



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:27 AM UTC

PDB ID : 3IOU / pdb_00003iou
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 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

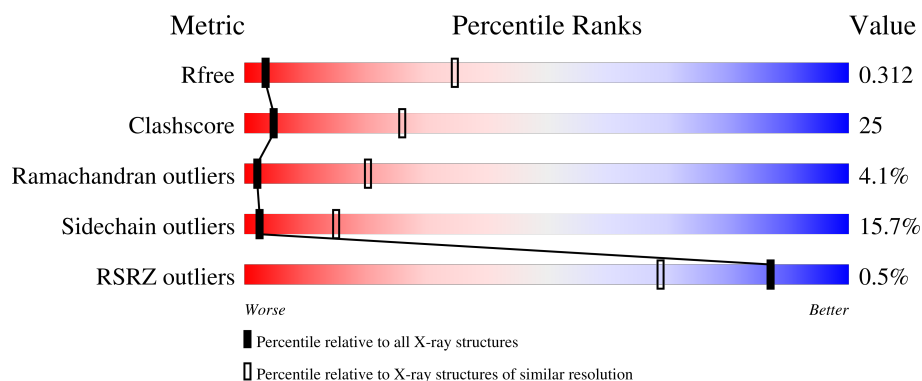
1 Overall quality at a glance

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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 $\leq 5\%$. 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	45% 34% 9% • 10%
1	B	449	47% 31% 7% • 13%
1	C	449	51% 32% 6% 11%

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 periplasmic protein,Huntingtin.

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 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
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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 (CCD ID: ZN) (formula: Zn).

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

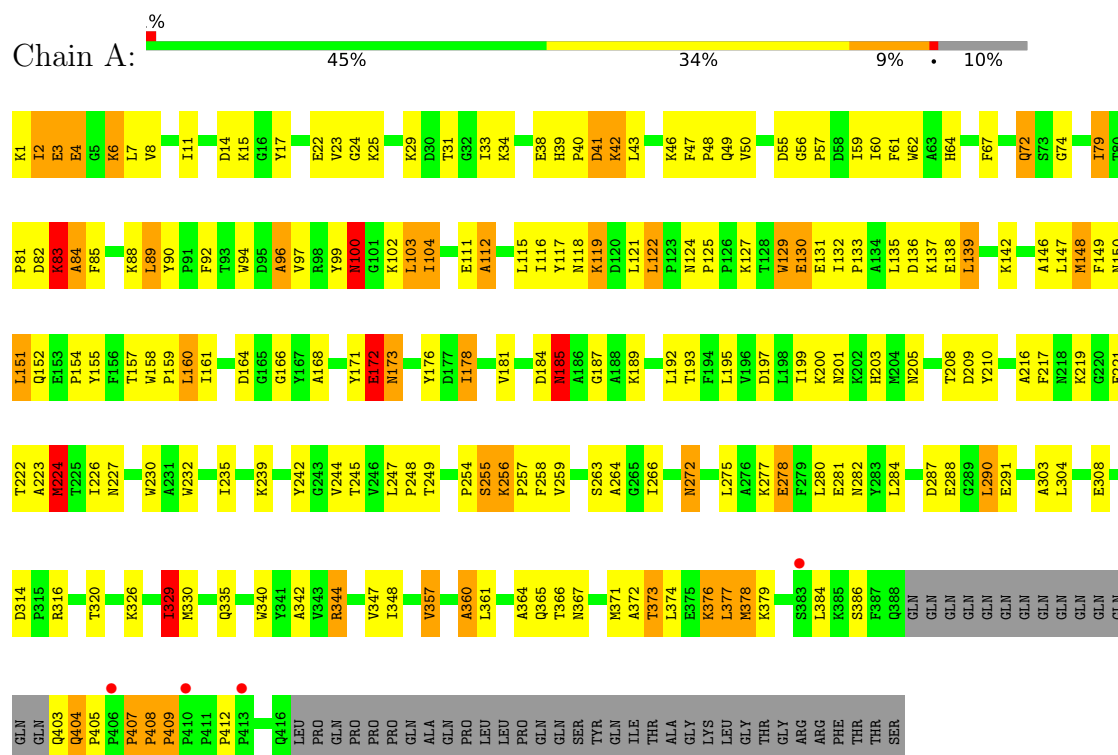
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

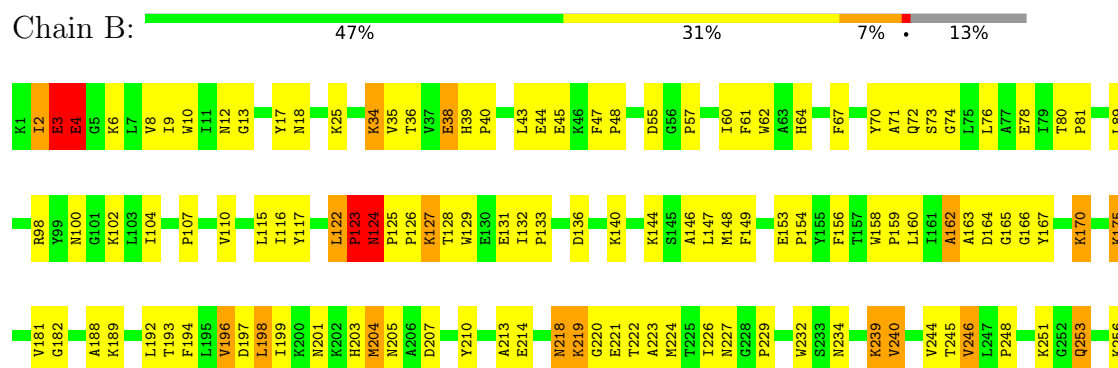
3 Residue-property plots [i](#)

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



- Molecule 1: Maltose-binding periplasmic protein,Huntingtin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.79Å 99.79Å 140.50Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	40.00 – 3.70 40.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	86.3 (40.00-3.70) 69.8 (40.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.272 , 0.299 0.286 , 0.312	Depositor DCC
R_{free} test set	1045 reflections (5.07%)	wwPDB-VP
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 , 101.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.52	2/3141 (0.1%)	0.98	14/4277 (0.3%)
1	B	0.47	0/3072	0.92	10/4171 (0.2%)
1	C	0.45	0/3085	0.89	8/4194 (0.2%)
All	All	0.48	2/9298 (0.0%)	0.93	32/12642 (0.3%)

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	224	MET	SD-CE	7.44	1.98	1.79
1	A	408	PRO	N-CD	5.56	1.55	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	PRO	N-CA-C	13.81	127.55	110.70
1	B	3	GLU	N-CA-C	8.87	122.64	109.24
1	A	104	ILE	N-CA-C	7.73	119.56	112.29
1	A	3	GLU	CA-C-N	7.58	135.35	121.70
1	A	3	GLU	C-N-CA	7.58	135.35	121.70
1	A	407	PRO	CA-C-N	-6.57	113.62	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	PRO	C-N-CA	-6.57	113.62	120.38
1	A	408	PRO	CB-CA-C	6.26	118.56	110.92
1	B	123	PRO	CA-C-N	6.20	132.85	121.70
1	B	123	PRO	C-N-CA	6.20	132.85	121.70
1	B	124	ASN	CA-C-N	6.17	126.73	120.38
1	B	124	ASN	C-N-CA	6.17	126.73	120.38
1	C	333	ILE	N-CA-CB	-5.91	102.94	111.21
1	C	153	GLU	CA-C-N	5.83	127.12	119.84
1	C	153	GLU	C-N-CA	5.83	127.12	119.84
1	A	83	LYS	N-CA-C	-5.75	94.89	111.00
1	A	405	PRO	N-CA-C	5.74	117.71	110.70
1	A	185	ASN	N-CA-C	5.73	117.30	110.19
1	B	220	GLY	N-CA-C	-5.47	107.65	115.64
1	A	124	ASN	CA-C-N	5.44	125.98	120.38
1	A	124	ASN	C-N-CA	5.44	125.98	120.38
1	B	4	GLU	N-CA-C	5.42	122.36	110.80
1	A	96	ALA	N-CA-C	-5.41	107.69	114.56
1	C	124	ASN	CA-C-N	5.37	123.58	119.66
1	C	124	ASN	C-N-CA	5.37	123.58	119.66
1	C	56	GLY	CA-C-N	5.25	125.16	119.85
1	C	56	GLY	C-N-CA	5.25	125.16	119.85
1	B	153	GLU	CA-C-N	5.13	124.58	119.24
1	B	153	GLU	C-N-CA	5.13	124.58	119.24
1	B	245	THR	N-CA-C	5.09	116.55	108.96
1	C	388	GLN	N-CA-C	-5.07	107.22	113.41
1	A	14	ASP	N-CA-C	-5.07	107.77	114.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	408	PRO	CA

All (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
1	B	2	ILE	Peptide
1	B	3	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	366	THR	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	194	1
1	B	2998	0	2967	142	0
1	C	3016	0	2913	135	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	456	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 25.

All (456) 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
1:A:147:LEU:HB2	1:A:224:MET:CE	1.68	1.22
1:A:2:ILE:HB	1:A:3:GLU:HA	1.19	1.14
1:A:3:GLU:HB2	1:A:4:GLU:CB	1.78	1.12
1:A:129:TRP:CH2	1:A:160:LEU:CG	2.36	1.09
1:A:3:GLU:HB2	1:A:4:GLU:HB2	1.17	1.08
1:A:3:GLU:HB3	1:A:4:GLU:HB2	1.35	1.07
1:A:147:LEU:HB2	1:A:224:MET:HE1	1.40	1.01
1:B:379:LYS:HE3	1:B:379:LYS:HA	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ASN:HA	1:B:43:LEU:HD21	1.46	0.98
1:B:257:PRO:HD2	1:B:327:GLY:HA2	1.44	0.97
1:C:247:LEU:H	1:C:247:LEU:HD23	1.29	0.95
1:A:133:PRO:HA	1:A:203:HIS:CD2	2.00	0.95
1:A:64:HIS:HE1	1:A:330:MET:O	1.49	0.92
1:B:62:TRP:HB3	1:B:67:PHE:HE1	1.35	0.92
1:A:152:GLN:HG3	1:A:209:ASP:HB3	1.51	0.92
1:A:72:GLN:CG	1:A:99:TYR:OH	2.18	0.91
1:B:123:PRO:HB2	1:B:124:ASN:CB	2.01	0.90
1:C:147:LEU:HD11	1:C:226:ILE:HD11	1.54	0.90
1:B:363:ALA:O	1:B:367:ASN:HB2	1.72	0.90
1:C:277:LYS:O	1:C:281:GLU:CG	2.20	0.89
1:A:147:LEU:HD13	1:A:224:MET:SD	2.13	0.89
1:A:64:HIS:CE1	1:A:330:MET:O	2.26	0.88
1:A:129:TRP:CZ3	1:A:160:LEU:CG	2.56	0.88
1:A:272:ASN:H	1:A:272:ASN:HD22	1.19	0.88
1:C:277:LYS:O	1:C:281:GLU:HG3	1.74	0.87
1:A:72:GLN:HG3	1:A:99:TYR:OH	1.74	0.87
1:A:147:LEU:HB2	1:A:224:MET:SD	2.13	0.86
1:B:246:VAL:HB	1:B:322:GLU:OE1	1.73	0.86
1:A:133:PRO:HA	1:A:203:HIS:NE2	1.91	0.85
1:A:372:ALA:O	1:A:376:LYS:HG3	1.75	0.85
1:B:288:GLU:HA	1:B:291:GLU:HB3	1.58	0.85
1:A:147:LEU:N	1:A:224:MET:HE3	1.92	0.85
1:B:123:PRO:HB2	1:B:124:ASN:HB3	1.60	0.84
1:A:82:ASP:HA	1:A:83:LYS:HB2	1.60	0.83
1:A:146:ALA:C	1:A:224:MET:HE3	2.01	0.83
1:A:335:GLN:HE21	1:A:376:LYS:HE3	1.41	0.83
1:A:2:ILE:HB	1:A:3:GLU:CA	2.06	0.82
1:B:380:ALA:HB2	1:C:370:ALA:HB1	1.61	0.81
1:A:147:LEU:CB	1:A:224:MET:CE	2.56	0.81
1:C:149:PHE:CD1	1:C:226:ILE:HG12	2.16	0.80
1:A:373:THR:O	1:A:377:LEU:HB3	1.81	0.79
1:C:247:LEU:HD23	1:C:247:LEU:N	1.98	0.79
1:B:62:TRP:HB3	1:B:67:PHE:CE1	2.17	0.78
1:A:136:ASP:HB3	1:A:203:HIS:HD2	1.49	0.76
1:A:377:LEU:HD12	1:B:374:LEU:HD21	1.66	0.76
1:C:277:LYS:O	1:C:281:GLU:HG2	1.86	0.76
1:B:147:LEU:HD11	1:B:226:ILE:HD12	1.66	0.76
1:B:304:LEU:H	1:B:304:LEU:HD12	1.50	0.75
1:A:378:MET:HE2	1:A:378:MET:HA	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HD11	1:C:226:ILE:CD1	2.17	0.74
1:A:129:TRP:CH2	1:A:160:LEU:CB	2.71	0.74
1:A:384:LEU:HA	1:B:341:TYR:OH	1.87	0.74
1:A:129:TRP:CH2	1:A:160:LEU:HB2	2.21	0.74
1:C:149:PHE:HD1	1:C:226:ILE:HG12	1.50	0.73
1:A:129:TRP:CZ3	1:A:160:LEU:CD1	2.72	0.73
1:C:94:TRP:HB3	1:C:98:ARG:HH22	1.53	0.72
1:B:162:ALA:O	1:B:164:ASP:N	2.22	0.72
1:C:285:LEU:HD12	1:C:285:LEU:O	1.88	0.72
1:A:278:GLU:O	1:A:282:ASN:HB2	1.89	0.72
1:B:379:LYS:HB2	1:B:379:LYS:NZ	2.04	0.72
1:A:38:GLU:C	1:A:40:PRO:HD3	2.15	0.71
1:A:377:LEU:CD1	1:B:374:LEU:HD21	2.19	0.71
1:A:72:GLN:HG2	1:A:99:TYR:OH	1.87	0.71
1:A:129:TRP:CZ2	1:A:160:LEU:HG	2.19	0.71
1:B:380:ALA:HB2	1:C:370:ALA:CB	2.20	0.71
1:A:129:TRP:HH2	1:A:160:LEU:HB2	1.54	0.71
1:C:85:PHE:CZ	1:C:285:LEU:HD23	2.26	0.70
1:A:129:TRP:O	1:A:131:GLU:N	2.25	0.69
1:B:132:ILE:N	1:B:133:PRO:HD2	2.08	0.69
1:A:373:THR:OG1	1:C:377:LEU:HD11	1.93	0.69
1:C:346:ALA:HA	1:C:360:ALA:HB1	1.73	0.69
1:B:89:LEU:HD13	1:B:107:PRO:HG2	1.72	0.68
1:C:242:TYR:OH	1:C:316:ARG:NH1	2.26	0.68
1:A:136:ASP:HB3	1:A:203:HIS:CD2	2.28	0.68
1:A:287:ASP:O	1:A:291:GLU:HB2	1.93	0.68
1:A:374:LEU:O	1:A:378:MET:HB2	1.93	0.68
1:A:129:TRP:CD1	1:A:248:PRO:HB2	2.28	0.68
1:A:344:ARG:O	1:A:348:ILE:HG12	1.94	0.68
1:B:149:PHE:H	1:B:204:MET:HE3	1.60	0.67
1:B:12:ASN:HB2	1:B:62:TRP:HZ3	1.59	0.67
1:C:288:GLU:H	1:C:288:GLU:CD	2.02	0.67
1:C:199:ILE:HD11	1:C:206:ALA:HA	1.76	0.66
1:A:147:LEU:CB	1:A:224:MET:HE1	2.22	0.66
1:C:9:ILE:HA	1:C:59:ILE:HG23	1.77	0.66
1:C:285:LEU:HD12	1:C:304:LEU:HD22	1.78	0.65
1:A:82:ASP:O	1:A:85:PHE:HB3	1.96	0.65
1:C:85:PHE:HZ	1:C:285:LEU:HD23	1.60	0.65
1:C:247:LEU:HD21	1:C:323:ASN:CG	2.21	0.65
1:C:109:ALA:HB3	1:C:262:LEU:HB3	1.78	0.64
1:A:367:ASN:O	1:A:371:MET:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:HIS:CD2	1:B:261:VAL:H	2.16	0.64
1:C:247:LEU:HD11	1:C:257:PRO:HG3	1.80	0.64
1:A:342:ALA:HB2	1:A:367:ASN:HB3	1.66	0.64
1:A:147:LEU:CD1	1:A:224:MET:SD	2.85	0.64
1:A:210:TYR:HH	1:A:230:TRP:CD1	2.16	0.63
1:A:272:ASN:H	1:A:272:ASN:ND2	1.93	0.63
1:A:83:LYS:H	1:A:85:PHE:H	1.46	0.63
1:C:225:THR:C	1:C:226:ILE:HD13	2.24	0.63
1:C:280:LEU:HA	1:C:284:LEU:HB3	1.81	0.63
1:A:43:LEU:HD13	1:A:60:ILE:HD11	1.80	0.63
1:A:133:PRO:CA	1:A:203:HIS:NE2	2.61	0.63
1:B:384:LEU:HB2	1:C:371:MET:HE1	1.80	0.63
1:A:374:LEU:HD23	1:A:377:LEU:HD21	1.80	0.62
1:A:3:GLU:CB	1:A:4:GLU:CB	2.44	0.62
1:A:72:GLN:HG2	1:A:99:TYR:CZ	2.34	0.62
1:A:72:GLN:HE22	1:B:366:THR:HG21	1.65	0.62
1:A:7:LEU:HD21	1:A:275:LEU:HB2	1.81	0.62
1:B:47:PHE:HB3	1:B:48:PRO:HD3	1.81	0.62
1:A:82:ASP:HA	1:A:83:LYS:CB	2.28	0.62
1:B:197:ASP:O	1:B:201:ASN:N	2.31	0.62
1:A:378:MET:HE2	1:A:378:MET:CA	2.30	0.61
1:C:40:PRO:HG2	1:C:43:LEU:HB3	1.82	0.61
1:A:280:LEU:HD23	1:A:284:LEU:HD23	1.82	0.61
1:A:277:LYS:O	1:A:281:GLU:HB2	2.01	0.61
1:B:218:ASN:N	1:B:218:ASN:HD22	1.99	0.61
1:B:280:LEU:HD23	1:B:284:LEU:HD23	1.83	0.61
1:A:116:ILE:HG12	1:A:244:VAL:HG22	1.83	0.60
1:B:64:HIS:HD2	1:B:261:VAL:H	1.49	0.60
1:A:39:HIS:CG	1:A:39:HIS:O	2.54	0.60
1:A:147:LEU:CB	1:A:224:MET:SD	2.89	0.60
1:A:374:LEU:HA	1:A:377:LEU:HD23	1.84	0.60
1:C:251:LYS:C	1:C:253:GLN:H	2.08	0.60
1:A:72:GLN:HE22	1:B:366:THR:CG2	2.16	0.59
1:C:61:PHE:O	1:C:62:TRP:HB2	2.01	0.59
1:C:331:PRO:HG2	1:C:336:MET:SD	2.42	0.59
1:B:89:LEU:CD1	1:B:107:PRO:HG2	2.32	0.59
1:C:358:ASP:HA	1:C:361:LEU:HB2	1.84	0.59
1:A:374:LEU:HG	1:C:377:LEU:CD1	2.33	0.58
1:B:285:LEU:HD23	1:B:290:LEU:HD11	1.85	0.58
1:B:367:ASN:O	1:B:370:ALA:N	2.36	0.58
1:A:304:LEU:O	1:A:308:GLU:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:HB1	1:B:321:MET:HE2	1.85	0.58
1:B:379:LYS:HE3	1:B:379:LYS:CA	2.20	0.58
1:A:72:GLN:NE2	1:B:366:THR:HG21	2.19	0.58
1:B:196:VAL:HA	1:B:199:ILE:HD12	1.86	0.58
1:A:146:ALA:O	1:A:224:MET:HG3	2.03	0.58
1:A:335:GLN:NE2	1:A:376:LYS:HE3	2.17	0.58
1:B:64:HIS:HE1	1:B:330:MET:O	1.86	0.58
1:B:100:ASN:HA	1:B:175:LYS:HE3	1.85	0.57
1:C:149:PHE:CD1	1:C:226:ILE:CG1	2.87	0.57
1:C:199:ILE:HG13	1:C:204:MET:HB3	1.85	0.57
1:A:226:ILE:HG23	1:A:247:LEU:HD21	1.86	0.57
1:B:127:LYS:HE2	1:B:127:LYS:HA	1.85	0.57
1:C:368:ALA:O	1:C:372:ALA:HB2	2.03	0.57
1:B:2:ILE:HG13	1:B:3:GLU:CG	2.34	0.57
1:C:67:PHE:HE2	1:C:265:GLY:HA3	1.70	0.57
1:B:166:GLY:HA3	1:B:188:ALA:HB2	1.86	0.57
1:A:172:GLU:O	1:A:173:ASN:HB3	2.04	0.57
1:C:129:TRP:HB3	1:C:194:PHE:HE2	1.69	0.57
1:C:279:PHE:C	1:C:279:PHE:CD2	2.81	0.57
1:A:171:TYR:HB2	1:A:176:TYR:CE1	2.40	0.57
1:A:254:PRO:HB3	1:A:326:LYS:HG2	1.85	0.56
1:B:132:ILE:H	1:B:133:PRO:HD2	1.69	0.56
1:B:144:LYS:HD2	1:B:221:GLU:HA	1.87	0.56
1:A:111:GLU:O	1:A:112:ALA:HB2	2.06	0.56
1:B:363:ALA:O	1:B:367:ASN:CB	2.52	0.56
1:A:181:VAL:HB	1:A:365:GLN:NE2	2.21	0.56
1:A:181:VAL:HB	1:A:365:GLN:HE22	1.70	0.56
1:A:2:ILE:CB	1:A:3:GLU:HA	2.12	0.55
1:B:39:HIS:CG	1:B:39:HIS:O	2.59	0.55
1:C:42:LYS:HE2	1:C:44:GLU:OE2	2.06	0.55
1:C:85:PHE:HZ	1:C:285:LEU:CD2	2.20	0.55
1:B:9:ILE:HD12	1:B:35:VAL:HG13	1.87	0.55
1:B:12:ASN:HB2	1:B:62:TRP:CZ3	2.40	0.55
1:C:10:TRP:CE2	1:C:40:PRO:HG3	2.42	0.55
1:A:147:LEU:HA	1:A:224:MET:O	2.06	0.55
1:A:149:PHE:HE2	1:A:157:THR:HG22	1.72	0.55
1:A:342:ALA:HB1	1:A:367:ASN:HB2	1.69	0.55
1:C:9:ILE:HD12	1:C:37:VAL:HG22	1.89	0.55
1:A:361:LEU:O	1:A:364:ALA:HB3	2.06	0.55
1:B:123:PRO:HB2	1:B:124:ASN:HB2	1.89	0.55
1:B:133:PRO:HA	1:B:203:HIS:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:HZ	1:A:284:LEU:HD21	1.72	0.55
1:A:374:LEU:HG	1:C:377:LEU:HD13	1.89	0.54
1:A:259:VAL:HB	1:A:329:ILE:HA	1.88	0.54
1:C:89:LEU:HD21	1:C:285:LEU:HD21	1.87	0.54
1:C:38:GLU:O	1:C:40:PRO:HD3	2.08	0.54
1:B:373:THR:O	1:B:377:LEU:HB2	2.08	0.54
1:C:68:GLY:HA3	1:C:332:ASN:HB2	1.89	0.54
1:C:170:LYS:HB3	1:C:180:ASP:HB3	1.90	0.54
1:A:232:TRP:HE1	1:A:244:VAL:HG21	1.73	0.53
1:A:377:LEU:CD1	1:A:378:MET:CE	2.86	0.53
1:B:40:PRO:O	1:B:43:LEU:HB3	2.08	0.53
1:B:367:ASN:O	1:B:368:ALA:C	2.52	0.53
1:A:148:MET:HE3	1:A:208:THR:HG23	1.91	0.53
1:C:216:ALA:O	1:C:221:GLU:HG3	2.08	0.53
1:A:377:LEU:CD1	1:B:374:LEU:CD2	2.86	0.53
1:C:184:ASP:O	1:C:189:LYS:HD3	2.08	0.53
1:B:219:LYS:HB3	1:B:221:GLU:H	1.73	0.53
1:A:62:TRP:HB3	1:A:67:PHE:HE1	1.73	0.53
1:A:72:GLN:HG2	1:A:99:TYR:CE2	2.44	0.53
1:A:256:LYS:HG3	1:A:326:LYS:O	2.09	0.53
1:C:9:ILE:HG12	1:C:59:ILE:HG21	1.90	0.53
1:B:45:GLU:O	1:B:48:PRO:HD2	2.08	0.53
1:C:151:LEU:C	1:C:153:GLU:H	2.16	0.53
1:A:72:GLN:HG3	1:A:99:TYR:HH	1.69	0.53
1:A:149:PHE:CE2	1:A:157:THR:HG22	2.44	0.53
1:B:289:GLY:O	1:B:293:VAL:HG23	2.09	0.53
1:B:129:TRP:CD1	1:B:248:PRO:O	2.62	0.52
1:A:38:GLU:O	1:A:40:PRO:HD3	2.08	0.52
1:A:185:ASN:HD22	1:A:185:ASN:H	1.56	0.52
1:C:7:LEU:HB2	1:C:35:VAL:HG22	1.91	0.52
1:C:62:TRP:HE1	1:C:66:ARG:HG3	1.74	0.52
1:C:85:PHE:CZ	1:C:285:LEU:CD2	2.92	0.52
1:B:375:GLU:HA	1:B:378:MET:HG2	1.90	0.52
1:C:129:TRP:HB3	1:C:194:PHE:CE2	2.44	0.52
1:B:133:PRO:HB3	1:B:203:HIS:CE1	2.45	0.52
1:B:384:LEU:HD12	1:C:371:MET:SD	2.50	0.52
1:C:85:PHE:O	1:C:86:GLN:C	2.53	0.52
1:A:195:LEU:O	1:A:199:ILE:HD12	2.10	0.52
1:C:66:ARG:HH11	1:C:66:ARG:HA	1.74	0.52
1:B:149:PHE:CD1	1:B:204:MET:HE1	2.45	0.52
1:C:7:LEU:HA	1:C:58:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:MET:O	1:C:225:THR:HA	2.09	0.51
1:A:60:ILE:O	1:A:264:ALA:HA	2.11	0.51
1:A:11:ILE:CG2	1:A:17:TYR:HB3	2.40	0.51
1:C:225:THR:O	1:C:226:ILE:HD13	2.09	0.51
1:C:247:LEU:CD2	1:C:323:ASN:CG	2.83	0.51
1:A:193:THR:HA	1:A:357:VAL:HG21	1.91	0.51
1:C:64:HIS:H	1:C:64:HIS:CD2	2.27	0.51
1:B:2:ILE:HG13	1:B:3:GLU:HG3	1.91	0.51
1:B:290:LEU:HD13	1:B:304:LEU:HD11	1.91	0.51
1:A:33:ILE:HG21	1:A:275:LEU:HD13	1.93	0.51
1:C:39:HIS:CG	1:C:39:HIS:O	2.64	0.51
1:C:118:ASN:OD1	1:C:121:LEU:N	2.43	0.51
1:A:129:TRP:CZ3	1:A:160:LEU:HD12	2.45	0.50
1:B:284:LEU:O	1:B:290:LEU:HD12	2.10	0.50
1:B:125:PRO:HB2	1:B:126:PRO:HD2	1.93	0.50
1:A:272:ASN:HD22	1:A:272:ASN:N	1.89	0.50
1:B:147:LEU:HD11	1:B:226:ILE:CD1	2.38	0.50
1:C:40:PRO:HD2	1:C:43:LEU:HD23	1.93	0.50
1:A:314:ASP:OD1	1:A:316:ARG:HG3	2.11	0.50
1:B:175:LYS:HE2	1:B:175:LYS:HA	1.94	0.50
1:B:251:LYS:O	1:B:253:GLN:NE2	2.44	0.50
1:C:85:PHE:O	1:C:88:LYS:N	2.42	0.50
1:A:342:ALA:HB1	1:A:367:ASN:HB3	0.57	0.50
1:B:2:ILE:HG22	1:B:55:ASP:HB3	1.93	0.50
1:B:167:TYR:CD1	1:B:182:GLY:HA3	2.47	0.50
1:A:83:LYS:O	1:A:84:ALA:HB3	2.12	0.49
1:B:78:GLU:HG3	1:B:102:LYS:HB3	1.93	0.49
1:C:94:TRP:HA	1:C:94:TRP:CE3	2.47	0.49
1:A:342:ALA:CB	1:A:367:ASN:CB	2.30	0.49
1:B:18:ASN:HB2	1:B:296:ASP:OD2	2.13	0.49
1:C:89:LEU:HD22	1:C:304:LEU:HA	1.94	0.49
1:A:372:ALA:O	1:A:376:LYS:CG	2.57	0.49
1:C:85:PHE:C	1:C:85:PHE:CD2	2.91	0.49
1:A:374:LEU:HA	1:A:377:LEU:CD2	2.42	0.49
1:A:72:GLN:C	1:A:74:GLY:H	2.20	0.49
1:A:130:GLU:O	1:A:133:PRO:HD2	2.13	0.49
1:A:72:GLN:CG	1:A:99:TYR:HH	2.24	0.49
1:B:287:ASP:HB3	1:B:307:TYR:CD1	2.48	0.49
1:C:64:HIS:CE1	1:C:330:MET:O	2.66	0.48
1:A:6:LYS:HD2	1:A:34:LYS:HE2	1.94	0.48
1:A:40:PRO:O	1:A:41:ASP:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:THR:HG23	1:B:131:GLU:OE1	2.13	0.48
1:C:259:VAL:HB	1:C:329:ILE:HA	1.94	0.48
1:B:4:GLU:HA	1:B:272:ASN:HD21	1.78	0.48
1:B:117:TYR:HB2	1:B:122:LEU:HD23	1.94	0.48
1:C:205:ASN:O	1:C:207:ASP:N	2.46	0.48
1:C:214:GLU:O	1:C:218:ASN:N	2.35	0.48
1:A:158:TRP:O	1:A:159:PRO:C	2.54	0.48
1:B:296:ASP:O	1:B:297:LYS:HD3	2.13	0.48
1:C:11:ILE:HG12	1:C:15:LYS:HB2	1.96	0.48
1:B:213:ALA:O	1:B:214:GLU:C	2.56	0.48
1:C:370:ALA:C	1:C:372:ALA:N	2.71	0.48
1:A:102:LYS:O	1:A:104:ILE:HG23	2.14	0.48
1:A:129:TRP:O	1:A:132:ILE:N	2.42	0.48
1:A:377:LEU:HD11	1:A:378:MET:CE	2.43	0.48
1:A:378:MET:HA	1:A:378:MET:CE	2.23	0.48
1:B:147:LEU:HB2	1:B:224:MET:HE3	1.96	0.48
1:B:302:VAL:N	1:B:308:GLU:OE1	2.40	0.48
1:C:116:ILE:HG12	1:C:244:VAL:HG22	1.96	0.48
1:C:195:LEU:HA	1:C:198:LEU:HD12	1.95	0.48
1:A:161:ILE:HG12	1:A:192:LEU:HB2	1.96	0.47
1:B:148:MET:HB2	1:B:222:THR:HG21	1.95	0.47
1:B:136:ASP:HB3	1:B:203:HIS:HD2	1.79	0.47
1:A:154:PRO:O	1:A:158:TRP:N	2.32	0.47
1:B:218:ASN:N	1:B:218:ASN:ND2	2.62	0.47
1:C:184:ASP:O	1:C:185:ASN:C	2.58	0.47
1:A:15:LYS:HE2	1:A:15:LYS:HA	1.96	0.47
1:A:122:LEU:HD21	1:A:125:PRO:HA	1.95	0.47
1:B:192:LEU:O	1:B:196:VAL:HG23	2.13	0.47
1:C:47:PHE:HB3	1:C:48:PRO:HD3	1.96	0.47
1:A:81:PRO:HA	1:A:281:GLU:OE2	2.15	0.47
1:C:67:PHE:CE2	1:C:265:GLY:HA3	2.49	0.47
1:C:355:GLN:HB3	1:C:360:ALA:HB2	1.97	0.47
1:B:234:ASN:HD22	1:B:234:ASN:H	1.63	0.47
1:A:61:PHE:HZ	1:A:284:LEU:CD2	2.28	0.47
1:A:118:ASN:HB3	1:A:121:LEU:HB2	1.95	0.47
1:A:272:ASN:ND2	1:A:272:ASN:N	2.56	0.47
1:B:132:ILE:N	1:B:133:PRO:CD	2.76	0.47
1:B:67:PHE:HA	1:B:70:TYR:CD2	2.50	0.47
1:C:90:TYR:CE2	1:C:305:LYS:HA	2.50	0.47
1:C:153:GLU:HA	1:C:154:PRO:HD2	1.80	0.47
1:A:118:ASN:N	1:A:223:ALA:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:O	1:A:257:PRO:HD3	2.15	0.47
1:A:377:LEU:HD13	1:B:374:LEU:CD2	2.44	0.47
1:A:96:ALA:HB2	1:A:329:ILE:CG2	2.45	0.46
1:B:64:HIS:CE1	1:B:330:MET:O	2.67	0.46
1:C:81:PRO:HB2	1:C:85:PHE:CD2	2.50	0.46
1:A:90:TYR:HB3	1:A:92:PHE:CE2	2.51	0.46
1:B:71:ALA:HB2	1:B:76:LEU:HD12	1.96	0.46
1:A:6:LYS:HB2	1:A:6:LYS:NZ	2.30	0.46
1:A:46:LYS:O	1:A:49:GLN:HB2	2.16	0.46
1:A:166:GLY:HA2	1:A:185:ASN:HD21	1.81	0.46
1:B:67:PHE:CD1	1:B:67:PHE:N	2.83	0.46
1:B:210[A]:TYR:HE1	1:B:227:ASN:HD21	1.62	0.46
1:B:364:ALA:O	1:B:365:GLN:C	2.57	0.46
1:C:66:ARG:HA	1:C:66:ARG:NH1	2.31	0.46
1:B:47:PHE:CE1	1:B:60:ILE:HB	2.51	0.46
1:B:375:GLU:O	1:B:378:MET:HG3	2.16	0.46
1:C:9:ILE:HG12	1:C:59:ILE:CG2	2.44	0.46
1:C:64:HIS:CD2	1:C:64:HIS:N	2.84	0.46
1:A:3:GLU:HB2	1:A:4:GLU:HB3	1.85	0.46
1:A:83:LYS:O	1:A:84:ALA:CB	2.64	0.46
1:A:89:LEU:HB3	1:A:94:TRP:HE1	1.81	0.46
1:B:61:PHE:HA	1:B:263:SER:O	2.16	0.46
1:C:72:GLN:C	1:C:74:GLY:H	2.24	0.45
1:A:178:ILE:H	1:A:178:ILE:HG13	1.59	0.45
1:C:251:LYS:C	1:C:253:GLN:N	2.75	0.45
1:C:344:ARG:HG3	1:C:348:ILE:HD13	1.98	0.45
1:B:341:TYR:HA	1:B:344:ARG:HB3	1.97	0.45
1:C:147:LEU:CD1	1:C:226:ILE:HD11	2.38	0.45
1:B:44:GLU:H	1:B:44:GLU:CD	2.24	0.45
1:B:282:ASN:HD22	1:B:282:ASN:N	2.15	0.45
1:B:333:ILE:HD13	1:B:333:ILE:H	1.81	0.45
1:C:31:THR:HG23	1:C:33:ILE:HG12	1.98	0.45
1:C:345:THR:O	1:C:349:ASN:OD1	2.35	0.45
1:A:8:VAL:HG13	1:A:57:PRO:HA	1.99	0.45
1:A:117:TYR:HE2	1:A:119:LYS:HG3	1.81	0.45
1:B:34:LYS:HG3	1:B:35:VAL:N	2.32	0.45
1:A:47:PHE:HB3	1:A:48:PRO:HD3	1.98	0.45
1:A:160:LEU:O	1:A:161:ILE:C	2.59	0.45
1:B:64:HIS:CE1	1:B:330:MET:HB3	2.52	0.45
1:B:378:MET:HG3	1:B:379:LYS:N	2.31	0.45
1:B:67:PHE:N	1:B:67:PHE:HD1	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:HB3	1:C:275:LEU:HD12	1.98	0.45
1:A:82:ASP:CA	1:A:83:LYS:CB	2.92	0.45
1:A:217:PHE:HD1	1:A:222:THR:HG23	1.82	0.45
1:B:60:ILE:O	1:B:264:ALA:HA	2.17	0.45
1:B:365:GLN:O	1:B:368:ALA:HB3	2.17	0.45
1:C:68:GLY:O	1:C:72:GLN:HB2	2.16	0.45
1:A:147:LEU:CA	1:A:224:MET:HE3	2.45	0.45
1:C:64:HIS:HA	1:C:67:PHE:HB2	1.98	0.45
1:B:140:LYS:HA	1:B:144:LYS:O	2.16	0.44
1:C:22:GLU:O	1:C:25:LYS:HB2	2.17	0.44
1:A:79:ILE:HG21	1:A:266:ILE:HD12	2.00	0.44
1:A:99:TYR:O	1:A:102:LYS:N	2.51	0.44
1:A:216:ALA:O	1:A:221:GLU:HB2	2.18	0.44
1:A:232:TRP:NE1	1:A:244:VAL:HG21	2.32	0.44
1:A:379:LYS:HD2	1:A:379:LYS:HA	1.73	0.44
1:B:156:PHE:O	1:B:159:PRO:HD2	2.18	0.44
1:C:68:GLY:CA	1:C:332:ASN:HB2	2.48	0.44
1:A:360:ALA:O	1:A:361:LEU:C	2.60	0.44
1:B:10:TRP:CD1	1:B:38:GLU:HG3	2.53	0.44
1:B:149:PHE:H	1:B:204:MET:CE	2.30	0.44
1:C:368:ALA:O	1:C:372:ALA:CB	2.64	0.44
1:B:34:LYS:HB2	1:B:34:LYS:HE2	1.62	0.44
1:B:147:LEU:HA	1:B:224:MET:O	2.18	0.44
1:A:89:LEU:HD21	1:A:303:ALA:HB1	1.99	0.44
1:B:194:PHE:CE2	1:B:198:LEU:HD21	2.53	0.44
1:A:39:HIS:O	1:A:39:HIS:CD2	2.70	0.44
1:A:129:TRP:HD1	1:A:249:THR:O	2.00	0.44
1:C:301:ALA:HB1	1:C:321:MET:HE2	2.00	0.44
1:A:335:GLN:HG2	1:A:372:ALA:HB1	2.00	0.43
1:B:291:GLU:O	1:B:291:GLU:HG3	2.16	0.43
1:A:288:GLU:HA	1:A:291:GLU:HB3	2.01	0.43
1:C:356:THR:HA	1:C:357:VAL:HA	1.88	0.43
1:A:55:ASP:HB3	1:A:56:GLY:H	1.41	0.43
1:B:287:ASP:OD1	1:B:287:ASP:N	2.51	0.43
1:C:283:TYR:O	1:C:286:THR:OG1	2.36	0.43
1:B:131:GLU:O	1:B:131:GLU:HG2	2.18	0.43
1:A:280:LEU:CD2	1:A:284:LEU:HD23	2.48	0.43
1:B:325:GLN:C	1:B:327:GLY:H	2.27	0.43
1:C:27:PHE:O	1:C:31:THR:HG22	2.19	0.43
1:C:129:TRP:CE3	1:C:132:ILE:HD12	2.53	0.43
1:B:136:ASP:HA	1:B:146:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD21	1:B:223:ALA:HB1	2.00	0.43
1:A:227:ASN:OD1	1:A:230:TRP:NE1	2.51	0.43
1:B:44:GLU:HB3	1:B:62:TRP:CZ2	2.54	0.43
1:C:58:ASP:OD2	1:C:58:ASP:N	2.52	0.43
1:C:199:ILE:HA	1:C:204:MET:HB3	2.01	0.43
1:B:72:GLN:C	1:B:74:GLY:N	2.77	0.42
1:B:13:GLY:HA2	1:B:39:HIS:HB2	2.00	0.42
1:B:239:LYS:O	1:B:240:VAL:C	2.62	0.42
1:A:151:LEU:HD11	1:A:199:ILE:HD11	2.02	0.42
1:C:64:HIS:O	1:C:67:PHE:HB2	2.19	0.42
1:B:34:LYS:HG3	1:B:35:VAL:H	1.85	0.42
1:B:332:ASN:OD1	1:B:332:ASN:N	2.53	0.42
1:C:371:MET:HE2	1:C:371:MET:HB2	1.89	0.42
1:A:342:ALA:CA	1:A:367:ASN:HB3	2.30	0.42
1:A:344:ARG:O	1:A:348:ILE:CG1	2.66	0.42
1:C:23:VAL:C	1:C:25:LYS:H	2.27	0.42
1:C:184:ASP:O	1:C:189:LYS:CD	2.67	0.42
1:A:111:GLU:O	1:A:112:ALA:CB	2.68	0.42
1:A:377:LEU:CD1	1:A:378:MET:HE2	2.50	0.41
1:B:219:LYS:HG2	1:B:221:GLU:HB2	2.01	0.41
1:C:96:ALA:HB2	1:C:329:ILE:HG21	2.02	0.41
1:A:242:TYR:CD2	1:A:242:TYR:C	2.98	0.41
1:B:149:PHE:CE1	1:B:204:MET:HE1	2.55	0.41
1:C:357:VAL:C	1:C:359:ALA:N	2.78	0.41
1:A:94:TRP:CZ3	1:A:103:LEU:HD11	2.55	0.41
1:A:99:TYR:O	1:A:100:ASN:C	2.63	0.41
1:B:128:THR:CG2	1:B:131:GLU:OE1	2.69	0.41
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.55	0.41
1:C:28:GLU:O	1:C:29:LYS:C	2.63	0.41
1:A:1:LYS:HE2	1:A:1:LYS:HB3	1.92	0.41
1:B:116:ILE:HG12	1:B:244:VAL:HG22	2.02	0.41
1:C:339:PHE:CE2	1:C:343:VAL:HG21	2.55	0.41
1:C:370:ALA:C	1:C:372:ALA:H	2.27	0.41
1:C:94:TRP:HA	1:C:94:TRP:HE3	1.85	0.41
1:C:132:ILE:N	1:C:133:PRO:HD2	2.35	0.41
1:A:94:TRP:HA	1:A:97:VAL:HG22	2.03	0.41
1:C:199:ILE:HD13	1:C:351:ALA:HB1	2.02	0.41
1:C:384:LEU:C	1:C:386:SER:H	2.29	0.41
1:A:164:ASP:HB3	1:A:187:GLY:O	2.21	0.41
1:C:9:ILE:HG22	1:C:10:TRP:N	2.36	0.41
1:C:129:TRP:NE1	1:C:248:PRO:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:TRP:O	1:A:130:GLU:C	2.64	0.41
1:B:10:TRP:CD1	1:B:57:PRO:HB3	2.56	0.41
1:B:258:PHE:HA	1:B:328:GLU:O	2.21	0.41
1:C:161:ILE:HA	1:C:191:GLY:HA3	2.01	0.41
1:A:6:LYS:HA	1:A:33:ILE:HG23	2.02	0.41
1:A:94:TRP:CE3	1:A:103:LEU:HD11	2.56	0.41
1:A:129:TRP:NE1	1:A:248:PRO:HB2	2.36	0.41
1:A:154:PRO:O	1:A:155:TYR:C	2.64	0.41
1:A:340:TRP:HA	1:A:340:TRP:CE3	2.56	0.41
1:B:61:PHE:O	1:B:62:TRP:HB2	2.21	0.41
1:B:170:LYS:HD3	1:B:170:LYS:HA	1.77	0.41
1:B:193:THR:OG1	1:B:357:VAL:HG11	2.21	0.41
1:C:352:SER:C	1:C:354:ARG:H	2.29	0.41
1:C:247:LEU:CD2	1:C:323:ASN:OD1	2.69	0.41
1:A:42:LYS:HE3	1:A:42:LYS:HA	2.02	0.40
1:B:154:PRO:O	1:B:158:TRP:N	2.52	0.40
1:B:339:PHE:CD1	1:B:339:PHE:C	2.99	0.40
1:A:72:GLN:C	1:A:74:GLY:N	2.79	0.40
1:A:139:LEU:O	1:A:142:LYS:N	2.37	0.40
1:A:284:LEU:O	1:A:290:LEU:HD23	2.22	0.40
1:C:179:LYS:HA	1:C:179:LYS:HE2	2.03	0.40
1:C:279:PHE:C	1:C:279:PHE:HD2	2.25	0.40
1:C:173:ASN:C	1:C:175:LYS:H	2.30	0.40
1:A:23:VAL:O	1:A:24:GLY:C	2.65	0.40
1:A:197:ASP:OD1	1:A:200:LYS:HE3	2.21	0.40
1:B:2:ILE:HG13	1:B:3:GLU:CB	2.51	0.40
1:B:124:ASN:HA	1:B:125:PRO:HD3	1.74	0.40
1:C:8:VAL:HG13	1:C:57:PRO:HA	2.03	0.40
1:C:22:GLU:HA	1:C:22:GLU:OE2	2.22	0.40
1:C:125:PRO:HA	1:C:126:PRO:HD3	2.00	0.40
1:A:130:GLU:OE1	1:A:130:GLU:N	2.53	0.40
1:C:184:ASP:HB2	1:C:365:GLN:CD	2.46	0.40
1:C:314:ASP:HA	1:C:315:PRO:HD2	1.92	0.40

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

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	398/449 (89%)	332 (83%)	46 (12%)	20 (5%)	1	17
1	B	388/449 (86%)	322 (83%)	51 (13%)	15 (4%)	2	21
1	C	396/449 (88%)	318 (80%)	64 (16%)	14 (4%)	3	24
All	All	1182/1347 (88%)	972 (82%)	161 (14%)	49 (4%)	2	20

All (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
1	B	4	GLU
1	B	163	ALA
1	B	240	VAL
1	B	357	VAL
1	B	367	ASN
1	C	206	ALA
1	C	399	GLN
1	A	100	ASN
1	A	150	ASN
1	A	168	ALA
1	B	388	GLN
1	C	4	GLU
1	C	168	ALA
1	C	185	ASN
1	C	233	SER
1	C	286	THR
1	C	400	GLN
1	A	84	ALA
1	A	112	ALA

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Mol	Chain	Res	Type
1	A	172	GLU
1	A	239	LYS
1	A	360	ALA
1	B	365	GLN
1	B	368	ALA
1	C	29	LYS
1	C	163	ALA
1	A	41	ASP
1	A	129	TRP
1	A	404	GLN
1	B	73	SER
1	B	124	ASN
1	B	162	ALA
1	C	165	GLY
1	A	2	ILE
1	A	409	PRO
1	B	387	PHE
1	B	165	GLY
1	C	2	ILE
1	B	123	PRO
1	A	329	ILE
1	B	81	PRO
1	A	412	PRO
1	C	16	GLY
1	C	40	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	312/363 (86%)	259 (83%)	53 (17%)	2	13
1	B	304/363 (84%)	256 (84%)	48 (16%)	2	15
1	C	295/363 (81%)	253 (86%)	42 (14%)	3	18
All	All	911/1089 (84%)	768 (84%)	143 (16%)	2	15

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	22	GLU
1	A	25	LYS
1	A	29	LYS
1	A	31	THR
1	A	42	LYS
1	A	50	VAL
1	A	59	ILE
1	A	72	GLN
1	A	79	ILE
1	A	83	LYS
1	A	88	LYS
1	A	89	LEU
1	A	100	ASN
1	A	103	LEU
1	A	115	LEU
1	A	119	LYS
1	A	122	LEU
1	A	127	LYS
1	A	135	LEU
1	A	137	LYS
1	A	139	LEU
1	A	148	MET
1	A	151	LEU
1	A	160	LEU
1	A	172	GLU
1	A	178	ILE
1	A	185	ASN
1	A	189	LYS
1	A	201	ASN
1	A	205	ASN
1	A	219	LYS
1	A	224	MET
1	A	235	ILE
1	A	245	THR
1	A	255	SER
1	A	256	LYS
1	A	258	PHE
1	A	263	SER
1	A	272	ASN
1	A	278	GLU
1	A	290	LEU

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Mol	Chain	Res	Type
1	A	320	THR
1	A	329	ILE
1	A	344	ARG
1	A	347	VAL
1	A	357	VAL
1	A	366	THR
1	A	373	THR
1	A	376	LYS
1	A	377	LEU
1	A	378	MET
1	A	386	SER
1	B	6	LYS
1	B	8	VAL
1	B	17	TYR
1	B	25	LYS
1	B	34	LYS
1	B	36	THR
1	B	38	GLU
1	B	80	THR
1	B	98	ARG
1	B	104	ILE
1	B	110	VAL
1	B	115	LEU
1	B	122	LEU
1	B	127	LYS
1	B	160	LEU
1	B	170	LYS
1	B	175	LYS
1	B	181	VAL
1	B	189	LYS
1	B	196	VAL
1	B	198	LEU
1	B	204	MET
1	B	205	ASN
1	B	207	ASP
1	B	218	ASN
1	B	219	LYS
1	B	239	LYS
1	B	246	VAL
1	B	253	GLN
1	B	256	LYS
1	B	274	GLU

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	287	ASP
1	B	291	GLU
1	B	293	VAL
1	B	304	LEU
1	B	317	ILE
1	B	332	ASN
1	B	333	ILE
1	B	335	GLN
1	B	341	TYR
1	B	344	ARG
1	B	348	ILE
1	B	354	ARG
1	B	366	THR
1	B	377	LEU
1	B	378	MET
1	B	379	LYS
1	C	10	TRP
1	C	29	LYS
1	C	36	THR
1	C	49	GLN
1	C	58	ASP
1	C	59	ILE
1	C	65	ASP
1	C	72	GLN
1	C	73	SER
1	C	79	ILE
1	C	82	ASP
1	C	86	GLN
1	C	104	ILE
1	C	108	ILE
1	C	115	LEU
1	C	148	MET
1	C	152	GLN
1	C	160	LEU
1	C	181	VAL
1	C	189	LYS
1	C	202	LYS
1	C	214	GLU
1	C	221	GLU
1	C	236	ASP
1	C	246	VAL

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Mol	Chain	Res	Type
1	C	247	LEU
1	C	251	LYS
1	C	256	LYS
1	C	273	LYS
1	C	277	LYS
1	C	278	GLU
1	C	279	PHE
1	C	281	GLU
1	C	285	LEU
1	C	288	GLU
1	C	329	ILE
1	C	339	PHE
1	C	344	ARG
1	C	354	ARG
1	C	358	ASP
1	C	377	LEU
1	C	384	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	49	GLN
1	A	64	HIS
1	A	72	GLN
1	A	86	GLN
1	A	100	ASN
1	A	118	ASN
1	A	185	ASN
1	A	201	ASN
1	A	218	ASN
1	A	272	ASN
1	A	294	ASN
1	A	335	GLN
1	A	404	GLN
1	B	64	HIS
1	B	72	GLN
1	B	86	GLN
1	B	201	ASN
1	B	203	HIS
1	B	205	ASN
1	B	218	ASN

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	282	ASN
1	C	49	GLN
1	C	64	HIS
1	C	72	GLN
1	C	86	GLN
1	C	100	ASN
1	C	201	ASN
1	C	272	ASN
1	C	325	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 oligosaccharides 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 ⓘ

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%)	-0.75	4 (0%) 79 55	21, 70, 70, 100	30 (7%)
1	B	389/449 (86%)	-0.86	0 100 100	39, 70, 70, 100	15 (3%)
1	C	400/449 (89%)	-0.85	2 (0%) 87 69	30, 70, 70, 100	31 (7%)
All	All	1191/1347 (88%)	-0.82	6 (0%) 87 69	21, 70, 70, 100	76 (6%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	SER	2.7
1	C	5	GLY	2.6
1	A	406	PRO	2.3
1	A	413	PRO	2.1
1	A	410	PRO	2.1
1	C	392	GLN	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	450	1/1	0.97	0.08	97,97,97,97	1
2	ZN	C	450	1/1	0.97	0.04	92,92,92,92	1
3	CA	C	451	1/1	0.97	0.04	99,99,99,99	0
2	ZN	B	451	1/1	0.98	0.04	100,100,100,100	0
2	ZN	A	451	1/1	0.98	0.05	100,100,100,100	0
3	CA	B	454	1/1	0.98	0.04	98,98,98,98	0
2	ZN	A	453	1/1	0.98	0.06	88,88,88,88	1
3	CA	A	454	1/1	0.99	0.05	96,96,96,96	0
3	CA	B	453	1/1	0.99	0.03	89,89,89,89	0
2	ZN	A	452	1/1	0.99	0.02	92,92,92,92	0
2	ZN	B	450	1/1	0.99	0.04	86,86,86,86	1
3	CA	C	452	1/1	0.99	0.04	98,98,98,98	0
2	ZN	B	452	1/1	1.00	0.03	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.