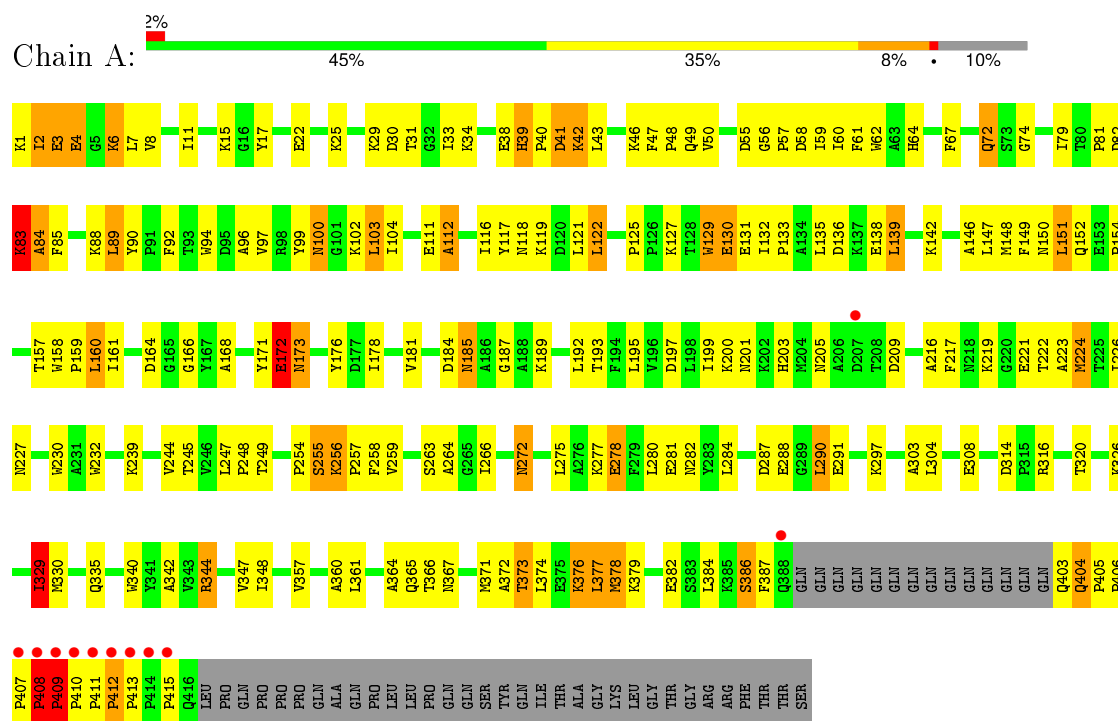
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

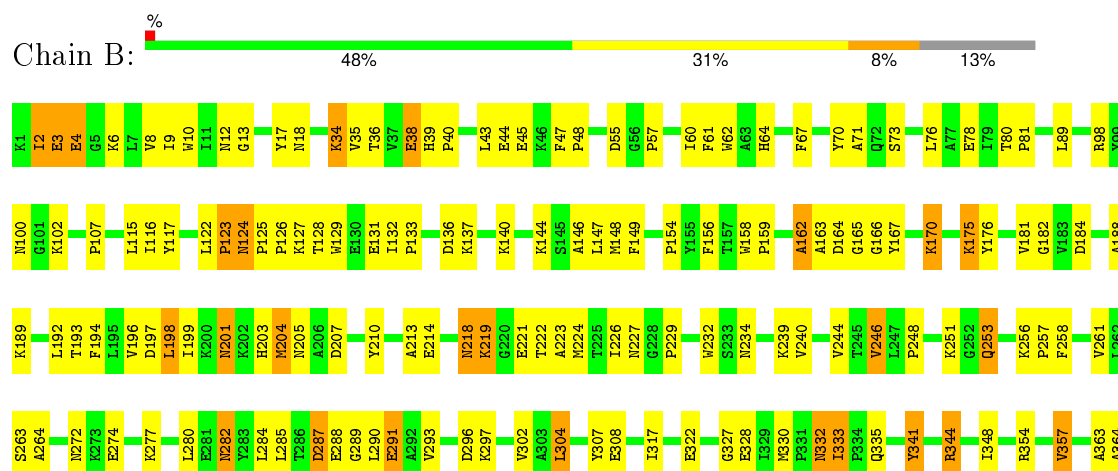
3 Residue-property plots

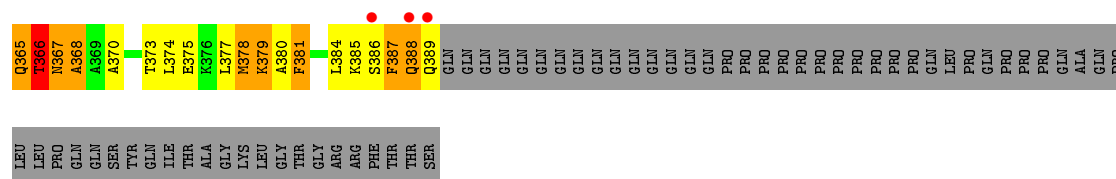
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Maltose-binding protein, huntingtin fusion protein

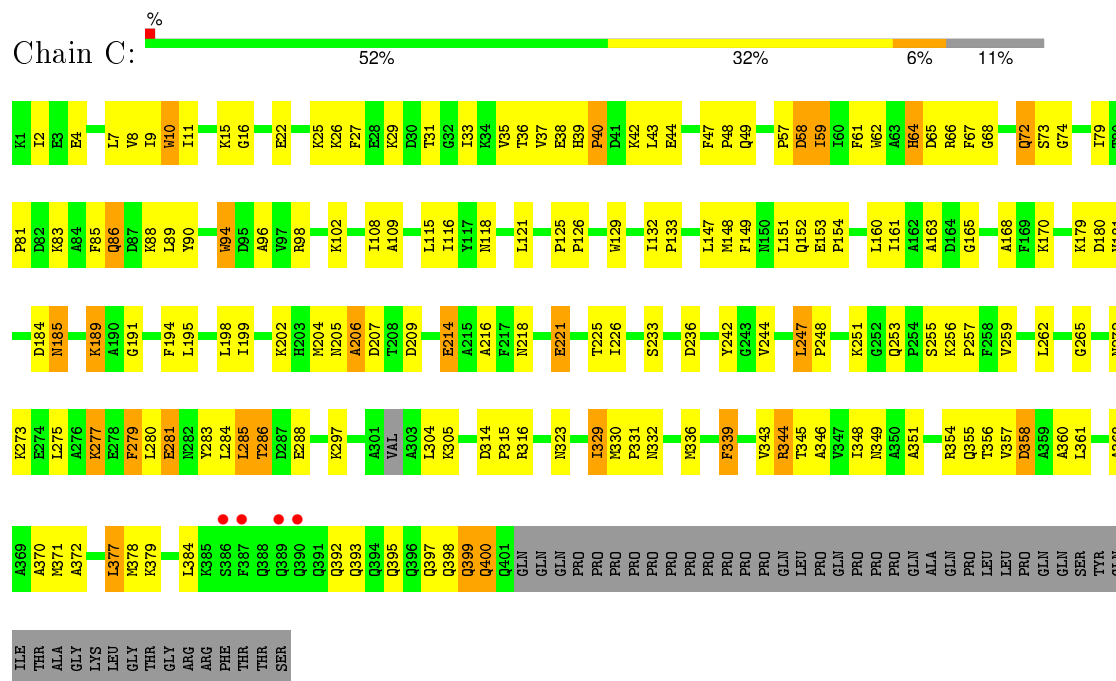


- Molecule 1: Maltose-binding protein, huntingtin fusion protein





- Molecule 1: Maltose-binding protein, huntingtin fusion protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.79 Å 99.79 Å 140.50 Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	40.00 – 3.70 29.70 – 3.70	Depositor EDS
% Data completeness (in resolution range)	86.3 (40.00-3.70) 69.9 (29.70-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 3.75 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.272 , 0.299 0.286 , 0.313	Depositor DCC
R_{free} test set	1045 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	118.8	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , -18.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	6 of 20610 reflections (0.029%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9089	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 ⓘ

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	0.42	2/3141 (0.1%)	0.59	3/4277 (0.1%)
1	B	0.38	0/3072	0.58	0/4171
1	C	0.36	0/3085	0.55	0/4194
All	All	0.39	2/9298 (0.0%)	0.57	3/12642 (0.0%)

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	1	5
1	B	0	3
All	All	1	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	PRO	N-CD	5.49	1.55	1.47
1	A	408	PRO	N-CA	-5.16	1.38	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	LYS	N-CA-C	-5.97	94.89	111.00
1	A	408	PRO	N-CA-C	5.94	127.55	112.10
1	A	3	GLU	C-N-CA	5.46	135.35	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	408	PRO	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ASP	Peptide
1	A	403	GLN	Peptide
1	A	404	GLN	Peptide
1	A	407	PRO	Peptide
1	A	409	PRO	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	3062	0	3016	245	1
1	B	2998	0	2967	147	0
1	C	3016	0	2913	146	0
2	A	4	0	0	0	0
2	B	3	0	0	0	1
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
All	All	9089	0	8896	498	1

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 28.

The worst 5 of 498 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:A:342:ALA:CB	1:A:367:ASN:HB3	1.34	1.55
1:A:129:TRP:CH2	1:A:160:LEU:HG	1.47	1.50
1:A:342:ALA:HB1	1:A:367:ASN:CB	1.40	1.49
1:A:3:GLU:CB	1:A:4:GLU:HB2	1.54	1.34
1:A:129:TRP:CZ3	1:A:160:LEU:HG	1.72	1.24

All (1) 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)
1:A:138:GLU:OE1	2:B:450:ZN:ZN[3_455]	1.64	0.56

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	398/449 (89%)	332 (83%)	46 (12%)	20 (5%)	3	31
1	B	388/449 (86%)	322 (83%)	51 (13%)	15 (4%)	4	38
1	C	396/449 (88%)	318 (80%)	64 (16%)	14 (4%)	4	43
All	All	1182/1347 (88%)	972 (82%)	161 (14%)	49 (4%)	3	37

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	83	LYS
1	A	130	GLU
1	A	173	ASN
1	A	408	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	312/363 (86%)	262 (84%)	50 (16%)	3	22
1	B	304/363 (84%)	259 (85%)	45 (15%)	4	26
1	C	295/363 (81%)	253 (86%)	42 (14%)	4	29
All	All	911/1089 (84%)	774 (85%)	137 (15%)	3	26

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	175	LYS
1	B	256	LYS
1	C	279	PHE
1	B	181	VAL
1	B	205	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	HIS
1	B	203	HIS
1	C	201	ASN
1	B	72	GLN
1	B	205	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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	402/449 (89%)	-0.40	11 (2%) 58 42	70, 70, 100, 100	30 (7%)
1	B	389/449 (86%)	-0.55	3 (0%) 87 77	56, 70, 73, 100	14 (3%)
1	C	400/449 (89%)	-0.52	4 (1%) 84 72	70, 70, 100, 100	31 (7%)
All	All	1191/1347 (88%)	-0.49	18 (1%) 76 62	56, 70, 100, 100	75 (6%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	SER	5.1
1	B	389	GLN	4.7
1	C	387	PHE	4.6
1	B	388	GLN	3.7
1	A	412	PRO	3.4

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	450	1/1	0.91	0.32	2.70	86,86,86,86	1
3	CA	C	452	1/1	0.50	0.12	-	98,98,98,98	0
3	CA	C	451	1/1	0.71	0.21	-	99,99,99,99	0
2	ZN	A	451	1/1	0.92	0.28	-	100,100,100,100	0
3	CA	B	453	1/1	0.96	0.25	-	89,89,89,89	0
2	ZN	B	452	1/1	0.94	0.25	-	100,100,100,100	0
3	CA	A	454	1/1	0.94	0.23	-	96,96,96,96	0
2	ZN	A	452	1/1	0.94	0.22	-	92,92,92,92	0
2	ZN	A	453	1/1	0.72	0.14	-	88,88,88,88	1
2	ZN	B	451	1/1	0.93	0.27	-	100,100,100,100	0
2	ZN	A	450	1/1	0.95	0.43	-	97,97,97,97	1
2	ZN	C	450	1/1	0.88	0.23	-	92,92,92,92	1
3	CA	B	454	1/1	0.88	0.20	-	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.