Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 09:32 PM EDT

PDB ID	:	3IOT
Title	:	Huntingtin amino-terminal region with 17 Gln residues - crystal C92-b
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

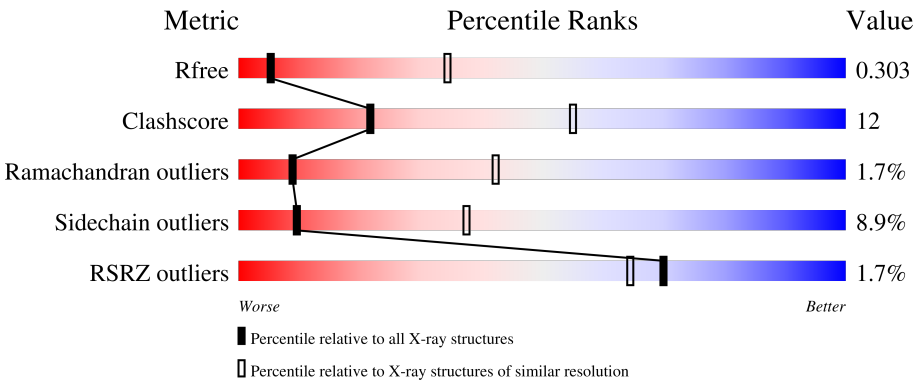
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 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	449	.% 63% 20% • 14%
1	B	449	2% 67% 19% • 11%
1	C	449	2% 67% 22% • • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9195 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 periplasmic protein,Huntingtin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	2967	1911	482	566	8	33	0	0
1	B	399	3044	1952	497	587	8	12	0	0
1	C	418	3166	2038	516	604	8	18	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	-	linker	UNP P0AEX9
A	360	ALA	-	linker	UNP P0AEX9
A	361	LEU	-	linker	UNP P0AEX9
A	362	ALA	-	linker	UNP P0AEX9
A	363	ALA	-	linker	UNP P0AEX9
A	364	ALA	-	linker	UNP P0AEX9
A	365	GLN	-	linker	UNP P0AEX9
A	366	THR	-	linker	UNP P0AEX9
A	367	ASN	-	linker	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
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	UNP P42858
A	432	SER	-	expression tag	UNP P42858
A	433	TYR	-	expression tag	UNP P42858
A	434	GLN	-	expression tag	UNP P42858
A	435	ILE	-	expression tag	UNP P42858
A	436	THR	-	expression tag	UNP P42858
A	437	ALA	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	expression tag	UNP P42858
A	439	LYS	-	expression tag	UNP P42858
A	440	LEU	-	expression tag	UNP P42858
A	441	GLY	-	expression tag	UNP P42858
A	442	THR	-	expression tag	UNP P42858
A	443	GLY	-	expression tag	UNP P42858
A	444	ARG	-	expression tag	UNP P42858
A	445	ARG	-	expression tag	UNP P42858
A	446	PHE	-	expression tag	UNP P42858
A	447	THR	-	expression tag	UNP P42858
A	448	THR	-	expression tag	UNP P42858
A	449	SER	-	expression tag	UNP P42858
B	359	ALA	-	linker	UNP P0AEX9
B	360	ALA	-	linker	UNP P0AEX9
B	361	LEU	-	linker	UNP P0AEX9
B	362	ALA	-	linker	UNP P0AEX9
B	363	ALA	-	linker	UNP P0AEX9
B	364	ALA	-	linker	UNP P0AEX9
B	365	GLN	-	linker	UNP P0AEX9
B	366	THR	-	linker	UNP P0AEX9
B	367	ASN	-	linker	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
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	UNP P42858
B	432	SER	-	expression tag	UNP P42858
B	433	TYR	-	expression tag	UNP P42858
B	434	GLN	-	expression tag	UNP P42858
B	435	ILE	-	expression tag	UNP P42858
B	436	THR	-	expression tag	UNP P42858
B	437	ALA	-	expression tag	UNP P42858
B	438	GLY	-	expression tag	UNP P42858
B	439	LYS	-	expression tag	UNP P42858
B	440	LEU	-	expression tag	UNP P42858
B	441	GLY	-	expression tag	UNP P42858
B	442	THR	-	expression tag	UNP P42858
B	443	GLY	-	expression tag	UNP P42858
B	444	ARG	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	ARG	-	expression tag	UNP P42858
B	446	PHE	-	expression tag	UNP P42858
B	447	THR	-	expression tag	UNP P42858
B	448	THR	-	expression tag	UNP P42858
B	449	SER	-	expression tag	UNP P42858
C	359	ALA	-	linker	UNP P0AEX9
C	360	ALA	-	linker	UNP P0AEX9
C	361	LEU	-	linker	UNP P0AEX9
C	362	ALA	-	linker	UNP P0AEX9
C	363	ALA	-	linker	UNP P0AEX9
C	364	ALA	-	linker	UNP P0AEX9
C	365	GLN	-	linker	UNP P0AEX9
C	366	THR	-	linker	UNP P0AEX9
C	367	ASN	-	linker	UNP P0AEX9
C	368	ALA	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
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	UNP P42858
C	432	SER	-	expression tag	UNP P42858
C	433	TYR	-	expression tag	UNP P42858
C	434	GLN	-	expression tag	UNP P42858
C	435	ILE	-	expression tag	UNP P42858
C	436	THR	-	expression tag	UNP P42858
C	437	ALA	-	expression tag	UNP P42858
C	438	GLY	-	expression tag	UNP P42858
C	439	LYS	-	expression tag	UNP P42858
C	440	LEU	-	expression tag	UNP P42858
C	441	GLY	-	expression tag	UNP P42858
C	442	THR	-	expression tag	UNP P42858
C	443	GLY	-	expression tag	UNP P42858
C	444	ARG	-	expression tag	UNP P42858
C	445	ARG	-	expression tag	UNP P42858
C	446	PHE	-	expression tag	UNP P42858
C	447	THR	-	expression tag	UNP P42858
C	448	THR	-	expression tag	UNP P42858
C	449	SER	-	expression tag	UNP P42858

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

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

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

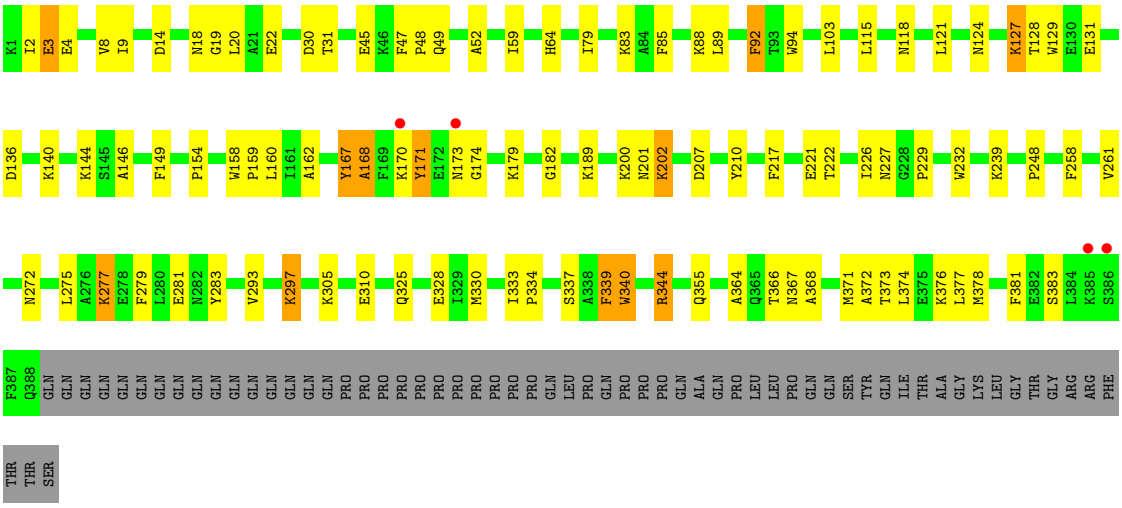
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	5	5	5	0	0
			Total	Ca		
3	B	2	2	2	0	0
			Total	Ca		
3	C	2	2	2	0	0

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.

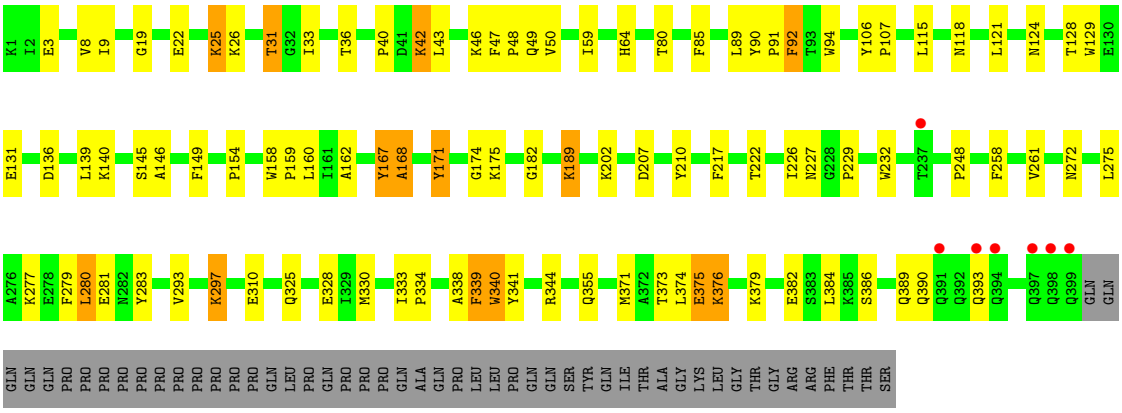
• Molecule 1: Maltose-binding periplasmic protein,Huntingtin

Chain A:



• Molecule 1: Maltose-binding periplasmic protein,Huntingtin

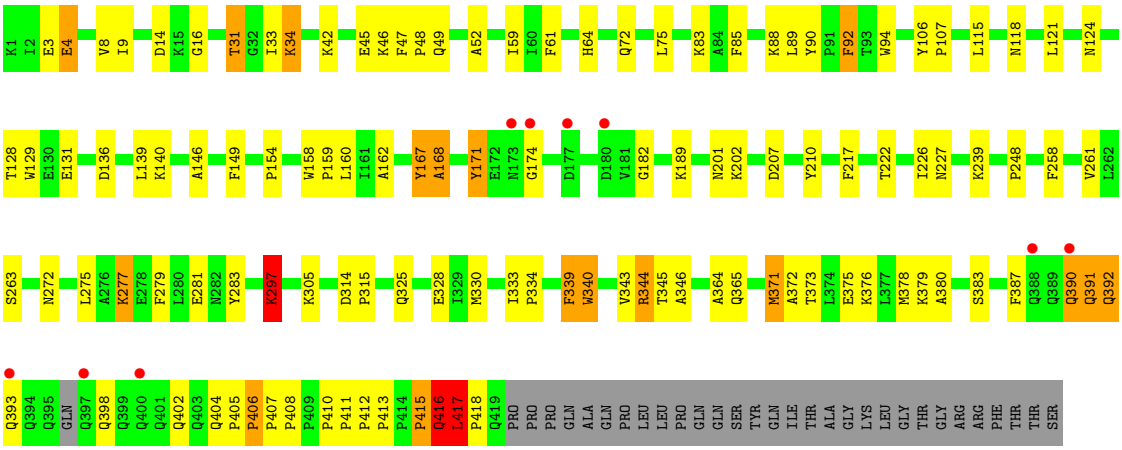
Chain B:



• Molecule 1: Maltose-binding periplasmic protein,Huntingtin

Chain C:

2%
67%
22%
7%


K1 I2 E3 E4 V8 I9 D14 K15 G16 T31 G32 I33 K34 K42 E45 K46 F47 P48 Q49 A52 I59 I60 F61 H64 Q72 L75 K83 A84 F85 K88 L89 Y90 P91 F92 T93 W94 Y106 P107 L115 N118 L121 N124
T128 W129 E130 E131 D136 L139 K140 A146 F149 P154 W158 P159 L160 I161 A162 Y167 A168 Y171 E172 N173 G174 D177 D180 V181 G182 K189 N201 K202 D207 Y210 F217 T222 I226 N227 K239 P248 F258 V261 L262
S263 N272 L275 A276 K277 E278 F279 L280 E281 N282 Y283 K287 K305 D314 P315 Q325 E328 I329 M330 I333 P334 F339 W340 V343 R344 T345 A346 A364 Q365 M371 A372 T373 L374 E375 K376 L377 M378 K379 A380 S383 F387 Q388 Q389 Q390 Q391 Q392
Q393 Q394 Q395 GLN Q397 Q398 Q399 Q400 Q401 Q402 Q403 Q404 P405 P406 P407 P408 P409 P410 P411 P412 P413 P414 P415 Q416 L417 P418 Q419 PRO PRO PRO GLN ALA GLN PRO LEU LEU PRO GLN GLN SER TYR GLN ILE THR ALA GLY LYS LEU GLY THR GLY ARG ARG PHE THR THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.25Å 101.36Å 137.03Å 90.00° 91.83° 90.00°	Depositor
Resolution (Å)	37.36 – 3.50 29.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	69.2 (37.36-3.50) 69.3 (29.87-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.247 , 0.295 0.258 , 0.303	Depositor DCC
R_{free} test set	975 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9195	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 (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	0.61	7/3038 (0.2%)	0.65	7/4130 (0.2%)
1	B	0.53	4/3115 (0.1%)	0.62	6/4238 (0.1%)
1	C	0.53	2/3248 (0.1%)	0.71	9/4430 (0.2%)
All	All	0.56	13/9401 (0.1%)	0.66	22/12798 (0.2%)

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	C	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	LYS	CB-CG	14.45	1.91	1.52
1	C	392	GLN	C-O	-13.95	0.96	1.23
1	B	26	LYS	CB-CG	11.75	1.84	1.52
1	A	378	MET	CB-CG	9.58	1.81	1.51
1	A	88	LYS	CB-CG	-8.86	1.28	1.52
1	B	175	LYS	CB-CG	-8.36	1.29	1.52
1	A	140	LYS	CB-CG	-7.70	1.31	1.52
1	C	391	GLN	C-O	7.04	1.36	1.23
1	B	310	GLU	CD-OE2	6.39	1.32	1.25
1	A	310	GLU	CD-OE1	5.66	1.31	1.25
1	B	25	LYS	CB-CG	-5.35	1.38	1.52
1	A	376	LYS	CB-CG	-5.33	1.38	1.52
1	A	221	GLU	CB-CG	-5.30	1.42	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	391	GLN	O-C-N	-18.06	93.80	122.70
1	C	46	LYS	CA-CB-CG	-14.82	80.79	113.40
1	A	378	MET	CA-CB-CG	-12.49	92.07	113.30
1	B	297	LYS	CD-CE-NZ	-11.26	85.80	111.70
1	A	297	LYS	CD-CE-NZ	-10.15	88.36	111.70
1	A	173	ASN	CB-CA-C	-9.42	91.56	110.40
1	C	46	LYS	CB-CG-CD	-8.87	88.53	111.60
1	C	392	GLN	O-C-N	8.53	136.35	122.70
1	B	26	LYS	CA-CB-CG	-8.12	95.54	113.40
1	C	297	LYS	CD-CE-NZ	-7.20	95.14	111.70
1	C	390	GLN	O-C-N	7.08	134.02	122.70
1	C	417	LEU	CA-CB-CG	6.91	131.18	115.30
1	C	392	GLN	CA-C-O	-6.81	105.81	120.10
1	A	144	LYS	CB-CG-CD	6.57	128.69	111.60
1	A	179	LYS	CB-CG-CD	-6.42	94.92	111.60
1	B	25	LYS	CB-CG-CD	-5.93	96.17	111.60
1	B	26	LYS	CB-CG-CD	-5.75	96.64	111.60
1	A	378	MET	CB-CG-SD	5.50	128.90	112.40
1	A	376	LYS	CB-CG-CD	5.33	125.47	111.60
1	B	341	TYR	OH-CZ-CE2	-5.22	106.00	120.10
1	B	189	LYS	CD-CE-NZ	5.09	123.42	111.70
1	C	390	GLN	CA-C-O	-5.09	109.40	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	391	GLN	Mainchain

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	2967	0	2908	64	0
1	B	3044	0	2946	65	0
1	C	3166	0	3062	90	0
2	A	3	0	0	0	1
2	B	3	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
3	A	5	0	0	0	1
3	B	2	0	0	0	0
3	C	2	0	0	0	0
All	All	9195	0	8916	213	2

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 12.

All (213) 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:C:404:GLN:C	1:C:406:PRO:HD3	1.53	1.28
1:C:404:GLN:O	1:C:406:PRO:HD3	1.45	1.16
1:C:404:GLN:O	1:C:406:PRO:CD	1.94	1.15
1:C:416:GLN:HA	1:C:417:LEU:CB	1.83	1.09
1:C:416:GLN:HA	1:C:417:LEU:HB3	1.49	0.95
1:B:210:TYR:HE1	1:B:227:ASN:HD21	1.14	0.93
1:A:210:TYR:HE1	1:A:227:ASN:HD21	1.17	0.91
1:C:210:TYR:HE1	1:C:227:ASN:HD21	1.19	0.91
1:C:404:GLN:O	1:C:406:PRO:HD2	1.72	0.89
1:C:416:GLN:HA	1:C:417:LEU:HB2	1.53	0.89
1:C:404:GLN:C	1:C:406:PRO:CD	2.40	0.84
1:C:417:LEU:H	1:C:418:PRO:HD3	1.42	0.84
1:C:416:GLN:CA	1:C:417:LEU:HB3	2.08	0.82
1:B:340:TRP:HA	1:B:340:TRP:CE3	2.16	0.80
1:C:340:TRP:CE3	1:C:340:TRP:HA	2.17	0.80
1:A:340:TRP:HA	1:A:340:TRP:CE3	2.18	0.79
1:B:210:TYR:HE1	1:B:227:ASN:ND2	1.82	0.77
1:C:416:GLN:CA	1:C:417:LEU:CB	2.64	0.76
1:A:210:TYR:HE1	1:A:227:ASN:ND2	1.84	0.76
1:C:339:PHE:CD1	1:C:339:PHE:C	2.61	0.74
1:B:339:PHE:CD1	1:B:339:PHE:C	2.61	0.74
1:C:210:TYR:HE1	1:C:227:ASN:ND2	1.86	0.73
1:C:167:TYR:HD2	1:C:167:TYR:O	1.71	0.73
1:B:167:TYR:HD2	1:B:167:TYR:O	1.72	0.72
1:A:339:PHE:CD1	1:A:339:PHE:C	2.62	0.72
1:B:375:GLU:O	1:B:379:LYS:HG2	1.90	0.71
1:A:167:TYR:HD2	1:A:167:TYR:O	1.73	0.71
1:C:128:THR:HG22	1:C:131:GLU:HG2	1.71	0.70
1:C:340:TRP:HA	1:C:340:TRP:HE3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:PHE:C	1:C:339:PHE:HD1	1.95	0.68
1:B:128:THR:HG22	1:B:131:GLU:HG2	1.76	0.68
1:A:339:PHE:C	1:A:339:PHE:HD1	1.97	0.68
1:B:340:TRP:HA	1:B:340:TRP:HE3	1.55	0.68
1:A:355:GLN:HA	1:C:52:ALA:O	1.94	0.68
1:B:339:PHE:C	1:B:339:PHE:HD1	1.96	0.68
1:A:128:THR:HG22	1:A:131:GLU:HG2	1.76	0.67
1:A:340:TRP:HA	1:A:340:TRP:HE3	1.58	0.67
1:C:346:ALA:HB2	1:C:364:ALA:HB2	1.78	0.66
1:C:14:ASP:O	1:C:297:LYS:HD3	1.96	0.65
1:A:168:ALA:HA	1:A:339:PHE:HE2	1.63	0.63
1:C:168:ALA:HA	1:C:339:PHE:HE2	1.64	0.63
1:B:9:ILE:HG12	1:B:59:ILE:HG12	1.81	0.63
1:B:168:ALA:HA	1:B:339:PHE:HE2	1.64	0.63
1:A:374:LEU:HD13	1:C:380:ALA:HB2	1.81	0.62
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.80	0.62
1:C:136:ASP:HA	1:C:146:ALA:HB2	1.81	0.62
1:B:167:TYR:CE2	1:B:182:GLY:HA3	2.35	0.61
1:B:136:ASP:HA	1:B:146:ALA:HB2	1.82	0.61
1:A:52:ALA:O	1:B:355:GLN:HA	2.00	0.61
1:A:171:TYR:CE1	1:A:174:GLY:HA2	2.36	0.60
1:C:371:MET:C	1:C:373:THR:H	2.05	0.60
1:A:377:LEU:HD22	1:B:373:THR:OG1	2.01	0.60
1:A:92:PHE:CE2	1:A:325:GLN:HG2	2.37	0.60
1:C:128:THR:CG2	1:C:131:GLU:HG2	2.31	0.59
1:C:129:TRP:CD1	1:C:248:PRO:HB2	2.37	0.59
1:C:31:THR:HB	1:C:33:ILE:HG12	1.83	0.59
1:C:417:LEU:H	1:C:418:PRO:CD	2.15	0.59
1:C:14:ASP:O	1:C:297:LYS:NZ	2.30	0.59
1:C:167:TYR:CE2	1:C:182:GLY:HA3	2.37	0.59
1:B:92:PHE:CE2	1:B:325:GLN:HG2	2.39	0.58
1:C:92:PHE:CE2	1:C:325:GLN:HG2	2.39	0.58
1:C:167:TYR:O	1:C:167:TYR:CD2	2.55	0.58
1:A:47:PHE:HB3	1:A:48:PRO:HD3	1.85	0.58
1:B:154:PRO:HG3	1:B:344:ARG:HA	1.86	0.57
1:A:167:TYR:CE2	1:A:182:GLY:HA3	2.39	0.57
1:B:171:TYR:HE1	1:B:174:GLY:H	1.52	0.57
1:B:42:LYS:HE3	1:B:42:LYS:HA	1.84	0.57
1:B:128:THR:CG2	1:B:131:GLU:HG2	2.34	0.57
1:C:154:PRO:HG3	1:C:344:ARG:HA	1.87	0.57
1:B:167:TYR:O	1:B:167:TYR:CD2	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HD3	1:A:128:THR:HB	1.86	0.57
1:A:171:TYR:HE1	1:A:174:GLY:H	1.52	0.56
1:A:368:ALA:O	1:A:372:ALA:HB2	2.05	0.56
1:A:154:PRO:HG3	1:A:344:ARG:HA	1.88	0.56
1:A:167:TYR:O	1:A:167:TYR:CD2	2.57	0.56
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.41	0.56
1:C:405:PRO:N	1:C:406:PRO:HD3	2.19	0.56
1:A:128:THR:CG2	1:A:131:GLU:HG2	2.35	0.56
1:B:92:PHE:HE2	1:B:325:GLN:HG2	1.71	0.56
1:C:92:PHE:HE2	1:C:325:GLN:HG2	1.71	0.55
1:A:217:PHE:HA	1:A:222:THR:HG22	1.89	0.55
1:A:366:THR:HG21	1:C:72:GLN:HE21	1.70	0.55
1:A:92:PHE:HE2	1:A:325:GLN:HG2	1.70	0.55
1:B:64:HIS:CD2	1:B:261:VAL:H	2.25	0.54
1:C:171:TYR:HE1	1:C:174:GLY:H	1.55	0.54
1:A:92:PHE:CD1	1:A:92:PHE:C	2.81	0.54
1:C:168:ALA:HA	1:C:339:PHE:CE2	2.43	0.53
1:A:129:TRP:CD1	1:A:248:PRO:HB2	2.44	0.53
1:C:417:LEU:N	1:C:418:PRO:HD3	2.17	0.53
1:B:217:PHE:HA	1:B:222:THR:HG22	1.91	0.53
1:B:140:LYS:HE3	1:B:145:SER:HA	1.91	0.52
1:A:14:ASP:O	1:A:297:LYS:HD3	2.09	0.52
1:B:92:PHE:CD1	1:B:92:PHE:C	2.82	0.52
1:B:64:HIS:HD2	1:B:261:VAL:H	1.57	0.52
1:B:376:LYS:HE3	1:B:376:LYS:HA	1.92	0.52
1:A:168:ALA:HA	1:A:339:PHE:CE2	2.43	0.52
1:C:171:TYR:CE1	1:C:174:GLY:HA2	2.45	0.52
1:C:217:PHE:HA	1:C:222:THR:HG22	1.91	0.52
1:C:92:PHE:CD1	1:C:92:PHE:C	2.82	0.52
1:B:171:TYR:CE1	1:B:174:GLY:HA2	2.45	0.51
1:A:339:PHE:HD1	1:A:340:TRP:N	2.09	0.51
1:A:19:GLY:HA3	1:A:293:VAL:HA	1.93	0.50
1:A:64:HIS:CD2	1:A:261:VAL:H	2.28	0.50
1:A:279:PHE:O	1:A:283:TYR:HB2	2.12	0.50
1:C:136:ASP:O	1:C:140:LYS:HG2	2.12	0.50
1:C:416:GLN:CB	1:C:417:LEU:HB3	2.41	0.50
1:A:64:HIS:HD2	1:A:261:VAL:H	1.59	0.49
1:A:89:LEU:HD12	1:A:94:TRP:CZ2	2.46	0.49
1:C:279:PHE:O	1:C:283:TYR:HB2	2.11	0.49
1:B:279:PHE:CD2	1:B:280:LEU:HD13	2.47	0.49
1:B:339:PHE:HD1	1:B:340:TRP:N	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:HIS:HE1	1:C:330:MET:O	1.93	0.49
1:C:258:PHE:CD2	1:C:330:MET:HG3	2.48	0.49
1:B:168:ALA:HA	1:B:339:PHE:CE2	2.44	0.49
1:C:201:ASN:O	1:C:202:LYS:HB2	2.13	0.49
1:A:207:ASP:N	1:A:207:ASP:OD1	2.46	0.49
1:B:258:PHE:CD2	1:B:330:MET:HG3	2.48	0.49
1:A:201:ASN:O	1:A:202:LYS:HB2	2.13	0.49
1:B:31:THR:HB	1:B:33:ILE:HG12	1.94	0.49
1:B:279:PHE:O	1:B:283:TYR:HB2	2.13	0.48
1:C:9:ILE:HG12	1:C:59:ILE:HG12	1.95	0.48
1:C:339:PHE:HD1	1:C:340:TRP:N	2.11	0.48
1:A:149:PHE:CD1	1:A:226:ILE:HD12	2.49	0.47
1:A:118:ASN:HB3	1:A:121:LEU:HD12	1.96	0.47
1:C:207:ASP:OD1	1:C:207:ASP:N	2.47	0.47
1:A:171:TYR:HE1	1:A:174:GLY:N	2.13	0.47
1:A:64:HIS:HE1	1:A:330:MET:O	1.98	0.47
1:C:64:HIS:CD2	1:C:261:VAL:H	2.33	0.47
1:B:149:PHE:CD1	1:B:226:ILE:HD12	2.49	0.47
1:B:390:GLN:HE22	1:C:345:THR:HA	1.80	0.47
1:A:277:LYS:O	1:A:281:GLU:HB2	2.15	0.47
1:B:64:HIS:HE1	1:B:330:MET:O	1.98	0.47
1:B:167:TYR:CD2	1:B:182:GLY:HA3	2.50	0.46
1:C:88:LYS:O	1:C:305:LYS:HG3	2.14	0.46
1:C:371:MET:O	1:C:373:THR:N	2.46	0.46
1:A:2:ILE:O	1:A:3:GLU:CB	2.63	0.46
1:B:89:LEU:HD12	1:B:94:TRP:CZ2	2.50	0.46
1:C:279:PHE:C	1:C:279:PHE:CD2	2.88	0.46
1:B:338:ALA:HB2	1:B:371:MET:HB2	1.98	0.46
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.51	0.46
1:B:47:PHE:HB3	1:B:48:PRO:HD3	1.97	0.46
1:B:207:ASP:OD1	1:B:207:ASP:N	2.48	0.46
1:C:167:TYR:CD2	1:C:182:GLY:HA3	2.51	0.46
1:A:272:ASN:HB3	1:A:275:LEU:HD12	1.97	0.45
1:C:415:PRO:O	1:C:416:GLN:HB3	2.17	0.45
1:A:9:ILE:HG23	1:A:59:ILE:HG13	1.99	0.45
1:A:167:TYR:CD2	1:A:182:GLY:HA3	2.51	0.45
1:C:64:HIS:HD2	1:C:261:VAL:H	1.65	0.45
1:A:364:ALA:HA	1:A:367:ASN:HB2	1.98	0.45
1:A:9:ILE:HG12	1:A:59:ILE:HG12	1.99	0.45
1:A:158:TRP:N	1:A:159:PRO:CD	2.79	0.45
1:C:404:GLN:N	1:C:405:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PHE:CD2	1:B:279:PHE:C	2.90	0.44
1:C:406:PRO:HD2	1:C:407:PRO:HD3	1.99	0.44
1:C:47:PHE:HB3	1:C:48:PRO:HD3	2.00	0.44
1:C:277:LYS:O	1:C:281:GLU:HB2	2.18	0.44
1:B:371:MET:HB3	1:B:374:LEU:HG	1.98	0.44
1:C:149:PHE:CD1	1:C:226:ILE:HD12	2.52	0.44
1:C:379:LYS:O	1:C:383:SER:N	2.50	0.44
1:A:279:PHE:CD2	1:A:279:PHE:C	2.91	0.44
1:C:34:LYS:HG2	1:C:34:LYS:O	2.18	0.44
1:B:158:TRP:N	1:B:159:PRO:CD	2.80	0.44
1:A:168:ALA:CA	1:A:339:PHE:HE2	2.29	0.43
1:A:85:PHE:CE2	1:A:281:GLU:HG2	2.53	0.43
1:A:154:PRO:HD3	1:A:344:ARG:HD3	2.00	0.43
1:B:386:SER:HA	1:B:389:GLN:HB2	2.00	0.43
1:C:85:PHE:CE2	1:C:281:GLU:HG2	2.52	0.43
1:C:168:ALA:CA	1:C:339:PHE:HE2	2.30	0.43
1:B:19:GLY:HA3	1:B:293:VAL:HA	1.99	0.43
1:B:118:ASN:HB3	1:B:121:LEU:HD12	2.00	0.43
1:B:272:ASN:HB3	1:B:275:LEU:HD12	2.00	0.43
1:C:411:PRO:HA	1:C:412:PRO:HD2	1.70	0.43
1:A:333:ILE:HB	1:A:334:PRO:HD2	2.01	0.43
1:B:40:PRO:HG2	1:B:43:LEU:HB3	2.01	0.43
1:B:171:TYR:HE1	1:B:174:GLY:N	2.17	0.43
1:C:158:TRP:CE2	1:C:162:ALA:HB2	2.54	0.43
1:C:90:TYR:CD1	1:C:305:LYS:HG2	2.53	0.43
1:C:4:GLU:H	1:C:272:ASN:HD21	1.66	0.42
1:A:258:PHE:CD2	1:A:330:MET:HG3	2.54	0.42
1:C:416:GLN:HB2	1:C:417:LEU:HB3	2.02	0.42
1:B:158:TRP:CE2	1:B:162:ALA:HB2	2.54	0.42
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.55	0.42
1:B:277:LYS:O	1:B:281:GLU:HB2	2.20	0.42
1:C:106:TYR:HA	1:C:107:PRO:HD3	1.92	0.42
1:C:118:ASN:HB3	1:C:121:LEU:HD12	2.00	0.42
1:B:85:PHE:CE2	1:B:281:GLU:HG2	2.54	0.42
1:C:16:GLY:CA	1:C:297:LYS:HB3	2.49	0.42
1:A:9:ILE:HG21	1:A:20:LEU:HD21	2.03	0.41
1:C:333:ILE:HB	1:C:334:PRO:HD2	2.02	0.41
1:C:89:LEU:HD12	1:C:94:TRP:CZ2	2.55	0.41
1:B:46:LYS:O	1:B:50:VAL:HG22	2.21	0.41
1:C:339:PHE:CE1	1:C:343:VAL:HG21	2.55	0.41
1:C:61:PHE:HA	1:C:263:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:HIS:CE1	1:C:330:MET:O	2.72	0.41
1:C:272:ASN:HB3	1:C:275:LEU:HD12	2.03	0.41
1:C:390:GLN:HA	1:C:393:GLN:HG2	2.03	0.41
1:A:171:TYR:CE1	1:A:174:GLY:CA	3.01	0.41
1:B:139:LEU:HD13	1:B:146:ALA:HA	2.02	0.41
1:C:139:LEU:HD13	1:C:146:ALA:HA	2.03	0.41
1:C:158:TRP:N	1:C:159:PRO:CD	2.84	0.41
1:C:167:TYR:CD2	1:C:167:TYR:C	2.94	0.41
1:C:314:ASP:HA	1:C:315:PRO:HD2	1.95	0.41
1:A:171:TYR:CZ	1:A:174:GLY:HA2	2.56	0.40
1:B:80:THR:O	1:B:277:LYS:NZ	2.54	0.40
1:A:79:ILE:HD11	1:A:103:LEU:HB3	2.03	0.40
1:A:18:ASN:O	1:A:22:GLU:HG2	2.20	0.40
1:B:90:TYR:HA	1:B:91:PRO:HD3	1.98	0.40
1:B:279:PHE:HD2	1:B:280:LEU:HD13	1.86	0.40
1:B:106:TYR:HA	1:B:107:PRO:HD3	1.92	0.40
1:C:375:GLU:OE2	1:C:375:GLU:HA	2.21	0.40
1:A:158:TRP:CE2	1:A:162:ALA:HB2	2.57	0.40
1:B:167:TYR:CD2	1:B:167:TYR:C	2.95	0.40
1:B:333:ILE:HB	1:B:334:PRO:HD2	2.03	0.40

All (2) 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)
2:A:502:ZN:ZN	2:B:503:ZN:ZN[3_455]	0.99	1.21
3:A:504:CA:CA	3:A:508:CA:CA[2_455]	1.40	0.80

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	386/449 (86%)	366 (95%)	16 (4%)	4 (1%)	15	54
1	B	397/449 (88%)	374 (94%)	20 (5%)	3 (1%)	19	58
1	C	414/449 (92%)	380 (92%)	21 (5%)	13 (3%)	4	30
All	All	1197/1347 (89%)	1120 (94%)	57 (5%)	20 (2%)	9	42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	B	3	GLU
1	C	3	GLU
1	C	415	PRO
1	C	417	LEU
1	A	168	ALA
1	B	168	ALA
1	C	168	ALA
1	C	372	ALA
1	C	416	GLN
1	A	4	GLU
1	C	4	GLU
1	C	398	GLN
1	A	202	LYS
1	C	402	GLN
1	C	406	PRO
1	C	410	PRO
1	B	202	LYS
1	C	413	PRO
1	C	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	298/363 (82%)	270 (91%)	28 (9%)	8	35
1	B	304/363 (84%)	280 (92%)	24 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	317/363 (87%)	287 (90%)	30 (10%)	8	34
All	All	919/1089 (84%)	837 (91%)	82 (9%)	9	37

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	30	ASP
1	A	31	THR
1	A	45	GLU
1	A	49	GLN
1	A	83	LYS
1	A	92	PHE
1	A	115	LEU
1	A	124	ASN
1	A	127	LYS
1	A	160	LEU
1	A	167	TYR
1	A	170	LYS
1	A	171	TYR
1	A	189	LYS
1	A	200	LYS
1	A	239	LYS
1	A	277	LYS
1	A	305	LYS
1	A	328	GLU
1	A	337	SER
1	A	339	PHE
1	A	340	TRP
1	A	344	ARG
1	A	371	MET
1	A	373	THR
1	A	381	PHE
1	A	383	SER
1	B	8	VAL
1	B	22	GLU
1	B	25	LYS
1	B	31	THR
1	B	36	THR
1	B	42	LYS
1	B	49	GLN
1	B	92	PHE

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Mol	Chain	Res	Type
1	B	115	LEU
1	B	124	ASN
1	B	160	LEU
1	B	167	TYR
1	B	171	TYR
1	B	189	LYS
1	B	280	LEU
1	B	297	LYS
1	B	328	GLU
1	B	339	PHE
1	B	340	TRP
1	B	375	GLU
1	B	376	LYS
1	B	382	GLU
1	B	384	LEU
1	B	393	GLN
1	C	8	VAL
1	C	31	THR
1	C	34	LYS
1	C	42	LYS
1	C	45	GLU
1	C	49	GLN
1	C	75	LEU
1	C	83	LYS
1	C	92	PHE
1	C	115	LEU
1	C	124	ASN
1	C	160	LEU
1	C	167	TYR
1	C	171	TYR
1	C	189	LYS
1	C	239	LYS
1	C	277	LYS
1	C	297	LYS
1	C	328	GLU
1	C	339	PHE
1	C	340	TRP
1	C	344	ARG
1	C	365	GLN
1	C	371	MET
1	C	376	LYS
1	C	378	MET

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Mol	Chain	Res	Type
1	C	387	PHE
1	C	392	GLN
1	C	416	GLN
1	C	417	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	64	HIS
1	A	201	ASN
1	A	218	ASN
1	A	282	ASN
1	B	18	ASN
1	B	64	HIS
1	B	201	ASN
1	B	218	ASN
1	B	390	GLN
1	B	393	GLN
1	B	394	GLN
1	C	18	ASN
1	C	64	HIS
1	C	72	GLN
1	C	201	ASN
1	C	218	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 18 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	388/449 (86%)	-0.45	4 (1%)	82	77	55, 55, 63, 88	24 (6%)
1	B	399/449 (88%)	-0.31	7 (1%)	68	62	55, 55, 87, 87	37 (9%)
1	C	418/449 (93%)	-0.36	9 (2%)	62	56	55, 55, 87, 88	43 (10%)
All	All	1205/1347 (89%)	-0.37	20 (1%)	70	64	55, 55, 87, 88	104 (8%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	397	GLN	4.1
1	B	397	GLN	3.4
1	B	399	GLN	3.2
1	C	388	GLN	3.0
1	B	391	GLN	2.8
1	B	398	GLN	2.8
1	C	390	GLN	2.6
1	A	386	SER	2.6
1	C	173	ASN	2.6
1	A	385	LYS	2.6
1	C	400	GLN	2.6
1	C	180	ASP	2.5
1	B	394	GLN	2.5
1	A	170	LYS	2.4
1	C	174	GLY	2.3
1	B	237	THR	2.3
1	C	177	ASP	2.2
1	C	393	GLN	2.1
1	B	393	GLN	2.1
1	A	173	ASN	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	ZN	C	501	1/1	0.85	0.11	132,132,132,132	0
3	CA	A	507	1/1	0.85	0.18	87,87,87,87	0
3	CA	B	504	1/1	0.85	0.32	70,70,70,70	0
2	ZN	C	502	1/1	0.87	0.12	103,103,103,103	0
3	CA	C	504	1/1	0.87	0.42	96,96,96,96	0
2	ZN	C	503	1/1	0.89	0.07	167,167,167,167	0
3	CA	C	505	1/1	0.89	0.29	75,75,75,75	0
2	ZN	A	503	1/1	0.93	0.12	98,98,98,98	0
2	ZN	B	501	1/1	0.94	0.20	98,98,98,98	0
2	ZN	B	503	1/1	0.95	0.12	110,110,110,110	0
2	ZN	A	502	1/1	0.95	0.12	99,99,99,99	0
3	CA	B	505	1/1	0.96	0.38	86,86,86,86	0
3	CA	A	506	1/1	0.97	0.28	62,62,62,62	0
3	CA	A	508	1/1	0.97	0.14	80,80,80,80	0
2	ZN	B	502	1/1	0.98	0.27	78,78,78,78	0
3	CA	A	505	1/1	0.98	0.28	32,32,32,32	0
2	ZN	A	501	1/1	0.98	0.16	76,76,76,76	0
3	CA	A	504	1/1	0.99	0.16	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.