wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2024 – 04:13 pm BST

PDB ID	:	8R3E
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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

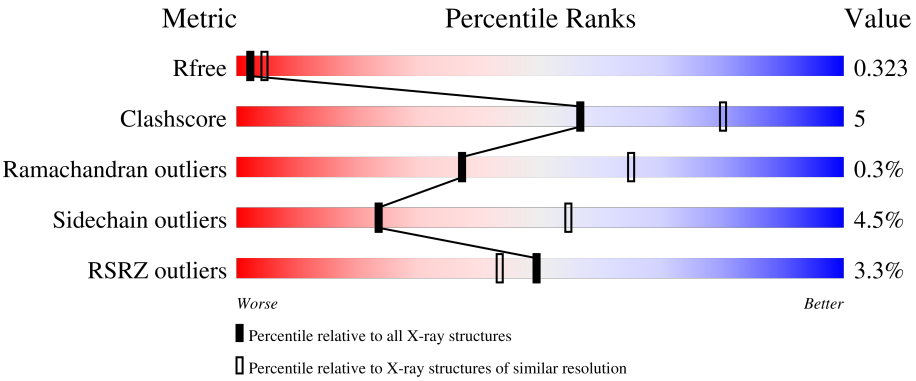
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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}	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (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 <=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	3% 86% 12%
1	B	399	2% 86% 12%
1	C	399	3% 84% 16%
1	D	399	5% 80% 18%
1	E	399	3% 84% 14%

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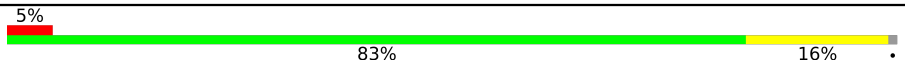
Mol	Chain	Length	Quality of chain
1	F	399	

2 Entry composition (i)

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 (three-letter code: ZN) (formula: Zn).

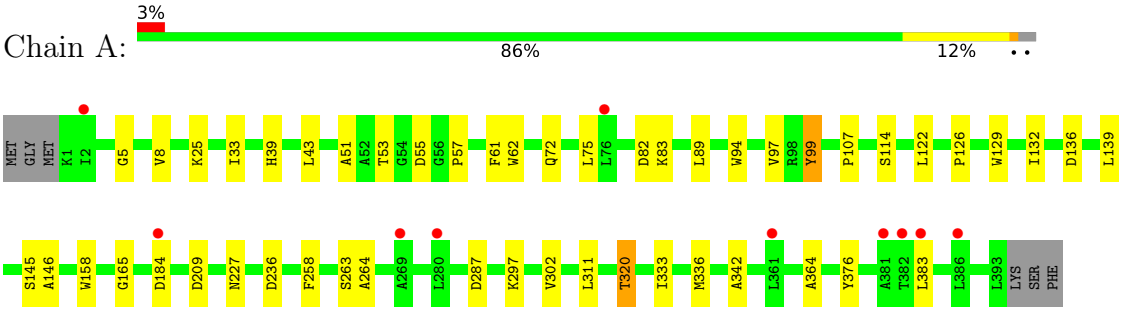
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	C	1	1	1	0	0

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.

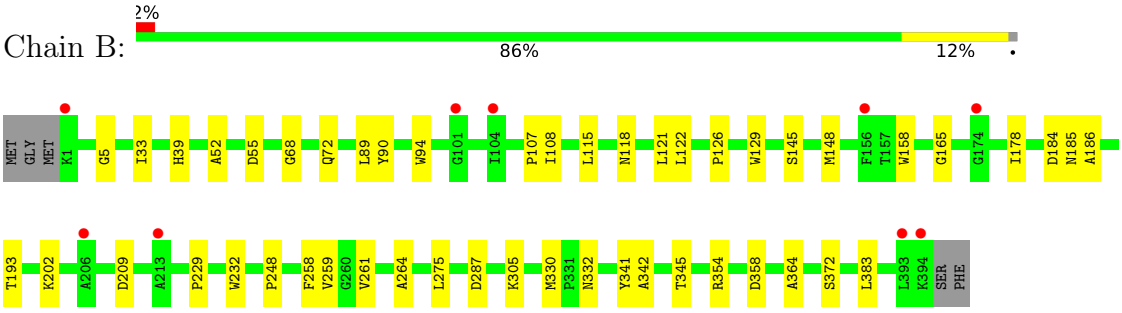
• Molecule 1: Maltodextrin-binding protein

Chain A:



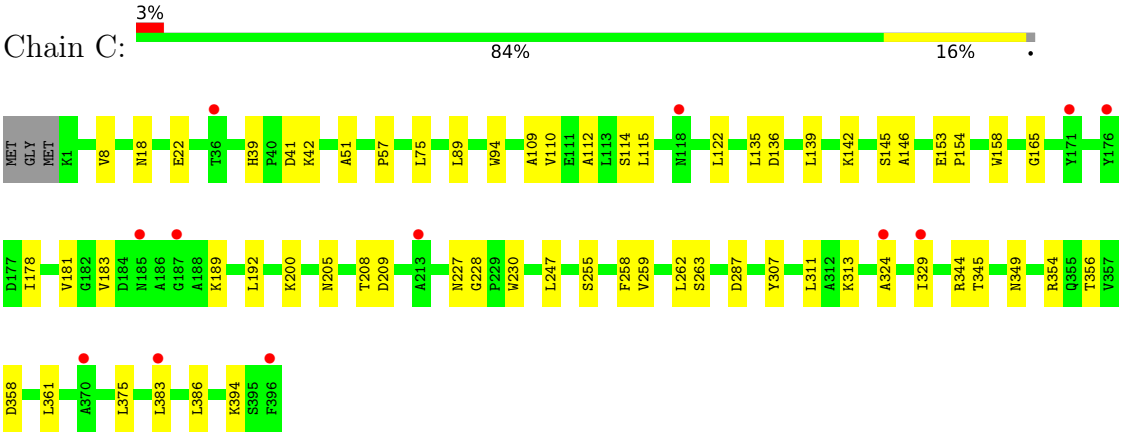
• Molecule 1: Maltodextrin-binding protein

Chain B:



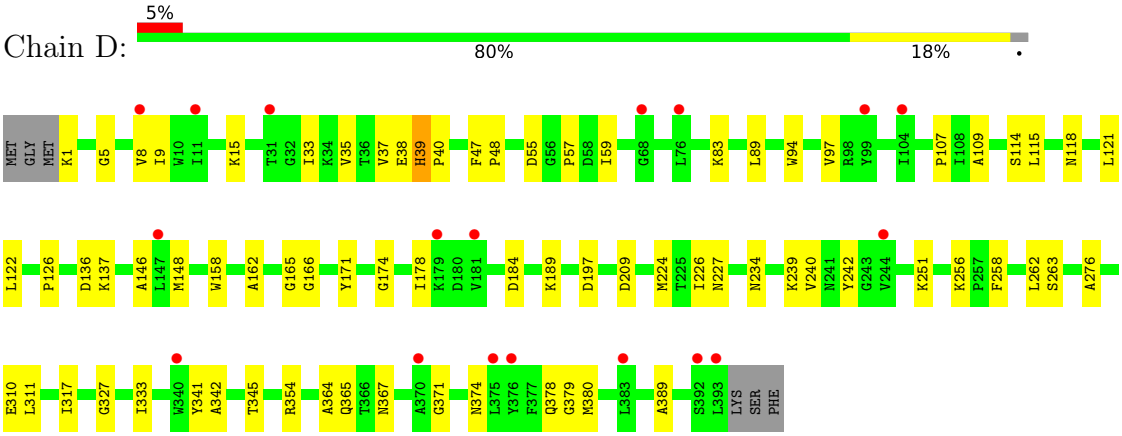
• Molecule 1: Maltodextrin-binding protein

Chain C:



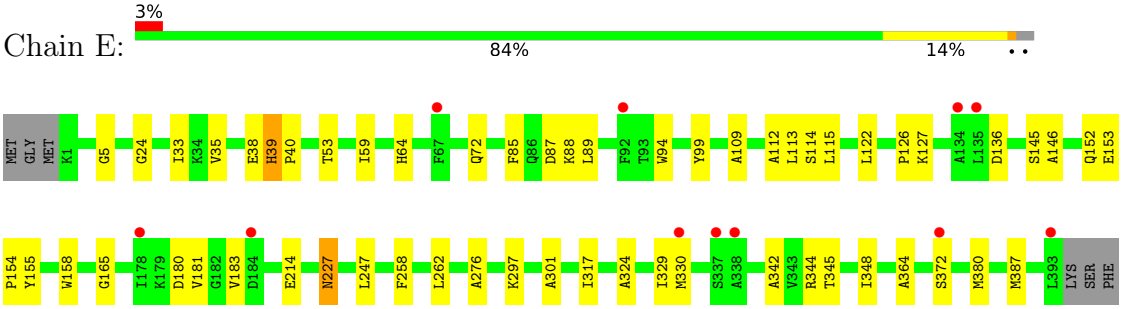
• Molecule 1: Maltodextrin-binding protein

Chain D:



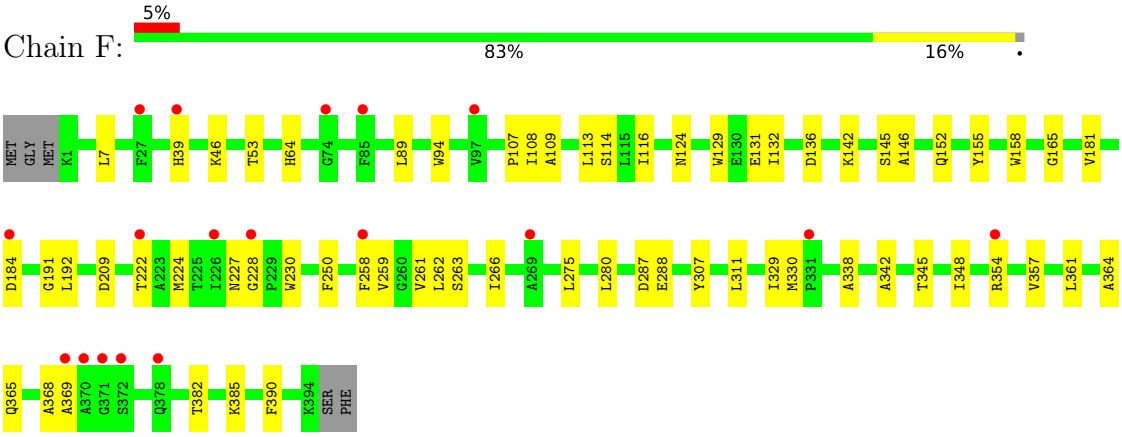
• Molecule 1: Maltodextrin-binding protein

Chain E:



• Molecule 1: Maltodextrin-binding protein

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	3273 reflections (5.04%)	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 , 22.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.74	0/3107	0.90	1/4216 (0.0%)
1	B	0.73	0/3116	0.88	0/4227
1	C	0.73	0/3134	0.88	0/4251
1	D	0.72	0/3107	0.87	0/4216
1	E	0.73	0/3107	0.88	0/4216
1	F	0.73	0/3116	0.89	0/4227
All	All	0.73	0/18687	0.88	1/25353 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	THR	CA-CB-OG1	-5.47	97.51	109.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	142	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	F	368	ALA	Peptide

5.2 Too-close contacts (i)

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	19	1
1	B	3044	0	3021	23	0
1	C	3061	0	3035	28	0
1	D	3035	0	3008	33	1
1	E	3035	0	3008	35	0
1	F	3044	0	3021	37	1
2	C	1	0	0	0	1
All	All	18255	0	18101	164	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.

The worst 5 of 164 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: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:E:380:MET:CE	1:F:382:THR:HG21	2.26	0.65

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%)	37	65
1	B	392/399 (98%)	370 (94%)	21 (5%)	1 (0%)	37	65
1	C	394/399 (99%)	373 (95%)	20 (5%)	1 (0%)	37	65
1	D	391/399 (98%)	365 (93%)	24 (6%)	2 (0%)	25	55
1	E	391/399 (98%)	369 (94%)	21 (5%)	1 (0%)	37	65
1	F	392/399 (98%)	366 (93%)	25 (6%)	1 (0%)	37	65
All	All	2351/2394 (98%)	2210 (94%)	134 (6%)	7 (0%)	37	65

5 of 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

5.3.2 Protein sidechains (i)

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%)	19	49
1	B	311/315 (99%)	297 (96%)	14 (4%)	23	54
1	C	313/315 (99%)	297 (95%)	16 (5%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	310/315 (98%)	292 (94%)	18 (6%)	17 44
1	E	310/315 (98%)	300 (97%)	10 (3%)	34 67
1	F	311/315 (99%)	301 (97%)	10 (3%)	34 67
All	All	1865/1890 (99%)	1781 (96%)	84 (4%)	23 54

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	251	LYS
1	E	297	LYS
1	D	310	GLU
1	E	87	ASP
1	F	114	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	12	ASN
1	D	39	HIS
1	D	374	ASN
1	F	227	ASN

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 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, 95^{th} 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%)	0.39	10 (2%)	58	52	15, 45, 74, 106	5 (1%)
1	B	394/399 (98%)	0.35	9 (2%)	61	55	17, 45, 73, 96	0
1	C	396/399 (99%)	0.49	12 (3%)	52	47	22, 49, 83, 120	4 (1%)
1	D	393/399 (98%)	0.48	18 (4%)	38	32	19, 46, 84, 129	0
1	E	393/399 (98%)	0.55	11 (2%)	55	49	19, 55, 82, 119	0
1	F	394/399 (98%)	0.49	18 (4%)	38	32	27, 49, 79, 130	5 (1%)
All	All	2363/2394 (98%)	0.46	78 (3%)	49	43	15, 48, 81, 130	14 (0%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	371	GLY	5.2
1	D	370	ALA	4.1
1	C	396	PHE	3.6
1	D	99	TYR	3.4
1	D	147	LEU	3.3

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

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	C	401	1/1	0.97	0.04	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.