



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:29 PM UTC

PDB ID : 3IOV / pdb_00003iov
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

<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

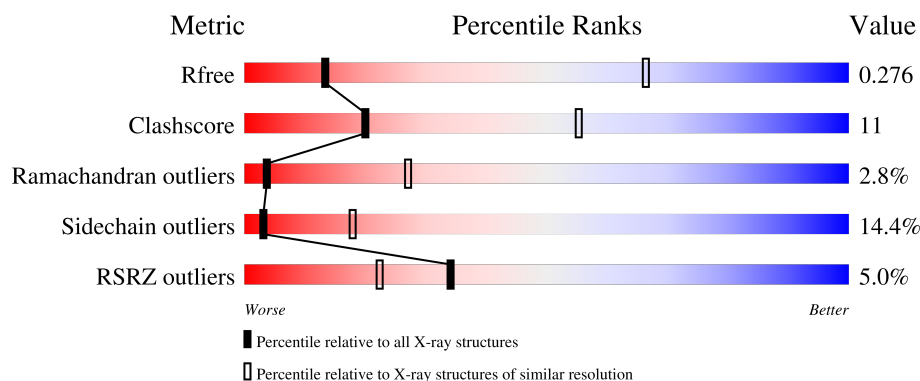
1 Overall quality at a glance

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	4% 58% 26% 5% 10%
1	B	449	4% 63% 22% • 11%
1	C	449	5% 60% 25% • 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 periplasmic protein,Huntingtin.

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 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	-	linker	UNP P0AEX9
A	360	ALA	-	linker	UNP P0AEX9
A	361	LEU	-	linker	UNP P0AEX9
A	362	ALA	-	linker	UNP P0AEX9
A	363	ALA	-	linker	UNP P0AEX9
A	364	ALA	-	linker	UNP P0AEX9
A	365	GLN	-	linker	UNP P0AEX9
A	366	THR	-	linker	UNP P0AEX9
A	367	ASN	-	linker	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	431	GLN	-	expression tag	UNP P42858
A	432	SER	-	expression tag	UNP P42858
A	433	TYR	-	expression tag	UNP P42858
A	434	GLN	-	expression tag	UNP P42858
A	435	ILE	-	expression tag	UNP P42858
A	436	THR	-	expression tag	UNP P42858
A	437	ALA	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	expression tag	UNP P42858
A	439	LYS	-	expression tag	UNP P42858
A	440	LEU	-	expression tag	UNP P42858
A	441	GLY	-	expression tag	UNP P42858
A	442	THR	-	expression tag	UNP P42858
A	443	GLY	-	expression tag	UNP P42858
A	444	ARG	-	expression tag	UNP P42858
A	445	ARG	-	expression tag	UNP P42858
A	446	PHE	-	expression tag	UNP P42858
A	447	THR	-	expression tag	UNP P42858
A	448	THR	-	expression tag	UNP P42858
A	449	SER	-	expression tag	UNP P42858
B	359	ALA	-	linker	UNP P0AEX9
B	360	ALA	-	linker	UNP P0AEX9
B	361	LEU	-	linker	UNP P0AEX9
B	362	ALA	-	linker	UNP P0AEX9
B	363	ALA	-	linker	UNP P0AEX9
B	364	ALA	-	linker	UNP P0AEX9
B	365	GLN	-	linker	UNP P0AEX9
B	366	THR	-	linker	UNP P0AEX9
B	367	ASN	-	linker	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	431	GLN	-	expression tag	UNP P42858
B	432	SER	-	expression tag	UNP P42858
B	433	TYR	-	expression tag	UNP P42858
B	434	GLN	-	expression tag	UNP P42858
B	435	ILE	-	expression tag	UNP P42858
B	436	THR	-	expression tag	UNP P42858
B	437	ALA	-	expression tag	UNP P42858
B	438	GLY	-	expression tag	UNP P42858
B	439	LYS	-	expression tag	UNP P42858
B	440	LEU	-	expression tag	UNP P42858
B	441	GLY	-	expression tag	UNP P42858
B	442	THR	-	expression tag	UNP P42858
B	443	GLY	-	expression tag	UNP P42858
B	444	ARG	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	ARG	-	expression tag	UNP P42858
B	446	PHE	-	expression tag	UNP P42858
B	447	THR	-	expression tag	UNP P42858
B	448	THR	-	expression tag	UNP P42858
B	449	SER	-	expression tag	UNP P42858
C	359	ALA	-	linker	UNP P0AEX9
C	360	ALA	-	linker	UNP P0AEX9
C	361	LEU	-	linker	UNP P0AEX9
C	362	ALA	-	linker	UNP P0AEX9
C	363	ALA	-	linker	UNP P0AEX9
C	364	ALA	-	linker	UNP P0AEX9
C	365	GLN	-	linker	UNP P0AEX9
C	366	THR	-	linker	UNP P0AEX9
C	367	ASN	-	linker	UNP P0AEX9
C	368	ALA	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	431	GLN	-	expression tag	UNP P42858
C	432	SER	-	expression tag	UNP P42858
C	433	TYR	-	expression tag	UNP P42858
C	434	GLN	-	expression tag	UNP P42858
C	435	ILE	-	expression tag	UNP P42858
C	436	THR	-	expression tag	UNP P42858
C	437	ALA	-	expression tag	UNP P42858
C	438	GLY	-	expression tag	UNP P42858
C	439	LYS	-	expression tag	UNP P42858
C	440	LEU	-	expression tag	UNP P42858
C	441	GLY	-	expression tag	UNP P42858
C	442	THR	-	expression tag	UNP P42858
C	443	GLY	-	expression tag	UNP P42858
C	444	ARG	-	expression tag	UNP P42858
C	445	ARG	-	expression tag	UNP P42858
C	446	PHE	-	expression tag	UNP P42858
C	447	THR	-	expression tag	UNP P42858
C	448	THR	-	expression tag	UNP P42858
C	449	SER	-	expression tag	UNP P42858

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

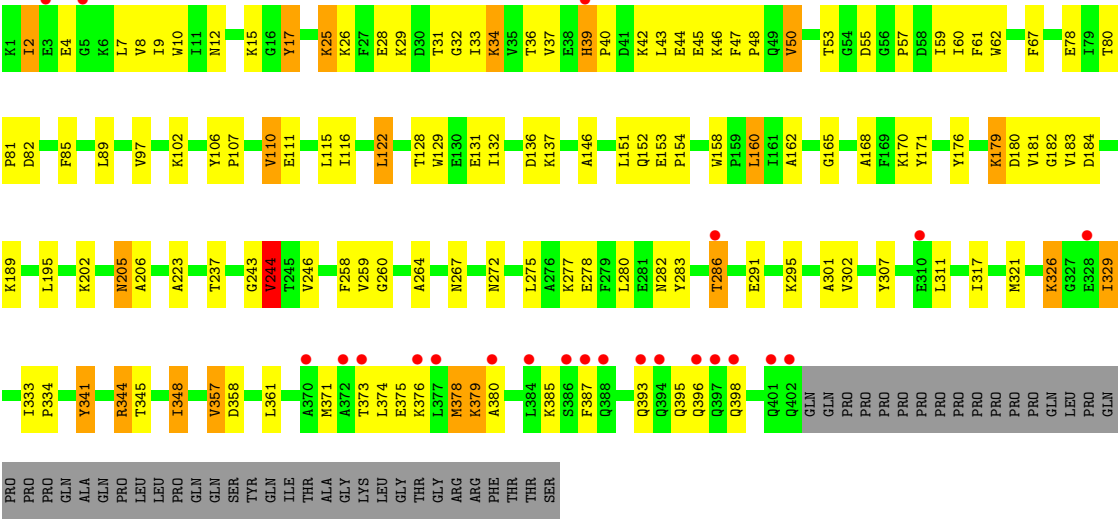
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	3	Total 3	Zn 3	0	0
2	C	1	Total 1	Zn 1	0	0

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

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

GLY
THR
GLY
ARG
ARG
PHE
THR
THR
SER

● 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	163.82Å 101.19Å 134.82Å 90.00° 99.23° 90.00°	Depositor
Resolution (Å)	38.00 – 3.70 38.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (38.00-3.70) 92.7 (38.00-3.70)	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 (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: CA, ZN

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	0.53	2/3164 (0.1%)	0.90	7/4307 (0.2%)
1	B	0.50	1/3120 (0.0%)	0.87	3/4236 (0.1%)
1	C	0.49	0/3136	0.82	2/4259 (0.0%)
All	All	0.50	3/9420 (0.0%)	0.86	12/12802 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	GLU	CB-CG	-8.10	1.28	1.52
1	A	6	LYS	CB-CG	-7.34	1.30	1.52
1	A	310	GLU	CB-CG	-6.28	1.33	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	PRO	CA-C-N	8.73	129.37	120.38
1	A	406	PRO	C-N-CA	8.73	129.37	120.38
1	A	310	GLU	CB-CG-CD	7.94	126.10	112.60
1	B	228	GLY	CA-C-N	7.69	129.45	119.84
1	B	228	GLY	C-N-CA	7.69	129.45	119.84
1	A	407	PRO	N-CA-C	7.32	119.63	110.70
1	A	415	PRO	N-CA-CB	5.95	109.49	103.25
1	A	124	ASN	CA-C-N	5.44	123.58	119.66
1	A	124	ASN	C-N-CA	5.44	123.58	119.66
1	C	12	ASN	N-CA-C	5.38	117.59	111.02
1	C	283	TYR	N-CA-C	5.24	117.00	111.28
1	B	259	VAL	N-CA-C	5.03	114.82	107.37

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	81	0
1	B	3049	0	2996	66	0
1	C	3065	0	2998	73	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	208	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 (208) 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:O	1:C:179:LYS:HG2	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: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:B:392:GLN:HG3	1:B:393:GLN:N	2.02	0.73
1:C:379:LYS:HZ3	1:C:380:ALA:N	1.89	0.71
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:B:381:PHE:HD1	1:C:374:LEU:HD12	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:O	1:A:285:LEU:HB2	1.90	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:379:LYS:HZ3	1:C:380:ALA:H	1.45	0.65
1:A:301:ALA:HB1	1:A:321:MET:HE2	1.77	0.65
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
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: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:308:GLU:HG3	1:A:321:MET:HE3	1.86	0.57
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: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:B:41:ASP:O	1:B:42:LYS:C	2.49	0.55
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:B:132:ILE:HD12	1:B:224:MET:HE1	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:LYS:HE3	1:B:385:LYS:C	2.33	0.53
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
1:A:45:GLU:OE1	1:A:66:ARG:NH2	2.42	0.52
1:B:370:ALA:HB3	1:B:371:MET:HE2	1.91	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:A:43:LEU:HA	1:A:46:LYS:HB2	1.93	0.51
1:C:122:LEU:HD23	1:C:223:ALA:HB1	1.92	0.51
1:A:164:ASP:HB3	1:A:187:GLY:HA2	1.92	0.51
1:A:411:PRO:C	1:A:413:PRO:HD3	2.36	0.51
1:B:210:TYR:HE2	1:B:227:ASN:HD21	1.57	0.50
1:B:299:LEU:CD1	1:B:302:VAL:HG12	2.41	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:B:128:THR:HG22	1:B:249:THR:O	2.13	0.49
1:C:9:ILE:HB	1:C:37:VAL:HG22	1.93	0.49
1:A:226:ILE:HG23	1:A:247:LEU:HD21	1.94	0.49
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.47	0.49
1:B:385:LYS:O	1:B:389:GLN:HG3	2.12	0.49
1:C:129:TRP:O	1:C:132:ILE:HG12	2.13	0.49
1:C:374:LEU:O	1:C:378:MET:HE2	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:A:177:ASP:O	1:A:180:ASP:HB2	2.14	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:1:LYS:C	1:A:3:GLU:H	2.21	0.48
1:C:106:TYR:CD2	1:C:280:LEU:HD23	2.49	0.48
1:A:129:TRP:NE1	1:A:248:PRO:O	2.47	0.48
1:C:28:GLU:O	1:C:32:GLY:HA2	2.14	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:B:392:GLN:HG3	1:B:393:GLN:HG2	1.95	0.48
1:A:409:PRO:CB	1:A:410:PRO:CA	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:34:LYS:HG3	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:A:363:ALA:HA	1:A:366:THR:HG22	1.96	0.47
1:C:158:TRP:CD1	1:C:258:PHE:CE2	3.03	0.47
1:B:249:THR:HG22	1:B:254:PRO:HA	1.97	0.47
1:B:384:LEU:C	1:B:384:LEU:HD22	2.40	0.47
1:A:378:MET:O	1:A:382:GLU:HB2	2.15	0.47
1:B:364:ALA:O	1:B:368:ALA:HB2	2.14	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:52:ALA:O	1:B:355:GLN:HA	2.16	0.46
1:A:381:PHE:HB2	1:B:371:MET:SD	2.56	0.46
1:A:410:PRO:CB	1:A:411:PRO:CD	2.74	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:B:385:LYS:HE3	1:B:386:SER:N	2.31	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:B:272:ASN:HB3	1:B:275:LEU:HD12	1.98	0.45
1:C:25:LYS:HA	1:C:25:LYS:NZ	2.32	0.45
1:B:258:PHE:CD2	1:B:340:TRP:HH2	2.35	0.44
1:A:373:THR:HA	1:A:376:LYS:NZ	2.31	0.44
1:A:410:PRO:CB	1:A:411:PRO:HD3	2.39	0.44
1:B:119:LYS:HB2	1:B:241:ASN:ND2	2.33	0.44
1:A:13:GLY:O	1:A:14:ASP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LYS:HB3	1:B:179:LYS:HE2	1.91	0.44
1:C:46:LYS:O	1:C:50:VAL:HG23	2.18	0.44
1:A:354:ARG:O	1:C:53:THR:HA	2.18	0.44
1:B:356:THR:O	1:B:357:VAL:C	2.60	0.44
1:A:361:LEU:HD12	1:A:361:LEU:HA	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: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
1:C:160:LEU:HD12	1:C:195:LEU:HB2	2.00	0.43
1:C:357:VAL:O	1:C:361:LEU:HB2	2.17	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:A:7:LEU:HA	1:A:58:ASP:OD2	2.18	0.43
1:A:159:PRO:HA	1:A:256:LYS:O	2.18	0.43
1:B:89:LEU:HB2	1:B:90:TYR:H	1.72	0.43
1:B:378:MET:O	1:B:382:GLU:HG2	2.19	0.43
1:C:81:PRO:HB2	1:C:85:PHE:CD2	2.53	0.43
1:C:62:TRP:HB3	1:C:67:PHE:HE1	1.82	0.43
1:A:363:ALA:HA	1:A:366:THR:CG2	2.49	0.43
1:C:61:PHE:CD2	1:C:264:ALA:HB2	2.53	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:C:151:LEU:C	1:C:153:GLU:H	2.26	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:A:108:ILE:N	1:A:262:LEU:O	2.44	0.42
1:A:286:THR:O	1:A:287:ASP:C	2.62	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:B:238:SER:C	1:B:240:VAL:H	2.27	0.42
1:C:44:GLU:HG2	1:C:45:GLU:OE2	2.20	0.42
1:C:179:LYS:O	1:C:179:LYS:CG	2.58	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:C:26:LYS:HD2	1:C:29:LYS:HZ1	1.84	0.41
1:B:377:LEU:HD12	1:C:373:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:ASP:O	1:A:181:VAL:C	2.64	0.41
1:A:349:ASN:HB3	1:A:355:GLN:HG2	2.02	0.41
1:A:371:MET:HE3	1:A:375:GLU:HG2	2.03	0.41
1:A:412:PRO:O	1:A:414:PRO:HD3	2.21	0.41
1:B:85:PHE:HD2	1:B:88:LYS:HD2	1.86	0.41
1:C:2:ILE:C	1:C:4:GLU:H	2.28	0.41
1:C:152:GLN:HA	1:C:348:ILE:HD11	2.03	0.41
1:C:301:ALA:HB1	1:C:321:MET:HE2	2.01	0.41
1:A:338:ALA:HB1	1:A:371:MET:HB3	2.03	0.41
1:B:381:PHE:HA	1:B:384:LEU:HD12	2.03	0.41
1:C:9:ILE:HG23	1:C:59:ILE:HG23	2.02	0.41
1:C:15:LYS:HA	1:C:15:LYS:HE2	2.03	0.41
1:A:158:TRP:CH2	1:A:183:VAL:HG12	2.56	0.40
1:A:405:PRO:HA	1:A:406:PRO:HD3	1.86	0.40
1:B:356:THR:O	1:B:358:ASP:N	2.54	0.40
1:B:158:TRP:N	1:B:159:PRO:CD	2.84	0.40
1:C:110:VAL:HG12	1:C:111:GLU:H	1.86	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:33:ILE:HG21	1:A:275:LEU:HD13	2.03	0.40
1:A:122:LEU:HA	1:A:123:PRO:HD2	1.97	0.40
1:A:164:ASP:HB3	1:A:187:GLY:CA	2.52	0.40
1:A:167:TYR:CE1	1:A:182:GLY:HA3	2.57	0.40
1:B:111:GLU:HG2	1:B:230:TRP:HZ3	1.86	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%)	2	18
1	B	396/449 (88%)	364 (92%)	25 (6%)	7 (2%)	6	34
1	C	400/449 (89%)	350 (88%)	42 (10%)	8 (2%)	6	32
All	All	1197/1347 (89%)	1060 (89%)	103 (9%)	34 (3%)	4	27

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
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%)	267 (86%)	44 (14%)	3	18
1	B	306/363 (84%)	263 (86%)	43 (14%)	3	18
1	C	305/363 (84%)	259 (85%)	46 (15%)	3	16
All	All	922/1089 (85%)	789 (86%)	133 (14%)	3	18

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
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	60	ILE
1	A	65	ASP
1	A	73	SER
1	A	80	THR
1	A	88	LYS
1	A	103	LEU
1	A	115	LEU
1	A	119	LYS
1	A	128	THR
1	A	137	LYS
1	A	140	LYS
1	A	160	LEU
1	A	179	LYS
1	A	189	LYS
1	A	200	LYS
1	A	201	ASN
1	A	202	LYS

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Mol	Chain	Res	Type
1	A	205	ASN
1	A	237	THR
1	A	272	ASN
1	A	277	LYS
1	A	278	GLU
1	A	297	LYS
1	A	308	GLU
1	A	310	GLU
1	A	322	GLU
1	A	329	ILE
1	A	348	ILE
1	A	357	VAL
1	A	361	LEU
1	A	374	LEU
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	43	LEU
1	B	80	THR
1	B	89	LEU
1	B	97	VAL
1	B	104	ILE
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	181	VAL
1	B	184	ASP
1	B	197	ASP
1	B	200	LYS
1	B	202	LYS
1	B	214	GLU
1	B	226	ILE

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Mol	Chain	Res	Type
1	B	235	ILE
1	B	236	ASP
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	325	GLN
1	B	332	ASN
1	B	335	GLN
1	B	345	THR
1	B	365	GLN
1	B	371	MET
1	B	376	LYS
1	B	384	LEU
1	B	385	LYS
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	78	GLU
1	C	80	THR
1	C	82	ASP
1	C	102	LYS
1	C	110	VAL
1	C	115	LEU
1	C	122	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	202	LYS

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Mol	Chain	Res	Type
1	C	205	ASN
1	C	237	THR
1	C	244	VAL
1	C	246	VAL
1	C	277	LYS
1	C	278	GLU
1	C	286	THR
1	C	291	GLU
1	C	295	LYS
1	C	311	LEU
1	C	317	ILE
1	C	326	LYS
1	C	329	ILE
1	C	341	TYR
1	C	344	ARG
1	C	345	THR
1	C	348	ILE
1	C	358	ASP
1	C	375	GLU
1	C	376	LYS
1	C	378	MET
1	C	379	LYS
1	C	385	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	72	GLN
1	A	86	GLN
1	A	124	ASN
1	A	185	ASN
1	A	201	ASN
1	A	234	ASN
1	A	365	GLN
1	B	18	ASN
1	B	64	HIS
1	B	86	GLN
1	B	173	ASN
1	B	218	ASN
1	B	294	ASN
1	B	332	ASN

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Mol	Chain	Res	Type
1	B	335	GLN
1	C	12	ASN
1	C	86	GLN
1	C	118	ASN
1	C	124	ASN
1	C	185	ASN
1	C	203	HIS
1	C	205	ASN
1	C	218	ASN
1	C	234	ASN
1	C	241	ASN
1	C	365	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 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%)	0.42	18 (4%) 39 25	37, 81, 93, 104	37 (9%)
1	B	398/449 (88%)	0.41	19 (4%) 35 23	42, 83, 94, 100	30 (7%)
1	C	402/449 (89%)	0.44	23 (5%) 29 20	32, 84, 98, 108	33 (8%)
All	All	1205/1347 (89%)	0.42	60 (4%) 34 22	32, 83, 96, 108	100 (8%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	387	PHE	7.3
1	C	402	GLN	5.5
1	A	403	GLN	4.7
1	B	390	GLN	4.6
1	B	130	GLU	4.0
1	B	380	ALA	3.6
1	A	373	THR	3.6
1	A	416	GLN	3.5
1	B	396	GLN	3.5
1	B	392	GLN	3.4
1	C	401	GLN	3.3
1	C	372	ALA	3.1
1	C	377	LEU	3.0
1	A	374	LEU	2.7
1	C	398	GLN	2.7
1	A	375	GLU	2.7
1	A	405	PRO	2.7
1	A	13	GLY	2.7
1	C	380	ALA	2.6
1	A	370	ALA	2.6
1	C	394	GLN	2.6
1	C	5	GLY	2.5
1	C	39	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	377	LEU	2.5
1	B	375	GLU	2.5
1	A	411	PRO	2.5
1	A	388	GLN	2.4
1	C	384	LEU	2.4
1	A	372	ALA	2.4
1	B	78	GLU	2.4
1	B	381	PHE	2.3
1	B	146	ALA	2.3
1	B	264	ALA	2.3
1	C	393	GLN	2.3
1	C	286	THR	2.3
1	B	379	LYS	2.3
1	B	374	LEU	2.3
1	C	397	GLN	2.2
1	C	3	GLU	2.2
1	A	171	TYR	2.2
1	B	371	MET	2.2
1	C	373	THR	2.2
1	A	390	GLN	2.2
1	A	376	LYS	2.2
1	C	370	ALA	2.2
1	B	382	GLU	2.1
1	C	310	GLU	2.1
1	A	391	GLN	2.1
1	A	1	LYS	2.1
1	C	396	GLN	2.1
1	B	387	PHE	2.1
1	B	397	GLN	2.1
1	C	328	GLU	2.1
1	A	381	PHE	2.1
1	C	388	GLN	2.1
1	A	378	MET	2.1
1	B	376	LYS	2.0
1	C	386	SER	2.0
1	C	376	LYS	2.0
1	B	370	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
2	ZN	B	501	1/1	0.68	0.12	105,105,105,105	0
2	ZN	B	502	1/1	0.91	0.23	99,99,99,99	0
2	ZN	A	502	1/1	0.92	0.05	116,116,116,116	0
3	CA	C	502	1/1	0.92	0.15	96,96,96,96	0
3	CA	B	504	1/1	0.93	0.05	74,74,74,74	0
2	ZN	C	501	1/1	0.94	0.06	110,110,110,110	0
3	CA	C	503	1/1	0.94	0.16	94,94,94,94	0
3	CA	A	505	1/1	0.95	0.11	89,89,89,89	0
3	CA	B	505	1/1	0.95	0.13	80,80,80,80	0
2	ZN	A	501	1/1	0.96	0.07	76,76,76,76	0
3	CA	A	504	1/1	0.98	0.14	58,58,58,58	0
2	ZN	B	503	1/1	0.98	0.06	65,65,65,65	0
3	CA	A	503	1/1	0.98	0.12	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.