



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:06 AM UTC

PDB ID : 3IO6 / pdb_00003io6
Title : Huntingtin amino-terminal region with 17 Gln residues - crystal C92-a
Authors : Kim, M.W.; Chelliah, Y.; Kim, S.W.; Otwinowski, Z.; Bezprozvanny, I.
Deposited on : 2009-08-13
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

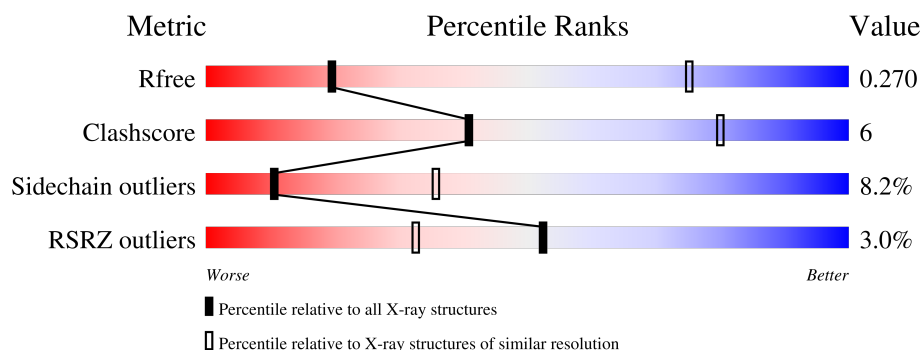
1 Overall quality at a glance

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)
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	 3% 71% 17% 11%
1	B	449	 2% 76% 13% 11%
1	C	449	 3% 71% 16% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9265 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	400	Total	C	N	O	S	8	0	0
			3059	1969	499	583	8			
1	C	397	Total	C	N	O	S	4	0	0
			3076	1976	504	588	8			
1	B	401	Total	C	N	O	S	20	0	0
			3116	1998	513	597	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	437	ALA	-	expression tag	UNP P42858
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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

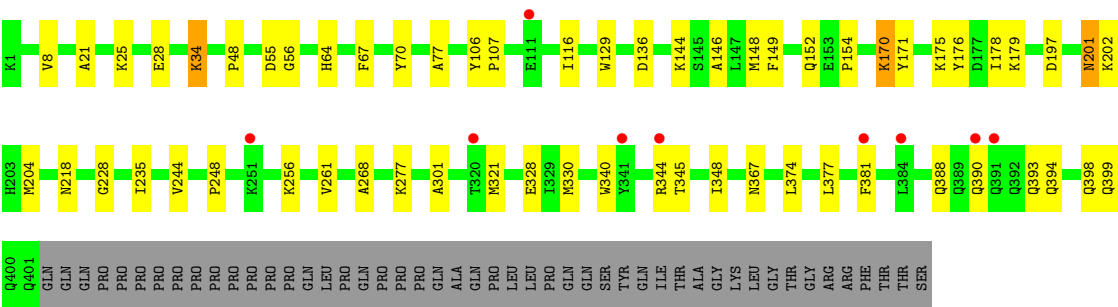
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	C	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0

- 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	C	4	Total 4	Ca 4	0	0
3	B	2	Total 2	Ca 2	0	0

- 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	163.40Å 101.24Å 138.19Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	38.67 – 3.70 38.67 – 3.70	Depositor EDS
% Data completeness (in resolution range)	92.4 (38.67-3.70) 92.3 (38.67-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.02	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.245 , 0.293 (Not available) , 0.270	Depositor DCC
R_{free} test set	1200 reflections (5.36%)	wwPDB-VP
Wilson B-factor (Å ²)	98.6	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9265	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: 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	0.48	1/3128 (0.0%)	0.91	13/4243 (0.3%)
1	B	0.52	2/3187 (0.1%)	0.90	12/4321 (0.3%)
1	C	0.50	1/3147 (0.0%)	0.85	2/4268 (0.0%)
All	All	0.50	4/9462 (0.0%)	0.89	27/12832 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	LYS	CB-CG	-11.96	1.16	1.52
1	C	144	LYS	CB-CG	-11.41	1.18	1.52
1	A	140	LYS	CB-CG	-9.28	1.24	1.52
1	B	277	LYS	CB-CG	8.16	1.76	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	LYS	CA-CB-CG	-10.52	93.07	114.10
1	B	328	GLU	CB-CG-CD	10.37	130.23	112.60
1	B	144	LYS	CA-CB-CG	10.05	134.20	114.10
1	B	34	LYS	CB-CG-CD	-9.79	88.79	111.30
1	B	256	LYS	CA-CB-CG	-8.73	96.64	114.10
1	A	408	PRO	N-CA-CB	8.61	111.43	103.08
1	B	277	LYS	CA-CB-CG	-8.35	97.41	114.10
1	A	413	PRO	N-CA-CB	8.01	110.85	103.08
1	A	406	PRO	N-CA-CB	7.99	110.83	103.08
1	A	405	PRO	N-CA-CB	7.98	110.82	103.08
1	A	409	PRO	N-CA-CB	7.62	110.47	103.08
1	A	407	PRO	N-CA-CB	7.45	110.31	103.08
1	A	414	PRO	N-CA-CB	7.34	110.20	103.08
1	B	277	LYS	CB-CG-CD	-7.26	94.59	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	GLU	CA-CB-CG	7.16	128.43	114.10
1	C	144	LYS	CA-CB-CG	6.99	128.09	114.10
1	A	415	PRO	N-CA-CB	6.96	110.56	103.25
1	A	410	PRO	N-CA-CB	6.79	110.47	103.00
1	B	256	LYS	CB-CG-CD	-6.68	95.93	111.30
1	B	228	GLY	CA-C-N	6.68	126.37	119.56
1	B	228	GLY	C-N-CA	6.68	126.37	119.56
1	B	144	LYS	CB-CG-CD	-6.67	95.97	111.30
1	A	412	PRO	N-CA-CB	6.61	110.28	103.00
1	A	414	PRO	N-CA-C	5.91	117.91	110.70
1	C	144	LYS	CB-CG-CD	-5.78	98.00	111.30
1	A	413	PRO	CA-C-N	5.17	125.70	120.38
1	A	413	PRO	C-N-CA	5.17	125.70	120.38

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	3059	0	2996	33	0
1	B	3116	0	3087	37	0
1	C	3076	0	3049	56	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
All	All	9265	0	9132	118	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 6.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:HA	1:C:305:LYS:HB2	1.43	0.98
1:B:64:HIS:HD2	1:B:261:VAL:H	1.27	0.83
1:C:27:PHE:CE1	1:C:279:PHE:HA	2.14	0.82
1:C:27:PHE:CZ	1:C:283:TYR:HB2	2.15	0.81
1:B:64:HIS:CD2	1:B:261:VAL:H	2.02	0.77
1:A:373:THR:HA	1:A:376:LYS:HE3	1.66	0.77
1:C:3:GLU:HG3	1:C:6:LYS:HE3	1.67	0.77
1:B:55:ASP:CG	1:B:56:GLY:H	1.96	0.73
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.23	0.72
1:C:72:GLN:HE21	1:C:99:TYR:HE2	1.36	0.72
1:B:148:MET:HE2	1:B:149:PHE:H	1.56	0.71
1:C:27:PHE:HE1	1:C:279:PHE:HA	1.58	0.66
1:C:89:LEU:HD12	1:C:94:TRP:CZ2	2.32	0.64
1:C:152:GLN:HA	1:C:348:ILE:HD11	1.80	0.64
1:A:209:ASP:H	1:A:212:ILE:HD12	1.63	0.63
1:C:301:ALA:HB1	1:C:321:MET:HE2	1.79	0.63
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.35	0.62
1:C:218:ASN:HD21	1:C:235:ILE:HG12	1.64	0.61
1:C:304:LEU:HA	1:C:305:LYS:CB	2.26	0.61
1:A:68:GLY:HA3	1:A:332:ASN:O	2.01	0.60
1:C:338:ALA:HB2	1:C:372:ALA:H	1.67	0.60
1:B:55:ASP:CG	1:B:56:GLY:N	2.59	0.60
1:A:301:ALA:HB1	1:A:321:MET:HE2	1.82	0.60
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.38	0.59
1:C:88:LYS:O	1:C:304:LEU:HD12	2.03	0.58
1:C:2:ILE:HG22	1:C:2:ILE:O	2.03	0.58
1:B:148:MET:HE2	1:B:148:MET:HA	1.86	0.58
1:C:305:LYS:N	1:C:308:GLU:OE1	2.37	0.57
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.68	0.57
1:C:374:LEU:HB3	1:B:381:PHE:HZ	1.69	0.57
1:B:48:PRO:HG3	1:B:70:TYR:CE1	2.39	0.57
1:C:304:LEU:CA	1:C:305:LYS:HB2	2.27	0.57
1:B:301:ALA:HB1	1:B:321:MET:HE2	1.88	0.55
1:A:45:GLU:O	1:A:49:GLN:NE2	2.39	0.55
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.42	0.55
1:C:64:HIS:HE1	1:C:330:MET:O	1.89	0.54
1:C:374:LEU:HB3	1:B:381:PHE:CZ	2.42	0.54
1:A:64:HIS:HE1	1:A:330:MET:O	1.91	0.54
1:A:89:LEU:HD12	1:A:94:TRP:CZ2	2.43	0.53
1:B:148:MET:HE2	1:B:149:PHE:N	2.22	0.53
1:A:89:LEU:HD23	1:A:304:LEU:HA	1.89	0.53
1:B:170:LYS:HE3	1:B:170:LYS:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:HIS:CD2	1:A:261:VAL:H	2.27	0.52
1:C:129:TRP:CD1	1:C:248:PRO:HB2	2.44	0.52
1:B:152:GLN:HA	1:B:348:ILE:HD11	1.90	0.52
1:A:387:PHE:HE1	1:B:345:THR:HG21	1.75	0.52
1:C:201:ASN:HB3	1:C:203:HIS:CE1	2.45	0.52
1:C:9:ILE:HG12	1:C:59:ILE:HB	1.91	0.52
1:C:90:TYR:CE2	1:C:308:GLU:OE1	2.63	0.52
1:C:116:ILE:HG12	1:C:244:VAL:HG22	1.93	0.51
1:A:104:ILE:O	1:A:105:ALA:HB2	2.10	0.51
1:C:23:VAL:HG12	1:C:27:PHE:CE2	2.46	0.50
1:C:23:VAL:HG12	1:C:27:PHE:HE2	1.77	0.49
1:C:153:GLU:HB2	1:C:156:PHE:HD1	1.78	0.49
1:C:18:ASN:O	1:C:22:GLU:HG2	2.13	0.48
1:C:64:HIS:CE1	1:C:330:MET:O	2.66	0.48
1:C:338:ALA:HB2	1:C:372:ALA:CB	2.42	0.48
1:B:48:PRO:HG3	1:B:70:TYR:HE1	1.78	0.48
1:C:89:LEU:HD12	1:C:94:TRP:HZ2	1.78	0.48
1:B:218:ASN:HD21	1:B:235:ILE:HG12	1.78	0.48
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.94	0.48
1:C:341:TYR:OH	1:B:388:GLN:HG3	2.14	0.47
1:C:302:VAL:HG21	1:C:307:TYR:HD2	1.80	0.47
1:C:27:PHE:HZ	1:C:283:TYR:HB2	1.77	0.47
1:B:394:GLN:O	1:B:398:GLN:HG3	2.13	0.47
1:B:116:ILE:HG12	1:B:244:VAL:HG22	1.96	0.47
1:C:136:ASP:HA	1:C:146:ALA:HB2	1.97	0.47
1:B:197:ASP:O	1:B:201:ASN:HB2	2.16	0.46
1:B:148:MET:HE3	1:B:204:MET:SD	2.56	0.46
1:B:340:TRP:O	1:B:344:ARG:HB2	2.16	0.46
1:A:2:ILE:HG22	1:A:2:ILE:O	2.16	0.46
1:C:48:PRO:HG3	1:C:70:TYR:HE1	1.80	0.46
1:A:387:PHE:HZ	1:B:367:ASN:ND2	2.14	0.46
1:A:129:TRP:HB3	1:A:194:PHE:CE2	2.51	0.45
1:A:192:LEU:HD23	1:A:357:VAL:HG13	1.99	0.45
1:A:370:ALA:HB1	1:C:380:ALA:HB2	1.98	0.45
1:B:77:ALA:HB2	1:B:268:ALA:HA	1.98	0.44
1:B:171:TYR:HB2	1:B:176:TYR:CE1	2.52	0.44
1:B:340:TRP:HA	1:B:340:TRP:CE3	2.53	0.44
1:A:127:LYS:HA	1:A:127:LYS:HD3	1.79	0.44
1:C:46:LYS:HA	1:C:46:LYS:HE2	2.00	0.44
1:C:374:LEU:C	1:C:374:LEU:HD13	2.42	0.44
1:B:148:MET:HA	1:B:148:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:PHE:HA	1:C:88:LYS:HE3	1.99	0.44
1:C:171:TYR:OH	1:C:174:GLY:HA2	2.17	0.44
1:B:21:ALA:O	1:B:25:LYS:HG3	2.18	0.44
1:B:154:PRO:HG3	1:B:344:ARG:HA	1.99	0.43
1:A:3:GLU:O	1:A:4:GLU:C	2.61	0.43
1:A:106:TYR:HA	1:A:107:PRO:HD3	1.86	0.43
1:A:47:PHE:HB3	1:A:48:PRO:HD3	2.00	0.43
1:C:27:PHE:CZ	1:C:283:TYR:CB	2.95	0.43
1:C:201:ASN:HD22	1:C:201:ASN:HA	1.65	0.43
1:C:305:LYS:O	1:C:306:SER:HB3	2.19	0.43
1:A:333:ILE:HB	1:A:334:PRO:HD2	2.01	0.42
1:C:127:LYS:HD3	1:C:127:LYS:HA	1.86	0.42
1:C:273:LYS:O	1:C:277:LYS:HB2	2.19	0.42
1:A:153:GLU:HA	1:A:154:PRO:HD3	1.96	0.42
1:C:64:HIS:O	1:C:67:PHE:HB2	2.19	0.42
1:C:305:LYS:H	1:C:308:GLU:CD	2.28	0.42
1:C:335:GLN:HA	1:C:372:ALA:CB	2.50	0.42
1:C:379:LYS:HE3	1:C:379:LYS:HA	2.01	0.42
1:C:28:GLU:O	1:C:32:GLY:HA2	2.20	0.42
1:A:377:LEU:HA	1:B:374:LEU:HD13	2.02	0.42
1:C:344:ARG:O	1:C:348:ILE:HG12	2.20	0.42
1:B:106:TYR:HA	1:B:107:PRO:HD3	1.84	0.42
1:B:64:HIS:HE1	1:B:330:MET:O	2.02	0.41
1:A:9:ILE:HG12	1:A:59:ILE:HB	2.02	0.41
1:A:12:ASN:ND2	1:A:14:ASP:OD1	2.53	0.41
1:B:28:GLU:CD	1:B:34:LYS:HA	2.45	0.41
1:A:77:ALA:HB2	1:A:268:ALA:HA	2.02	0.41
1:B:136:ASP:HA	1:B:146:ALA:HB2	2.02	0.41
1:C:291:GLU:HA	1:C:307:TYR:OH	2.20	0.41
1:A:178:ILE:H	1:A:178:ILE:HG13	1.77	0.41
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.56	0.41
1:C:374:LEU:HB2	1:B:377:LEU:HD22	2.03	0.41
1:A:373:THR:HG22	1:A:376:LYS:NZ	2.36	0.40
1:A:129:TRP:CD1	1:A:248:PRO:HB2	2.56	0.40
1:B:67:PHE:HD1	1:B:70:TYR:CD2	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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%)	288 (94%)	19 (6%)	16	44
1	B	132/363 (36%)	122 (92%)	10 (8%)	12	38
1	C	119/363 (33%)	102 (86%)	17 (14%)	3	18
All	All	558/1089 (51%)	512 (92%)	46 (8%)	10	36

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	15	LYS
1	A	29	LYS
1	A	36	THR
1	A	60	ILE
1	A	102	LYS
1	A	104	ILE
1	A	160	LEU
1	A	179	LYS
1	A	200	LYS
1	A	202	LYS
1	A	277	LYS
1	A	288	GLU
1	A	326	LYS
1	A	328	GLU
1	A	358	ASP
1	A	377	LEU
1	A	381	PHE
1	A	385	LYS

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Mol	Chain	Res	Type
1	C	1	LYS
1	C	3	GLU
1	C	4	GLU
1	C	8	VAL
1	C	23	VAL
1	C	29	LYS
1	C	34	LYS
1	C	42	LYS
1	C	43	LEU
1	C	83	LYS
1	C	344	ARG
1	C	374	LEU
1	C	379	LYS
1	C	384	LEU
1	C	385	LYS
1	C	388	GLN
1	C	394	GLN
1	B	8	VAL
1	B	170	LYS
1	B	175	LYS
1	B	178	ILE
1	B	179	LYS
1	B	201	ASN
1	B	202	LYS
1	B	390	GLN
1	B	393	GLN
1	B	399	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	72	GLN
1	A	86	GLN
1	A	201	ASN
1	A	205	ASN
1	A	218	ASN
1	A	234	ASN
1	C	64	HIS
1	C	72	GLN
1	C	86	GLN
1	C	367	ASN

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Mol	Chain	Res	Type
1	C	388	GLN
1	C	389	GLN
1	C	394	GLN
1	C	395	GLN
1	B	201	ASN
1	B	218	ASN
1	B	396	GLN
1	B	399	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 ⓘ

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	400/449 (89%)	0.20	15 (3%) 44 28	40, 80, 80, 108	27 (6%)
1	B	401/449 (89%)	0.19	9 (2%) 62 39	41, 80, 80, 108	33 (8%)
1	C	397/449 (88%)	0.20	12 (3%) 52 32	41, 80, 80, 108	23 (5%)
All	All	1198/1347 (88%)	0.19	36 (3%) 52 32	40, 80, 80, 108	83 (6%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	LYS	5.2
1	C	392	GLN	4.8
1	B	341	TYR	4.2
1	A	341	TYR	4.1
1	B	381	PHE	4.0
1	C	34	LYS	3.9
1	C	385	LYS	3.9
1	B	344	ARG	3.7
1	C	46	LYS	3.6
1	B	251	LYS	3.5
1	C	391	GLN	3.2
1	C	111	GLU	3.2
1	A	405	PRO	3.1
1	A	406	PRO	3.0
1	A	354	ARG	3.0
1	A	221	GLU	3.0
1	B	111	GLU	2.8
1	C	344	ARG	2.7
1	A	407	PRO	2.7
1	C	4	GLU	2.7
1	C	180	ASP	2.7
1	A	4	GLU	2.6
1	A	381	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	410	PRO	2.5
1	B	391	GLN	2.2
1	A	371	MET	2.2
1	A	288	GLU	2.1
1	A	404	GLN	2.1
1	B	384	LEU	2.1
1	B	320	THR	2.1
1	C	27	PHE	2.1
1	C	265	GLY	2.0
1	B	390	GLN	2.0
1	A	413	PRO	2.0
1	A	387	PHE	2.0
1	C	383	SER	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($\text{\AA}^2$)	Q<0.9
3	CA	C	454	1/1	0.84	0.11	107,107,107,107	0
3	CA	C	455	1/1	0.87	0.07	107,107,107,107	0
3	CA	B	452	1/1	0.90	0.10	107,107,107,107	0
3	CA	A	453	1/1	0.92	0.20	107,107,107,107	0
2	ZN	C	451	1/1	0.92	0.12	107,107,107,107	0
3	CA	B	453	1/1	0.93	0.24	107,107,107,107	0
3	CA	A	451	1/1	0.94	0.17	107,107,107,107	0
3	CA	C	452	1/1	0.94	0.11	107,107,107,107	0
2	ZN	B	450	1/1	0.95	0.05	107,107,107,107	0
2	ZN	A	450	1/1	0.96	0.06	107,107,107,107	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	0.97	0.11	107,107,107,107	0
3	CA	A	452	1/1	0.99	0.03	107,107,107,107	0
3	CA	C	453	1/1	0.99	0.20	107,107,107,107	0
2	ZN	B	451	1/1	0.99	0.02	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.