



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:30 AM GMT

PDB ID : 3IOW  
Title : Huntingtin amino-terminal region with 17 Gln residues - crystal C99-Hg  
Authors : Kim, M.W.  
Deposited on : 2009-08-14  
Resolution : 3.50 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](mailto: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.

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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

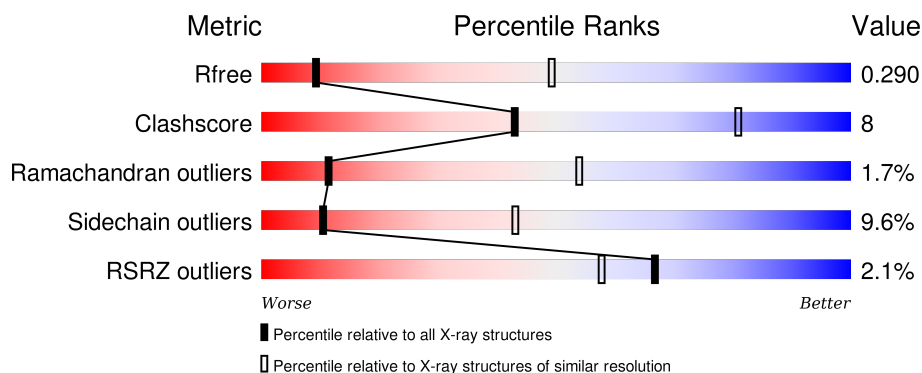
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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  $\geq 3$ , 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>76%</div> <div>12%</div> <div>8%</div> </div>
1	B	449	<div> <div>3%</div> <div>73%</div> <div>14%</div> <div>10%</div> </div>
1	C	449	<div> <div>%</div> <div>72%</div> <div>12%</div> <div>12%</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
3	CA	A	506	-	-	-	X
3	CA	C	505	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9280 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	414	Total	C	N	O	S	0	1	0
			3135	2018	514	595	8			
1	B	404	Total	C	N	O	S	0	1	0
			3111	1999	512	592	8			
1	C	393	Total	C	N	O	S	0	3	0
			3017	1943	491	575	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	2	Total Zn 2 2	0	0
2	A	3	Total Zn 3 3	0	0
2	C	2	Total Zn 2 2	0	0

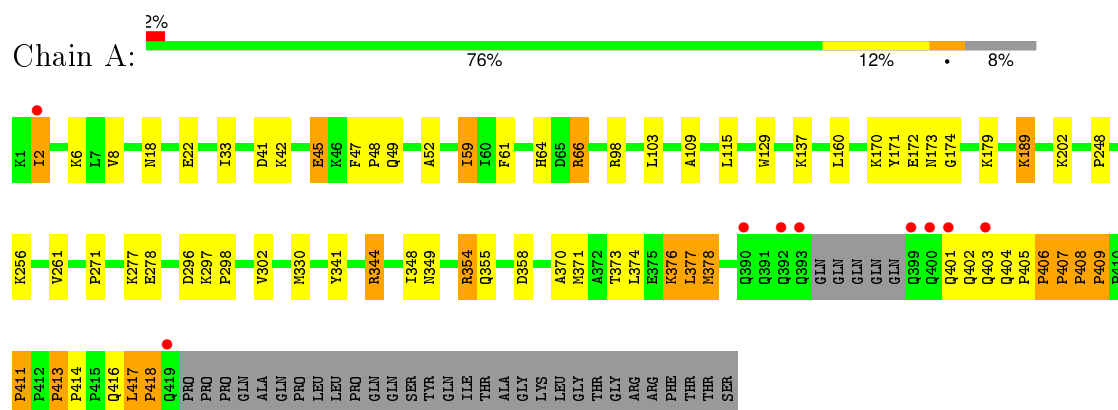
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	5	Total Ca 5 5	0	0
3	C	4	Total Ca 4 4	0	0

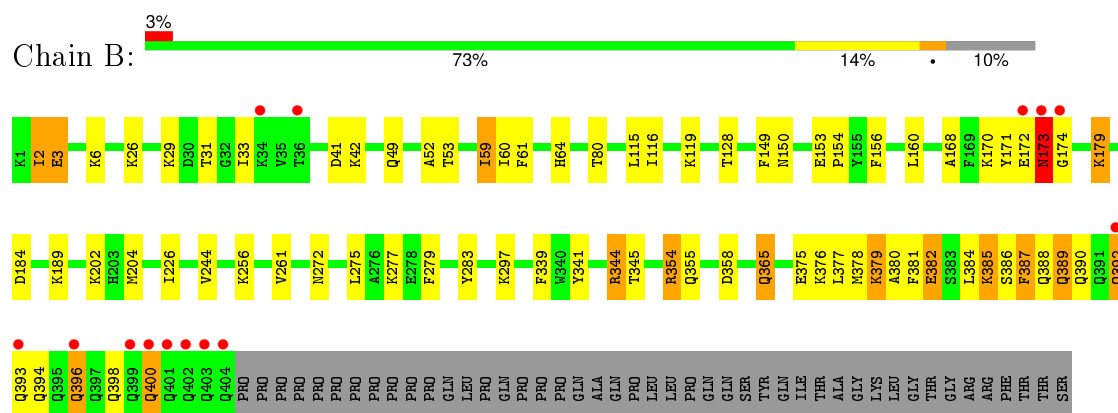
### 3 Residue-property plots

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: Maltose-binding protein, huntingtin fusion protein



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





[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.10Å 162.77Å 139.66Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 39.25 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (40.00-3.50) 91.7 (39.25-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.243 , 0.281 0.251 , 0.290	Depositor DCC
$R_{free}$ test set	1316 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 14.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 25830 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.34	0/3218	0.49	0/4386
1	B	0.35	0/3186	0.48	0/4324
1	C	0.35	0/3097	0.50	0/4209
All	All	0.35	0/9501	0.49	0/12919

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3135	0	3058	64	0
1	B	3111	0	3053	60	0
1	C	3017	0	2960	45	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
All	All	9280	0	9071	151	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 8.

All (151) 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:376:LYS:CE	1:A:377:LEU:HD23	1.39	1.52
1:A:376:LYS:HE3	1:A:377:LEU:CD2	1.62	1.27
1:C:373:THR:CG2	1:C:376:LYS:HD2	1.67	1.24
1:A:378:MET:HA	1:A:378:MET:HE3	1.09	1.08
1:C:373:THR:HG23	1:C:376:LYS:HD2	1.30	1.08
1:A:377:LEU:HD22	1:C:373:THR:HG21	1.37	1.06
1:A:378:MET:CE	1:A:378:MET:HA	1.88	1.03
1:A:370:ALA:HB1	1:B:380:ALA:HB2	1.42	1.00
1:C:373:THR:HG22	1:C:376:LYS:HD2	1.43	1.00
1:B:396:GLN:O	1:B:400:GLN:HB3	1.66	0.96
1:A:376:LYS:CE	1:A:377:LEU:CD2	2.34	0.91
1:A:354:ARG:HH12	1:B:389:GLN:CD	1.74	0.90
1:C:373:THR:HG22	1:C:376:LYS:CD	2.02	0.89
1:C:373:THR:CG2	1:C:376:LYS:CD	2.55	0.84
1:A:354:ARG:NH1	1:B:389:GLN:OE1	2.11	0.82
1:B:149[B]:PHE:CZ	1:B:156:PHE:CD2	2.68	0.81
1:A:376:LYS:HE2	1:A:377:LEU:HD23	1.57	0.80
1:C:344:ARG:HG2	1:C:344:ARG:HH11	1.47	0.79
1:B:149[B]:PHE:CE2	1:B:226:ILE:HB	2.19	0.78
1:B:376:LYS:NZ	1:B:376:LYS:HB3	2.00	0.77
1:B:149[B]:PHE:CD2	1:B:226:ILE:HB	2.20	0.77
1:A:376:LYS:HE3	1:A:377:LEU:HD23	0.78	0.77
1:A:378:MET:CA	1:A:378:MET:HE3	2.04	0.74
1:C:64:HIS:CD2	1:C:261:VAL:H	2.07	0.73
1:B:172:GLU:O	1:B:173:ASN:HB2	1.87	0.73
1:A:18:ASN:O	1:A:22:GLU:HG3	1.88	0.72
1:B:345:THR:HG21	1:C:387:PHE:CE1	2.26	0.70
1:A:349:ASN:OD1	1:A:354:ARG:HD2	1.90	0.70
1:A:341:TYR:OH	1:B:387:PHE:HB2	1.92	0.70
1:C:183:VAL:HG22	1:C:365:GLN:HG3	1.73	0.69
1:B:149[B]:PHE:HZ	1:B:156:PHE:CD2	2.09	0.69
1:C:296:ASP:O	1:C:297:LYS:HD3	1.92	0.69
1:A:407:PRO:N	1:A:408:PRO:HD3	2.07	0.68
1:A:417:LEU:N	1:A:418:PRO:HD2	2.08	0.68
1:A:401:GLN:O	1:A:403:GLN:N	2.26	0.67
1:A:376:LYS:C	1:A:376:LYS:HD2	2.16	0.66
1:B:376:LYS:HZ3	1:B:376:LYS:HB3	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:CD1	1:B:387:PHE:C	2.68	0.66
1:B:354:ARG:HA	1:B:354:ARG:NE	2.09	0.66
1:C:64:HIS:HD2	1:C:261:VAL:H	1.42	0.65
1:B:385:LYS:HA	1:B:385:LYS:HE3	1.78	0.65
1:B:6:LYS:HA	1:B:33:ILE:HG23	1.80	0.64
1:B:341:TYR:OH	1:C:387:PHE:HB2	1.98	0.64
1:B:388:GLN:O	1:B:392:GLN:HB2	1.98	0.63
1:A:406:PRO:C	1:A:408:PRO:HD3	2.18	0.63
1:B:59:ILE:HD11	1:B:61:PHE:CE1	2.33	0.63
1:B:149[B]:PHE:CE1	1:B:226:ILE:O	2.52	0.63
1:B:189:LYS:HE2	1:B:358:ASP:HA	1.82	0.62
1:B:26:LYS:O	1:B:29:LYS:HG2	2.00	0.61
1:B:184:ASP:HB2	1:B:365:GLN:HG3	1.83	0.61
1:C:344:ARG:HH11	1:C:344:ARG:CG	2.14	0.60
1:B:355:GLN:HA	1:C:52:ALA:O	2.02	0.60
1:A:378:MET:CE	1:A:378:MET:CA	2.71	0.60
1:A:407:PRO:O	1:A:409:PRO:HD3	2.02	0.59
1:C:379:LYS:O	1:C:383:SER:HB3	2.02	0.59
1:C:59:ILE:HD11	1:C:61:PHE:CE1	2.37	0.59
1:B:168:ALA:HA	1:B:339:PHE:CE2	2.38	0.59
1:A:371:MET:SD	1:B:384:LEU:HD21	2.43	0.59
1:B:386:SER:O	1:B:389:GLN:HG3	2.03	0.58
1:B:345:THR:HG21	1:C:387:PHE:CD1	2.39	0.57
1:A:64:HIS:CD2	1:A:261:VAL:H	2.23	0.57
1:C:340:TRP:O	1:C:344:ARG:HB3	2.05	0.56
1:A:354:ARG:HH22	1:B:389:GLN:HE22	1.54	0.56
1:A:376:LYS:C	1:A:376:LYS:CD	2.74	0.56
1:B:272:ASN:HB3	1:B:275:LEU:HD12	1.88	0.56
1:C:371:MET:O	1:C:374[A]:LEU:HB3	2.06	0.56
1:C:171:TYR:OH	1:C:174:GLY:HA2	2.06	0.55
1:A:297[A]:LYS:HD3	1:A:298:PRO:HD2	1.89	0.55
1:B:172:GLU:O	1:B:173:ASN:CB	2.54	0.54
1:B:2:ILE:O	1:B:3:GLU:CB	2.55	0.53
1:A:349:ASN:CG	1:A:354:ARG:HD2	2.28	0.53
1:A:377:LEU:CD2	1:C:373:THR:HG21	2.26	0.53
1:A:354:ARG:HH12	1:B:389:GLN:NE2	2.07	0.53
1:A:64:HIS:HE1	1:A:330:MET:O	1.94	0.51
1:B:379:LYS:HA	1:B:382:GLU:OE2	2.10	0.51
1:B:393:GLN:HA	1:B:396:GLN:HG2	1.93	0.51
1:A:59:ILE:HD11	1:A:61:PHE:CE1	2.46	0.50
1:A:407:PRO:C	1:A:409:PRO:HD3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:HIS:HD2	1:B:261:VAL:H	1.59	0.50
1:C:31:THR:HG22	1:C:33:ILE:HG12	1.93	0.50
1:A:297[B]:LYS:HE3	1:A:298:PRO:HG2	1.93	0.49
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.13	0.49
1:C:344:ARG:NH1	1:C:344:ARG:CG	2.73	0.49
1:B:179:LYS:HE3	1:B:179:LYS:HA	1.94	0.49
1:A:417:LEU:H	1:A:418:PRO:HD2	1.75	0.49
1:A:6:LYS:HA	1:A:33:ILE:HG23	1.94	0.49
1:B:64:HIS:CD2	1:B:261:VAL:H	2.30	0.48
1:A:98:ARG:HG3	1:A:103:LEU:HD12	1.95	0.48
1:A:373:THR:O	1:A:376:LYS:HE2	2.13	0.48
1:B:376:LYS:NZ	1:B:376:LYS:CB	2.75	0.48
1:C:373:THR:HG22	1:C:376:LYS:HD3	1.91	0.48
1:A:414:PRO:HG2	1:A:416:GLN:HE22	1.79	0.48
1:A:64:HIS:HD2	1:A:261:VAL:H	1.62	0.47
1:C:16:GLY:HA2	1:C:297:LYS:HE2	1.96	0.47
1:A:18:ASN:HB2	1:A:296:ASP:OD2	2.15	0.47
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.50	0.47
1:A:52:ALA:O	1:C:355:GLN:HA	2.15	0.47
1:B:389:GLN:OE1	1:B:390:GLN:CB	2.63	0.47
1:A:47:PHE:HB3	1:A:48:PRO:HD3	1.95	0.47
1:A:374:LEU:HA	1:A:377:LEU:HG	1.97	0.47
1:B:378:MET:C	1:B:380:ALA:H	2.18	0.46
1:B:149[B]:PHE:CD1	1:B:150:ASN:N	2.82	0.46
1:C:154:PRO:HG3	1:C:344:ARG:HA	1.96	0.46
1:B:154:PRO:HG3	1:B:344:ARG:HA	1.98	0.46
1:C:129:TRP:CD1	1:C:248:PRO:HB2	2.50	0.46
1:A:129:TRP:CD1	1:A:248:PRO:HB2	2.51	0.46
1:A:370:ALA:HB1	1:B:380:ALA:CB	2.30	0.46
1:A:297[B]:LYS:HE3	1:A:298:PRO:CD	2.46	0.46
1:C:128:THR:O	1:C:131:GLU:HG2	2.17	0.45
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.52	0.45
1:A:2:ILE:CB	1:A:271:PRO:HD3	2.47	0.45
1:B:31:THR:HG22	1:B:33:ILE:HG12	1.99	0.45
1:A:407:PRO:N	1:A:408:PRO:CD	2.78	0.45
1:A:411:PRO:O	1:A:413:PRO:HD3	2.17	0.44
1:C:256:LYS:HG3	1:C:326:LYS:O	2.17	0.44
1:A:414:PRO:HB2	1:A:416:GLN:HE22	1.83	0.44
1:C:341:TYR:CE1	1:C:371:MET:HG3	2.52	0.44
1:A:45:GLU:OE1	1:A:66:ARG:NH2	2.47	0.44
1:A:354:ARG:HB2	1:A:354:ARG:HE	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLN:CG	1:B:390:GLN:N	2.81	0.43
1:C:170:LYS:HB3	1:C:180:ASP:HB3	1.99	0.43
1:B:376:LYS:HZ2	1:B:376:LYS:HB3	1.82	0.43
1:B:279:PHE:O	1:B:283:TYR:HB2	2.18	0.43
1:C:381:PHE:CD1	1:C:381:PHE:C	2.91	0.43
1:C:189:LYS:HD2	1:C:358:ASP:HA	1.99	0.43
1:C:249:THR:HG22	1:C:254:PRO:HA	2.01	0.42
1:B:171:TYR:OH	1:B:174:GLY:HA2	2.18	0.42
1:B:387:PHE:HD1	1:B:388:GLN:N	2.17	0.42
1:C:375:GLU:O	1:C:379:LYS:CB	2.68	0.42
1:B:396:GLN:HB3	1:B:396:GLN:HE21	1.66	0.42
1:A:354:ARG:O	1:B:53:THR:HG22	2.18	0.42
1:C:381:PHE:HD1	1:C:381:PHE:C	2.22	0.42
1:B:116:ILE:HG12	1:B:244:VAL:HG22	2.01	0.42
1:A:109:ALA:HA	1:A:302:VAL:HA	2.01	0.42
1:A:376:LYS:HE2	1:A:376:LYS:HB3	1.68	0.42
1:B:149[B]:PHE:CE2	1:B:156:PHE:HB3	2.55	0.42
1:A:377:LEU:HD11	1:B:377:LEU:HD22	2.00	0.42
1:C:122:LEU:HA	1:C:123:PRO:HD2	1.87	0.41
1:A:355:GLN:HA	1:B:52:ALA:O	2.20	0.41
1:A:417:LEU:N	1:A:418:PRO:CD	2.79	0.41
1:B:150:ASN:ND2	1:B:153:GLU:OE2	2.54	0.41
1:C:344:ARG:O	1:C:348:ILE:HD13	2.20	0.41
1:C:183:VAL:CG2	1:C:365:GLN:HG3	2.47	0.41
1:A:344:ARG:O	1:A:348:ILE:HD13	2.21	0.41
1:C:46:LYS:O	1:C:50:VAL:HG22	2.21	0.41
1:B:189:LYS:HE3	1:B:189:LYS:HB2	1.88	0.40
1:B:384:LEU:O	1:B:387:PHE:HB3	2.21	0.40
1:A:189:LYS:HD2	1:A:358:ASP:HA	2.03	0.40
1:C:158:TRP:CE2	1:C:162:ALA:HB2	2.56	0.40
1:A:374:LEU:HD23	1:A:377:LEU:HD12	2.04	0.40
1:A:376:LYS:NZ	1:A:377:LEU:HD23	2.21	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	411/449 (92%)	381 (93%)	18 (4%)	12 (3%)	6	42
1	B	403/449 (90%)	381 (94%)	19 (5%)	3 (1%)	26	72
1	C	394/449 (88%)	379 (96%)	10 (2%)	5 (1%)	15	60
All	All	1208/1347 (90%)	1141 (94%)	47 (4%)	20 (2%)	11	54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	402	GLN
1	A	406	PRO
1	A	409	PRO
1	A	418	PRO
1	B	173	ASN
1	C	3	GLU
1	C	173	ASN
1	A	2	ILE
1	A	405	PRO
1	B	3	GLU
1	A	408	PRO
1	A	413	PRO
1	A	407	PRO
1	B	2	ILE
1	C	4	GLU
1	C	168	ALA
1	C	123	PRO
1	A	404	GLN
1	A	411	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	314/363 (86%)	290 (92%)	24 (8%)	16	55
1	B	313/363 (86%)	280 (90%)	33 (10%)	8	38
1	C	303/363 (84%)	269 (89%)	34 (11%)	7	35
All	All	930/1089 (85%)	839 (90%)	91 (10%)	10	42

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	41	ASP
1	A	42	LYS
1	A	45	GLU
1	A	49	GLN
1	A	59	ILE
1	A	66	ARG
1	A	115	LEU
1	A	137	LYS
1	A	160	LEU
1	A	170	LYS
1	A	172	GLU
1	A	179	LYS
1	A	189	LYS
1	A	202	LYS
1	A	256	LYS
1	A	277	LYS
1	A	278	GLU
1	A	344	ARG
1	A	354	ARG
1	A	376	LYS
1	A	377	LEU
1	A	378	MET
1	A	417	LEU
1	B	41	ASP
1	B	42	LYS
1	B	49	GLN
1	B	59	ILE
1	B	60	ILE
1	B	80	THR
1	B	115	LEU
1	B	119	LYS
1	B	128	THR
1	B	160	LEU

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Mol	Chain	Res	Type
1	B	170	LYS
1	B	173	ASN
1	B	179	LYS
1	B	202	LYS
1	B	204	MET
1	B	256	LYS
1	B	277	LYS
1	B	297	LYS
1	B	344	ARG
1	B	354	ARG
1	B	365	GLN
1	B	375	GLU
1	B	379	LYS
1	B	381	PHE
1	B	382	GLU
1	B	385	LYS
1	B	387	PHE
1	B	389	GLN
1	B	392	GLN
1	B	394	GLN
1	B	396	GLN
1	B	398	GLN
1	B	400	GLN
1	C	6	LYS
1	C	8	VAL
1	C	38	GLU
1	C	45	GLU
1	C	49	GLN
1	C	59	ILE
1	C	66	ARG
1	C	115	LEU
1	C	128	THR
1	C	137	LYS
1	C	153[A]	GLU
1	C	153[B]	GLU
1	C	160	LEU
1	C	170	LYS
1	C	172	GLU
1	C	179	LYS
1	C	189	LYS
1	C	202	LYS
1	C	204	MET

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Mol	Chain	Res	Type
1	C	256	LYS
1	C	277	LYS
1	C	278	GLU
1	C	297	LYS
1	C	341	TYR
1	C	344	ARG
1	C	365	GLN
1	C	373	THR
1	C	374[A]	LEU
1	C	374[B]	LEU
1	C	375	GLU
1	C	376	LYS
1	C	377	LEU
1	C	381	PHE
1	C	383	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	201	ASN
1	A	203	HIS
1	A	218	ASN
1	A	325	GLN
1	A	365	GLN
1	A	416	GLN
1	B	49	GLN
1	B	64	HIS
1	B	173	ASN
1	B	218	ASN
1	B	234	ASN
1	B	325	GLN
1	B	394	GLN
1	B	396	GLN
1	C	64	HIS
1	C	201	ASN
1	C	218	ASN
1	C	325	GLN
1	C	392	GLN

### 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 17 ligands modelled in this entry, 17 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	414/449 (92%)	-0.09	9 (2%) 65 55	78, 78, 97, 97	45 (10%)
1	B	404/449 (89%)	-0.02	14 (3%) 48 38	78, 78, 97, 97	33 (8%)
1	C	393/449 (87%)	-0.15	3 (0%) 87 80	78, 78, 96, 97	23 (5%)
All	All	1211/1347 (89%)	-0.08	26 (2%) 67 58	78, 78, 97, 97	101 (8%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	GLN	6.2
1	A	392	GLN	4.8
1	B	396	GLN	4.0
1	B	400	GLN	3.7
1	B	403	GLN	3.6
1	A	399	GLN	3.6
1	B	401	GLN	3.6
1	B	402	GLN	3.4
1	B	174	GLY	3.3
1	B	404	GLN	3.3
1	A	390	GLN	3.0
1	A	2	ILE	3.0
1	A	419	GLN	2.9
1	A	403	GLN	2.8
1	B	399	GLN	2.6
1	A	400	GLN	2.5
1	B	393	GLN	2.5
1	B	36	THR	2.4
1	C	328	GLU	2.3
1	C	141	ALA	2.3
1	A	401	GLN	2.2
1	B	172	GLU	2.2
1	B	34	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	173	ASN	2.1
1	C	177	ASP	2.0
1	B	392	GLN	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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	CA	C	505	1/1	0.88	0.46	7.52	78,78,78,78	0
3	CA	A	506	1/1	0.92	0.43	4.58	83,83,83,83	0
2	ZN	B	502	1/1	0.96	0.23	-	92,92,92,92	0
2	ZN	A	502	1/1	0.96	0.24	-	75,75,75,75	0
3	CA	A	505	1/1	0.86	0.72	-	73,73,73,73	1
2	ZN	A	503	1/1	0.94	0.28	-	103,103,103,103	0
3	CA	C	506	1/1	0.75	0.46	-	70,70,70,70	1
2	ZN	B	501	1/1	0.92	0.23	-	102,102,102,102	1
3	CA	B	503	1/1	0.89	0.24	-	86,86,86,86	0
3	CA	C	504	1/1	0.94	0.26	-	94,94,94,94	0
3	CA	C	503	1/1	0.86	0.28	-	94,94,94,94	0
3	CA	A	507	1/1	0.76	0.37	-	80,80,80,80	1
3	CA	A	508	1/1	0.89	0.22	-	105,105,105,105	0
2	ZN	C	501	1/1	0.96	0.27	-	73,73,73,73	0
2	ZN	A	501	1/1	0.81	0.27	-	108,108,108,108	0
3	CA	A	504	1/1	0.73	0.32	-	73,73,73,73	1
2	ZN	C	502	1/1	0.98	0.28	-	96,96,96,96	0

## 6.5 Other polymers

There are no such residues in this entry.