



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:11 AM EDT

PDB ID : 8R3E / pdb_00008r3e
Title : Huntingtin, 1-17, MBP-N
Authors : Steinbacher, S.; Toledo-Sherman, L.; Dominguez, C.
Deposited on : 2023-11-08
Resolution : 2.91 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

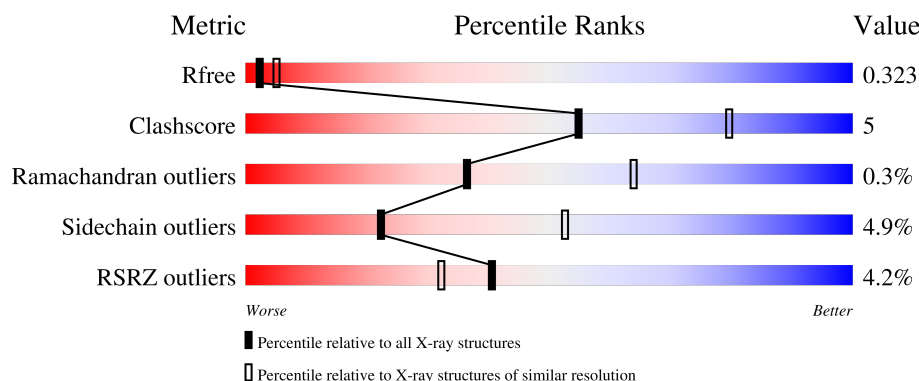
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	399	5% 83% 15% ..
1	B	399	3% 85% 13% ..
1	C	399	4% 84% 15% ..
1	D	399	5% 78% 20% ..
1	E	399	3% 82% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	399	5% 80% 18% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18255 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 Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	18	0	0
			3035	1955	492	580	8			
1	B	394	Total	C	N	O	S	0	0	0
			3044	1961	494	581	8			
1	C	396	Total	C	N	O	S	13	0	0
			3061	1973	496	584	8			
1	D	393	Total	C	N	O	S	0	0	0
			3035	1955	492	580	8			
1	E	393	Total	C	N	O	S	0	0	0
			3035	1955	492	580	8			
1	F	394	Total	C	N	O	S	17	0	0
			3044	1961	494	581	8			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
A	-1	GLY	-	expression tag	UNP A0A4P1LXE0
A	0	MET	-	expression tag	UNP A0A4P1LXE0
A	359	ALA	GLU	conflict	UNP A0A4P1LXE0
A	362	ALA	LYS	conflict	UNP A0A4P1LXE0
A	363	ALA	ASP	conflict	UNP A0A4P1LXE0
A	371	GLY	-	expression tag	UNP A0A4P1LXE0
A	372	SER	-	expression tag	UNP A0A4P1LXE0
A	373	GLU	-	expression tag	UNP A0A4P1LXE0
A	374	ASN	-	expression tag	UNP A0A4P1LXE0
A	375	LEU	-	expression tag	UNP A0A4P1LXE0
A	376	TYR	-	expression tag	UNP A0A4P1LXE0
A	377	PHE	-	expression tag	UNP A0A4P1LXE0
A	378	GLN	-	expression tag	UNP A0A4P1LXE0
A	379	GLY	-	expression tag	UNP A0A4P1LXE0
A	380	MET	-	expression tag	UNP A0A4P1LXE0
A	381	ALA	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	382	THR	-	expression tag	UNP A0A4P1LXE0
A	383	LEU	-	expression tag	UNP A0A4P1LXE0
A	384	GLU	-	expression tag	UNP A0A4P1LXE0
A	385	LYS	-	expression tag	UNP A0A4P1LXE0
A	386	LEU	-	expression tag	UNP A0A4P1LXE0
A	387	MET	-	expression tag	UNP A0A4P1LXE0
A	388	LYS	-	expression tag	UNP A0A4P1LXE0
A	389	ALA	-	expression tag	UNP A0A4P1LXE0
A	390	PHE	-	expression tag	UNP A0A4P1LXE0
A	391	GLU	-	expression tag	UNP A0A4P1LXE0
A	392	SER	-	expression tag	UNP A0A4P1LXE0
A	393	LEU	-	expression tag	UNP A0A4P1LXE0
A	394	LYS	-	expression tag	UNP A0A4P1LXE0
A	395	SER	-	expression tag	UNP A0A4P1LXE0
A	396	PHE	-	expression tag	UNP A0A4P1LXE0
B	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
B	-1	GLY	-	expression tag	UNP A0A4P1LXE0
B	0	MET	-	expression tag	UNP A0A4P1LXE0
B	359	ALA	GLU	conflict	UNP A0A4P1LXE0
B	362	ALA	LYS	conflict	UNP A0A4P1LXE0
B	363	ALA	ASP	conflict	UNP A0A4P1LXE0
B	371	GLY	-	expression tag	UNP A0A4P1LXE0
B	372	SER	-	expression tag	UNP A0A4P1LXE0
B	373	GLU	-	expression tag	UNP A0A4P1LXE0
B	374	ASN	-	expression tag	UNP A0A4P1LXE0
B	375	LEU	-	expression tag	UNP A0A4P1LXE0
B	376	TYR	-	expression tag	UNP A0A4P1LXE0
B	377	PHE	-	expression tag	UNP A0A4P1LXE0
B	378	GLN	-	expression tag	UNP A0A4P1LXE0
B	379	GLY	-	expression tag	UNP A0A4P1LXE0
B	380	MET	-	expression tag	UNP A0A4P1LXE0
B	381	ALA	-	expression tag	UNP A0A4P1LXE0
B	382	THR	-	expression tag	UNP A0A4P1LXE0
B	383	LEU	-	expression tag	UNP A0A4P1LXE0
B	384	GLU	-	expression tag	UNP A0A4P1LXE0
B	385	LYS	-	expression tag	UNP A0A4P1LXE0
B	386	LEU	-	expression tag	UNP A0A4P1LXE0
B	387	MET	-	expression tag	UNP A0A4P1LXE0
B	388	LYS	-	expression tag	UNP A0A4P1LXE0
B	389	ALA	-	expression tag	UNP A0A4P1LXE0
B	390	PHE	-	expression tag	UNP A0A4P1LXE0
B	391	GLU	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	SER	-	expression tag	UNP A0A4P1LXE0
B	393	LEU	-	expression tag	UNP A0A4P1LXE0
B	394	LYS	-	expression tag	UNP A0A4P1LXE0
B	395	SER	-	expression tag	UNP A0A4P1LXE0
B	396	PHE	-	expression tag	UNP A0A4P1LXE0
C	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
C	-1	GLY	-	expression tag	UNP A0A4P1LXE0
C	0	MET	-	expression tag	UNP A0A4P1LXE0
C	359	ALA	GLU	conflict	UNP A0A4P1LXE0
C	362	ALA	LYS	conflict	UNP A0A4P1LXE0
C	363	ALA	ASP	conflict	UNP A0A4P1LXE0
C	371	GLY	-	expression tag	UNP A0A4P1LXE0
C	372	SER	-	expression tag	UNP A0A4P1LXE0
C	373	GLU	-	expression tag	UNP A0A4P1LXE0
C	374	ASN	-	expression tag	UNP A0A4P1LXE0
C	375	LEU	-	expression tag	UNP A0A4P1LXE0
C	376	TYR	-	expression tag	UNP A0A4P1LXE0
C	377	PHE	-	expression tag	UNP A0A4P1LXE0
C	378	GLN	-	expression tag	UNP A0A4P1LXE0
C	379	GLY	-	expression tag	UNP A0A4P1LXE0
C	380	MET	-	expression tag	UNP A0A4P1LXE0
C	381	ALA	-	expression tag	UNP A0A4P1LXE0
C	382	THR	-	expression tag	UNP A0A4P1LXE0
C	383	LEU	-	expression tag	UNP A0A4P1LXE0
C	384	GLU	-	expression tag	UNP A0A4P1LXE0
C	385	LYS	-	expression tag	UNP A0A4P1LXE0
C	386	LEU	-	expression tag	UNP A0A4P1LXE0
C	387	MET	-	expression tag	UNP A0A4P1LXE0
C	388	LYS	-	expression tag	UNP A0A4P1LXE0
C	389	ALA	-	expression tag	UNP A0A4P1LXE0
C	390	PHE	-	expression tag	UNP A0A4P1LXE0
C	391	GLU	-	expression tag	UNP A0A4P1LXE0
C	392	SER	-	expression tag	UNP A0A4P1LXE0
C	393	LEU	-	expression tag	UNP A0A4P1LXE0
C	394	LYS	-	expression tag	UNP A0A4P1LXE0
C	395	SER	-	expression tag	UNP A0A4P1LXE0
C	396	PHE	-	expression tag	UNP A0A4P1LXE0
D	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
D	-1	GLY	-	expression tag	UNP A0A4P1LXE0
D	0	MET	-	expression tag	UNP A0A4P1LXE0
D	359	ALA	GLU	conflict	UNP A0A4P1LXE0
D	362	ALA	LYS	conflict	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	363	ALA	ASP	conflict	UNP A0A4P1LXE0
D	371	GLY	-	expression tag	UNP A0A4P1LXE0
D	372	SER	-	expression tag	UNP A0A4P1LXE0
D	373	GLU	-	expression tag	UNP A0A4P1LXE0
D	374	ASN	-	expression tag	UNP A0A4P1LXE0
D	375	LEU	-	expression tag	UNP A0A4P1LXE0
D	376	TYR	-	expression tag	UNP A0A4P1LXE0
D	377	PHE	-	expression tag	UNP A0A4P1LXE0
D	378	GLN	-	expression tag	UNP A0A4P1LXE0
D	379	GLY	-	expression tag	UNP A0A4P1LXE0
D	380	MET	-	expression tag	UNP A0A4P1LXE0
D	381	ALA	-	expression tag	UNP A0A4P1LXE0
D	382	THR	-	expression tag	UNP A0A4P1LXE0
D	383	LEU	-	expression tag	UNP A0A4P1LXE0
D	384	GLU	-	expression tag	UNP A0A4P1LXE0
D	385	LYS	-	expression tag	UNP A0A4P1LXE0
D	386	LEU	-	expression tag	UNP A0A4P1LXE0
D	387	MET	-	expression tag	UNP A0A4P1LXE0
D	388	LYS	-	expression tag	UNP A0A4P1LXE0
D	389	ALA	-	expression tag	UNP A0A4P1LXE0
D	390	PHE	-	expression tag	UNP A0A4P1LXE0
D	391	GLU	-	expression tag	UNP A0A4P1LXE0
D	392	SER	-	expression tag	UNP A0A4P1LXE0
D	393	LEU	-	expression tag	UNP A0A4P1LXE0
D	394	LYS	-	expression tag	UNP A0A4P1LXE0
D	395	SER	-	expression tag	UNP A0A4P1LXE0
D	396	PHE	-	expression tag	UNP A0A4P1LXE0
E	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
E	-1	GLY	-	expression tag	UNP A0A4P1LXE0
E	0	MET	-	expression tag	UNP A0A4P1LXE0
E	359	ALA	GLU	conflict	UNP A0A4P1LXE0
E	362	ALA	LYS	conflict	UNP A0A4P1LXE0
E	363	ALA	ASP	conflict	UNP A0A4P1LXE0
E	371	GLY	-	expression tag	UNP A0A4P1LXE0
E	372	SER	-	expression tag	UNP A0A4P1LXE0
E	373	GLU	-	expression tag	UNP A0A4P1LXE0
E	374	ASN	-	expression tag	UNP A0A4P1LXE0
E	375	LEU	-	expression tag	UNP A0A4P1LXE0
E	376	TYR	-	expression tag	UNP A0A4P1LXE0
E	377	PHE	-	expression tag	UNP A0A4P1LXE0
E	378	GLN	-	expression tag	UNP A0A4P1LXE0
E	379	GLY	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	380	MET	-	expression tag	UNP A0A4P1LXE0
E	381	ALA	-	expression tag	UNP A0A4P1LXE0
E	382	THR	-	expression tag	UNP A0A4P1LXE0
E	383	LEU	-	expression tag	UNP A0A4P1LXE0
E	384	GLU	-	expression tag	UNP A0A4P1LXE0
E	385	LYS	-	expression tag	UNP A0A4P1LXE0
E	386	LEU	-	expression tag	UNP A0A4P1LXE0
E	387	MET	-	expression tag	UNP A0A4P1LXE0
E	388	LYS	-	expression tag	UNP A0A4P1LXE0
E	389	ALA	-	expression tag	UNP A0A4P1LXE0
E	390	PHE	-	expression tag	UNP A0A4P1LXE0
E	391	GLU	-	expression tag	UNP A0A4P1LXE0
E	392	SER	-	expression tag	UNP A0A4P1LXE0
E	393	LEU	-	expression tag	UNP A0A4P1LXE0
E	394	LYS	-	expression tag	UNP A0A4P1LXE0
E	395	SER	-	expression tag	UNP A0A4P1LXE0
E	396	PHE	-	expression tag	UNP A0A4P1LXE0
F	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
F	-1	GLY	-	expression tag	UNP A0A4P1LXE0
F	0	MET	-	expression tag	UNP A0A4P1LXE0
F	359	ALA	GLU	conflict	UNP A0A4P1LXE0
F	362	ALA	LYS	conflict	UNP A0A4P1LXE0
F	363	ALA	ASP	conflict	UNP A0A4P1LXE0
F	371	GLY	-	expression tag	UNP A0A4P1LXE0
F	372	SER	-	expression tag	UNP A0A4P1LXE0
F	373	GLU	-	expression tag	UNP A0A4P1LXE0
F	374	ASN	-	expression tag	UNP A0A4P1LXE0
F	375	LEU	-	expression tag	UNP A0A4P1LXE0
F	376	TYR	-	expression tag	UNP A0A4P1LXE0
F	377	PHE	-	expression tag	UNP A0A4P1LXE0
F	378	GLN	-	expression tag	UNP A0A4P1LXE0
F	379	GLY	-	expression tag	UNP A0A4P1LXE0
F	380	MET	-	expression tag	UNP A0A4P1LXE0
F	381	ALA	-	expression tag	UNP A0A4P1LXE0
F	382	THR	-	expression tag	UNP A0A4P1LXE0
F	383	LEU	-	expression tag	UNP A0A4P1LXE0
F	384	GLU	-	expression tag	UNP A0A4P1LXE0
F	385	LYS	-	expression tag	UNP A0A4P1LXE0
F	386	LEU	-	expression tag	UNP A0A4P1LXE0
F	387	MET	-	expression tag	UNP A0A4P1LXE0
F	388	LYS	-	expression tag	UNP A0A4P1LXE0
F	389	ALA	-	expression tag	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	390	PHE	-	expression tag	UNP A0A4P1LXE0
F	391	GLU	-	expression tag	UNP A0A4P1LXE0
F	392	SER	-	expression tag	UNP A0A4P1LXE0
F	393	LEU	-	expression tag	UNP A0A4P1LXE0
F	394	LYS	-	expression tag	UNP A0A4P1LXE0
F	395	SER	-	expression tag	UNP A0A4P1LXE0
F	396	PHE	-	expression tag	UNP A0A4P1LXE0

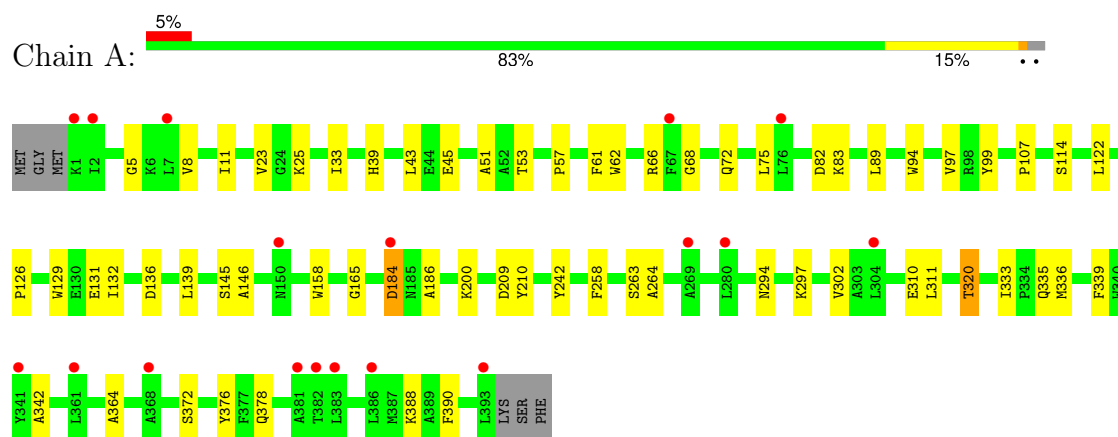
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

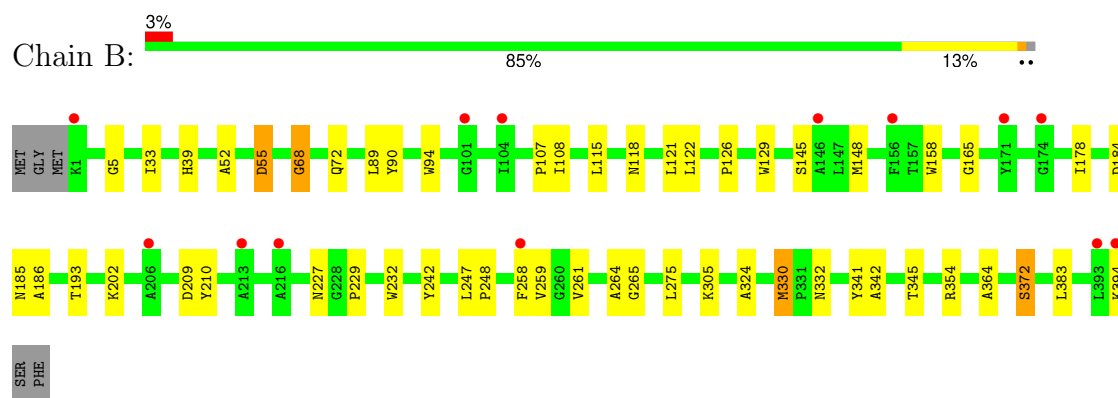
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

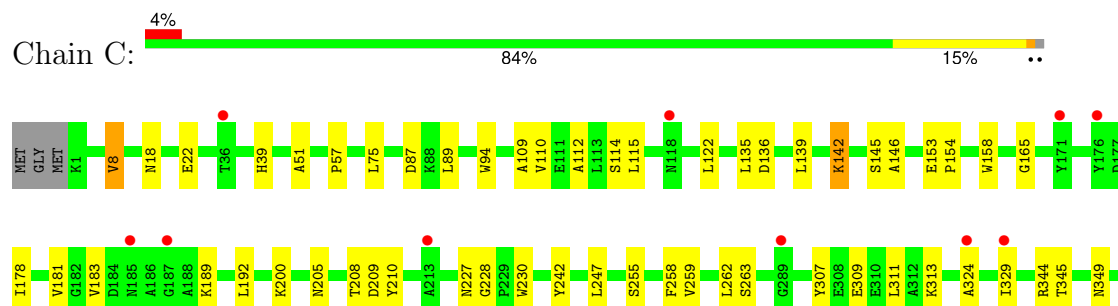
• Molecule 1: Maltodextrin-binding protein



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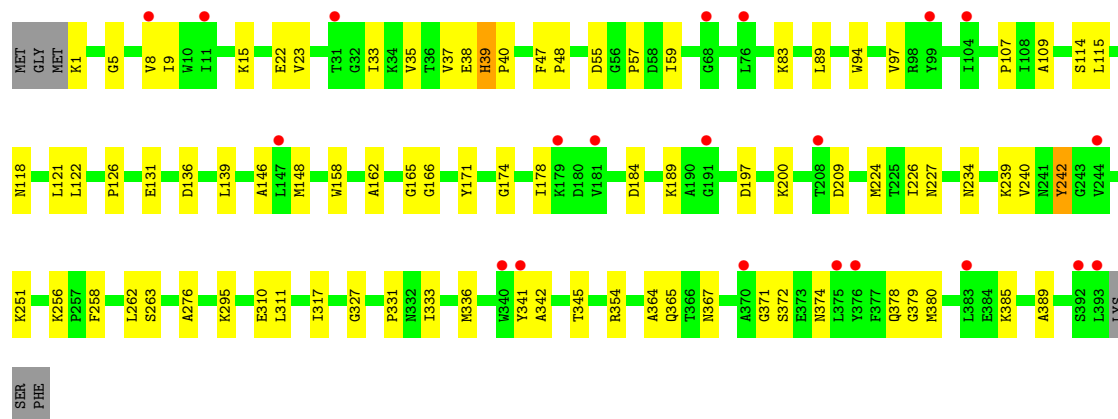
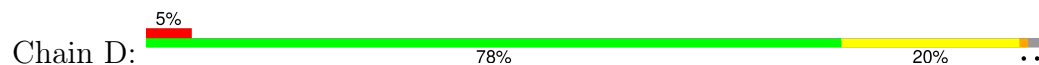


• Molecule 1: Maltodextrin-binding protein

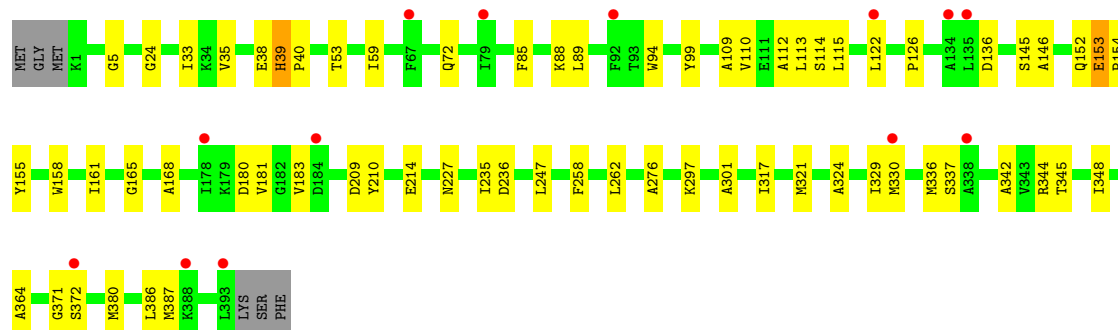
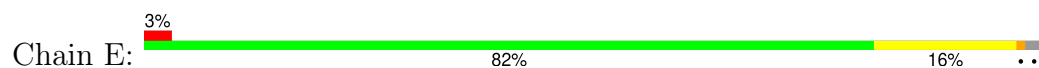




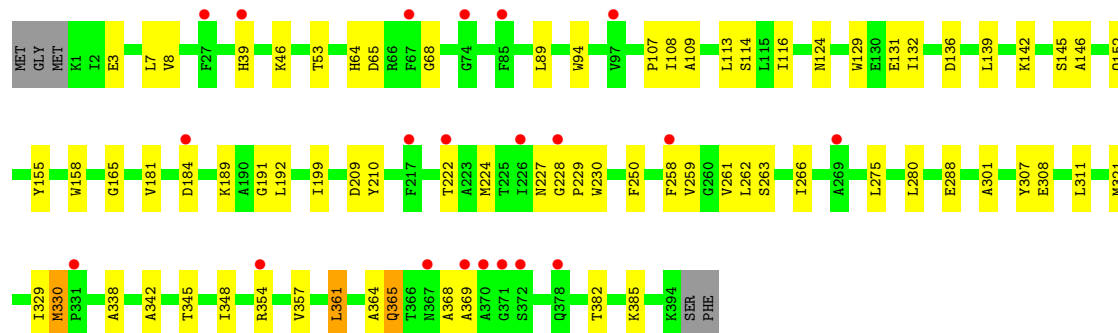
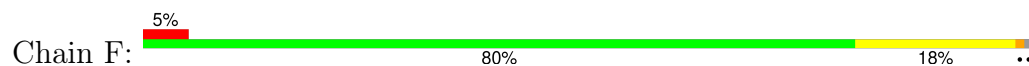
● Molecule 1: Maltodextrin-binding protein



● Molecule 1: Maltodextrin-binding protein



● Molecule 1: Maltodextrin-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.04Å 96.11Å 97.67Å 76.40° 80.72° 63.19°	Depositor
Resolution (Å)	45.79 – 2.91 45.79 – 2.91	Depositor EDS
% Data completeness (in resolution range)	48.0 (45.79-2.91) 48.0 (45.79-2.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.252 , 0.329 0.254 , 0.323	Depositor DCC
R_{free} test set	1602 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	18255	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.11	0/3107	1.66	20/4216 (0.5%)
1	B	1.10	0/3116	1.67	11/4227 (0.3%)
1	C	1.11	0/3134	1.64	5/4251 (0.1%)
1	D	1.11	0/3107	1.63	7/4216 (0.2%)
1	E	1.10	0/3107	1.66	11/4216 (0.3%)
1	F	1.11	0/3116	1.64	7/4227 (0.2%)
All	All	1.11	0/18687	1.65	61/25353 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ASP	CA-CB-CG	9.16	121.76	112.60
1	A	320	THR	CA-CB-OG1	-8.06	97.51	109.60
1	E	153	GLU	CB-CG-CD	6.82	124.19	112.60
1	A	390	PHE	CA-CB-CG	6.24	120.04	113.80
1	A	131	GLU	CA-C-N	6.18	124.14	120.24
1	A	131	GLU	C-N-CA	6.18	124.14	120.24
1	C	242	TYR	CA-C-N	5.91	126.65	122.33
1	C	242	TYR	C-N-CA	5.91	126.65	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	GLN	CA-C-N	5.89	126.48	119.94
1	A	378	GLN	C-N-CA	5.89	126.48	119.94
1	D	23	VAL	CA-C-N	5.65	126.25	119.98
1	D	23	VAL	C-N-CA	5.65	126.25	119.98
1	F	199	ILE	CA-C-N	5.60	127.72	120.44
1	F	199	ILE	C-N-CA	5.60	127.72	120.44
1	A	242	TYR	CA-C-N	5.56	126.39	122.33
1	A	242	TYR	C-N-CA	5.56	126.39	122.33
1	D	22	GLU	CB-CG-CD	5.55	122.04	112.60
1	D	242	TYR	CA-C-N	5.54	125.87	121.61
1	D	242	TYR	C-N-CA	5.54	125.87	121.61
1	A	335	GLN	CA-C-N	5.40	127.78	120.38
1	A	335	GLN	C-N-CA	5.40	127.78	120.38
1	E	209	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	23	VAL	CA-C-N	5.36	125.92	119.98
1	A	23	VAL	C-N-CA	5.36	125.92	119.98
1	E	161	ILE	CA-C-N	5.35	127.44	120.28
1	E	161	ILE	C-N-CA	5.35	127.44	120.28
1	D	131	GLU	CA-C-N	5.26	123.56	120.24
1	D	131	GLU	C-N-CA	5.26	123.56	120.24
1	A	11	ILE	CA-C-O	-5.26	116.78	121.09
1	B	324	ALA	CA-C-N	5.20	127.24	120.28
1	B	324	ALA	C-N-CA	5.20	127.24	120.28
1	C	87	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	210	TYR	CA-C-N	5.18	127.54	120.54
1	C	210	TYR	C-N-CA	5.18	127.54	120.54
1	A	184	ASP	CA-CB-CG	5.16	117.76	112.60
1	E	337	SER	CA-C-N	5.15	127.13	120.44
1	E	337	SER	C-N-CA	5.15	127.13	120.44
1	A	186	ALA	CA-C-N	5.13	125.65	120.00
1	A	186	ALA	C-N-CA	5.13	125.65	120.00
1	F	65	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	68	GLY	CA-C-N	5.08	125.72	120.03
1	A	68	GLY	C-N-CA	5.08	125.72	120.03
1	B	68	GLY	CA-C-N	5.08	125.61	119.98
1	B	68	GLY	C-N-CA	5.08	125.61	119.98
1	E	210	TYR	CA-C-N	5.06	127.38	120.54
1	E	210	TYR	C-N-CA	5.06	127.38	120.54
1	A	210	TYR	CA-C-N	5.06	127.37	120.54
1	A	210	TYR	C-N-CA	5.06	127.37	120.54
1	B	184	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	242	TYR	CA-C-N	5.04	125.66	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	TYR	C-N-CA	5.04	125.66	122.18
1	E	236	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	371	GLY	CA-C-N	5.04	127.34	120.54
1	E	371	GLY	C-N-CA	5.04	127.34	120.54
1	F	68	GLY	CA-C-N	5.03	125.66	120.03
1	F	68	GLY	C-N-CA	5.03	125.66	120.03
1	B	265	GLY	CA-C-O	-5.02	116.35	120.92
1	B	210	TYR	CA-C-N	5.01	127.30	120.54
1	B	210	TYR	C-N-CA	5.01	127.30	120.54
1	F	210	TYR	CA-C-N	5.01	127.30	120.54
1	F	210	TYR	C-N-CA	5.01	127.30	120.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	142	LYS	Peptide
1	F	368	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3035	0	3008	20	1
1	B	3044	0	3021	25	0
1	C	3061	0	3035	28	0
1	D	3035	0	3008	37	1
1	E	3035	0	3008	37	0
1	F	3044	0	3021	39	1
2	C	1	0	0	0	1
All	All	18255	0	18101	174	2

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 5.

All (174) 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:F:184:ASP:HB2	1:F:365:GLN:HG3	1.56	0.85
1:E:380:MET:HE1	1:F:382:THR:HG21	1.56	0.84
1:F:181:VAL:HG21	1:F:369:ALA:HA	1.73	0.71
1:D:342:ALA:HB1	1:D:364:ALA:HA	1.77	0.67
1:D:39:HIS:CG	1:D:39:HIS:O	2.48	0.66
1:F:192:LEU:HD23	1:F:357:VAL:HG13	1.80	0.64
1:E:122:LEU:HD21	1:E:126:PRO:HD3	1.80	0.63
1:E:152:GLN:HA	1:E:348:ILE:HD11	1.79	0.63
1:C:115:LEU:HB2	1:C:247:LEU:HD23	1.80	0.63
1:D:380:MET:HE1	1:F:338:ALA:HB2	1.80	0.61
1:E:380:MET:CE	1:F:382:THR:HG21	2.26	0.61
1:A:51:ALA:HB3	1:A:75:LEU:HD13	1.82	0.61
1:C:8:VAL:HG13	1:C:57:PRO:HA	1.82	0.61
1:D:122:LEU:HD21	1:D:126:PRO:HD3	1.83	0.61
1:E:39:HIS:CG	1:E:39:HIS:O	2.54	0.61
1:D:115:LEU:HD11	1:D:224:MET:HB3	1.83	0.61
1:E:342:ALA:HB1	1:E:364:ALA:HA	1.84	0.60
1:F:184:ASP:HB2	1:F:365:GLN:CG	2.31	0.60
1:C:89:LEU:HD12	1:C:94:TRP:CZ2	2.37	0.60
1:D:136:ASP:HA	1:D:146:ALA:HB2	1.84	0.59
1:D:109:ALA:HB3	1:D:262:LEU:HB3	1.84	0.59
1:C:122:LEU:HD22	1:C:135:LEU:HD11	1.85	0.59
1:E:109:ALA:HB3	1:E:262:LEU:HB3	1.86	0.57
1:C:39:HIS:O	1:C:39:HIS:CG	2.58	0.56
1:A:97:VAL:HG21	1:A:107:PRO:HD3	1.87	0.56
1:C:136:ASP:HA	1:C:146:ALA:HB2	1.88	0.56
1:F:109:ALA:HB3	1:F:262:LEU:HB3	1.87	0.56
1:B:89:LEU:HD12	1:B:94:TRP:CZ2	2.41	0.55
1:D:39:HIS:O	1:D:39:HIS:CD2	2.59	0.55
1:B:39:HIS:O	1:B:39:HIS:CG	2.59	0.54
1:B:108:ILE:HD11	1:B:264:ALA:HB2	1.90	0.53
1:D:178:ILE:HD11	1:D:371:GLY:CA	2.38	0.53
1:D:389:ALA:HB2	1:E:387:MET:HE3	1.90	0.52
1:F:89:LEU:HD12	1:F:94:TRP:CZ2	2.44	0.52
1:E:89:LEU:HD12	1:E:94:TRP:CZ2	2.44	0.52
1:E:158:TRP:CD1	1:E:258:PHE:CE2	2.98	0.52
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.92	0.52
1:E:59:ILE:HD11	1:E:276:ALA:CB	2.40	0.52
1:D:178:ILE:HG22	1:D:333:ILE:HD12	1.91	0.52
1:E:330:MET:HE3	1:E:330:MET:HA	1.92	0.52
1:D:59:ILE:HD11	1:D:276:ALA:CB	2.40	0.52
1:C:192:LEU:HD22	1:C:361:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:VAL:HG13	1:D:57:PRO:HA	1.91	0.51
1:F:228:GLY:HA3	1:F:230:TRP:CZ3	2.46	0.51
1:B:158:TRP:CD1	1:B:258:PHE:CE2	2.99	0.51
1:F:116:ILE:HD12	1:F:116:ILE:N	2.25	0.51
1:C:228:GLY:HA3	1:C:230:TRP:CZ3	2.46	0.50
1:E:85:PHE:HA	1:E:88:LYS:HG2	1.92	0.50
1:E:168:ALA:CB	1:E:336:MET:HE1	2.41	0.50
1:F:308:GLU:HG2	1:F:321:MET:HE3	1.92	0.50
1:C:329:ILE:N	1:C:329:ILE:HD12	2.27	0.50
1:D:35:VAL:HG12	1:D:37:VAL:HG23	1.94	0.50
1:D:97:VAL:HG21	1:D:107:PRO:HD3	1.94	0.50
1:D:311:LEU:HB3	1:D:317:ILE:HD13	1.93	0.50
1:A:89:LEU:HD12	1:A:94:TRP:CZ2	2.47	0.50
1:C:205:ASN:HB3	1:C:208:THR:HG23	1.94	0.50
1:D:158:TRP:CD1	1:D:258:PHE:CE2	2.99	0.50
1:B:122:LEU:HD21	1:B:126:PRO:HD3	1.93	0.49
1:E:38:GLU:C	1:E:40:PRO:HD3	2.37	0.49
1:E:113:LEU:HD11	1:E:155:TYR:CE1	2.47	0.49
1:A:139:LEU:HD13	1:A:146:ALA:HA	1.94	0.49
1:D:47:PHE:HB3	1:D:48:PRO:HD3	1.95	0.49
1:D:59:ILE:HD11	1:D:276:ALA:HB1	1.94	0.49
1:D:184:ASP:HB2	1:D:365:GLN:HB2	1.95	0.49
1:F:158:TRP:CD1	1:F:258:PHE:CE2	3.01	0.49
1:B:33:ILE:HD13	1:B:275:LEU:HD22	1.93	0.48
1:E:136:ASP:HA	1:E:146:ALA:HB2	1.94	0.48
1:F:191:GLY:HA2	1:F:250:PHE:CE2	2.48	0.48
1:C:158:TRP:CD1	1:C:258:PHE:CE2	3.01	0.48
1:B:90:TYR:CE2	1:B:305:LYS:HA	2.48	0.48
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.48	0.48
1:E:24:GLY:HA2	1:E:35:VAL:HG21	1.94	0.48
1:F:152:GLN:HA	1:F:348:ILE:HD11	1.94	0.48
1:D:256:LYS:HA	1:D:327:GLY:HA2	1.96	0.48
1:C:139:LEU:HD13	1:C:146:ALA:HA	1.96	0.48
1:D:118:ASN:CG	1:D:121:LEU:HD12	2.38	0.48
1:F:39:HIS:O	1:F:39:HIS:CD2	2.67	0.48
1:F:64:HIS:CE1	1:F:330:MET:O	2.67	0.48
1:A:158:TRP:CD1	1:A:258:PHE:CE2	3.01	0.47
1:B:5:GLY:O	1:B:33:ILE:HG23	2.14	0.47
1:B:68:GLY:CA	1:B:332:ASN:HD22	2.28	0.47
1:B:259:VAL:HG12	1:B:261:VAL:HG23	1.96	0.47
1:D:385:LYS:HG2	1:E:387:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:ALA:HB1	1:F:364:ALA:HA	1.95	0.47
1:F:131:GLU:O	1:F:131:GLU:HG2	2.14	0.47
1:A:72:GLN:HG2	1:A:99:TYR:CE2	2.49	0.47
1:A:72:GLN:HG2	1:A:99:TYR:CZ	2.50	0.47
1:D:342:ALA:HB2	1:D:367:ASN:HB3	1.97	0.47
1:B:89:LEU:HD13	1:B:107:PRO:HG2	1.96	0.47
1:D:38:GLU:C	1:D:40:PRO:HD3	2.39	0.47
1:F:301:ALA:HB1	1:F:321:MET:HE2	1.96	0.47
1:A:122:LEU:HD21	1:A:126:PRO:HD3	1.97	0.46
1:E:153:GLU:OE1	1:E:344:ARG:NH1	2.48	0.46
1:C:307:TYR:CE2	1:C:311:LEU:HD11	2.50	0.46
1:F:259:VAL:HG12	1:F:261:VAL:HG23	1.97	0.46
1:B:178:ILE:HD13	1:B:372:SER:OG	2.15	0.46
1:C:51:ALA:HB3	1:C:75:LEU:HD13	1.96	0.46
1:E:329:ILE:HD12	1:E:329:ILE:N	2.30	0.46
1:A:5:GLY:O	1:A:33:ILE:HG23	2.15	0.46
1:C:110:VAL:HG13	1:C:259:VAL:HG13	1.97	0.46
1:A:43:LEU:HD11	1:A:62:TRP:CE3	2.51	0.46
1:D:89:LEU:HD12	1:D:94:TRP:CZ2	2.51	0.46
1:D:5:GLY:O	1:D:33:ILE:HG23	2.16	0.45
1:A:302:VAL:HG22	1:A:311:LEU:HD12	1.97	0.45
1:F:108:ILE:HG12	1:F:263:SER:HA	1.98	0.45
1:E:301:ALA:HA	1:E:317:ILE:HG23	1.97	0.45
1:D:1:LYS:HB2	1:D:55:ASP:HB3	1.98	0.45
1:D:354:ARG:O	1:F:53:THR:HG22	2.17	0.45
1:B:185:ASN:OD1	1:B:186:ALA:N	2.51	0.44
1:E:72:GLN:HG2	1:E:99:TYR:CE2	2.52	0.44
1:E:181:VAL:CG1	1:E:183:VAL:HG23	2.46	0.44
1:D:171:TYR:CZ	1:D:174:GLY:HA2	2.53	0.44
1:F:329:ILE:HD12	1:F:329:ILE:N	2.32	0.44
1:F:192:LEU:HD22	1:F:361:LEU:CD1	2.47	0.44
1:F:382:THR:HG22	1:F:385:LYS:NZ	2.33	0.44
1:E:112:ALA:HB2	1:E:324:ALA:HB2	1.99	0.44
1:B:129:TRP:CE2	1:B:248:PRO:HG2	2.52	0.44
1:B:342:ALA:HB1	1:B:364:ALA:HA	1.98	0.44
1:D:9:ILE:HB	1:D:37:VAL:HG22	2.00	0.44
1:D:240:VAL:HG23	1:D:242:TYR:HB3	1.99	0.43
1:F:7:LEU:HD21	1:F:275:LEU:HB2	2.00	0.43
1:B:115:LEU:HD22	1:B:248:PRO:HD3	1.99	0.43
1:B:178:ILE:HD12	1:B:178:ILE:C	2.43	0.43
1:B:122:LEU:HD21	1:B:126:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:LEU:HD23	1:C:386:LEU:HD12	2.00	0.43
1:A:53:THR:HG22	1:B:354:ARG:O	2.19	0.43
1:D:331:PRO:HD2	1:D:336:MET:HE2	2.01	0.43
1:E:59:ILE:HD11	1:E:276:ALA:HB1	2.01	0.43
1:F:307:TYR:CD2	1:F:311:LEU:HD11	2.54	0.43
1:C:18:ASN:O	1:C:22:GLU:HG2	2.19	0.43
1:F:181:VAL:HG21	1:F:369:ALA:CA	2.46	0.43
1:A:342:ALA:HB1	1:A:364:ALA:HA	2.00	0.43
1:D:379:GLY:HA2	1:E:380:MET:HG3	2.01	0.43
1:E:72:GLN:HG2	1:E:99:TYR:CZ	2.53	0.43
1:D:178:ILE:C	1:D:178:ILE:HD12	2.43	0.43
1:B:52:ALA:O	1:C:356:THR:N	2.51	0.42
1:C:349:ASN:OD1	1:C:354:ARG:NH2	2.52	0.42
1:E:214:GLU:OE1	1:E:227:ASN:ND2	2.52	0.42
1:F:136:ASP:HA	1:F:146:ALA:HB2	2.01	0.42
1:E:115:LEU:HB2	1:E:247:LEU:HD23	2.01	0.42
1:F:113:LEU:HD11	1:F:155:TYR:CE1	2.53	0.42
1:B:39:HIS:O	1:B:39:HIS:ND1	2.52	0.42
1:A:129:TRP:HA	1:A:132:ILE:HD12	2.00	0.42
1:C:189:LYS:HA	1:C:361:LEU:HD12	2.02	0.42
1:D:389:ALA:HB2	1:E:387:MET:CE	2.50	0.42
1:E:154:PRO:HG3	1:E:344:ARG:HA	2.02	0.42
1:D:162:ALA:HA	1:D:166:GLY:HA3	2.01	0.42
1:F:307:TYR:CE2	1:F:311:LEU:HD11	2.55	0.42
1:A:8:VAL:HG13	1:A:57:PRO:HA	2.02	0.41
1:C:189:LYS:HA	1:C:361:LEU:CD1	2.50	0.41
1:E:110:VAL:HG21	1:E:321:MET:HE1	2.02	0.41
1:F:382:THR:HG22	1:F:385:LYS:HZ1	1.84	0.41
1:A:376:TYR:OH	1:C:375:LEU:HG	2.20	0.41
1:B:118:ASN:ND2	1:B:121:LEU:HD12	2.34	0.41
1:A:82:ASP:OD1	1:A:83:LYS:N	2.53	0.41
1:C:112:ALA:HB2	1:C:324:ALA:HB2	2.02	0.41
1:E:39:HIS:O	1:E:39:HIS:ND1	2.53	0.41
1:B:330:MET:HE3	1:B:330:MET:HA	2.03	0.41
1:C:39:HIS:O	1:C:39:HIS:ND1	2.53	0.41
1:F:222:THR:HG22	1:F:224:MET:H	1.85	0.41
1:F:266:ILE:HD11	1:F:280:LEU:HD12	2.01	0.41
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.56	0.41
1:C:89:LEU:HB2	1:C:94:TRP:HE1	1.86	0.41
1:C:109:ALA:HB3	1:C:262:LEU:HB3	2.01	0.41
1:C:154:PRO:HG3	1:C:344:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:HIS:O	1:F:39:HIS:CG	2.73	0.41
1:F:89:LEU:HD13	1:F:107:PRO:HG2	2.02	0.41
1:F:129:TRP:CE3	1:F:132:ILE:HD12	2.56	0.41
1:C:181:VAL:CG1	1:C:183:VAL:HG23	2.51	0.41
1:E:5:GLY:O	1:E:33:ILE:HG23	2.21	0.41
1:B:68:GLY:HA2	1:B:332:ASN:HD22	1.86	0.40
1:A:336:MET:HE3	1:A:339:PHE:CD1	2.56	0.40
1:E:183:VAL:HG11	1:E:364:ALA:HB3	2.04	0.40
1:E:53:THR:HG22	1:F:354:ARG:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:ND1	2:C:401:ZN:ZN[1_545]	1.61	0.59
1:D:15:LYS:O	1:F:124:ASN:ND2[1_455]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	391/399 (98%)	367 (94%)	23 (6%)	1 (0%)	36	64
1	B	392/399 (98%)	370 (94%)	21 (5%)	1 (0%)	36	64
1	C	394/399 (99%)	373 (95%)	20 (5%)	1 (0%)	36	64
1	D	391/399 (98%)	365 (93%)	24 (6%)	2 (0%)	24	53
1	E	391/399 (98%)	369 (94%)	21 (5%)	1 (0%)	36	64
1	F	392/399 (98%)	366 (93%)	25 (6%)	1 (0%)	36	64
All	All	2351/2394 (98%)	2210 (94%)	134 (6%)	7 (0%)	36	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	239	LYS
1	A	165	GLY
1	C	165	GLY
1	D	165	GLY
1	F	165	GLY
1	E	165	GLY
1	B	165	GLY

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	310/315 (98%)	294 (95%)	16 (5%)	21	50
1	B	311/315 (99%)	296 (95%)	15 (5%)	23	54
1	C	313/315 (99%)	299 (96%)	14 (4%)	24	56
1	D	310/315 (98%)	289 (93%)	21 (7%)	14	40
1	E	310/315 (98%)	301 (97%)	9 (3%)	37	69
1	F	311/315 (99%)	295 (95%)	16 (5%)	21	51
All	All	1865/1890 (99%)	1774 (95%)	91 (5%)	22	52

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	45	GLU
1	A	66	ARG
1	A	114	SER
1	A	145	SER
1	A	184	ASP
1	A	200	LYS
1	A	209	ASP
1	A	263	SER
1	A	294	ASN
1	A	297	LYS
1	A	310	GLU

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Mol	Chain	Res	Type
1	A	320	THR
1	A	333	ILE
1	A	372	SER
1	A	388	LYS
1	B	55	ASP
1	B	72	GLN
1	B	145	SER
1	B	148	MET
1	B	193	THR
1	B	202	LYS
1	B	209	ASP
1	B	227	ASN
1	B	247	LEU
1	B	330	MET
1	B	341	TYR
1	B	345	THR
1	B	372	SER
1	B	383	LEU
1	B	394	LYS
1	C	8	VAL
1	C	114	SER
1	C	142	LYS
1	C	145	SER
1	C	153	GLU
1	C	178	ILE
1	C	200	LYS
1	C	209	ASP
1	C	227	ASN
1	C	255	SER
1	C	263	SER
1	C	309	GLU
1	C	313	LYS
1	C	345	THR
1	D	39	HIS
1	D	83	LYS
1	D	114	SER
1	D	139	LEU
1	D	148	MET
1	D	189	LYS
1	D	197	ASP
1	D	200	LYS
1	D	209	ASP

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Mol	Chain	Res	Type
1	D	226	ILE
1	D	227	ASN
1	D	234	ASN
1	D	251	LYS
1	D	263	SER
1	D	295	LYS
1	D	310	GLU
1	D	341	TYR
1	D	345	THR
1	D	372	SER
1	D	374	ASN
1	D	378	GLN
1	E	39	HIS
1	E	114	SER
1	E	145	SER
1	E	180	ASP
1	E	235	ILE
1	E	297	LYS
1	E	345	THR
1	E	372	SER
1	E	386	LEU
1	F	3	GLU
1	F	8	VAL
1	F	46	LYS
1	F	114	SER
1	F	139	LEU
1	F	142	LYS
1	F	145	SER
1	F	189	LYS
1	F	209	ASP
1	F	227	ASN
1	F	229	PRO
1	F	288	GLU
1	F	330	MET
1	F	345	THR
1	F	361	LEU
1	F	365	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN

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Mol	Chain	Res	Type
1	B	18	ASN
1	B	72	GLN
1	B	201	ASN
1	B	253	GLN
1	B	282	ASN
1	C	18	ASN
1	C	100	ASN
1	C	272	ASN
1	C	282	ASN
1	C	325	GLN
1	D	12	ASN
1	D	18	ASN
1	D	185	ASN
1	D	201	ASN
1	D	282	ASN
1	D	367	ASN
1	D	374	ASN
1	E	18	ASN
1	E	49	GLN
1	E	86	GLN
1	E	100	ASN
1	E	152	GLN
1	E	227	ASN
1	E	282	ASN
1	F	39	HIS
1	F	49	GLN
1	F	152	GLN
1	F	173	ASN
1	F	201	ASN
1	F	234	ASN
1	F	367	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

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	393/399 (98%)	0.54	18 (4%)	37	29	15, 45, 74, 106	5 (1%)
1	B	394/399 (98%)	0.52	13 (3%)	49	39	17, 45, 73, 96	0
1	C	396/399 (99%)	0.62	14 (3%)	47	38	22, 49, 83, 120	4 (1%)
1	D	393/399 (98%)	0.64	21 (5%)	32	25	19, 46, 84, 129	0
1	E	393/399 (98%)	0.72	13 (3%)	49	39	19, 55, 82, 119	0
1	F	394/399 (98%)	0.63	21 (5%)	32	25	27, 49, 79, 130	5 (1%)
All	All	2363/2394 (98%)	0.61	100 (4%)	40	32	15, 48, 81, 130	14 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	371	GLY	5.4
1	D	370	ALA	4.2
1	C	396	PHE	3.7
1	D	99	TYR	3.5
1	D	147	LEU	3.4
1	F	258	PHE	3.4
1	E	393	LEU	3.4
1	A	361	LEU	3.3
1	E	134	ALA	3.2
1	B	206	ALA	3.0
1	D	393	LEU	3.0
1	F	331	PRO	2.9
1	C	176	TYR	2.9
1	A	383	LEU	2.9
1	C	171	TYR	2.9
1	D	376	TYR	2.9
1	C	213	ALA	2.8
1	F	39	HIS	2.8
1	E	372	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	36	THR	2.7
1	C	370	ALA	2.7
1	D	68	GLY	2.7
1	F	74	GLY	2.7
1	E	338	ALA	2.6
1	E	184	ASP	2.6
1	F	369	ALA	2.6
1	C	383	LEU	2.6
1	F	97	VAL	2.6
1	D	8	VAL	2.6
1	E	178	ILE	2.5
1	C	185	ASN	2.5
1	A	184	ASP	2.5
1	E	135	LEU	2.5
1	E	67	PHE	2.5
1	A	269	ALA	2.5
1	A	381	ALA	2.5
1	B	213	ALA	2.5
1	D	179	LYS	2.4
1	D	392	SER	2.4
1	C	329	ILE	2.4
1	A	76	LEU	2.4
1	A	2	ILE	2.4
1	D	11	ILE	2.4
1	E	92	PHE	2.4
1	F	354	ARG	2.3
1	F	370	ALA	2.3
1	D	340	TRP	2.3
1	D	181	VAL	2.3
1	D	383	LEU	2.3
1	B	104	ILE	2.3
1	F	226	ILE	2.3
1	C	187	GLY	2.3
1	D	191	GLY	2.3
1	F	27	PHE	2.3
1	F	372	SER	2.3
1	D	31	THR	2.3
1	F	228	GLY	2.3
1	B	156	PHE	2.3
1	A	280	LEU	2.3
1	A	386	LEU	2.3
1	B	393	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	375	LEU	2.3
1	B	394	LYS	2.3
1	B	174	GLY	2.3
1	E	330	MET	2.2
1	F	378	GLN	2.2
1	F	184	ASP	2.2
1	B	258	PHE	2.2
1	E	388	LYS	2.2
1	B	1	LYS	2.2
1	D	76	LEU	2.2
1	A	341	TYR	2.2
1	E	122	LEU	2.2
1	B	216	ALA	2.2
1	C	118	ASN	2.2
1	A	382	THR	2.2
1	F	222	THR	2.2
1	D	341	TYR	2.2
1	F	269	ALA	2.2
1	D	104	ILE	2.1
1	B	101	GLY	2.1
1	A	393	LEU	2.1
1	C	324	ALA	2.1
1	A	368	ALA	2.1
1	B	146	ALA	2.1
1	F	367	ASN	2.1
1	D	208	THR	2.1
1	F	67	PHE	2.1
1	D	244	VAL	2.1
1	C	390	PHE	2.1
1	A	7	LEU	2.0
1	A	304	LEU	2.0
1	C	289	GLY	2.0
1	E	79	ILE	2.0
1	A	150	ASN	2.0
1	A	67	PHE	2.0
1	F	85	PHE	2.0
1	F	217	PHE	2.0
1	A	1	LYS	2.0
1	B	171	TYR	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
2	ZN	C	401	1/1	0.97	0.04	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.