



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 8PR9 / pdb_00008pr9
Title : The structure of v13Bagel2
Authors : Vandebroek, L.; Voet, A.R.D.; Lee, X.Y.
Deposited on : 2023-07-12
Resolution : 2.35 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:

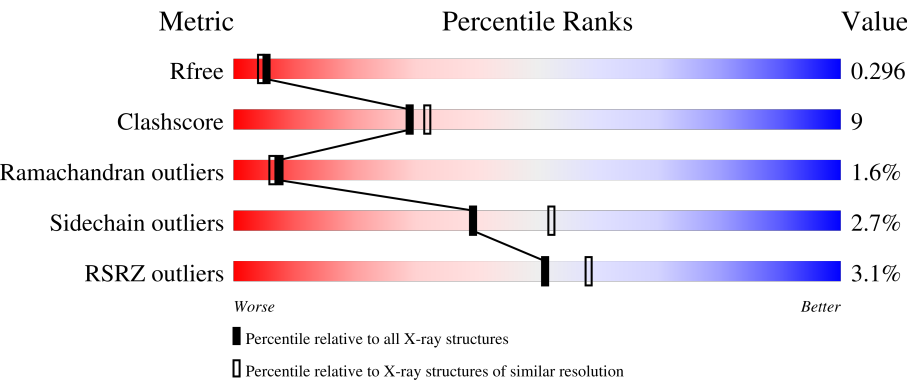
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	85	69%24%6%
1	B	85	2% 73%19%6%
1	C	85	4% 71%18%6%6%
1	D	85	2% 75%18%6%
1	E	85	2% 78%14%6%

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Mol	Chain	Length	Quality of chain
1	F	85	4% 69% 20% 5% 6%
1	G	85	2% 75% 18% • 6%
1	H	85	7% 73% 19% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4969 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 Cell surface protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	0	0	0
			612	390	104	118			
1	B	80	Total	C	N	O	0	0	0
			612	390	104	118			
1	C	80	Total	C	N	O	0	0	0
			612	390	104	118			
1	D	80	Total	C	N	O	0	0	0
			612	390	104	118			
1	E	80	Total	C	N	O	0	0	0
			612	390	104	118			
1	F	80	Total	C	N	O	0	0	0
			612	390	104	118			
1	G	80	Total	C	N	O	0	0	0
			612	390	104	118			
1	H	80	Total	C	N	O	0	0	0
			612	390	104	118			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP B5YBJ6
A	-2	SER	-	expression tag	UNP B5YBJ6
A	-1	HIS	-	expression tag	UNP B5YBJ6
A	0	MET	-	expression tag	UNP B5YBJ6
A	1	ASN	ASP	conflict	UNP B5YBJ6
A	3	LYS	THR	conflict	UNP B5YBJ6
A	9	GLU	LYS	conflict	UNP B5YBJ6
A	31	ASN	ASP	conflict	UNP B5YBJ6
A	52	GLY	ARG	conflict	UNP B5YBJ6
A	53	SER	PRO	conflict	UNP B5YBJ6
A	71	ASN	MET	conflict	UNP B5YBJ6
A	81	GLY	ASP	conflict	UNP B5YBJ6
B	-3	GLY	-	expression tag	UNP B5YBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP B5YBJ6
B	-1	HIS	-	expression tag	UNP B5YBJ6
B	0	MET	-	expression tag	UNP B5YBJ6
B	1	ASN	ASP	conflict	UNP B5YBJ6
B	3	LYS	THR	conflict	UNP B5YBJ6
B	9	GLU	LYS	conflict	UNP B5YBJ6
B	31	ASN	ASP	conflict	UNP B5YBJ6
B	52	GLY	ARG	conflict	UNP B5YBJ6
B	53	SER	PRO	conflict	UNP B5YBJ6
B	71	ASN	MET	conflict	UNP B5YBJ6
B	81	GLY	ASP	conflict	UNP B5YBJ6
C	-3	GLY	-	expression tag	UNP B5YBJ6
C	-2	SER	-	expression tag	UNP B5YBJ6
C	-1	HIS	-	expression tag	UNP B5YBJ6
C	0	MET	-	expression tag	UNP B5YBJ6
C	1	ASN	ASP	conflict	UNP B5YBJ6
C	3	LYS	THR	conflict	UNP B5YBJ6
C	9	GLU	LYS	conflict	UNP B5YBJ6
C	31	ASN	ASP	conflict	UNP B5YBJ6
C	52	GLY	ARG	conflict	UNP B5YBJ6
C	53	SER	PRO	conflict	UNP B5YBJ6
C	71	ASN	MET	conflict	UNP B5YBJ6
C	81	GLY	ASP	conflict	UNP B5YBJ6
D	-3	GLY	-	expression tag	UNP B5YBJ6
D	-2	SER	-	expression tag	UNP B5YBJ6
D	-1	HIS	-	expression tag	UNP B5YBJ6
D	0	MET	-	expression tag	UNP B5YBJ6
D	1	ASN	ASP	conflict	UNP B5YBJ6
D	3	LYS	THR	conflict	UNP B5YBJ6
D	9	GLU	LYS	conflict	UNP B5YBJ6
D	31	ASN	ASP	conflict	UNP B5YBJ6
D	52	GLY	ARG	conflict	UNP B5YBJ6
D	53	SER	PRO	conflict	UNP B5YBJ6
D	71	ASN	MET	conflict	UNP B5YBJ6
D	81	GLY	ASP	conflict	UNP B5YBJ6
E	-3	GLY	-	expression tag	UNP B5YBJ6
E	-2	SER	-	expression tag	UNP B5YBJ6
E	-1	HIS	-	expression tag	UNP B5YBJ6
E	0	MET	-	expression tag	UNP B5YBJ6
E	1	ASN	ASP	conflict	UNP B5YBJ6
E	3	LYS	THR	conflict	UNP B5YBJ6
E	9	GLU	LYS	conflict	UNP B5YBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	31	ASN	ASP	conflict	UNP B5YBJ6
E	52	GLY	ARG	conflict	UNP B5YBJ6
E	53	SER	PRO	conflict	UNP B5YBJ6
E	71	ASN	MET	conflict	UNP B5YBJ6
E	81	GLY	ASP	conflict	UNP B5YBJ6
F	-3	GLY	-	expression tag	UNP B5YBJ6
F	-2	SER	-	expression tag	UNP B5YBJ6
F	-1	HIS	-	expression tag	UNP B5YBJ6
F	0	MET	-	expression tag	UNP B5YBJ6
F	1	ASN	ASP	conflict	UNP B5YBJ6
F	3	LYS	THR	conflict	UNP B5YBJ6
F	9	GLU	LYS	conflict	UNP B5YBJ6
F	31	ASN	ASP	conflict	UNP B5YBJ6
F	52	GLY	ARG	conflict	UNP B5YBJ6
F	53	SER	PRO	conflict	UNP B5YBJ6
F	71	ASN	MET	conflict	UNP B5YBJ6
F	81	GLY	ASP	conflict	UNP B5YBJ6
G	-3	GLY	-	expression tag	UNP B5YBJ6
G	-2	SER	-	expression tag	UNP B5YBJ6
G	-1	HIS	-	expression tag	UNP B5YBJ6
G	0	MET	-	expression tag	UNP B5YBJ6
G	1	ASN	ASP	conflict	UNP B5YBJ6
G	3	LYS	THR	conflict	UNP B5YBJ6
G	9	GLU	LYS	conflict	UNP B5YBJ6
G	31	ASN	ASP	conflict	UNP B5YBJ6
G	52	GLY	ARG	conflict	UNP B5YBJ6
G	53	SER	PRO	conflict	UNP B5YBJ6
G	71	ASN	MET	conflict	UNP B5YBJ6
G	81	GLY	ASP	conflict	UNP B5YBJ6
H	-3	GLY	-	expression tag	UNP B5YBJ6
H	-2	SER	-	expression tag	UNP B5YBJ6
H	-1	HIS	-	expression tag	UNP B5YBJ6
H	0	MET	-	expression tag	UNP B5YBJ6
H	1	ASN	ASP	conflict	UNP B5YBJ6
H	3	LYS	THR	conflict	UNP B5YBJ6
H	9	GLU	LYS	conflict	UNP B5YBJ6
H	31	ASN	ASP	conflict	UNP B5YBJ6
H	52	GLY	ARG	conflict	UNP B5YBJ6
H	53	SER	PRO	conflict	UNP B5YBJ6
H	71	ASN	MET	conflict	UNP B5YBJ6
H	81	GLY	ASP	conflict	UNP B5YBJ6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total 5	O 5	0	0
2	B	8	Total 8	O 8	0	0
2	C	7	Total 7	O 7	0	0
2	D	9	Total 9	O 9	0	0
2	E	12	Total 12	O 12	0	0
2	F	13	Total 13	O 13	0	0
2	G	8	Total 8	O 8	0	0
2	H	11	Total 11	O 11	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: Cell surface protein

Chain A: 



- Molecule 1: Cell surface protein

Chain B: 



- Molecule 1: Cell surface protein

Chain C: 



- Molecule 1: Cell surface protein

Chain D: 

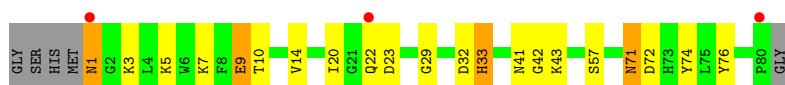


- Molecule 1: Cell surface protein

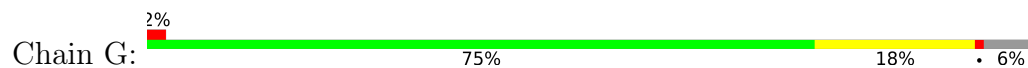
Chain E: 



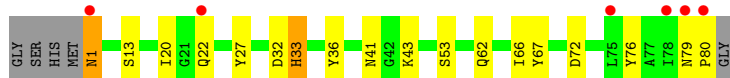
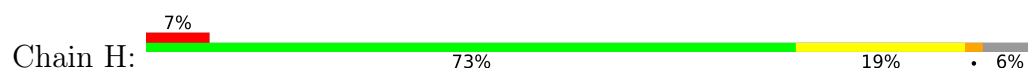
- Molecule 1: Cell surface protein



- Molecule 1: Cell surface protein



- Molecule 1: Cell surface protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.52Å 83.52Å 96.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.35 – 2.35 63.27 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.35-2.35) 100.0 (63.27-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.236 , 0.294 0.248 , 0.296	Depositor DCC
R_{free} test set	1264 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4969	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6366e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.18	1/631 (0.2%)	1.49	3/857 (0.4%)
1	B	1.25	5/631 (0.8%)	1.48	3/857 (0.4%)
1	C	1.10	0/631	1.52	5/857 (0.6%)
1	D	1.16	2/631 (0.3%)	1.50	1/857 (0.1%)
1	E	1.22	1/631 (0.2%)	1.50	2/857 (0.2%)
1	F	1.27	2/631 (0.3%)	1.52	4/857 (0.5%)
1	G	1.23	2/631 (0.3%)	1.49	3/857 (0.4%)
1	H	1.24	3/631 (0.5%)	1.48	1/857 (0.1%)
All	All	1.21	16/5048 (0.3%)	1.50	22/6856 (0.3%)

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	H	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	ASP	CG-OD2	7.24	1.39	1.25
1	D	8	PHE	C-O	-6.01	1.16	1.24
1	B	47	LYS	C-O	-6.01	1.16	1.23
1	G	33	HIS	ND1-CE1	6.01	1.38	1.32
1	B	7	LYS	C-O	-5.95	1.17	1.23
1	F	9	GLU	CD-OE2	5.83	1.36	1.25
1	H	53	SER	C-O	-5.67	1.17	1.23
1	G	33	HIS	CD2-NE2	5.59	1.44	1.37
1	B	63	ASP	CG-OD2	5.52	1.35	1.25
1	H	13	SER	CA-CB	-5.26	1.45	1.53
1	B	63	ASP	CG-OD1	5.25	1.35	1.25
1	H	53	SER	CA-CB	-5.23	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	HIS	CG-CD2	-5.14	1.30	1.35
1	B	15	HIS	CD2-NE2	-5.08	1.32	1.37
1	E	20	ILE	C-O	-5.07	1.18	1.24
1	F	10	THR	C-O	-5.03	1.17	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	22	GLN	CB-CG-CD	7.21	124.86	112.60
1	F	20	ILE	CA-C-O	-6.56	113.65	120.27
1	E	71	ASN	OD1-CG-ND2	6.32	128.92	122.60
1	A	3	LYS	CB-CG-CD	6.21	125.58	111.30
1	A	9	GLU	CB-CG-CD	5.97	122.75	112.60
1	G	71	ASN	CA-CB-CG	5.95	118.55	112.60
1	F	71	ASN	OD1-CG-ND2	5.88	128.48	122.60
1	A	63	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	7	LYS	CB-CA-C	5.85	119.88	109.65
1	B	15	HIS	CA-CB-CG	-5.81	107.99	113.80
1	C	20	ILE	CA-C-O	-5.73	114.43	120.39
1	D	43	LYS	CA-C-O	5.73	127.64	121.16
1	F	42	GLY	O-C-N	-5.57	115.92	122.38
1	G	33	HIS	CA-CB-CG	5.41	119.21	113.80
1	C	45	LYS	CB-CA-C	5.38	120.41	110.56
1	F	22	GLN	N-CA-CB	5.27	118.45	110.28
1	B	63	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	71	ASN	OD1-CG-ND2	5.25	127.85	122.60
1	C	22	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	E	18	PRO	CA-C-O	-5.22	115.30	121.67
1	G	22	GLN	CB-CG-CD	5.18	121.41	112.60
1	C	3	LYS	CB-CG-CD	5.07	122.97	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	66	ILE	Mainchain

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	612	0	578	16	0
1	B	612	0	578	12	0
1	C	612	0	578	16	0
1	D	612	0	578	10	0
1	E	612	0	578	11	0
1	F	612	0	578	14	0
1	G	612	0	578	11	0
1	H	612	0	578	13	0
2	A	5	0	0	0	0
2	B	8	0	0	0	0
2	C	7	0	0	1	0
2	D	9	0	0	0	0
2	E	12	0	0	2	0
2	F	13	0	0	2	0
2	G	8	0	0	2	0
2	H	11	0	0	0	0
All	All	4969	0	4624	83	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 9.

All (83) 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:80:PRO:C	1:H:1:ASN:H2	1.66	1.04
1:F:7:LYS:NZ	2:F:101:HOH:O	1.70	1.01
1:G:3:LYS:HE3	2:G:108:HOH:O	1.70	0.91
1:C:80:PRO:C	1:H:1:ASN:N	2.30	0.88
1:E:7:LYS:NZ	2:E:101:HOH:O	2.07	0.88
1:B:80:PRO:C	1:C:1:ASN:H2	1.83	0.85
1:C:41:ASN:HD21	1:C:43:LYS:HD2	1.46	0.81
1:B:80:PRO:C	1:C:1:ASN:N	2.43	0.77
1:C:80:PRO:O	1:H:1:ASN:N	2.15	0.77
1:F:41:ASN:HD21	1:F:43:LYS:HD2	1.50	0.76
1:C:45:LYS:HE2	2:C:104:HOH:O	1.85	0.75
1:A:41:ASN:HD21	1:A:43:LYS:HD2	1.51	0.75
1:B:41:ASN:HD21	1:B:43:LYS:HD2	1.55	0.72
1:G:41:ASN:HD21	1:G:43:LYS:HD2	1.56	0.70
1:G:3:LYS:CE	2:G:108:HOH:O	2.37	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:C	1:D:1:ASN:H2	2.04	0.66
1:A:74:TYR:CE2	1:D:9:GLU:HB2	2.31	0.65
1:A:80:PRO:C	1:D:1:ASN:N	2.56	0.63
1:F:41:ASN:ND2	1:F:43:LYS:HD2	2.13	0.63
1:E:1:ASN:H2	1:H:80:PRO:C	2.07	0.62
1:B:41:ASN:ND2	1:B:43:LYS:HD2	2.16	0.60
1:A:65:THR:HG21	1:D:5:LYS:HE2	1.84	0.59
1:H:41:ASN:HD21	1:H:43:LYS:HD2	1.68	0.58
1:A:41:ASN:ND2	1:A:43:LYS:HD2	2.20	0.56
1:H:41:ASN:ND2	1:H:43:LYS:HD2	2.22	0.55
1:B:74:TYR:CD2	1:C:7:LYS:HG3	2.43	0.54
1:G:41:ASN:ND2	1:G:43:LYS:HD2	2.22	0.53
1:A:7:LYS:HG3	1:F:74:TYR:CD2	2.43	0.53
1:E:1:ASN:N	1:H:80:PRO:C	2.66	0.53
1:C:41:ASN:ND2	1:C:43:LYS:HD2	2.22	0.53
1:E:43:LYS:NZ	2:E:102:HOH:O	2.42	0.52
1:D:27:TYR:HA	1:D:36:TYR:O	2.11	0.51
1:F:9:GLU:HB2	1:G:74:TYR:CE2	2.45	0.51
1:B:74:TYR:CE2	1:C:9:GLU:HB2	2.45	0.51
1:D:41:ASN:HD21	1:D:43:LYS:HD2	1.76	0.51
1:D:72:ASP:OD2	1:D:76:TYR:OH	2.28	0.51
1:B:7:LYS:HG3	1:E:74:TYR:CD2	2.47	0.50
1:A:76:TYR:CE2	1:D:7:LYS:HE3	2.46	0.50
1:H:72:ASP:OD2	1:H:76:TYR:OH	2.27	0.49
1:B:72:ASP:OD2	1:B:76:TYR:OH	2.29	0.49
1:F:72:ASP:OD2	1:F:76:TYR:OH	2.29	0.49
1:A:34:TYR:CE1	1:A:49:GLU:HB2	2.49	0.48
1:F:1:ASN:OD1	1:F:3:LYS:HD2	2.14	0.48
1:G:72:ASP:OD2	1:G:76:TYR:OH	2.29	0.48
1:C:72:ASP:OD2	1:C:76:TYR:OH	2.28	0.48
1:D:34:TYR:CE2	1:D:49:GLU:HB2	2.49	0.47
1:D:41:ASN:ND2	1:D:43:LYS:HD2	2.29	0.47
1:A:72:ASP:OD2	1:A:76:TYR:OH	2.29	0.47
1:G:34:TYR:CE2	1:G:49:GLU:HB2	2.52	0.45
1:E:5:LYS:HD3	1:H:79:ASN:OD1	2.18	0.44
1:A:32:ASP:O	1:A:33:HIS:HB2	2.18	0.44
1:E:34:TYR:CE2	1:E:49:GLU:HB2	2.52	0.44
1:F:32:ASP:O	1:F:33:HIS:HB2	2.17	0.44
1:H:32:ASP:O	1:H:33:HIS:HB2	2.18	0.44
1:A:17:SER:HG	1:F:57:SER:H	1.61	0.43
1:F:32:ASP:OD1	1:F:32:ASP:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ASP:OD2	1:E:76:TYR:OH	2.29	0.43
1:C:27:TYR:HA	1:C:36:TYR:O	2.19	0.43
1:A:27:TYR:HA	1:A:36:TYR:O	2.18	0.43
1:E:32:ASP:O	1:E:33:HIS:HB2	2.19	0.43
1:G:72:ASP:OD1	1:G:72:ASP:C	2.62	0.43
1:A:32:ASP:C	1:A:32:ASP:OD1	2.61	0.43
1:H:27:TYR:HA	1:H:36:TYR:O	2.19	0.43
1:F:14:VAL:HG13	1:F:29:GLY:O	2.19	0.42
1:B:32:ASP:O	1:B:33:HIS:HB2	2.19	0.42
1:F:23:ASP:N	2:F:103:HOH:O	2.32	0.42
1:G:32:ASP:OD1	1:G:32:ASP:C	2.62	0.42
1:C:32:ASP:OD1	1:C:32:ASP:C	2.61	0.42
1:A:17:SER:OG	1:F:57:SER:N	2.35	0.42
1:C:32:ASP:O	1:C:33:HIS:HB2	2.20	0.42
1:H:67:TYR:HA	1:H:76:TYR:O	2.20	0.42
1:E:32:ASP:C	1:E:32:ASP:OD1	2.62	0.41
1:G:32:ASP:O	1:G:33:HIS:HB2	2.20	0.41
1:A:67:TYR:HA	1:A:76:TYR:O	2.20	0.41
1:B:32:ASP:C	1:B:32:ASP:OD1	2.63	0.41
1:E:72:ASP:OD1	1:E:72:ASP:C	2.64	0.41
1:H:32:ASP:OD1	1:H:32:ASP:C	2.63	0.41
1:B:27:TYR:HA	1:B:36:TYR:O	2.21	0.41
1:C:34:TYR:CE1	1:C:49:GLU:HB2	2.56	0.41
1:G:27:TYR:HA	1:G:36:TYR:O	2.21	0.41
1:B:34:TYR:CE2	1:B:49:GLU:HB2	2.55	0.40
1:F:32:ASP:O	1:F:33:HIS:CB	2.69	0.40
1:C:67:TYR:HA	1:C:76:TYR:O	2.22	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	78/85 (92%)	73 (94%)	3 (4%)	2 (3%)	4	2
1	B	78/85 (92%)	74 (95%)	3 (4%)	1 (1%)	9	8
1	C	78/85 (92%)	75 (96%)	1 (1%)	2 (3%)	4	2
1	D	78/85 (92%)	74 (95%)	3 (4%)	1 (1%)	9	8
1	E	78/85 (92%)	73 (94%)	4 (5%)	1 (1%)	9	8
1	F	78/85 (92%)	74 (95%)	3 (4%)	1 (1%)	9	8
1	G	78/85 (92%)	75 (96%)	2 (3%)	1 (1%)	9	8
1	H	78/85 (92%)	74 (95%)	3 (4%)	1 (1%)	9	8
All	All	624/680 (92%)	592 (95%)	22 (4%)	10 (2%)	7	6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	33	HIS
1	F	33	HIS
1	G	33	HIS
1	A	33	HIS
1	B	33	HIS
1	C	33	HIS
1	E	33	HIS
1	H	33	HIS
1	A	73	HIS
1	C	73	HIS

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	64/67 (96%)	63 (98%)	1 (2%)	55	70
1	B	64/67 (96%)	63 (98%)	1 (2%)	55	70
1	C	64/67 (96%)	62 (97%)	2 (3%)	35	47
1	D	64/67 (96%)	63 (98%)	1 (2%)	55	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	64/67 (96%)	63 (98%)	1 (2%)	55	70
1	F	64/67 (96%)	61 (95%)	3 (5%)	23	30
1	G	64/67 (96%)	62 (97%)	2 (3%)	35	47
1	H	64/67 (96%)	61 (95%)	3 (5%)	23	30
All	All	512/536 (96%)	498 (97%)	14 (3%)	39	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	B	5	LYS
1	C	1	ASN
1	C	3	LYS
1	D	3	LYS
1	E	1	ASN
1	F	1	ASN
1	F	5	LYS
1	F	71	ASN
1	G	1	ASN
1	G	20	ILE
1	H	1	ASN
1	H	20	ILE
1	H	62	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	41	ASN
1	A	62	GLN
1	B	33	HIS
1	B	41	ASN
1	B	62	GLN
1	B	79	ASN
1	C	39	ASN
1	C	41	ASN
1	D	41	ASN
1	D	73	HIS
1	E	33	HIS
1	E	62	GLN

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Mol	Chain	Res	Type
1	E	73	HIS
1	F	33	HIS
1	F	41	ASN
1	F	62	GLN
1	F	73	HIS
1	G	41	ASN
1	G	62	GLN
1	G	73	HIS
1	H	39	ASN
1	H	41	ASN
1	H	73	HIS

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](#)

There are no ligands in this entry.

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	80/85 (94%)	0.14	0 100 100	27, 40, 67, 86	0
1	B	80/85 (94%)	0.20	2 (2%) 58 64	27, 40, 69, 80	0
1	C	80/85 (94%)	0.34	3 (3%) 44 50	29, 42, 64, 92	0
1	D	80/85 (94%)	0.37	2 (2%) 58 64	28, 42, 63, 88	0
1	E	80/85 (94%)	0.32	2 (2%) 58 64	25, 42, 69, 102	0
1	F	80/85 (94%)	0.44	3 (3%) 44 50	25, 42, 77, 93	0
1	G	80/85 (94%)	0.46	2 (2%) 58 64	27, 42, 79, 101	0
1	H	80/85 (94%)	0.55	6 (7%) 20 23	27, 45, 78, 98	0
All	All	640/680 (94%)	0.35	20 (3%) 51 58	25, 42, 75, 102	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	80	PRO	3.9
1	G	22	GLN	3.6
1	H	1	ASN	3.2
1	G	1	ASN	3.2
1	D	1	ASN	3.0
1	F	80	PRO	3.0
1	C	1	ASN	2.9
1	E	1	ASN	2.8
1	H	75	LEU	2.4
1	H	78	ILE	2.3
1	F	1	ASN	2.3
1	B	22	GLN	2.3
1	H	22	GLN	2.2
1	C	3	LYS	2.1
1	D	41	ASN	2.1
1	E	80	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	22	GLN	2.0
1	H	79	ASN	2.0
1	B	55	HIS	2.0
1	C	60	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.