



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:31 AM GMT

PDB ID : 3IOV
Title : Huntingtin amino-terminal region with 17 Gln residues - crystal C99
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

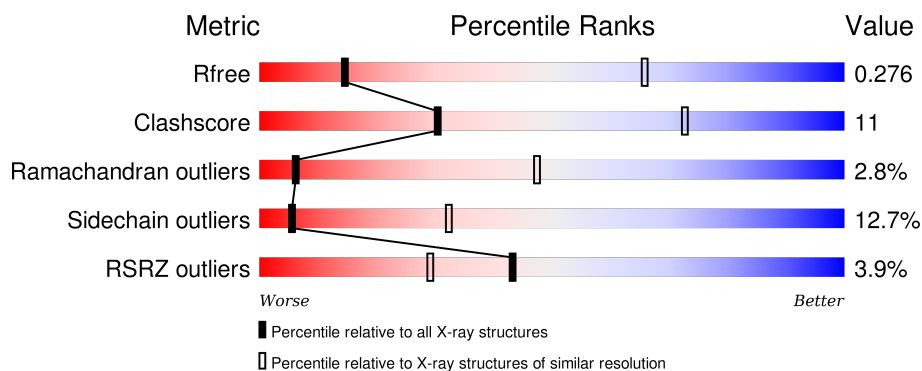
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

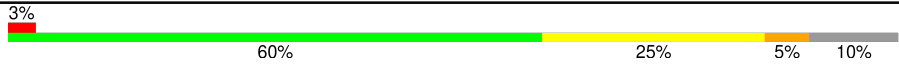


The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	 3% 60% 25% 5% 10%
1	B	449	 4% 64% 21% •• 11%
1	C	449	 4% 63% 23% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9211 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	405	Total	C	N	O	S	8	0	0
			3084	1992	502	582	8			
1	B	398	Total	C	N	O	S	4	0	0
			3049	1961	500	580	8			
1	C	402	Total	C	N	O	S	0	0	0
			3065	1971	503	583	8			

There are 111 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

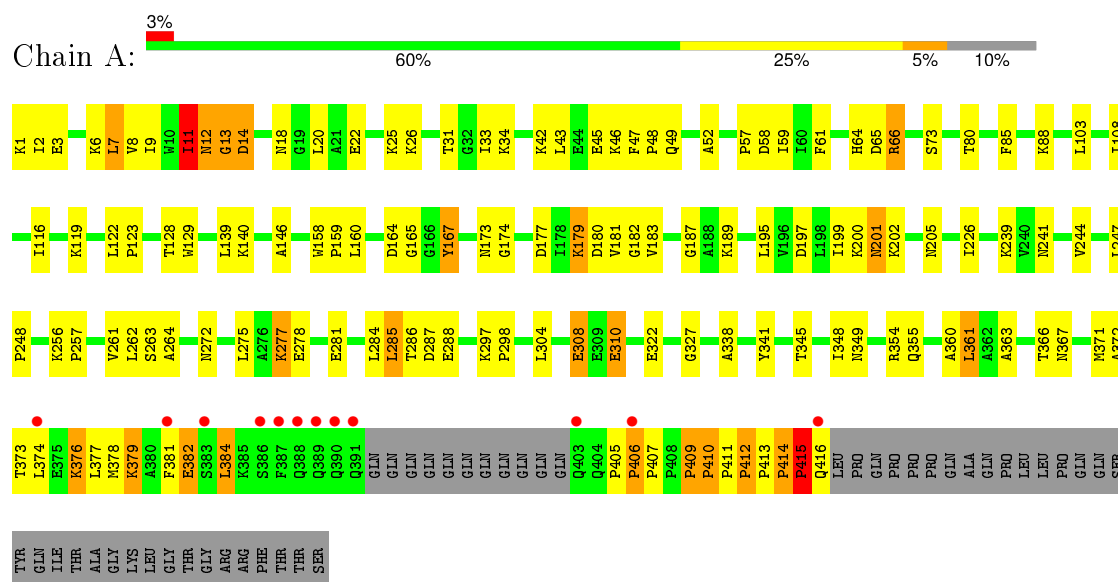
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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



THR	L374	A223	K102	K1
ALA	E375	T237	Y106	I2
GLY	M378	G243	P107	L7
LYS	K379	V244	V110	V8
LEU	A380	F258	E111	I9
GLY	S383	V259	L115	W10
THR	L384	G260	I116	K15
GLY	K385	A264	L122	G16
ARG	S386	N267	T128	Y17
PHE	F387	N272	W129	K25
THR	Q388	L275	E131	E28
THR	Q389	A276	I132	T31
SER	Q390	K277	D136	G32
	Q391	E278	K137	I33
	Q392	F279	A146	K34
	Q393	L280	Q152	V35
	Q394	E281	E153	T36
	Q395	N282	P154	V37
	Q396	T286	G165	E38
	Q397	K295	A168	H39
	Q398	D296	F169	P40
	Q399	K297	K170	D41
	Q400	T302	Y171	K42
	Q401	V307	E172	L43
	Q402	Y307	N173	E44
	GLN	L311	G174	E45
	GLN	K326	K175	K46
	PRO	I329	Y176	F47
	PRO	I333	K179	P48
	PRO	P334	D180	Q49
	PRO	Y341	V181	V50
	PRO	R344	G182	T53
	PRO	T345	V183	G54
	GLN	I348	D184	D55
	LEU	V357	K189	G56
	PRO	D358	L196	P57
	GLN	L361	N205	D58
	GLN	SER	A372	I59
	SER	TTR	T373	I60
	GLN	ILE		F61
				W62
				F67
				T80
				P81
				D82
				F85
				L89
				V97

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.82Å 101.19Å 134.82Å 90.00° 99.23° 90.00°	Depositor
Resolution (Å)	38.00 – 3.70 37.53 – 3.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (38.00-3.70) 92.8 (37.53-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.264 , 0.280 0.260 , 0.276	Depositor DCC
R_{free} test set	1095 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 21724 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9211	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	2/3164 (0.1%)	0.52	1/4307 (0.0%)
1	B	0.43	1/3120 (0.0%)	0.51	1/4236 (0.0%)
1	C	0.37	0/3136	0.49	0/4259
All	All	0.40	3/9420 (0.0%)	0.51	2/12802 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	GLU	CB-CG	-12.62	1.28	1.52
1	A	310	GLU	CB-CG	-9.75	1.33	1.52
1	A	6	LYS	CB-CG	-8.20	1.30	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	PRO	N-CA-CB	5.16	109.49	103.30
1	B	384	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3084	0	3028	80	0
1	B	3049	0	2996	65	0
1	C	3065	0	2998	70	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
All	All	9211	0	9022	201	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 11.

All (201) 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:415:PRO:CB	1:A:416:GLN:HA	1.84	1.05
1:A:410:PRO:HB2	1:A:411:PRO:CD	1.88	1.04
1:B:381:PHE:HE2	1:C:371:MET:HG2	1.30	0.94
1:C:205:ASN:HD22	1:C:206:ALA:H	1.06	0.93
1:A:11:ILE:HG23	1:A:12:ASN:H	1.39	0.86
1:B:381:PHE:CE2	1:C:371:MET:HG2	2.12	0.84
1:A:410:PRO:HB2	1:A:411:PRO:HD3	1.59	0.82
1:C:179:LYS:HG2	1:C:179:LYS:O	1.79	0.80
1:B:381:PHE:CD1	1:C:374:LEU:HD12	2.19	0.78
1:C:205:ASN:HD22	1:C:206:ALA:N	1.84	0.76
1:B:392:GLN:HG3	1:B:393:GLN:N	2.02	0.74
1:B:89:LEU:O	1:B:305:LYS:HG3	1.88	0.73
1:B:335:GLN:H	1:B:335:GLN:HE21	1.34	0.73
1:C:57:PRO:O	1:C:267:ASN:ND2	2.24	0.71
1:B:110:VAL:HG12	1:B:301:ALA:HB3	1.73	0.70
1:C:39:HIS:CG	1:C:39:HIS:O	2.44	0.69
1:A:284:LEU:O	1:A:285:LEU:HB2	1.90	0.69
1:B:381:PHE:HD1	1:C:374:LEU:HD12	1.56	0.69
1:A:415:PRO:CB	1:A:416:GLN:CA	2.65	0.69
1:A:367:ASN:O	1:A:371:MET:HB2	1.91	0.68
1:B:387:PHE:O	1:B:391:GLN:HG2	1.93	0.68
1:A:18:ASN:O	1:A:22:GLU:HG2	1.95	0.66
1:A:409:PRO:CB	1:A:410:PRO:HA	2.26	0.66
1:C:116:ILE:HG12	1:C:244:VAL:HG22	1.79	0.64
1:C:341:TYR:CE1	1:C:371:MET:HG3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:PRO:HB2	1:A:411:PRO:HD2	1.74	0.64
1:C:50:VAL:HG12	1:C:55:ASP:HB2	1.78	0.64
1:C:171:TYR:HB2	1:C:176:TYR:HE1	1.62	0.64
1:C:171:TYR:HB2	1:C:176:TYR:CE1	2.32	0.63
1:A:20:LEU:HD13	1:A:284:LEU:HD13	1.81	0.63
1:C:243:GLY:O	1:C:244:VAL:HG23	1.99	0.62
1:A:413:PRO:HG2	1:B:385:LYS:HE2	1.82	0.61
1:B:392:GLN:HG3	1:B:393:GLN:H	1.64	0.61
1:C:379:LYS:HZ3	1:C:380:ALA:N	1.99	0.60
1:A:197:ASP:O	1:A:201:ASN:HB2	2.01	0.60
1:C:17:TYR:H	1:C:17:TYR:HD2	1.47	0.60
1:C:9:ILE:HG12	1:C:59:ILE:CG2	2.32	0.60
1:A:47:PHE:HB3	1:A:48:PRO:HD3	1.84	0.59
1:C:7:LEU:HD21	1:C:275:LEU:HB2	1.85	0.59
1:A:409:PRO:HB3	1:A:410:PRO:HA	1.84	0.58
1:B:64:HIS:HE1	1:B:330:MET:O	1.87	0.58
1:C:333:ILE:HB	1:C:334:PRO:HD2	1.86	0.58
1:A:381:PHE:CD2	1:B:371:MET:HB3	2.39	0.58
1:A:345:THR:HG21	1:C:387:PHE:HB3	1.85	0.57
1:A:8:VAL:HG13	1:A:57:PRO:HA	1.85	0.57
1:A:411:PRO:O	1:A:413:PRO:HD3	2.03	0.57
1:A:286:THR:O	1:A:288:GLU:N	2.38	0.57
1:A:381:PHE:HD2	1:B:371:MET:HB3	1.69	0.57
1:B:270:SER:O	1:B:273:LYS:HG2	2.05	0.57
1:C:89:LEU:HD13	1:C:107:PRO:HG2	1.88	0.56
1:C:393:GLN:O	1:C:398:GLN:HB2	2.06	0.56
1:A:381:PHE:CD2	1:A:384:LEU:HD22	2.41	0.56
1:B:183:VAL:HG23	1:B:365:GLN:HG3	1.88	0.55
1:A:9:ILE:HG12	1:A:59:ILE:HG12	1.88	0.55
1:C:379:LYS:HZ3	1:C:380:ALA:H	1.54	0.55
1:A:116:ILE:HG13	1:A:244:VAL:HG22	1.88	0.54
1:A:297:LYS:HD3	1:A:298:PRO:HD2	1.88	0.54
1:C:128:THR:HB	1:C:131:GLU:OE1	2.07	0.54
1:C:302:VAL:HG21	1:C:307:TYR:HD2	1.73	0.54
1:C:60:ILE:O	1:C:264:ALA:HA	2.07	0.54
1:A:195:LEU:O	1:A:199:ILE:HD12	2.08	0.54
1:B:332:ASN:H	1:B:332:ASN:ND2	2.06	0.53
1:A:410:PRO:O	1:A:412:PRO:HD3	2.09	0.53
1:A:277:LYS:O	1:A:281:GLU:HB2	2.09	0.53
1:A:349:ASN:HA	1:A:354:ARG:HH21	1.74	0.53
1:A:377:LEU:HG	1:B:374:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:OE1	1:A:66:ARG:NH2	2.42	0.52
1:C:282:ASN:O	1:C:286:THR:HG23	2.09	0.52
1:C:8:VAL:HG13	1:C:57:PRO:HA	1.92	0.52
1:C:122:LEU:HD23	1:C:223:ALA:HB1	1.92	0.51
1:A:43:LEU:HA	1:A:46:LYS:HB2	1.93	0.51
1:C:383:SER:O	1:C:387:PHE:HD2	1.94	0.51
1:B:41:ASP:O	1:B:42:LYS:C	2.49	0.51
1:A:164:ASP:HB3	1:A:187:GLY:HA2	1.92	0.51
1:B:299:LEU:CD1	1:B:302:VAL:HG12	2.41	0.50
1:B:210:TYR:HE2	1:B:227:ASN:HD21	1.57	0.50
1:C:158:TRP:CE2	1:C:162:ALA:HB2	2.46	0.50
1:B:132:ILE:N	1:B:133:PRO:HD2	2.28	0.49
1:C:9:ILE:HB	1:C:37:VAL:HG22	1.93	0.49
1:B:128:THR:HG22	1:B:249:THR:O	2.13	0.49
1:A:226:ILE:HG23	1:A:247:LEU:HD21	1.94	0.49
1:B:385:LYS:O	1:B:389:GLN:HG3	2.12	0.49
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.47	0.49
1:C:129:TRP:O	1:C:132:ILE:HG12	2.13	0.49
1:A:304:LEU:O	1:A:308:GLU:HB2	2.12	0.48
1:B:204:MET:HG2	1:B:205:ASN:H	1.78	0.48
1:B:385:LYS:C	1:B:385:LYS:HE3	2.33	0.48
1:C:47:PHE:HB3	1:C:48:PRO:HD3	1.95	0.48
1:C:259:VAL:HG12	1:C:260:GLY:N	2.28	0.48
1:A:177:ASP:O	1:A:180:ASP:HB2	2.14	0.48
1:C:106:TYR:CD2	1:C:280:LEU:HD23	2.49	0.48
1:C:28:GLU:O	1:C:32:GLY:HA2	2.14	0.48
1:A:129:TRP:NE1	1:A:248:PRO:O	2.47	0.48
1:B:392:GLN:HG3	1:B:393:GLN:HG2	1.95	0.48
1:A:377:LEU:CD1	1:B:370:ALA:HB1	2.43	0.48
1:B:116:ILE:HG12	1:B:244:VAL:HG22	1.96	0.48
1:A:409:PRO:CB	1:A:410:PRO:CA	2.92	0.48
1:B:129:TRP:CE2	1:B:248:PRO:HG2	2.49	0.48
1:A:372:ALA:O	1:A:376:LYS:HB3	2.13	0.47
1:A:284:LEU:O	1:A:285:LEU:CB	2.61	0.47
1:C:34:LYS:HG3	1:C:34:LYS:O	2.15	0.47
1:A:11:ILE:HD12	1:A:61:PHE:CB	2.44	0.47
1:C:272:ASN:HB3	1:C:275:LEU:HD13	1.97	0.47
1:C:158:TRP:CD1	1:C:258:PHE:CE2	3.03	0.47
1:A:363:ALA:HA	1:A:366:THR:HG22	1.96	0.47
1:B:249:THR:HG22	1:B:254:PRO:HA	1.97	0.47
1:B:364:ALA:O	1:B:368:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:MET:O	1:A:382:GLU:HB2	2.15	0.47
1:C:10:TRP:CE3	1:C:40:PRO:HG3	2.50	0.46
1:B:119:LYS:HD3	1:B:241:ASN:OD1	2.16	0.46
1:C:9:ILE:HG12	1:C:59:ILE:HG22	1.98	0.46
1:A:381:PHE:HB2	1:B:371:MET:SD	2.56	0.46
1:A:52:ALA:O	1:B:355:GLN:HA	2.16	0.46
1:A:411:PRO:C	1:A:413:PRO:HD3	2.36	0.46
1:A:410:PRO:CB	1:A:411:PRO:CD	2.74	0.46
1:B:385:LYS:HE3	1:B:386:SER:N	2.31	0.46
1:A:11:ILE:HG23	1:A:12:ASN:N	2.18	0.46
1:B:196:VAL:HA	1:B:199:ILE:HD12	1.98	0.46
1:A:355:GLN:HG3	1:A:360:ALA:HB2	1.98	0.46
1:C:326:LYS:HA	1:C:326:LYS:NZ	2.31	0.46
1:A:376:LYS:NZ	1:A:377:LEU:HB2	2.31	0.45
1:C:81:PRO:HB2	1:C:85:PHE:HD2	1.80	0.45
1:C:183:VAL:O	1:C:361:LEU:HG	2.16	0.45
1:A:45:GLU:O	1:A:48:PRO:HD2	2.17	0.45
1:A:257:PRO:HD2	1:A:327:GLY:HA2	1.97	0.45
1:B:333:ILE:HB	1:B:334:PRO:HD2	1.99	0.45
1:A:179:LYS:HA	1:A:179:LYS:NZ	2.32	0.45
1:B:107:PRO:HA	1:B:263:SER:HB3	1.98	0.45
1:B:110:VAL:HG23	1:B:261:VAL:HG22	1.99	0.45
1:C:181:VAL:HG12	1:C:182:GLY:H	1.82	0.45
1:B:128:THR:OG1	1:B:131:GLU:OE2	2.28	0.45
1:C:25:LYS:HA	1:C:25:LYS:NZ	2.32	0.45
1:B:272:ASN:HB3	1:B:275:LEU:HD12	1.98	0.45
1:B:258:PHE:CD2	1:B:340:TRP:HH2	2.35	0.44
1:A:410:PRO:CB	1:A:411:PRO:HD3	2.39	0.44
1:A:373:THR:HA	1:A:376:LYS:NZ	2.31	0.44
1:B:119:LYS:HB2	1:B:241:ASN:ND2	2.33	0.44
1:C:46:LYS:O	1:C:50:VAL:HG23	2.18	0.44
1:B:179:LYS:HB3	1:B:179:LYS:HE2	1.91	0.44
1:A:13:GLY:O	1:A:14:ASP:HB3	2.18	0.44
1:A:354:ARG:O	1:C:53:THR:HA	2.18	0.44
1:A:361:LEU:HA	1:A:361:LEU:HD12	1.90	0.44
1:A:379:LYS:HE2	1:A:379:LYS:HA	1.98	0.44
1:C:259:VAL:HB	1:C:329:ILE:HA	1.99	0.44
1:B:41:ASP:O	1:B:46:LYS:HE3	2.18	0.43
1:C:357:VAL:O	1:C:361:LEU:HB2	2.17	0.43
1:A:139:LEU:HD12	1:A:146:ALA:HA	2.00	0.43
1:B:85:PHE:CD2	1:B:88:LYS:HD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LEU:HD12	1:C:195:LEU:HB2	2.00	0.43
1:A:1:LYS:C	1:A:3:GLU:H	2.21	0.43
1:B:385:LYS:HG3	1:B:386:SER:N	2.33	0.43
1:C:97:VAL:HG21	1:C:107:PRO:HD3	2.00	0.43
1:B:89:LEU:HB2	1:B:90:TYR:H	1.72	0.43
1:A:381:PHE:CD2	1:A:384:LEU:CD2	3.01	0.43
1:C:81:PRO:HB2	1:C:85:PHE:CD2	2.53	0.43
1:A:159:PRO:HA	1:A:256:LYS:O	2.18	0.43
1:A:7:LEU:HA	1:A:58:ASP:OD2	2.18	0.43
1:B:378:MET:O	1:B:382:GLU:HG2	2.19	0.43
1:C:62:TRP:HB3	1:C:67:PHE:HE1	1.82	0.43
1:C:61:PHE:CD2	1:C:264:ALA:HB2	2.53	0.43
1:A:363:ALA:HA	1:A:366:THR:CG2	2.49	0.43
1:C:136:ASP:HA	1:C:146:ALA:HB2	2.01	0.43
1:B:279:PHE:O	1:B:283:TYR:HB2	2.19	0.43
1:B:389:GLN:HA	1:B:392:GLN:HG2	2.01	0.42
1:C:43:LEU:HA	1:C:46:LYS:HB2	2.01	0.42
1:B:332:ASN:H	1:B:332:ASN:HD22	1.65	0.42
1:B:368:ALA:O	1:B:372:ALA:HB2	2.18	0.42
1:A:108:ILE:N	1:A:262:LEU:O	2.44	0.42
1:C:44:GLU:HG2	1:C:45:GLU:OE2	2.20	0.42
1:C:179:LYS:CG	1:C:179:LYS:O	2.58	0.42
1:B:384:LEU:C	1:B:384:LEU:HD22	2.40	0.42
1:A:85:PHE:HZ	1:A:285:LEU:HD13	1.85	0.42
1:C:43:LEU:H	1:C:43:LEU:HD23	1.85	0.42
1:A:64:HIS:CD2	1:A:261:VAL:H	2.37	0.42
1:B:382:GLU:HA	1:B:382:GLU:OE1	2.18	0.42
1:B:6:LYS:HA	1:B:33:ILE:HG23	2.01	0.41
1:B:377:LEU:HD12	1:C:373:THR:HG21	2.02	0.41
1:C:154:PRO:HD3	1:C:344:ARG:HD3	2.01	0.41
1:B:258:PHE:CD2	1:B:340:TRP:CH2	3.09	0.41
1:A:412:PRO:O	1:A:414:PRO:HD3	2.21	0.41
1:C:383:SER:O	1:C:387:PHE:CD2	2.73	0.41
1:A:349:ASN:HB3	1:A:355:GLN:HG2	2.02	0.41
1:B:85:PHE:HD2	1:B:88:LYS:HD2	1.86	0.41
1:C:152:GLN:HA	1:C:348:ILE:HD11	2.03	0.41
1:B:381:PHE:HA	1:B:384:LEU:HD12	2.03	0.41
1:A:338:ALA:HB1	1:A:371:MET:HB3	2.03	0.41
1:C:9:ILE:HG23	1:C:59:ILE:HG23	2.02	0.41
1:B:370:ALA:HB3	1:B:371:MET:HE2	2.03	0.41
1:C:15:LYS:HA	1:C:15:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:PRO:HA	1:A:406:PRO:HD3	1.86	0.40
1:A:158:TRP:CH2	1:A:183:VAL:HG12	2.56	0.40
1:B:356:THR:O	1:B:358:ASP:N	2.54	0.40
1:C:110:VAL:HG12	1:C:111:GLU:H	1.86	0.40
1:B:158:TRP:N	1:B:159:PRO:CD	2.84	0.40
1:A:61:PHE:HA	1:A:263:SER:O	2.21	0.40
1:C:10:TRP:CD1	1:C:57:PRO:HB3	2.56	0.40
1:A:164:ASP:HB3	1:A:187:GLY:CA	2.52	0.40
1:B:111:GLU:HG2	1:B:230:TRP:HZ3	1.86	0.40
1:A:33:ILE:HG21	1:A:275:LEU:HD13	2.03	0.40
1:A:167:TYR:CE1	1:A:182:GLY:HA3	2.57	0.40
1:A:122:LEU:HA	1:A:123:PRO:HD2	1.97	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	401/449 (89%)	346 (86%)	36 (9%)	19 (5%)	3	33
1	B	396/449 (88%)	364 (92%)	25 (6%)	7 (2%)	11	56
1	C	400/449 (89%)	350 (88%)	42 (10%)	8 (2%)	9	55
All	All	1197/1347 (89%)	1060 (89%)	103 (9%)	34 (3%)	6	47

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	14	ASP
1	A	181	VAL
1	A	285	LEU
1	A	287	ASP

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Mol	Chain	Res	Type
1	A	406	PRO
1	A	407	PRO
1	A	415	PRO
1	B	357	VAL
1	A	173	ASN
1	B	42	LYS
1	C	168	ALA
1	C	357	VAL
1	C	396	GLN
1	A	12	ASN
1	A	174	GLY
1	A	241	ASN
1	A	410	PRO
1	B	4	GLU
1	B	165	GLY
1	C	180	ASP
1	A	13	GLY
1	A	165	GLY
1	A	409	PRO
1	C	165	GLY
1	C	244	VAL
1	A	412	PRO
1	B	89	LEU
1	B	180	ASP
1	C	2	ILE
1	C	395	GLN
1	B	229	PRO
1	A	11	ILE
1	A	414	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	311/363 (86%)	271 (87%)	40 (13%)	5	32
1	B	306/363 (84%)	267 (87%)	39 (13%)	5	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	305/363 (84%)	267 (88%)	38 (12%)	6	33
All	All	922/1089 (85%)	805 (87%)	117 (13%)	5	32

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	ILE
1	A	25	LYS
1	A	26	LYS
1	A	31	THR
1	A	34	LYS
1	A	42	LYS
1	A	49	GLN
1	A	65	ASP
1	A	66	ARG
1	A	73	SER
1	A	80	THR
1	A	88	LYS
1	A	103	LEU
1	A	119	LYS
1	A	128	THR
1	A	140	LYS
1	A	160	LEU
1	A	167	TYR
1	A	179	LYS
1	A	189	LYS
1	A	200	LYS
1	A	201	ASN
1	A	202	LYS
1	A	205	ASN
1	A	239	LYS
1	A	272	ASN
1	A	277	LYS
1	A	278	GLU
1	A	308	GLU
1	A	310	GLU
1	A	322	GLU
1	A	341	TYR
1	A	348	ILE
1	A	361	LEU
1	A	374	LEU

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Mol	Chain	Res	Type
1	A	376	LYS
1	A	379	LYS
1	A	382	GLU
1	A	384	LEU
1	B	8	VAL
1	B	22	GLU
1	B	25	LYS
1	B	41	ASP
1	B	42	LYS
1	B	80	THR
1	B	89	LEU
1	B	97	VAL
1	B	100	ASN
1	B	110	VAL
1	B	115	LEU
1	B	121	LEU
1	B	128	THR
1	B	139	LEU
1	B	148	MET
1	B	160	LEU
1	B	173	ASN
1	B	184	ASP
1	B	197	ASP
1	B	200	LYS
1	B	214	GLU
1	B	235	ILE
1	B	259	VAL
1	B	272	ASN
1	B	277	LYS
1	B	282	ASN
1	B	286	THR
1	B	297	LYS
1	B	299	LEU
1	B	332	ASN
1	B	335	GLN
1	B	345	THR
1	B	365	GLN
1	B	367	ASN
1	B	375	GLU
1	B	376	LYS
1	B	384	LEU
1	B	385	LYS

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Mol	Chain	Res	Type
1	B	389	GLN
1	C	17	TYR
1	C	25	LYS
1	C	31	THR
1	C	33	ILE
1	C	34	LYS
1	C	36	THR
1	C	39	HIS
1	C	42	LYS
1	C	50	VAL
1	C	80	THR
1	C	82	ASP
1	C	102	LYS
1	C	115	LEU
1	C	137	LYS
1	C	160	LEU
1	C	170	LYS
1	C	179	LYS
1	C	184	ASP
1	C	189	LYS
1	C	205	ASN
1	C	237	THR
1	C	267	ASN
1	C	277	LYS
1	C	278	GLU
1	C	286	THR
1	C	295	LYS
1	C	297	LYS
1	C	311	LEU
1	C	326	LYS
1	C	329	ILE
1	C	341	TYR
1	C	344	ARG
1	C	345	THR
1	C	358	ASP
1	C	375	GLU
1	C	378	MET
1	C	379	LYS
1	C	385	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	86	GLN
1	A	124	ASN
1	A	201	ASN
1	A	203	HIS
1	A	234	ASN
1	A	365	GLN
1	B	64	HIS
1	B	72	GLN
1	B	86	GLN
1	B	100	ASN
1	B	218	ASN
1	B	332	ASN
1	B	335	GLN
1	C	118	ASN
1	C	124	ASN
1	C	152	GLN
1	C	203	HIS
1	C	205	ASN
1	C	218	ASN
1	C	396	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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 ⓘ

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

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, 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	405/449 (90%)	-0.07	12 (2%) 54 37	58, 83, 93, 104	37 (9%)
1	B	398/449 (88%)	-0.05	19 (4%) 34 22	72, 84, 94, 100	30 (7%)
1	C	402/449 (89%)	-0.04	16 (3%) 42 28	74, 85, 98, 108	33 (8%)
All	All	1205/1347 (89%)	-0.05	47 (3%) 43 29	58, 84, 96, 108	100 (8%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	GLN	5.0
1	B	390	GLN	4.6
1	C	395	GLN	4.6
1	B	387	PHE	4.5
1	C	394	GLN	4.2
1	B	391	GLN	4.1
1	B	388	GLN	4.0
1	B	382	GLU	3.8
1	A	389	GLN	3.6
1	A	403	GLN	3.6
1	B	386	SER	3.5
1	A	386	SER	3.5
1	C	400	GLN	3.4
1	C	399	GLN	3.3
1	A	406	PRO	3.3
1	A	383	SER	3.3
1	C	396	GLN	3.2
1	A	416	GLN	3.1
1	B	393	GLN	3.0
1	A	381	PHE	3.0
1	B	394	GLN	2.9
1	C	397	GLN	2.8
1	A	391	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	387	PHE	2.7
1	C	385	LYS	2.7
1	C	389	GLN	2.6
1	C	174	GLY	2.6
1	B	398	GLN	2.6
1	B	130	GLU	2.4
1	A	390	GLN	2.4
1	B	389	GLN	2.4
1	B	381	PHE	2.4
1	C	391	GLN	2.3
1	C	393	GLN	2.3
1	B	395	GLN	2.3
1	B	383	SER	2.3
1	B	392	GLN	2.2
1	C	401	GLN	2.2
1	B	102	LYS	2.2
1	B	4	GLU	2.2
1	A	374	LEU	2.1
1	C	173	ASN	2.1
1	C	1	LYS	2.1
1	C	390	GLN	2.1
1	B	378	MET	2.1
1	B	397	GLN	2.1
1	C	2	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	A	503	1/1	0.94	0.21	-	54,54,54,54	0
3	CA	A	504	1/1	0.95	0.23	-	58,58,58,58	0
2	ZN	B	501	1/1	0.74	0.12	-	105,105,105,105	0
2	ZN	B	502	1/1	0.97	0.42	-	99,99,99,99	0
2	ZN	A	502	1/1	0.93	0.09	-	116,116,116,116	0
2	ZN	A	501	1/1	0.99	0.21	-	76,76,76,76	0
3	CA	B	504	1/1	0.84	0.12	-	74,74,74,74	0
2	ZN	B	503	1/1	0.98	0.15	-	65,65,65,65	0
3	CA	A	505	1/1	0.94	0.15	-	89,89,89,89	0
3	CA	B	505	1/1	0.83	0.16	-	80,80,80,80	0
2	ZN	C	501	1/1	0.92	0.06	-	110,110,110,110	0
3	CA	C	503	1/1	0.96	0.31	-	94,94,94,94	0
3	CA	C	502	1/1	0.93	0.22	-	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.