



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 PM UTC

PDB ID : 3IO4 / pdb_00003io4
Title : Huntingtin amino-terminal region with 17 Gln residues - Crystal C90
Authors : Kim, M.W.; Chelliah, Y.; Kim, S.W.; Otwinowski, Z.; Bezprozvanny, I.
Deposited on : 2009-08-13
Resolution : 3.63 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

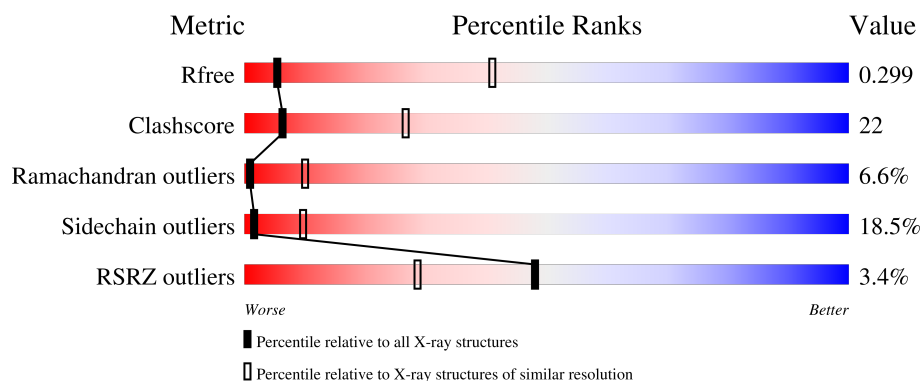
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.63 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	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

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	4% 47% 36% 8% • 7%
1	B	449	4% 42% 34% 11% • 12%
1	C	449	2% 49% 33% 6% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9331 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 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	4	0	0
			3176	2046	520	602	8			
1	B	397	Total	C	N	O	S	20	1	0
			3076	1974	506	588	8			
1	C	398	Total	C	N	O	S	8	0	0
			3065	1969	503	585	8			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	-	linker	UNP P0AEY0
A	360	ALA	-	linker	UNP P0AEY0
A	361	LEU	-	linker	UNP P0AEY0
A	362	ALA	-	linker	UNP P0AEY0
A	363	ALA	-	linker	UNP P0AEY0
A	364	ALA	-	linker	UNP P0AEY0
A	365	GLN	-	linker	UNP P0AEY0
A	366	THR	-	linker	UNP P0AEY0
A	367	ASN	-	linker	UNP P0AEY0
A	368	ALA	-	linker	UNP P0AEY0
A	369	ALA	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
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 P0AEY0
B	360	ALA	-	linker	UNP P0AEY0
B	361	LEU	-	linker	UNP P0AEY0
B	362	ALA	-	linker	UNP P0AEY0
B	363	ALA	-	linker	UNP P0AEY0
B	364	ALA	-	linker	UNP P0AEY0
B	365	GLN	-	linker	UNP P0AEY0
B	366	THR	-	linker	UNP P0AEY0
B	367	ASN	-	linker	UNP P0AEY0
B	368	ALA	-	linker	UNP P0AEY0
B	369	ALA	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
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 P0AEY0
C	360	ALA	-	linker	UNP P0AEY0
C	361	LEU	-	linker	UNP P0AEY0
C	362	ALA	-	linker	UNP P0AEY0
C	363	ALA	-	linker	UNP P0AEY0
C	364	ALA	-	linker	UNP P0AEY0
C	365	GLN	-	linker	UNP P0AEY0
C	366	THR	-	linker	UNP P0AEY0
C	367	ASN	-	linker	UNP P0AEY0
C	368	ALA	-	linker	UNP P0AEY0
C	369	ALA	-	linker	UNP P0AEY0
C	370	ALA	-	linker	UNP P0AEY0
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
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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	3	Total 3	Zn 3	0	0
2	B	3	Total 3	Zn 3	0	0
2	C	2	Total 2	Zn 2	0	0

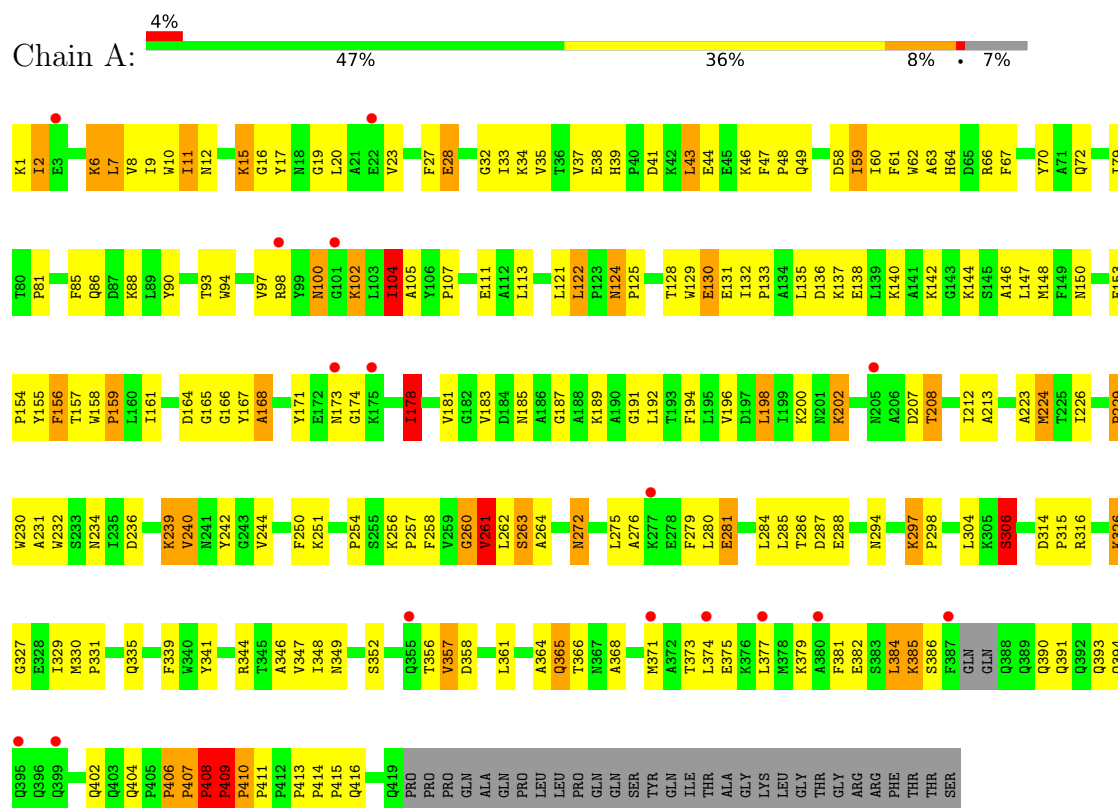
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

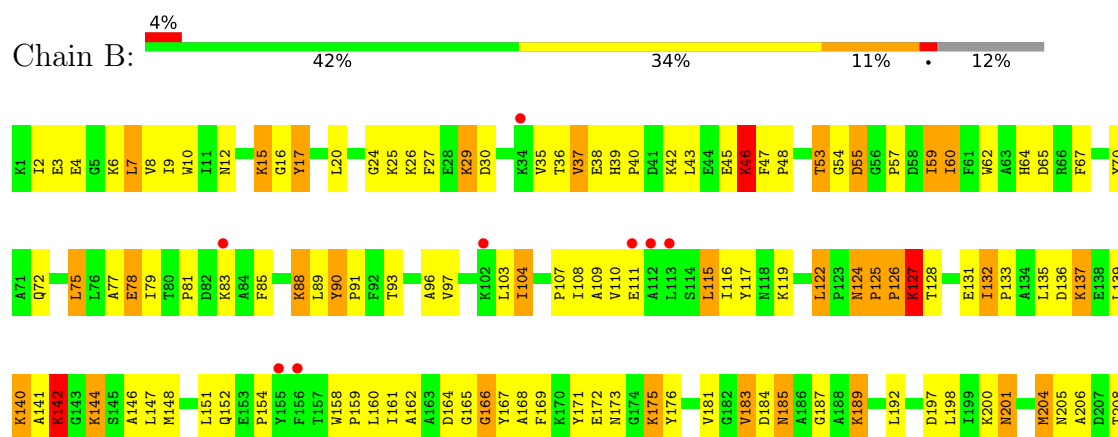
3 Residue-property plots

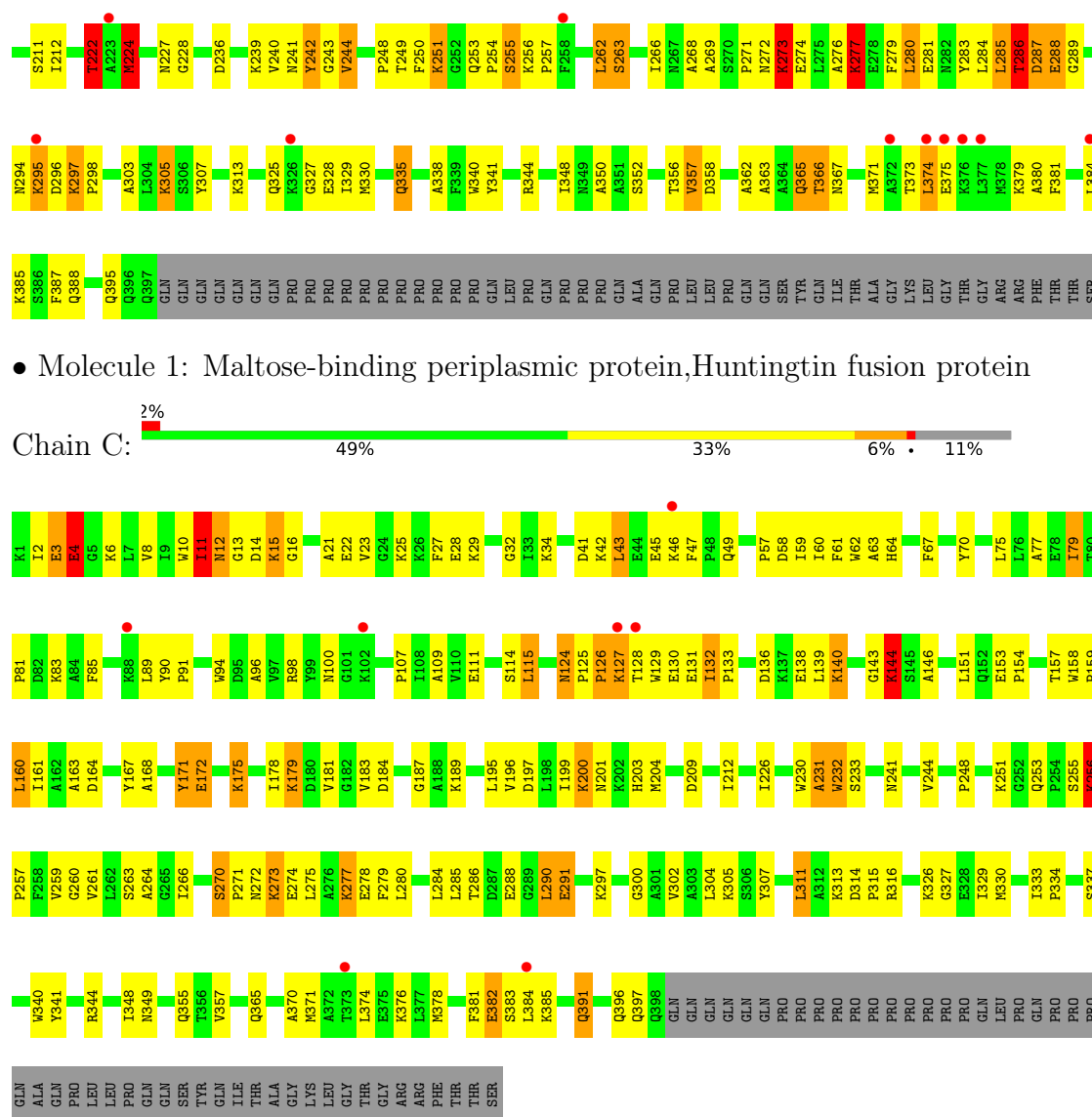
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 fusion protein



- Molecule 1: Maltose-binding periplasmic protein,Huntingtin fusion protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.95Å 101.21Å 142.05Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	37.42 – 3.63 37.42 – 3.63	Depositor EDS
% Data completeness (in resolution range)	64.4 (37.42-3.63) 64.3 (37.42-3.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.02	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.251 , 0.304 (Not available) , 0.299	Depositor DCC
R_{free} test set	842 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	135.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.041 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9331	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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 [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	0.64	3/3258 (0.1%)	1.00	12/4436 (0.3%)
1	B	0.80	7/3147 (0.2%)	1.06	15/4270 (0.4%)
1	C	0.68	1/3136 (0.0%)	0.95	6/4256 (0.1%)
All	All	0.71	11/9541 (0.1%)	1.01	33/12962 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	LYS	CB-CG	-22.92	0.83	1.52
1	B	140	LYS	CB-CG	18.20	2.07	1.52
1	B	15	LYS	CB-CG	-17.83	0.98	1.52
1	B	111	GLU	CB-CG	-11.77	1.17	1.52
1	A	202	LYS	CB-CG	-11.40	1.18	1.52
1	B	46	LYS	CB-CG	-8.71	1.26	1.52
1	B	88	LYS	CB-CG	-7.34	1.30	1.52
1	B	142	LYS	CE-NZ	7.03	1.70	1.49
1	B	142	LYS	CD-CE	6.45	1.71	1.52
1	A	411	PRO	CA-C	5.70	1.57	1.52
1	A	408	PRO	CA-C	5.39	1.57	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	LYS	CA-CB-CG	17.82	149.75	114.10
1	B	46	LYS	CB-CG-CD	-14.71	77.47	111.30
1	A	411	PRO	N-CA-C	10.88	123.98	110.70
1	B	140	LYS	CA-CB-CG	-10.86	92.39	114.10
1	B	111	GLU	CA-CB-CG	10.53	135.16	114.10
1	B	15	LYS	CB-CG-CD	-9.72	88.94	111.30
1	C	15	LYS	CA-CB-CG	8.50	131.10	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	LYS	CA-CB-CG	8.31	130.71	114.10
1	A	408	PRO	CA-C-N	8.09	128.72	120.38
1	A	408	PRO	C-N-CA	8.09	128.72	120.38
1	B	124	ASN	CA-C-N	7.72	128.34	120.38
1	B	124	ASN	C-N-CA	7.72	128.34	120.38
1	B	111	GLU	CB-CG-CD	-7.57	99.74	112.60
1	B	228	GLY	CA-C-N	7.18	128.82	119.84
1	B	228	GLY	C-N-CA	7.18	128.82	119.84
1	A	409	PRO	N-CA-C	7.04	119.29	110.70
1	A	414	PRO	N-CA-C	6.88	119.10	110.70
1	A	124	ASN	CA-C-N	6.55	127.13	120.38
1	A	124	ASN	C-N-CA	6.55	127.13	120.38
1	A	202	LYS	CB-CG-CD	-6.23	96.97	111.30
1	C	124	ASN	CA-C-N	6.13	126.70	120.38
1	C	124	ASN	C-N-CA	6.13	126.70	120.38
1	A	409	PRO	CA-C-N	5.97	126.53	120.38
1	A	409	PRO	C-N-CA	5.97	126.53	120.38
1	A	104	ILE	N-CA-C	5.81	118.04	111.88
1	B	173	ASN	N-CA-C	5.58	117.44	110.91
1	A	406	PRO	N-CA-C	5.42	117.31	110.70
1	B	88	LYS	CB-CG-CD	5.38	123.67	111.30
1	C	333	ILE	CA-C-N	5.29	126.46	119.84
1	C	333	ILE	C-N-CA	5.29	126.46	119.84
1	C	98	ARG	N-CA-C	5.15	115.83	107.23
1	B	90	TYR	N-CA-C	5.07	115.80	109.57
1	B	266	ILE	N-CA-C	5.00	115.65	107.24

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	3176	0	3103	166	0
1	B	3076	0	3033	145	0
1	C	3065	0	3018	112	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	1
2	B	3	0	0	0	0
2	C	2	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
All	All	9331	0	9154	409	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 22.

All (409) 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:239:LYS:HA	1:A:239:LYS:HE2	1.20	1.09
1:C:381:PHE:CD1	1:C:385:LYS:HE3	1.87	1.09
1:A:11:ILE:HG13	1:A:12:ASN:H	1.19	1.06
1:A:406:PRO:HB2	1:C:381:PHE:HE2	0.99	1.06
1:A:406:PRO:HB2	1:C:381:PHE:CE2	1.91	1.05
1:A:85:PHE:HE2	1:A:281:GLU:HB2	1.20	1.04
1:B:148:MET:HB2	1:B:222:THR:HG21	1.39	1.03
1:A:85:PHE:CE2	1:A:281:GLU:HB2	1.98	0.99
1:A:15:LYS:HA	1:A:297:LYS:HD3	1.43	0.96
1:A:239:LYS:HA	1:A:239:LYS:CE	1.94	0.96
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.48	0.95
1:A:62:TRP:CD1	1:A:63:ALA:H	1.85	0.95
1:B:9:ILE:HG12	1:B:59:ILE:HG12	1.48	0.93
1:B:122:LEU:HD11	1:B:125:PRO:HA	1.51	0.91
1:B:54:GLY:O	1:B:55:ASP:HB2	1.69	0.91
1:A:62:TRP:HD1	1:A:63:ALA:H	0.99	0.90
1:A:62:TRP:HD1	1:A:63:ALA:N	1.71	0.87
1:A:239:LYS:HE2	1:A:239:LYS:CA	2.05	0.87
1:B:126:PRO:HD3	1:B:224:MET:HE3	1.56	0.87
1:A:257:PRO:HD2	1:A:327:GLY:HA2	1.55	0.86
1:A:406:PRO:CB	1:C:381:PHE:HE2	1.86	0.86
1:A:374:LEU:HD11	1:C:376:LYS:HB3	1.56	0.85
1:A:408:PRO:CB	1:A:409:PRO:HD2	2.07	0.84
1:C:381:PHE:CE1	1:C:385:LYS:HE3	2.13	0.84
1:C:151:LEU:HD11	1:C:204:MET:HE2	1.59	0.83
1:A:408:PRO:HB2	1:A:409:PRO:HD2	1.61	0.82
1:B:107:PRO:HA	1:B:263:SER:HB2	1.58	0.82
1:B:192:LEU:HD11	1:B:350:ALA:HB1	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:PHE:HD1	1:C:385:LYS:HE3	1.43	0.81
1:B:242:TYR:HB2	1:B:243:GLY:HA3	1.62	0.80
1:A:229:PRO:O	1:A:231:ALA:N	2.14	0.79
1:B:126:PRO:HD3	1:B:224:MET:CE	2.13	0.78
1:A:132:ILE:HB	1:A:133:PRO:HD3	1.65	0.77
1:C:11:ILE:O	1:C:12:ASN:HB2	1.83	0.77
1:A:11:ILE:HG13	1:A:12:ASN:N	1.92	0.76
1:A:384:LEU:HD11	1:B:371:MET:SD	2.25	0.76
1:C:201:ASN:HB3	1:C:203:HIS:CE1	2.21	0.76
1:B:348:ILE:O	1:B:352:SER:HB2	1.84	0.75
1:B:64:HIS:CE1	1:B:330:MET:O	2.40	0.74
1:A:11:ILE:CG1	1:A:12:ASN:H	1.99	0.74
1:A:128:THR:HG23	1:A:131:GLU:HG3	1.70	0.74
1:A:236:ASP:HA	1:A:239:LYS:CE	2.16	0.74
1:A:223:ALA:O	1:A:224:MET:HB2	1.88	0.73
1:A:155:TYR:CE1	1:A:258:PHE:HB2	2.24	0.73
1:A:62:TRP:CD1	1:A:63:ALA:N	2.51	0.72
1:C:128:THR:HG23	1:C:131:GLU:HB2	1.70	0.72
1:C:164:ASP:HB3	1:C:187:GLY:HA2	1.71	0.71
1:A:260:GLY:O	1:A:261:VAL:HB	1.89	0.71
1:B:136:ASP:HA	1:B:146:ALA:HB2	1.71	0.70
1:B:128:THR:HG22	1:B:131:GLU:HG3	1.73	0.70
1:B:64:HIS:HE1	1:B:330:MET:O	1.75	0.69
1:A:90:TYR:HB2	1:A:93:THR:HG23	1.74	0.69
1:B:272:ASN:O	1:B:274:GLU:N	2.25	0.69
1:C:129:TRP:HA	1:C:132:ILE:HD12	1.75	0.68
1:B:89:LEU:HD13	1:B:303:ALA:HB1	1.75	0.68
1:A:9:ILE:HG12	1:A:59:ILE:HG12	1.74	0.68
1:A:154:PRO:HG3	1:A:344:ARG:HB2	1.77	0.67
1:B:12:ASN:HB2	1:B:62:TRP:CZ3	2.30	0.67
1:C:62:TRP:HB3	1:C:67:PHE:HE2	1.60	0.67
1:A:181:VAL:HB	1:A:365:GLN:HE22	1.60	0.67
1:A:406:PRO:O	1:A:408:PRO:HD3	1.95	0.66
1:A:297:LYS:HE2	1:A:298:PRO:O	1.96	0.66
1:C:126:PRO:O	1:C:127:LYS:HB2	1.96	0.66
1:A:261:VAL:HG12	1:A:261:VAL:O	1.95	0.66
1:A:167:TYR:O	1:A:168:ALA:HB3	1.96	0.66
1:B:12:ASN:HB2	1:B:62:TRP:HZ3	1.61	0.66
1:B:17:TYR:C	1:B:17:TYR:CD2	2.73	0.66
1:B:108:ILE:HG12	1:B:263:SER:HA	1.77	0.66
1:A:16:GLY:H	1:A:297:LYS:HZ2	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ALA:O	1:C:233:SER:N	2.29	0.66
1:A:19:GLY:O	1:A:23:VAL:HG23	1.96	0.65
1:A:155:TYR:HE1	1:A:258:PHE:HB2	1.62	0.65
1:B:54:GLY:O	1:B:55:ASP:CB	2.45	0.65
1:A:44:GLU:HB3	1:A:62:TRP:CZ3	2.32	0.64
1:B:142:LYS:HG3	1:B:144:LYS:HG2	1.78	0.64
1:B:96:ALA:HB2	1:B:329:ILE:HD12	1.80	0.64
1:B:222:THR:HG22	1:B:222:THR:O	1.98	0.64
1:C:158:TRP:N	1:C:159:PRO:HD2	2.13	0.64
1:A:150:ASN:HB3	1:A:156:PHE:HD2	1.62	0.64
1:A:121:LEU:HD12	1:A:223:ALA:HB2	1.78	0.63
1:B:171:TYR:HB2	1:B:175:LYS:O	1.99	0.63
1:B:189:LYS:HZ1	1:B:358:ASP:HA	1.64	0.63
1:A:43:LEU:HA	1:A:46:LYS:HB2	1.80	0.62
1:B:107:PRO:HA	1:B:263:SER:CB	2.28	0.62
1:A:377:LEU:HD22	1:B:373:THR:CG2	2.28	0.62
1:A:171:TYR:CE1	1:A:174:GLY:HA2	2.33	0.62
1:C:21:ALA:O	1:C:25:LYS:HG2	1.98	0.62
1:C:10:TRP:HE3	1:C:43:LEU:HD13	1.66	0.61
1:C:334:PRO:O	1:C:337:SER:OG	2.17	0.61
1:B:276:ALA:O	1:B:280:LEU:HB2	2.00	0.61
1:C:272:ASN:O	1:C:274:GLU:N	2.34	0.61
1:A:393:GLN:HG3	1:A:394:GLN:H	1.66	0.60
1:B:295:LYS:HG3	1:B:296:ASP:N	2.15	0.60
1:A:382:GLU:HA	1:A:385:LYS:HZ2	1.67	0.60
1:C:91:PRO:HA	1:C:94:TRP:HD1	1.67	0.60
1:A:236:ASP:HA	1:A:239:LYS:HE3	1.83	0.59
1:C:270:SER:O	1:C:273:LYS:HG2	2.03	0.59
1:B:338:ALA:HB1	1:B:371:MET:HG2	1.84	0.59
1:B:189:LYS:NZ	1:B:358:ASP:HA	2.17	0.59
1:B:381:PHE:HA	1:B:384:LEU:HD12	1.84	0.59
1:B:248:PRO:O	1:B:255:SER:OG	2.21	0.58
1:C:349:ASN:HB3	1:C:355:GLN:HG2	1.84	0.58
1:C:64:HIS:O	1:C:67:PHE:HB2	2.04	0.58
1:A:12:ASN:HB3	1:A:15:LYS:HG2	1.85	0.58
1:C:125:PRO:HG2	1:C:127:LYS:HE2	1.85	0.58
1:A:272:ASN:HB3	1:A:275:LEU:HD12	1.84	0.58
1:A:85:PHE:HE2	1:A:281:GLU:CB	2.04	0.58
1:A:167:TYR:O	1:A:168:ALA:CB	2.50	0.58
1:A:377:LEU:HD22	1:B:373:THR:HG21	1.85	0.58
1:C:89:LEU:CD1	1:C:107:PRO:HG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:TYR:O	1:C:172:GLU:HB3	2.04	0.58
1:B:183:VAL:O	1:B:185[A]:ASN:N	2.37	0.58
1:C:11:ILE:HG23	1:C:12:ASN:H	1.68	0.58
1:B:158:TRP:CE2	1:B:162:ALA:HB2	2.38	0.57
1:C:129:TRP:O	1:C:132:ILE:HB	2.04	0.57
1:C:114:SER:HB3	1:C:244:VAL:HG13	1.85	0.57
1:A:107:PRO:HA	1:A:263:SER:HB3	1.85	0.57
1:A:130:GLU:O	1:A:133:PRO:HD2	2.04	0.57
1:B:164:ASP:HB3	1:B:187:GLY:HA2	1.86	0.57
1:A:150:ASN:HB3	1:A:156:PHE:CD2	2.39	0.57
1:B:148:MET:HB2	1:B:222:THR:CG2	2.25	0.57
1:B:204:MET:HE2	1:B:205:ASN:H	1.69	0.56
1:A:404:GLN:O	1:A:406:PRO:HD3	2.04	0.56
1:A:61:PHE:CE1	1:A:264:ALA:HB2	2.40	0.56
1:B:185[A]:ASN:C	1:B:185[A]:ASN:ND2	2.60	0.56
1:C:11:ILE:HD12	1:C:61:PHE:HB2	1.87	0.56
1:B:136:ASP:CA	1:B:146:ALA:HB2	2.35	0.56
1:A:161:ILE:HA	1:A:191:GLY:HA3	1.87	0.56
1:C:11:ILE:HG23	1:C:12:ASN:N	2.19	0.56
1:A:382:GLU:HA	1:A:385:LYS:NZ	2.21	0.56
1:C:10:TRP:CE3	1:C:43:LEU:HD13	2.40	0.56
1:B:251:LYS:C	1:B:253:GLN:H	2.14	0.55
1:C:136:ASP:O	1:C:140:LYS:HB3	2.06	0.55
1:B:116:ILE:HA	1:B:244:VAL:H	1.71	0.55
1:B:29:LYS:O	1:B:29:LYS:HG3	2.05	0.55
1:C:168:ALA:O	1:C:181:VAL:HA	2.07	0.55
1:B:151:LEU:HD11	1:B:204:MET:SD	2.46	0.55
1:B:158:TRP:HZ2	1:B:167:TYR:HA	1.71	0.55
1:A:159:PRO:HA	1:A:256:LYS:O	2.07	0.55
1:A:285:LEU:O	1:A:304:LEU:HD22	2.07	0.54
1:B:147:LEU:HD12	1:B:224:MET:HB3	1.89	0.54
1:A:17:TYR:O	1:A:20:LEU:HB3	2.08	0.54
1:A:346:ALA:HB2	1:A:364:ALA:HB2	1.88	0.54
1:A:229:PRO:HA	1:A:232:TRP:CZ3	2.42	0.54
1:B:242:TYR:HD1	1:B:242:TYR:H	1.56	0.54
1:A:63:ALA:HA	1:A:262:LEU:HA	1.89	0.54
1:B:183:VAL:O	1:B:185[B]:ASN:N	2.37	0.54
1:A:279:PHE:HD1	1:A:280:LEU:HD12	1.73	0.54
1:B:185[A]:ASN:C	1:B:185[A]:ASN:HD22	2.16	0.54
1:A:131:GLU:HB3	1:A:135:LEU:HD13	1.90	0.53
1:C:11:ILE:HD12	1:C:61:PHE:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:LYS:HB2	1:C:327:GLY:HA2	1.91	0.53
1:A:373:THR:O	1:A:377:LEU:HG	2.08	0.53
1:B:77:ALA:HB2	1:B:268:ALA:HA	1.90	0.53
1:B:162:ALA:HB3	1:B:256:LYS:HB2	1.91	0.53
1:B:189:LYS:HA	1:B:189:LYS:HZ3	1.74	0.53
1:A:192:LEU:HD11	1:A:347:VAL:HG23	1.91	0.52
1:C:136:ASP:HB3	1:C:203:HIS:HD2	1.75	0.52
1:B:126:PRO:CD	1:B:224:MET:HE3	2.34	0.52
1:A:124:ASN:HD22	1:A:125:PRO:HD2	1.73	0.52
1:A:183:VAL:O	1:A:361:LEU:HD22	2.08	0.52
1:B:249:THR:HG22	1:B:254:PRO:HA	1.91	0.52
1:C:286:THR:O	1:C:290:LEU:HD23	2.10	0.52
1:B:371:MET:SD	1:B:374:LEU:HD13	2.49	0.52
1:B:45:GLU:O	1:B:46:LYS:C	2.52	0.52
1:A:406:PRO:CD	1:A:407:PRO:HD3	2.39	0.52
1:A:409:PRO:HG2	1:B:384:LEU:HD13	1.92	0.52
1:B:158:TRP:N	1:B:159:PRO:HD2	2.24	0.52
1:B:197:ASP:HA	1:B:200:LYS:HG2	1.92	0.52
1:A:168:ALA:O	1:A:181:VAL:HA	2.10	0.51
1:A:223:ALA:O	1:A:224:MET:CB	2.56	0.51
1:C:61:PHE:CE1	1:C:264:ALA:HB2	2.46	0.51
1:C:378:MET:O	1:C:382:GLU:HB2	2.10	0.51
1:A:166:GLY:HA2	1:A:185:ASN:HD22	1.75	0.51
1:B:344:ARG:O	1:B:348:ILE:HG12	2.11	0.51
1:A:286:THR:O	1:A:287:ASP:C	2.53	0.51
1:A:240:VAL:O	1:A:242:TYR:HD2	1.94	0.51
1:C:11:ILE:O	1:C:12:ASN:CB	2.55	0.51
1:B:147:LEU:HD12	1:B:224:MET:HG3	1.93	0.50
1:C:115:LEU:HD12	1:C:248:PRO:HD3	1.92	0.50
1:A:366:THR:C	1:A:368:ALA:H	2.20	0.50
1:B:384:LEU:O	1:B:388:GLN:HB2	2.11	0.50
1:A:9:ILE:HG23	1:A:59:ILE:HG13	1.93	0.50
1:A:408:PRO:CB	1:A:409:PRO:CD	2.84	0.50
1:A:132:ILE:HB	1:A:133:PRO:CD	2.37	0.50
1:C:60:ILE:O	1:C:264:ALA:HA	2.10	0.50
1:A:6:LYS:O	1:A:7:LEU:HB2	2.11	0.50
1:B:242:TYR:CB	1:B:243:GLY:HA3	2.37	0.50
1:A:171:TYR:CZ	1:A:174:GLY:HA2	2.47	0.50
1:B:53:THR:HA	1:C:355:GLN:HA	1.93	0.50
1:B:59:ILE:HG13	1:B:60:ILE:N	2.24	0.50
1:B:24:GLY:HA2	1:B:35:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TRP:N	1:A:159:PRO:HD2	2.27	0.50
1:B:274:GLU:O	1:B:277:LYS:HB3	2.12	0.49
1:C:89:LEU:HD12	1:C:107:PRO:HG2	1.94	0.49
1:A:12:ASN:HB3	1:A:15:LYS:CG	2.42	0.49
1:B:135:LEU:O	1:B:139:LEU:HG	2.11	0.49
1:B:122:LEU:HD11	1:B:125:PRO:CA	2.33	0.49
1:B:373:THR:OG1	1:B:374:LEU:N	2.46	0.49
1:B:128:THR:CG2	1:B:131:GLU:HG3	2.42	0.49
1:B:151:LEU:HD12	1:B:208:THR:HB	1.93	0.49
1:A:408:PRO:HB2	1:A:409:PRO:CD	2.39	0.49
1:B:205:ASN:CG	1:B:206:ALA:H	2.20	0.49
1:A:148:MET:HE3	1:A:208:THR:HG23	1.94	0.49
1:A:155:TYR:CD1	1:A:155:TYR:O	2.66	0.49
1:B:338:ALA:CB	1:B:371:MET:HG2	2.43	0.49
1:C:383:SER:OG	1:C:384:LEU:N	2.44	0.49
1:C:70:TYR:HA	1:C:75:LEU:HD12	1.94	0.49
1:A:121:LEU:HD12	1:A:223:ALA:CB	2.42	0.48
1:A:207:ASP:O	1:A:208:THR:C	2.56	0.48
1:B:10:TRP:CD1	1:B:38:GLU:HB2	2.48	0.48
1:A:104:ILE:O	1:A:105:ALA:HB2	2.12	0.48
1:A:164:ASP:HB3	1:A:187:GLY:HA2	1.95	0.48
1:A:229:PRO:HB3	1:A:232:TRP:CZ3	2.48	0.48
1:A:154:PRO:HA	1:A:157:THR:OG1	2.12	0.48
1:C:302:VAL:HG21	1:C:307:TYR:HD2	1.79	0.48
1:B:192:LEU:HD12	1:B:357:VAL:HG13	1.96	0.48
1:C:158:TRP:HZ2	1:C:167:TYR:HA	1.78	0.48
1:A:136:ASP:CA	1:A:146:ALA:HB2	2.34	0.48
1:A:349:ASN:O	1:A:352:SER:HB2	2.14	0.48
1:A:377:LEU:HB3	1:B:373:THR:HB	1.96	0.48
1:B:90:TYR:HB2	1:B:93:THR:HG23	1.95	0.48
1:B:136:ASP:O	1:B:140:LYS:N	2.35	0.48
1:B:257:PRO:HD2	1:B:327:GLY:HA2	1.95	0.48
1:B:363:ALA:O	1:B:366:THR:HG22	2.14	0.48
1:A:344:ARG:NH2	1:A:348:ILE:HD12	2.28	0.48
1:A:356:THR:O	1:A:357:VAL:C	2.57	0.48
1:A:28:GLU:O	1:A:32:GLY:HA2	2.14	0.47
1:B:67:PHE:HD2	1:B:70:TYR:CD1	2.32	0.47
1:B:64:HIS:NE2	1:B:330:MET:HB3	2.29	0.47
1:B:7:LEU:HB3	1:B:35:VAL:HG22	1.95	0.47
1:A:373:THR:C	1:A:377:LEU:HG	2.40	0.47
1:C:109:ALA:O	1:C:261:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:O	1:A:264:ALA:HA	2.15	0.47
1:B:204:MET:HE2	1:B:204:MET:HA	1.96	0.47
1:C:307:TYR:CD2	1:C:311:LEU:HD21	2.50	0.47
1:C:381:PHE:CD1	1:C:385:LYS:CE	2.79	0.47
1:A:59:ILE:HD13	1:A:280:LEU:HD11	1.96	0.47
1:A:168:ALA:HB2	1:A:339:PHE:CE1	2.49	0.47
1:B:159:PRO:HA	1:B:256:LYS:O	2.14	0.47
1:A:60:ILE:HG13	1:A:61:PHE:N	2.30	0.47
1:A:236:ASP:HA	1:A:239:LYS:HE2	1.92	0.47
1:A:276:ALA:O	1:A:280:LEU:HD13	2.14	0.47
1:A:384:LEU:HD22	1:B:341:TYR:HE2	1.80	0.47
1:B:348:ILE:O	1:B:352:SER:CB	2.58	0.47
1:B:387:PHE:HB2	1:C:341:TYR:CE1	2.50	0.47
1:A:261:VAL:O	1:A:261:VAL:CG1	2.61	0.46
1:A:27:PHE:CE1	1:A:33:ILE:HB	2.51	0.46
1:C:64:HIS:HE1	1:C:330:MET:O	1.98	0.46
1:C:64:HIS:CE1	1:C:330:MET:O	2.68	0.46
1:C:154:PRO:HA	1:C:157:THR:OG1	2.14	0.46
1:B:169:PHE:CZ	1:B:335:GLN:HB3	2.50	0.46
1:A:304:LEU:HG	1:A:306:SER:H	1.80	0.46
1:B:10:TRP:CD1	1:B:57:PRO:HB3	2.50	0.46
1:B:146:ALA:O	1:B:224:MET:HB2	2.14	0.46
1:A:11:ILE:HD12	1:A:61:PHE:HB3	1.97	0.46
1:A:124:ASN:HA	1:A:125:PRO:HD2	1.78	0.46
1:A:156:PHE:CD1	1:A:156:PHE:N	2.81	0.46
1:B:115:LEU:O	1:B:244:VAL:HA	2.15	0.46
1:A:377:LEU:HD22	1:B:373:THR:HG22	1.95	0.46
1:C:111:GLU:OE1	1:C:230:TRP:HZ3	1.99	0.46
1:A:60:ILE:HG13	1:A:61:PHE:H	1.80	0.46
1:A:79:ILE:HD12	1:A:81:PRO:HG3	1.96	0.46
1:A:250:PHE:O	1:A:251:LYS:C	2.59	0.46
1:C:96:ALA:HB2	1:C:329:ILE:HD12	1.98	0.46
1:A:64:HIS:CE1	1:A:330:MET:O	2.69	0.46
1:A:406:PRO:HD2	1:A:407:PRO:HD3	1.97	0.46
1:B:27:PHE:CE2	1:B:279:PHE:HB2	2.51	0.45
1:A:148:MET:HE2	1:A:213:ALA:HA	1.96	0.45
1:B:295:LYS:HG3	1:B:296:ASP:H	1.80	0.45
1:C:158:TRP:HA	1:C:161:ILE:HD12	1.98	0.45
1:A:44:GLU:OE2	1:A:62:TRP:HZ3	1.99	0.45
1:A:159:PRO:HA	1:A:256:LYS:C	2.42	0.45
1:C:85:PHE:HZ	1:C:285:LEU:HD13	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLU:HA	1:A:154:PRO:HD3	1.86	0.45
1:B:81:PRO:HB2	1:B:85:PHE:HB3	1.97	0.45
1:A:67:PHE:HA	1:A:70:TYR:HD1	1.81	0.45
1:A:86:GLN:HA	1:A:94:TRP:CZ2	2.52	0.45
1:A:158:TRP:HB3	1:A:159:PRO:CD	2.46	0.45
1:B:78:GLU:CB	1:B:103:LEU:O	2.65	0.45
1:B:127:LYS:HA	1:B:127:LYS:HD3	1.71	0.45
1:C:272:ASN:HB3	1:C:275:LEU:HD12	1.98	0.45
1:B:17:TYR:HA	1:B:20:LEU:HD23	1.99	0.45
1:B:62:TRP:O	1:B:262:LEU:O	2.34	0.45
1:C:259:VAL:HG12	1:C:260:GLY:H	1.81	0.45
1:C:85:PHE:CZ	1:C:285:LEU:HD13	2.52	0.45
1:A:232:TRP:HE1	1:A:244:VAL:HG21	1.81	0.45
1:B:286:THR:O	1:B:287:ASP:C	2.59	0.45
1:B:363:ALA:O	1:B:367:ASN:HB2	2.17	0.45
1:B:128:THR:HG22	1:B:131:GLU:OE1	2.17	0.44
1:C:288:GLU:HA	1:C:291:GLU:HB3	1.99	0.44
1:A:196:VAL:HG12	1:A:200:LYS:HE2	1.98	0.44
1:C:43:LEU:O	1:C:47:PHE:HB3	2.17	0.44
1:A:63:ALA:HA	1:A:261:VAL:O	2.18	0.44
1:A:100:ASN:O	1:A:102:LYS:HE2	2.17	0.44
1:A:147:LEU:HD21	1:A:226:ILE:HD11	2.00	0.44
1:A:371:MET:O	1:A:375:GLU:HB2	2.18	0.44
1:A:409:PRO:HA	1:A:410:PRO:HD3	1.55	0.44
1:B:171:TYR:HA	1:B:176:TYR:HA	2.00	0.44
1:A:9:ILE:O	1:A:10:TRP:HD1	2.00	0.44
1:A:194:PHE:CZ	1:A:198:LEU:HD21	2.53	0.44
1:A:254:PRO:HG2	1:A:326:LYS:HG2	2.00	0.44
1:C:89:LEU:HD22	1:C:304:LEU:HA	2.00	0.44
1:A:11:ILE:CD1	1:A:61:PHE:HB3	2.48	0.43
1:B:109:ALA:H	1:B:262:LEU:HB3	1.83	0.43
1:C:274:GLU:HA	1:C:277:LYS:HD2	1.99	0.43
1:B:26:LYS:O	1:B:30:ASP:HB2	2.19	0.43
1:B:340:TRP:HA	1:B:340:TRP:CE3	2.53	0.43
1:B:380:ALA:HA	1:C:370:ALA:HB1	1.99	0.43
1:C:62:TRP:CD1	1:C:63:ALA:H	2.37	0.43
1:B:204:MET:HA	1:B:204:MET:CE	2.48	0.43
1:C:10:TRP:CD1	1:C:57:PRO:HB3	2.54	0.43
1:B:9:ILE:O	1:B:37:VAL:HA	2.18	0.43
1:B:67:PHE:HD2	1:B:70:TYR:HD1	1.66	0.43
1:A:329:ILE:O	1:A:331:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:TYR:HA	1:B:91:PRO:HD3	1.88	0.43
1:B:269:ALA:O	1:B:271:PRO:HD3	2.19	0.43
1:B:164:ASP:C	1:B:187:GLY:HA3	2.44	0.43
1:B:268:ALA:O	1:B:273:LYS:HE2	2.19	0.43
1:C:28:GLU:O	1:C:32:GLY:HA2	2.19	0.42
1:C:143:GLY:O	1:C:144:LYS:HB2	2.18	0.42
1:C:195:LEU:O	1:C:196:VAL:C	2.61	0.42
1:A:47:PHE:HD1	1:A:70:TYR:CE2	2.38	0.42
1:C:27:PHE:CE2	1:C:279:PHE:HA	2.54	0.42
1:C:90:TYR:HA	1:C:91:PRO:HD2	1.77	0.42
1:B:117:TYR:CD2	1:B:117:TYR:N	2.87	0.42
1:B:158:TRP:NE1	1:B:162:ALA:HB2	2.34	0.42
1:B:284:LEU:O	1:B:289:GLY:HA3	2.19	0.42
1:B:286:THR:O	1:B:288:GLU:N	2.51	0.42
1:C:130:GLU:O	1:C:133:PRO:HD2	2.19	0.42
1:A:279:PHE:CD1	1:A:280:LEU:HD12	2.53	0.42
1:B:126:PRO:HD3	1:B:224:MET:HE1	1.97	0.42
1:B:250:PHE:O	1:B:253:GLN:HB2	2.19	0.42
1:C:179:LYS:HE3	1:C:179:LYS:HA	2.00	0.42
1:C:199:ILE:HA	1:C:204:MET:O	2.20	0.42
1:B:162:ALA:HA	1:B:166:GLY:O	2.19	0.42
1:B:362:ALA:O	1:B:366:THR:HB	2.19	0.42
1:C:4:GLU:HG2	1:C:271:PRO:HB2	2.02	0.42
1:C:139:LEU:O	1:C:140:LYS:C	2.63	0.42
1:C:199:ILE:H	1:C:199:ILE:HD12	1.85	0.42
1:A:10:TRP:CD1	1:A:38:GLU:HB2	2.55	0.42
1:C:21:ALA:O	1:C:25:LYS:CG	2.66	0.42
1:C:60:ILE:HG12	1:C:61:PHE:N	2.35	0.42
1:A:260:GLY:O	1:A:261:VAL:CB	2.65	0.42
1:B:201:ASN:HD22	1:B:201:ASN:HA	1.71	0.42
1:A:41:ASP:O	1:A:46:LYS:NZ	2.53	0.41
1:A:47:PHE:HB3	1:A:48:PRO:HD3	2.01	0.41
1:C:3:GLU:O	1:C:4:GLU:HB2	2.20	0.41
1:B:279:PHE:O	1:B:283:TYR:HB2	2.20	0.41
1:B:287:ASP:HA	1:B:307:TYR:CD1	2.56	0.41
1:C:77:ALA:HB3	1:C:266:ILE:HB	2.01	0.41
1:C:307:TYR:CE2	1:C:311:LEU:HD21	2.54	0.41
1:A:196:VAL:C	1:A:198:LEU:H	2.28	0.41
1:A:314:ASP:HA	1:A:315:PRO:HD3	1.87	0.41
1:A:44:GLU:OE2	1:A:62:TRP:CZ3	2.73	0.41
1:A:90:TYR:HB2	1:A:93:THR:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TYR:OH	1:A:316:ARG:NH2	2.53	0.41
1:B:38:GLU:C	1:B:40:PRO:HD3	2.45	0.41
1:B:297:LYS:HA	1:B:298:PRO:HD2	1.90	0.41
1:C:12:ASN:CG	1:C:13:GLY:H	2.28	0.41
1:C:391:GLN:HE21	1:C:391:GLN:HB2	1.59	0.41
1:A:1:LYS:O	1:A:2:ILE:CB	2.68	0.41
1:A:147:LEU:HA	1:A:224:MET:O	2.20	0.41
1:A:413:PRO:HB2	1:A:415:PRO:HD2	2.03	0.41
1:C:160:LEU:O	1:C:163:ALA:CB	2.69	0.41
1:C:280:LEU:HD23	1:C:284:LEU:HD23	2.01	0.41
1:C:314:ASP:HA	1:C:315:PRO:HD2	1.89	0.41
1:A:297:LYS:NZ	1:A:297:LYS:HB3	2.35	0.41
1:B:85:PHE:CE1	1:B:285:LEU:HD12	2.56	0.41
1:C:153:GLU:HA	1:C:154:PRO:HD3	1.86	0.41
1:C:154:PRO:HG3	1:C:344:ARG:HA	2.02	0.41
1:A:178:ILE:HG21	1:A:335:GLN:NE2	2.36	0.41
1:B:90:TYR:CE1	1:B:305:LYS:HA	2.55	0.41
1:C:100:ASN:HD22	1:C:175:LYS:HD3	1.86	0.41
1:C:290:LEU:HD12	1:C:302:VAL:HG11	2.02	0.41
1:C:340:TRP:CE3	1:C:340:TRP:HA	2.56	0.41
1:A:147:LEU:HD12	1:A:224:MET:O	2.20	0.41
1:A:366:THR:C	1:A:368:ALA:N	2.79	0.41
1:C:197:ASP:HA	1:C:200:LYS:HB3	2.03	0.41
1:B:39:HIS:O	1:B:39:HIS:CG	2.74	0.41
1:B:132:ILE:N	1:B:133:PRO:CD	2.84	0.41
1:B:365:GLN:HE21	1:B:365:GLN:HB3	1.65	0.41
1:C:124:ASN:HD22	1:C:125:PRO:HD2	1.85	0.41
1:C:181:VAL:HG12	1:C:183:VAL:HG22	2.03	0.41
1:C:209:ASP:H	1:C:212:ILE:HB	1.86	0.41
1:A:140:LYS:HA	1:A:144:LYS:O	2.21	0.41
1:B:17:TYR:C	1:B:17:TYR:HD2	2.27	0.41
1:B:296:ASP:O	1:B:297:LYS:HE2	2.21	0.41
1:C:251:LYS:C	1:C:253:GLN:H	2.28	0.41
1:A:39:HIS:O	1:A:39:HIS:CG	2.73	0.40
1:C:42:LYS:HD3	1:C:45:GLU:HG3	2.03	0.40
1:C:79:ILE:HG22	1:C:266:ILE:HD12	2.03	0.40
1:C:139:LEU:HD12	1:C:146:ALA:HA	2.03	0.40
1:C:270:SER:HA	1:C:271:PRO:HD2	1.91	0.40
1:C:383:SER:O	1:C:384:LEU:C	2.64	0.40
1:A:229:PRO:HB3	1:A:232:TRP:HZ3	1.86	0.40
1:B:75:LEU:O	1:B:268:ALA:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LYS:O	1:B:141:ALA:HB2	2.21	0.40
1:B:158:TRP:HA	1:B:161:ILE:HD12	2.03	0.40
1:C:90:TYR:CE1	1:C:305:LYS:HA	2.56	0.40
1:C:126:PRO:O	1:C:127:LYS:CB	2.68	0.40
1:A:148:MET:HE3	1:A:208:THR:CG2	2.50	0.40
1:B:107:PRO:CA	1:B:263:SER:HB2	2.40	0.40
1:C:232:TRP:CH2	1:C:316:ARG:HB3	2.56	0.40
1:A:64:HIS:HE1	1:A:330:MET:O	2.04	0.40
1:B:47:PHE:HB3	1:B:48:PRO:CD	2.51	0.40
1:B:96:ALA:HA	1:B:329:ILE:HG21	2.02	0.40
1:C:256:LYS:HB2	1:C:326:LYS:O	2.22	0.40
1:A:406:PRO:N	1:A:407:PRO:HD3	2.37	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:C:138:GLU:OE2	2:A:452:ZN:ZN[3_445]	1.54	0.66

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	413/449 (92%)	332 (80%)	56 (14%)	25 (6%)	1	11
1	B	396/449 (88%)	308 (78%)	57 (14%)	31 (8%)	1	7
1	C	396/449 (88%)	325 (82%)	47 (12%)	24 (6%)	1	11
All	All	1205/1347 (90%)	965 (80%)	160 (13%)	80 (7%)	1	10

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	168	ALA
1	A	224	MET
1	A	229	PRO
1	A	230	TRP
1	A	261	VAL
1	A	357	VAL
1	B	2	ILE
1	B	55	ASP
1	B	125	PRO
1	B	127	LYS
1	B	165	GLY
1	B	184	ASP
1	B	224	MET
1	B	273	LYS
1	B	277	LYS
1	B	281	GLU
1	C	12	ASN
1	C	232	TRP
1	C	273	LYS
1	A	409	PRO
1	A	410	PRO
1	B	126	PRO
1	B	166	GLY
1	B	287	ASP
1	C	2	ILE
1	C	4	GLU
1	C	11	ILE
1	C	81	PRO
1	C	300	GLY
1	A	100	ASN
1	A	129	TRP
1	A	173	ASN
1	A	208	THR
1	A	402	GLN
1	B	4	GLU
1	B	168	ALA
1	B	172	GLU
1	B	241	ASN
1	B	262	LEU
1	B	286	THR
1	B	357	VAL
1	C	3	GLU

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Mol	Chain	Res	Type
1	C	126	PRO
1	C	171	TYR
1	C	255	SER
1	A	165	GLY
1	A	416	GLN
1	B	78	GLU
1	B	154	PRO
1	B	222	THR
1	B	285	LEU
1	C	140	LYS
1	C	144	LYS
1	C	231	ALA
1	C	256	LYS
1	C	397	GLN
1	A	11	ILE
1	A	178	ILE
1	A	306	SER
1	A	408	PRO
1	B	3	GLU
1	B	42	LYS
1	B	124	ASN
1	B	244	VAL
1	B	288	GLU
1	C	15	LYS
1	C	241	ASN
1	A	7	LEU
1	A	122	LEU
1	A	159	PRO
1	A	260	GLY
1	C	257	PRO
1	C	270	SER
1	C	396	GLN
1	B	16	GLY
1	C	357	VAL
1	A	407	PRO
1	C	16	GLY
1	B	104	ILE

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	307/363 (85%)	253 (82%)	54 (18%)	2	11
1	B	313/363 (86%)	239 (76%)	74 (24%)	1	5
1	C	310/363 (85%)	265 (86%)	45 (14%)	3	16
All	All	930/1089 (85%)	757 (81%)	173 (19%)	1	9

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	8	VAL
1	A	15	LYS
1	A	28	GLU
1	A	34	LYS
1	A	35	VAL
1	A	37	VAL
1	A	43	LEU
1	A	49	GLN
1	A	58	ASP
1	A	59	ILE
1	A	66	ARG
1	A	72	GLN
1	A	88	LYS
1	A	97	VAL
1	A	98	ARG
1	A	102	LYS
1	A	104	ILE
1	A	111	GLU
1	A	113	LEU
1	A	122	LEU
1	A	130	GLU
1	A	137	LYS
1	A	138	GLU
1	A	142	LYS
1	A	156	PHE
1	A	178	ILE
1	A	189	LYS
1	A	198	LEU
1	A	202	LYS

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Mol	Chain	Res	Type
1	A	212	ILE
1	A	234	ASN
1	A	239	LYS
1	A	240	VAL
1	A	261	VAL
1	A	263	SER
1	A	272	ASN
1	A	281	GLU
1	A	284	LEU
1	A	288	GLU
1	A	294	ASN
1	A	297	LYS
1	A	306	SER
1	A	326	LYS
1	A	341	TYR
1	A	358	ASP
1	A	365	GLN
1	A	379	LYS
1	A	381	PHE
1	A	384	LEU
1	A	385	LYS
1	A	386	SER
1	A	390	GLN
1	A	391	GLN
1	B	6	LYS
1	B	7	LEU
1	B	8	VAL
1	B	15	LYS
1	B	17	TYR
1	B	25	LYS
1	B	29	LYS
1	B	36	THR
1	B	37	VAL
1	B	43	LEU
1	B	46	LYS
1	B	53	THR
1	B	59	ILE
1	B	60	ILE
1	B	65	ASP
1	B	72	GLN
1	B	75	LEU
1	B	79	ILE

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Mol	Chain	Res	Type
1	B	83	LYS
1	B	88	LYS
1	B	97	VAL
1	B	104	ILE
1	B	110	VAL
1	B	115	LEU
1	B	119	LYS
1	B	122	LEU
1	B	127	LYS
1	B	132	ILE
1	B	137	LYS
1	B	142	LYS
1	B	144	LYS
1	B	152	GLN
1	B	160	LEU
1	B	175	LYS
1	B	181	VAL
1	B	183	VAL
1	B	185[A]	ASN
1	B	185[B]	ASN
1	B	189	LYS
1	B	198	LEU
1	B	201	ASN
1	B	204	MET
1	B	211	SER
1	B	212	ILE
1	B	222	THR
1	B	224	MET
1	B	227	ASN
1	B	236	ASP
1	B	239	LYS
1	B	240	VAL
1	B	242	TYR
1	B	251	LYS
1	B	255	SER
1	B	263	SER
1	B	273	LYS
1	B	277	LYS
1	B	280	LEU
1	B	286	THR
1	B	294	ASN
1	B	295	LYS

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Mol	Chain	Res	Type
1	B	297	LYS
1	B	305	LYS
1	B	313	LYS
1	B	325	GLN
1	B	328	GLU
1	B	335	GLN
1	B	356	THR
1	B	365	GLN
1	B	366	THR
1	B	374	LEU
1	B	375	GLU
1	B	379	LYS
1	B	385	LYS
1	B	395	GLN
1	C	4	GLU
1	C	6	LYS
1	C	8	VAL
1	C	11	ILE
1	C	14	ASP
1	C	22	GLU
1	C	23	VAL
1	C	29	LYS
1	C	34	LYS
1	C	41	ASP
1	C	43	LEU
1	C	46	LYS
1	C	49	GLN
1	C	58	ASP
1	C	59	ILE
1	C	79	ILE
1	C	83	LYS
1	C	115	LEU
1	C	127	LYS
1	C	132	ILE
1	C	144	LYS
1	C	160	LEU
1	C	172	GLU
1	C	175	LYS
1	C	178	ILE
1	C	179	LYS
1	C	184	ASP
1	C	189	LYS

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Mol	Chain	Res	Type
1	C	200	LYS
1	C	226	ILE
1	C	256	LYS
1	C	263	SER
1	C	277	LYS
1	C	278	GLU
1	C	290	LEU
1	C	291	GLU
1	C	297	LYS
1	C	311	LEU
1	C	313	LYS
1	C	348	ILE
1	C	365	GLN
1	C	371	MET
1	C	374	LEU
1	C	382	GLU
1	C	391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	39	HIS
1	A	86	GLN
1	A	100	ASN
1	A	124	ASN
1	A	152	GLN
1	A	185	ASN
1	A	203	HIS
1	A	218	ASN
1	A	267	ASN
1	A	325	GLN
1	A	365	GLN
1	B	64	HIS
1	B	72	GLN
1	B	86	GLN
1	B	100	ASN
1	B	118	ASN
1	B	152	GLN
1	B	173	ASN
1	B	201	ASN
1	B	203	HIS

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	294	ASN
1	B	323	ASN
1	B	325	GLN
1	B	355	GLN
1	B	365	GLN
1	B	389	GLN
1	B	390	GLN
1	B	395	GLN
1	B	396	GLN
1	C	49	GLN
1	C	64	HIS
1	C	100	ASN
1	C	124	ASN
1	C	201	ASN
1	C	203	HIS
1	C	218	ASN
1	C	267	ASN
1	C	391	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	396:GLN	C	399:GLN	N	21.49

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	417/449 (92%)	0.04	16 (3%) 44 26	40, 103, 104, 135	49 (11%)
1	B	397/449 (88%)	0.05	18 (4%) 38 23	51, 103, 103, 123	43 (10%)
1	C	398/449 (88%)	-0.07	7 (1%) 67 41	57, 103, 103, 112	36 (9%)
All	All	1212/1347 (89%)	0.01	41 (3%) 48 28	40, 103, 103, 135	128 (10%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	LYS	5.0
1	A	395	GLN	4.9
1	B	112	ALA	4.3
1	A	399	GLN	4.1
1	A	175	LYS	4.0
1	B	156	PHE	4.0
1	C	46	LYS	3.8
1	C	127	LYS	3.7
1	A	98	ARG	3.4
1	B	377	LEU	3.2
1	A	22	GLU	3.2
1	B	83	LYS	3.1
1	C	373	THR	3.1
1	B	295	LYS	3.1
1	B	326	LYS	3.1
1	C	88	LYS	2.7
1	B	258	PHE	2.7
1	A	371	MET	2.7
1	B	372	ALA	2.7
1	B	375	GLU	2.7
1	B	155	TYR	2.6
1	A	374	LEU	2.6
1	A	377	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	102	LYS	2.5
1	B	374	LEU	2.5
1	C	128	THR	2.4
1	A	101	GLY	2.3
1	A	355	GLN	2.2
1	C	102	LYS	2.2
1	B	111	GLU	2.2
1	A	205	ASN	2.2
1	A	387	PHE	2.2
1	B	34	LYS	2.2
1	B	223	ALA	2.2
1	B	113	LEU	2.2
1	A	173	ASN	2.1
1	C	384	LEU	2.1
1	A	380	ALA	2.1
1	A	3	GLU	2.0
1	B	376	LYS	2.0
1	B	384	LEU	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 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(Å ²)	Q<0.9
3	CA	C	453	1/1	0.65	0.18	141,141,141,141	0
3	CA	B	454	1/1	0.75	0.31	153,153,153,153	0
3	CA	B	453	1/1	0.77	0.09	137,137,137,137	0
2	ZN	B	452	1/1	0.84	0.06	203,203,203,203	0
2	ZN	C	451	1/1	0.88	0.11	185,185,185,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	450	1/1	0.91	0.12	170,170,170,170	0
3	CA	C	452	1/1	0.92	0.10	132,132,132,132	0
2	ZN	B	451	1/1	0.94	0.12	109,109,109,109	0
3	CA	B	455	1/1	0.95	0.12	147,147,147,147	0
2	ZN	A	451	1/1	0.97	0.06	179,179,179,179	0
2	ZN	A	452	1/1	0.97	0.07	149,149,149,149	0
2	ZN	B	450	1/1	0.97	0.15	128,128,128,128	0
2	ZN	A	450	1/1	0.98	0.08	151,151,151,151	0
3	CA	C	454	1/1	0.98	0.12	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.