



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:40 AM UTC

PDB ID : 8QFB / pdb_00008qfb
Title : Crystal structure of human MPP8 C-terminal region (residues 565-860)
Authors : Prigozhin, D.M.; Modis, Y.
Deposited on : 2023-09-04
Resolution : 3.04 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

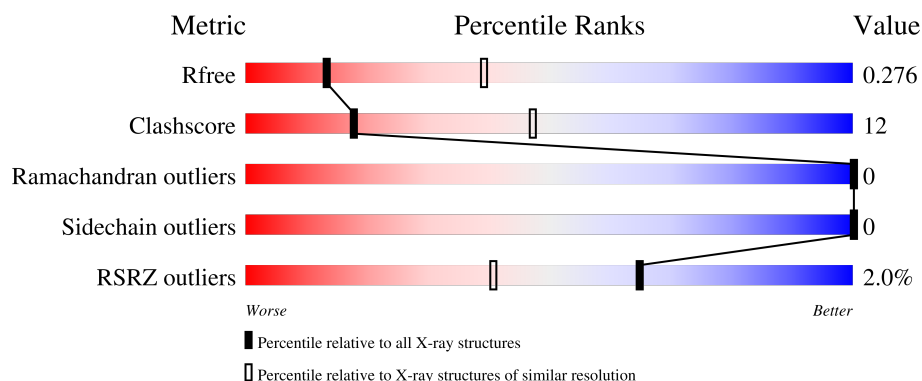
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

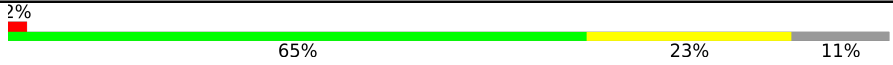
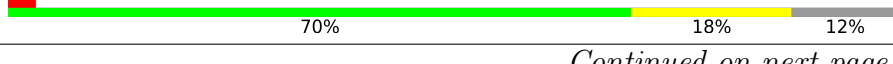
The reported resolution of this entry is 3.04 Å.

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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	336	
1	B	336	
1	C	336	
1	D	336	
1	E	336	

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Mol	Chain	Length	Quality of chain
1	F	336	% 65% 23% 12%
1	G	336	2% 69% 18% 12%
1	H	336	% 67% 21% 12%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 35246 atoms, of which 17506 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 M-phase phosphoprotein 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	294	Total	C	H	N	O	S	0	0	0
			4370	1399	2170	379	412	10			
1	A	298	Total	C	H	N	O	S	0	0	0
			4456	1427	2217	384	418	10			
1	C	294	Total	C	H	N	O	S	0	0	0
			4323	1390	2139	375	409	10			
1	D	298	Total	C	H	N	O	S	0	0	0
			4523	1440	2260	390	423	10			
1	E	296	Total	C	H	N	O	S	0	0	0
			4387	1407	2179	379	412	10			
1	F	294	Total	C	H	N	O	S	0	0	0
			4382	1405	2169	380	418	10			
1	G	295	Total	C	H	N	O	S	0	0	0
			4423	1411	2202	386	414	10			
1	H	296	Total	C	H	N	O	S	0	0	0
			4382	1407	2170	380	415	10			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	525	MET	-	initiating methionine	UNP Q99549
B	526	GLY	-	expression tag	UNP Q99549
B	527	SER	-	expression tag	UNP Q99549
B	528	SER	-	expression tag	UNP Q99549
B	529	HIS	-	expression tag	UNP Q99549
B	530	HIS	-	expression tag	UNP Q99549
B	531	HIS	-	expression tag	UNP Q99549
B	532	HIS	-	expression tag	UNP Q99549
B	533	HIS	-	expression tag	UNP Q99549
B	534	HIS	-	expression tag	UNP Q99549
B	535	SER	-	expression tag	UNP Q99549
B	536	SER	-	expression tag	UNP Q99549
B	537	GLY	-	expression tag	UNP Q99549

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Chain	Residue	Modelled	Actual	Comment	Reference
B	538	LEU	-	expression tag	UNP Q99549
B	539	VAL	-	expression tag	UNP Q99549
B	540	PRO	-	expression tag	UNP Q99549
B	541	ARG	-	expression tag	UNP Q99549
B	542	GLY	-	expression tag	UNP Q99549
B	543	SER	-	expression tag	UNP Q99549
B	544	HIS	-	expression tag	UNP Q99549
B	545	MET	-	expression tag	UNP Q99549
A	525	MET	-	initiating methionine	UNP Q99549
A	526	GLY	-	expression tag	UNP Q99549
A	527	SER	-	expression tag	UNP Q99549
A	528	SER	-	expression tag	UNP Q99549
A	529	HIS	-	expression tag	UNP Q99549
A	530	HIS	-	expression tag	UNP Q99549
A	531	HIS	-	expression tag	UNP Q99549
A	532	HIS	-	expression tag	UNP Q99549
A	533	HIS	-	expression tag	UNP Q99549
A	534	HIS	-	expression tag	UNP Q99549
A	535	SER	-	expression tag	UNP Q99549
A	536	SER	-	expression tag	UNP Q99549
A	537	GLY	-	expression tag	UNP Q99549
A	538	LEU	-	expression tag	UNP Q99549
A	539	VAL	-	expression tag	UNP Q99549
A	540	PRO	-	expression tag	UNP Q99549
A	541	ARG	-	expression tag	UNP Q99549
A	542	GLY	-	expression tag	UNP Q99549
A	543	SER	-	expression tag	UNP Q99549
A	544	HIS	-	expression tag	UNP Q99549
A	545	MET	-	expression tag	UNP Q99549
C	525	MET	-	initiating methionine	UNP Q99549
C	526	GLY	-	expression tag	UNP Q99549
C	527	SER	-	expression tag	UNP Q99549
C	528	SER	-	expression tag	UNP Q99549
C	529	HIS	-	expression tag	UNP Q99549
C	530	HIS	-	expression tag	UNP Q99549
C	531	HIS	-	expression tag	UNP Q99549
C	532	HIS	-	expression tag	UNP Q99549
C	533	HIS	-	expression tag	UNP Q99549
C	534	HIS	-	expression tag	UNP Q99549
C	535	SER	-	expression tag	UNP Q99549
C	536	SER	-	expression tag	UNP Q99549
C	537	GLY	-	expression tag	UNP Q99549

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Chain	Residue	Modelled	Actual	Comment	Reference
C	538	LEU	-	expression tag	UNP Q99549
C	539	VAL	-	expression tag	UNP Q99549
C	540	PRO	-	expression tag	UNP Q99549
C	541	ARG	-	expression tag	UNP Q99549
C	542	GLY	-	expression tag	UNP Q99549
C	543	SER	-	expression tag	UNP Q99549
C	544	HIS	-	expression tag	UNP Q99549
C	545	MET	-	expression tag	UNP Q99549
D	525	MET	-	initiating methionine	UNP Q99549
D	526	GLY	-	expression tag	UNP Q99549
D	527	SER	-	expression tag	UNP Q99549
D	528	SER	-	expression tag	UNP Q99549
D	529	HIS	-	expression tag	UNP Q99549
D	530	HIS	-	expression tag	UNP Q99549
D	531	HIS	-	expression tag	UNP Q99549
D	532	HIS	-	expression tag	UNP Q99549
D	533	HIS	-	expression tag	UNP Q99549
D	534	HIS	-	expression tag	UNP Q99549
D	535	SER	-	expression tag	UNP Q99549
D	536	SER	-	expression tag	UNP Q99549
D	537	GLY	-	expression tag	UNP Q99549
D	538	LEU	-	expression tag	UNP Q99549
D	539	VAL	-	expression tag	UNP Q99549
D	540	PRO	-	expression tag	UNP Q99549
D	541	ARG	-	expression tag	UNP Q99549
D	542	GLY	-	expression tag	UNP Q99549
D	543	SER	-	expression tag	UNP Q99549
D	544	HIS	-	expression tag	UNP Q99549
D	545	MET	-	expression tag	UNP Q99549
E	525	MET	-	initiating methionine	UNP Q99549
E	526	GLY	-	expression tag	UNP Q99549
E	527	SER	-	expression tag	UNP Q99549
E	528	SER	-	expression tag	UNP Q99549
E	529	HIS	-	expression tag	UNP Q99549
E	530	HIS	-	expression tag	UNP Q99549
E	531	HIS	-	expression tag	UNP Q99549
E	532	HIS	-	expression tag	UNP Q99549
E	533	HIS	-	expression tag	UNP Q99549
E	534	HIS	-	expression tag	UNP Q99549
E	535	SER	-	expression tag	UNP Q99549
E	536	SER	-	expression tag	UNP Q99549
E	537	GLY	-	expression tag	UNP Q99549

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Chain	Residue	Modelled	Actual	Comment	Reference
E	538	LEU	-	expression tag	UNP Q99549
E	539	VAL	-	expression tag	UNP Q99549
E	540	PRO	-	expression tag	UNP Q99549
E	541	ARG	-	expression tag	UNP Q99549
E	542	GLY	-	expression tag	UNP Q99549
E	543	SER	-	expression tag	UNP Q99549
E	544	HIS	-	expression tag	UNP Q99549
E	545	MET	-	expression tag	UNP Q99549
F	525	MET	-	initiating methionine	UNP Q99549
F	526	GLY	-	expression tag	UNP Q99549
F	527	SER	-	expression tag	UNP Q99549
F	528	SER	-	expression tag	UNP Q99549
F	529	HIS	-	expression tag	UNP Q99549
F	530	HIS	-	expression tag	UNP Q99549
F	531	HIS	-	expression tag	UNP Q99549
F	532	HIS	-	expression tag	UNP Q99549
F	533	HIS	-	expression tag	UNP Q99549
F	534	HIS	-	expression tag	UNP Q99549
F	535	SER	-	expression tag	UNP Q99549
F	536	SER	-	expression tag	UNP Q99549
F	537	GLY	-	expression tag	UNP Q99549
F	538	LEU	-	expression tag	UNP Q99549
F	539	VAL	-	expression tag	UNP Q99549
F	540	PRO	-	expression tag	UNP Q99549
F	541	ARG	-	expression tag	UNP Q99549
F	542	GLY	-	expression tag	UNP Q99549
F	543	SER	-	expression tag	UNP Q99549
F	544	HIS	-	expression tag	UNP Q99549
F	545	MET	-	expression tag	UNP Q99549
G	525	MET	-	initiating methionine	UNP Q99549
G	526	GLY	-	expression tag	UNP Q99549
G	527	SER	-	expression tag	UNP Q99549
G	528	SER	-	expression tag	UNP Q99549
G	529	HIS	-	expression tag	UNP Q99549
G	530	HIS	-	expression tag	UNP Q99549
G	531	HIS	-	expression tag	UNP Q99549
G	532	HIS	-	expression tag	UNP Q99549
G	533	HIS	-	expression tag	UNP Q99549
G	534	HIS	-	expression tag	UNP Q99549
G	535	SER	-	expression tag	UNP Q99549
G	536	SER	-	expression tag	UNP Q99549
G	537	GLY	-	expression tag	UNP Q99549

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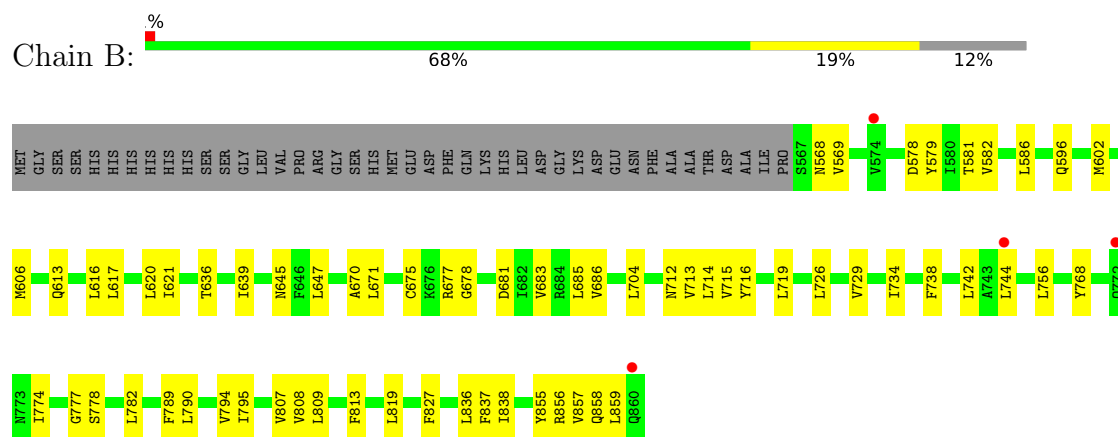
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Chain	Residue	Modelled	Actual	Comment	Reference
G	538	LEU	-	expression tag	UNP Q99549
G	539	VAL	-	expression tag	UNP Q99549
G	540	PRO	-	expression tag	UNP Q99549
G	541	ARG	-	expression tag	UNP Q99549
G	542	GLY	-	expression tag	UNP Q99549
G	543	SER	-	expression tag	UNP Q99549
G	544	HIS	-	expression tag	UNP Q99549
G	545	MET	-	expression tag	UNP Q99549
H	525	MET	-	initiating methionine	UNP Q99549
H	526	GLY	-	expression tag	UNP Q99549
H	527	SER	-	expression tag	UNP Q99549
H	528	SER	-	expression tag	UNP Q99549
H	529	HIS	-	expression tag	UNP Q99549
H	530	HIS	-	expression tag	UNP Q99549
H	531	HIS	-	expression tag	UNP Q99549
H	532	HIS	-	expression tag	UNP Q99549
H	533	HIS	-	expression tag	UNP Q99549
H	534	HIS	-	expression tag	UNP Q99549
H	535	SER	-	expression tag	UNP Q99549
H	536	SER	-	expression tag	UNP Q99549
H	537	GLY	-	expression tag	UNP Q99549
H	538	LEU	-	expression tag	UNP Q99549
H	539	VAL	-	expression tag	UNP Q99549
H	540	PRO	-	expression tag	UNP Q99549
H	541	ARG	-	expression tag	UNP Q99549
H	542	GLY	-	expression tag	UNP Q99549
H	543	SER	-	expression tag	UNP Q99549
H	544	HIS	-	expression tag	UNP Q99549
H	545	MET	-	expression tag	UNP Q99549

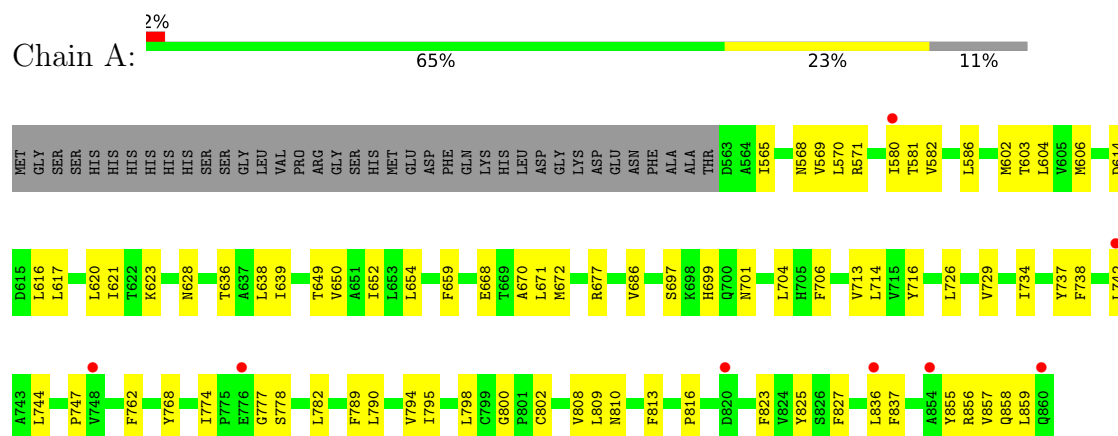
3 Residue-property plots [i](#)

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.

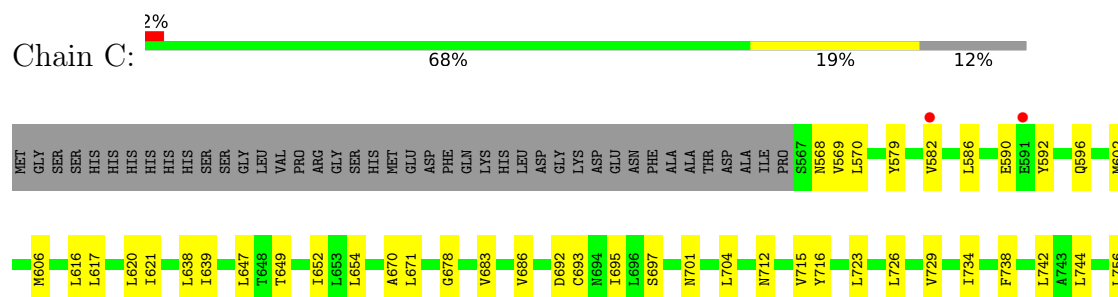
- Molecule 1: M-phase phosphoprotein 8



- Molecule 1: M-phase phosphoprotein 8



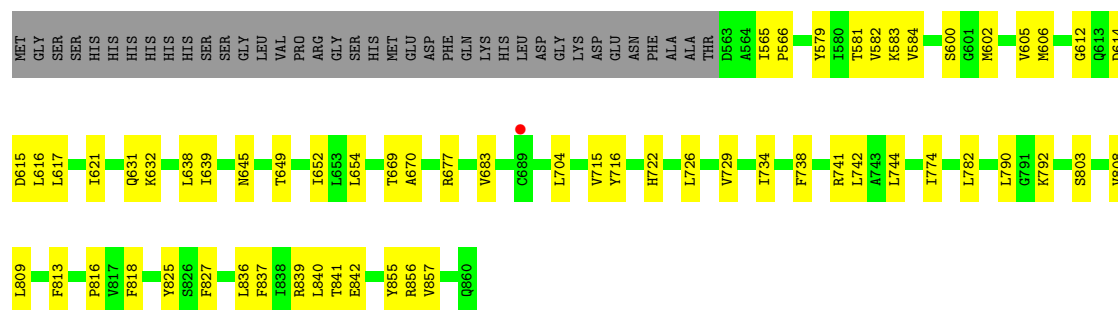
- Molecule 1: M-phase phosphoprotein 8





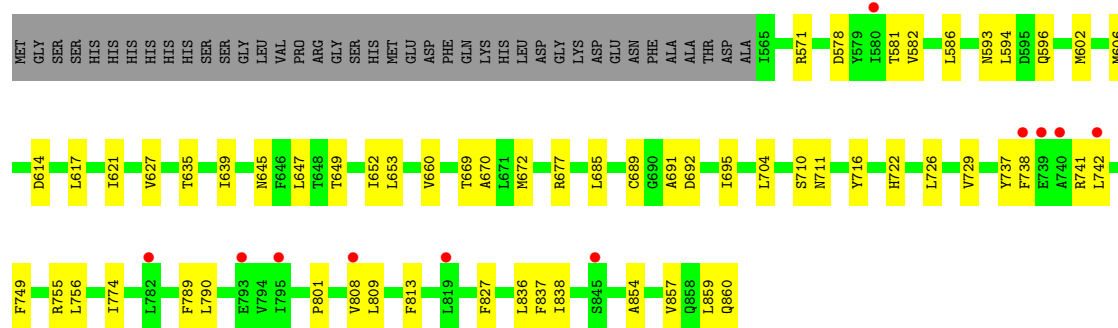
• Molecule 1: M-phase phosphoprotein 8

Chain D: 71% 18% 11%



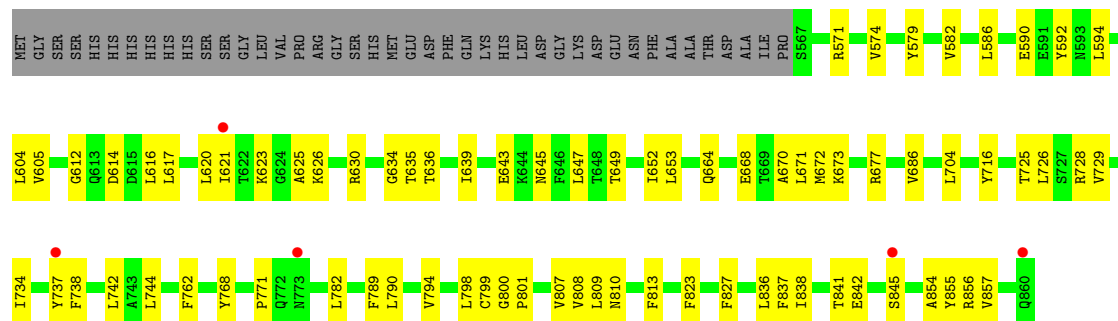
• Molecule 1: M-phase phosphoprotein 8

Chain E: 3% 70% 18% 12%



• Molecule 1: M-phase phosphoprotein 8

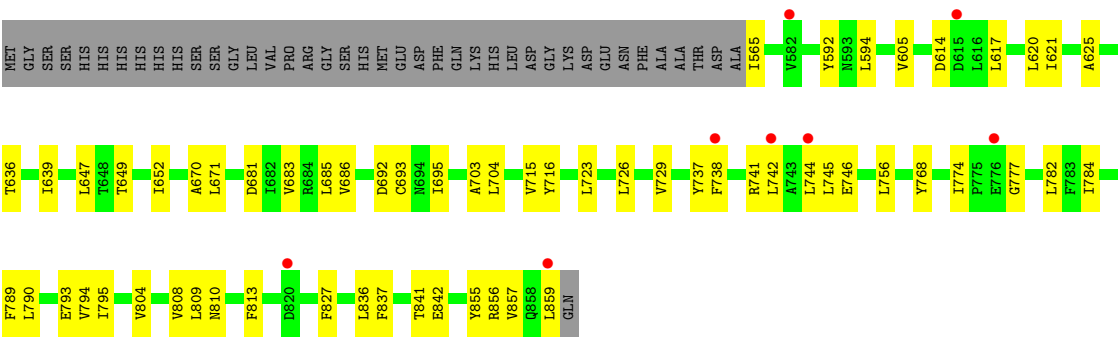
Chain F: % 65% 23% 12%



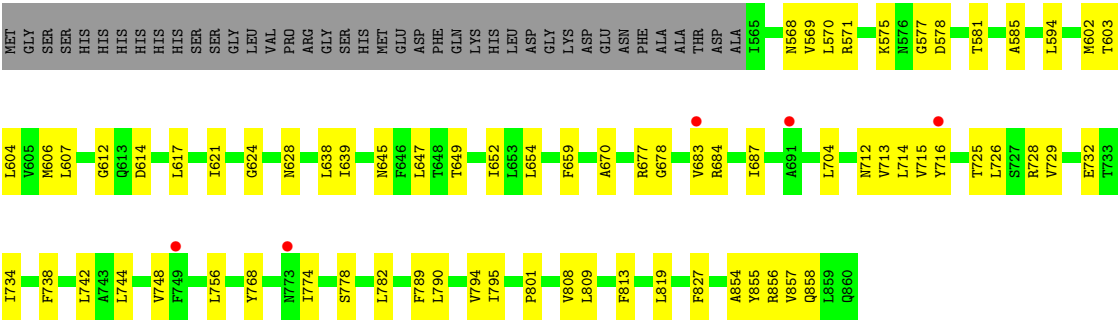
• Molecule 1: M-phase phosphoprotein 8

Chain G: 2% 69% 18% 12%





● Molecule 1: M-phase phosphoprotein 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.56Å 179.53Å 228.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.54 – 3.04 93.54 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.8 (93.54-3.04) 98.8 (93.54-3.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.256 , 0.295 (Not available) , 0.276	Depositor DCC
R_{free} test set	4361 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	100.7	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35246	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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](#)

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	0.28	0/2279	0.53	0/3101
1	B	0.23	0/2238	0.46	0/3044
1	C	0.22	0/2222	0.47	0/3026
1	D	0.29	0/2303	0.54	0/3129
1	E	0.23	0/2246	0.48	0/3056
1	F	0.24	0/2252	0.50	0/3065
1	G	0.22	0/2260	0.48	0/3073
1	H	0.22	0/2251	0.48	0/3065
All	All	0.24	0/18051	0.49	0/24559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2239	2217	2217	67	0
1	B	2200	2170	2170	46	0
1	C	2184	2139	2139	53	0
1	D	2263	2260	2260	56	0
1	E	2208	2179	2179	48	0
1	F	2213	2169	2169	70	2
1	G	2221	2202	2202	58	0
1	H	2212	2170	2170	57	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17740	17506	17506	434	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 12.

All (434) 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:D:645:ASN:OD1	1:D:677:ARG:NE	2.01	0.91
1:H:778:SER:OG	1:H:858:GLN:OE1	1.94	0.84
1:D:617:LEU:HD23	1:D:652:ILE:HD11	1.59	0.83
1:C:738:PHE:CD2	1:C:742:LEU:HD22	2.14	0.82
1:G:745:LEU:HD23	1:G:746:GLU:HG2	1.65	0.79
1:B:645:ASN:OD1	1:B:677:ARG:NE	2.17	0.78
1:C:697:SER:OG	1:C:701:ASN:OD1	2.02	0.77
1:A:704:LEU:HD11	1:A:716:TYR:HD1	1.50	0.76
1:A:704:LEU:HD11	1:A:716:TYR:CD1	2.21	0.76
1:G:795:ILE:HD11	1:H:795:ILE:HD11	1.67	0.75
1:G:795:ILE:CD1	1:H:795:ILE:HD11	2.17	0.75
1:E:790:LEU:CB	1:F:790:LEU:HD13	2.16	0.75
1:F:768:TYR:OH	1:F:856:ARG:NH2	2.19	0.74
1:A:617:LEU:HD13	1:A:652:ILE:HD11	1.70	0.74
1:F:571:ARG:HD3	1:F:604:LEU:HD21	1.68	0.73
1:D:566:PRO:HD3	1:F:837:PHE:CE2	2.23	0.73
1:C:596:GLN:N	1:C:596:GLN:OE1	2.22	0.73
1:H:617:LEU:HD13	1:H:652:ILE:HD11	1.70	0.73
1:H:819:LEU:HD13	1:H:819:LEU:O	1.87	0.73
1:A:697:SER:OG	1:A:701:ASN:OD1	2.06	0.73
1:F:645:ASN:OD1	1:F:677:ARG:NH2	2.21	0.73
1:H:768:TYR:OH	1:H:856:ARG:NH2	2.22	0.71
1:B:671:LEU:HD23	1:B:686:VAL:CG2	2.21	0.71
1:B:790:LEU:HB3	1:A:790:LEU:HD22	1.73	0.71
1:F:614:ASP:OD1	1:F:649:THR:HG22	1.89	0.71
1:D:614:ASP:OD1	1:D:649:THR:HG22	1.91	0.71
1:A:768:TYR:OH	1:A:856:ARG:NH2	2.24	0.70
1:B:819:LEU:HD13	1:B:819:LEU:O	1.91	0.70
1:B:795:ILE:HD11	1:A:795:ILE:CD1	2.21	0.69
1:G:744:LEU:HD22	1:G:855:TYR:HD2	1.54	0.69
1:C:738:PHE:HD2	1:C:742:LEU:HD22	1.57	0.69
1:D:734:ILE:HD12	1:D:744:LEU:HD11	1.74	0.69
1:D:602:MET:HE2	1:D:631:GLN:HE22	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:742:LEU:HD21	1:E:857:VAL:HG21	1.74	0.68
1:B:582:VAL:O	1:B:586:LEU:HD13	1.92	0.68
1:B:768:TYR:OH	1:B:856:ARG:NH2	2.26	0.67
1:G:768:TYR:OH	1:G:856:ARG:NH2	2.27	0.67
1:B:596:GLN:N	1:B:596:GLN:OE1	2.28	0.67
1:H:602:MET:SD	1:H:602:MET:N	2.68	0.67
1:H:617:LEU:CD1	1:H:652:ILE:HD11	2.24	0.67
1:F:742:LEU:HD21	1:F:857:VAL:HG21	1.75	0.66
1:A:614:ASP:OD1	1:A:649:THR:HG22	1.94	0.66
1:C:671:LEU:HD23	1:C:686:VAL:CG2	2.25	0.66
1:G:793:GLU:OE1	1:H:790:LEU:HD21	1.96	0.66
1:E:578:ASP:OD2	1:E:581:THR:OG1	2.12	0.66
1:B:808:VAL:HG22	1:B:813:PHE:CD1	2.31	0.65
1:B:795:ILE:HD11	1:A:795:ILE:HD12	1.78	0.65
1:C:639:ILE:HD13	1:C:670:ALA:HB2	1.78	0.65
1:A:639:ILE:HD13	1:A:670:ALA:HB2	1.78	0.65
1:E:639:ILE:HD13	1:E:670:ALA:HB2	1.79	0.65
1:G:565:ILE:O	1:G:592:TYR:OH	2.15	0.65
1:A:617:LEU:CD1	1:A:652:ILE:HD11	2.26	0.64
1:A:742:LEU:HD21	1:A:857:VAL:HG21	1.79	0.64
1:C:819:LEU:HD13	1:C:819:LEU:O	1.98	0.64
1:A:734:ILE:HG21	1:A:744:LEU:HD11	1.80	0.64
1:G:639:ILE:HD13	1:G:670:ALA:HB2	1.79	0.64
1:G:745:LEU:CD2	1:G:746:GLU:HG2	2.28	0.64
1:H:570:LEU:HD21	1:H:585:ALA:HB1	1.80	0.64
1:C:693:CYS:HB2	1:C:723:LEU:HD21	1.79	0.63
1:H:614:ASP:OD1	1:H:649:THR:HG22	1.99	0.63
1:A:734:ILE:HG21	1:A:744:LEU:CD1	2.28	0.63
1:E:738:PHE:HD2	1:E:742:LEU:HD22	1.64	0.63
1:F:586:LEU:HD22	1:F:623:LYS:HD2	1.80	0.63
1:F:594:LEU:HD23	1:F:623:LYS:HD3	1.79	0.63
1:C:569:VAL:HG23	1:C:570:LEU:HD12	1.80	0.63
1:B:671:LEU:HD23	1:B:686:VAL:HG21	1.82	0.62
1:D:639:ILE:HD13	1:D:670:ALA:HB2	1.82	0.62
1:B:681:ASP:O	1:B:685:LEU:HD23	2.00	0.62
1:A:671:LEU:HD23	1:A:686:VAL:CG2	2.29	0.62
1:E:669:THR:HG22	1:E:670:ALA:N	2.14	0.61
1:E:692:ASP:OD2	1:E:695:ILE:HD11	2.00	0.61
1:B:639:ILE:HD13	1:B:670:ALA:HB2	1.82	0.61
1:A:778:SER:OG	1:A:858:GLN:OE1	2.18	0.61
1:C:790:LEU:HD13	1:D:790:LEU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:836:LEU:HD23	1:F:837:PHE:N	2.15	0.61
1:F:639:ILE:HD13	1:F:670:ALA:HB2	1.83	0.61
1:D:669:THR:HG22	1:D:670:ALA:N	2.16	0.61
1:F:594:LEU:HD22	1:F:625:ALA:HB2	1.82	0.61
1:A:565:ILE:HD11	1:A:569:VAL:HG11	1.83	0.60
1:G:742:LEU:HD11	1:G:857:VAL:HG21	1.83	0.60
1:H:603:THR:H	1:H:606:MET:HE3	1.66	0.60
1:G:790:LEU:HD22	1:H:790:LEU:HB2	1.84	0.60
1:H:704:LEU:HD11	1:H:716:TYR:CE1	2.37	0.60
1:D:742:LEU:HD11	1:D:857:VAL:HG11	1.84	0.60
1:F:734:ILE:HD13	1:F:744:LEU:HD11	1.83	0.59
1:H:569:VAL:HG23	1:H:570:LEU:HD12	1.84	0.59
1:G:742:LEU:HD21	1:G:857:VAL:HG21	1.85	0.59
1:B:616:LEU:O	1:B:620:LEU:HD13	2.03	0.59
1:A:809:LEU:HD12	1:A:827:PHE:CE1	2.37	0.59
1:C:802:CYS:HB2	1:C:823:PHE:HE1	1.68	0.59
1:D:582:VAL:HG21	1:D:616:LEU:HD22	1.85	0.59
1:A:582:VAL:O	1:A:586:LEU:HD13	2.02	0.59
1:C:809:LEU:HD12	1:C:827:PHE:CE1	2.37	0.59
1:G:777:GLY:O	1:G:859:LEU:HD13	2.03	0.59
1:D:581:THR:O	1:D:584:VAL:HG12	2.03	0.58
1:C:774:ILE:HD12	1:C:774:ILE:O	2.03	0.58
1:D:809:LEU:HD12	1:D:827:PHE:CE1	2.37	0.58
1:F:582:VAL:O	1:F:586:LEU:HG	2.04	0.58
1:F:789:PHE:CD2	1:F:794:VAL:HG12	2.38	0.58
1:A:603:THR:HG22	1:A:606:MET:HE3	1.85	0.58
1:B:713:VAL:HG13	1:B:714:LEU:HD22	1.85	0.58
1:D:704:LEU:HD11	1:D:716:TYR:CE1	2.38	0.58
1:E:645:ASN:OD1	1:E:677:ARG:NH2	2.37	0.58
1:B:742:LEU:HD21	1:B:857:VAL:HG21	1.86	0.57
1:E:808:VAL:HG22	1:E:813:PHE:CD1	2.39	0.57
1:H:742:LEU:HD21	1:H:857:VAL:HG21	1.87	0.57
1:C:798:LEU:HA	1:C:823:PHE:HD2	1.70	0.57
1:B:809:LEU:HD12	1:B:827:PHE:CE1	2.40	0.57
1:B:789:PHE:CD2	1:B:794:VAL:HG12	2.39	0.57
1:C:582:VAL:O	1:C:586:LEU:HD13	2.03	0.57
1:H:568:ASN:OD1	1:H:569:VAL:N	2.38	0.57
1:E:614:ASP:OD1	1:E:649:THR:HG22	2.05	0.57
1:E:859:LEU:O	1:E:860:GLN:HG3	2.04	0.56
1:H:639:ILE:HD13	1:H:670:ALA:HB2	1.86	0.56
1:A:789:PHE:CD1	1:A:794:VAL:HG12	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:LEU:O	1:B:729:VAL:HG12	2.05	0.56
1:A:617:LEU:O	1:A:621:ILE:HG12	2.06	0.56
1:A:774:ILE:HD12	1:A:774:ILE:O	2.06	0.56
1:F:579:TYR:O	1:F:582:VAL:HG22	2.05	0.56
1:H:809:LEU:HD12	1:H:827:PHE:CE1	2.40	0.56
1:B:704:LEU:HD11	1:B:716:TYR:CE1	2.40	0.56
1:B:778:SER:OG	1:B:858:GLN:OE1	2.24	0.55
1:A:628:ASN:HD21	1:A:659:PHE:H	1.54	0.55
1:E:738:PHE:CD2	1:E:742:LEU:HD22	2.41	0.55
1:E:809:LEU:HD12	1:E:827:PHE:CE1	2.41	0.55
1:G:671:LEU:HD23	1:G:686:VAL:CG2	2.36	0.55
1:F:623:LYS:O	1:F:623:LYS:HG2	2.06	0.55
1:F:809:LEU:HD12	1:F:827:PHE:CE1	2.41	0.55
1:C:762:PHE:O	1:C:837:PHE:HD1	1.90	0.55
1:C:616:LEU:O	1:C:620:LEU:HD13	2.07	0.55
1:C:742:LEU:HD21	1:C:857:VAL:HG21	1.89	0.55
1:C:798:LEU:C	1:C:823:PHE:CD2	2.85	0.55
1:H:571:ARG:HD3	1:H:604:LEU:HD21	1.89	0.55
1:B:738:PHE:HD2	1:B:742:LEU:HD22	1.72	0.54
1:G:681:ASP:O	1:G:685:LEU:HD23	2.06	0.54
1:H:704:LEU:HD11	1:H:716:TYR:CD1	2.42	0.54
1:A:671:LEU:HD23	1:A:686:VAL:HG21	1.89	0.54
1:D:638:LEU:HD11	1:D:654:LEU:HD11	1.89	0.54
1:E:647:LEU:HD11	1:E:685:LEU:HD12	1.89	0.54
1:G:744:LEU:HD22	1:G:855:TYR:CD2	2.40	0.53
1:B:795:ILE:HD11	1:A:795:ILE:HD11	1.89	0.53
1:D:744:LEU:HD22	1:D:855:TYR:HD2	1.73	0.53
1:E:741:ARG:O	1:E:741:ARG:HG2	2.05	0.53
1:A:744:LEU:HD23	1:A:855:TYR:HD2	1.73	0.53
1:H:594:LEU:HD12	1:H:624:GLY:O	2.09	0.53
1:E:774:ILE:O	1:E:774:ILE:HD12	2.07	0.53
1:H:789:PHE:CD1	1:H:794:VAL:HG12	2.42	0.53
1:G:693:CYS:HB2	1:G:723:LEU:HD21	1.90	0.53
1:A:777:GLY:O	1:A:859:LEU:HD13	2.09	0.53
1:A:713:VAL:HG13	1:A:714:LEU:HD22	1.91	0.53
1:G:790:LEU:HB2	1:H:790:LEU:HD22	1.90	0.53
1:E:859:LEU:O	1:E:860:GLN:CG	2.57	0.52
1:B:774:ILE:HD12	1:B:774:ILE:O	2.09	0.52
1:G:614:ASP:OD1	1:G:649:THR:HG22	2.09	0.52
1:H:808:VAL:HG22	1:H:813:PHE:CD1	2.44	0.52
1:F:744:LEU:CD2	1:F:855:TYR:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:744:LEU:HD23	1:D:857:VAL:HG22	1.91	0.51
1:A:744:LEU:HD23	1:A:855:TYR:CD2	2.44	0.51
1:C:692:ASP:OD2	1:C:695:ILE:HD11	2.09	0.51
1:E:756:LEU:HD13	1:E:756:LEU:O	2.10	0.51
1:D:774:ILE:HD12	1:D:774:ILE:O	2.11	0.51
1:B:617:LEU:O	1:B:621:ILE:HG12	2.10	0.51
1:C:836:LEU:HD23	1:C:837:PHE:N	2.25	0.51
1:G:789:PHE:C	1:G:790:LEU:HD12	2.35	0.51
1:D:839:ARG:NH1	1:D:840:LEU:O	2.44	0.51
1:D:808:VAL:HG22	1:D:813:PHE:CD1	2.45	0.51
1:H:683:VAL:HG21	1:H:715:VAL:HG13	1.93	0.51
1:D:738:PHE:CD2	1:D:742:LEU:HD13	2.45	0.51
1:G:809:LEU:HD12	1:G:827:PHE:CE1	2.46	0.51
1:A:636:THR:CG2	1:A:639:ILE:HG12	2.42	0.50
1:C:802:CYS:CB	1:C:823:PHE:HE1	2.24	0.50
1:A:628:ASN:ND2	1:A:659:PHE:H	2.09	0.50
1:D:565:ILE:HG22	1:D:566:PRO:HD2	1.93	0.50
1:E:737:TYR:CE1	1:F:801:PRO:HD3	2.46	0.50
1:F:808:VAL:HG22	1:F:813:PHE:CD1	2.47	0.50
1:G:617:LEU:O	1:G:621:ILE:HG12	2.12	0.50
1:H:738:PHE:HD2	1:H:742:LEU:HD22	1.76	0.50
1:C:671:LEU:HD23	1:C:686:VAL:HG21	1.93	0.50
1:B:602:MET:HA	1:B:606:MET:SD	2.52	0.50
1:G:647:LEU:C	1:G:647:LEU:HD23	2.37	0.50
1:G:738:PHE:CE2	1:G:742:LEU:HD13	2.46	0.50
1:H:726:LEU:O	1:H:729:VAL:HG12	2.12	0.50
1:F:734:ILE:HD12	1:F:744:LEU:HD21	1.93	0.49
1:A:616:LEU:O	1:A:620:LEU:HD13	2.11	0.49
1:H:617:LEU:O	1:H:621:ILE:HG12	2.13	0.49
1:A:570:LEU:HD23	1:A:570:LEU:O	2.12	0.49
1:A:586:LEU:HB3	1:A:623:LYS:HE3	1.92	0.49
1:D:638:LEU:HD11	1:D:654:LEU:CD1	2.43	0.49
1:H:725:THR:HA	1:H:728:ARG:HG2	1.94	0.49
1:F:742:LEU:HG	1:F:857:VAL:HG22	1.94	0.49
1:D:738:PHE:O	1:D:741:ARG:HG2	2.13	0.49
1:C:602:MET:HA	1:C:606:MET:SD	2.53	0.49
1:E:749:PHE:HE1	1:E:854:ALA:HB3	1.76	0.49
1:E:836:LEU:HD23	1:E:837:PHE:N	2.28	0.49
1:D:816:PRO:HB2	1:D:818:PHE:O	2.13	0.48
1:E:742:LEU:CD2	1:E:857:VAL:HG21	2.43	0.48
1:F:809:LEU:HD23	1:F:810:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:774:ILE:HD12	1:H:774:ILE:O	2.13	0.48
1:F:762:PHE:O	1:F:837:PHE:CD1	2.66	0.48
1:G:692:ASP:OD2	1:G:695:ILE:HD11	2.14	0.48
1:C:617:LEU:O	1:C:621:ILE:HG12	2.13	0.48
1:E:660:VAL:HG11	1:E:691:ALA:HB2	1.94	0.48
1:F:630:ARG:HG2	1:F:634:GLY:HA2	1.94	0.48
1:H:645:ASN:OD1	1:H:677:ARG:NE	2.40	0.48
1:G:605:VAL:HG22	1:G:620:LEU:HD23	1.96	0.48
1:A:734:ILE:HD13	1:A:744:LEU:HD11	1.96	0.48
1:D:836:LEU:HD23	1:D:837:PHE:N	2.29	0.48
1:G:683:VAL:HG21	1:G:715:VAL:HG13	1.95	0.48
1:A:726:LEU:O	1:A:729:VAL:HG12	2.14	0.48
1:D:605:VAL:HG13	1:D:617:LEU:HD11	1.96	0.48
1:G:742:LEU:HG	1:G:857:VAL:HG22	1.96	0.48
1:A:580:ILE:HG13	1:A:581:THR:N	2.29	0.48
1:F:837:PHE:HD1	1:F:838:ILE:N	2.11	0.48
1:G:795:ILE:HD12	1:H:795:ILE:HD11	1.92	0.48
1:E:593:ASN:O	1:E:596:GLN:OE1	2.31	0.47
1:E:710:SER:O	1:E:711:ASN:OD1	2.31	0.47
1:B:675:CYS:SG	1:B:719:LEU:HD11	2.54	0.47
1:D:566:PRO:HD3	1:F:837:PHE:CD2	2.49	0.47
1:F:617:LEU:O	1:F:621:ILE:HG12	2.14	0.47
1:F:800:GLY:O	1:F:823:PHE:HZ	1.97	0.47
1:G:605:VAL:CG2	1:G:625:ALA:HB1	2.45	0.47
1:G:742:LEU:HD21	1:G:857:VAL:CG2	2.43	0.47
1:G:809:LEU:HD23	1:G:810:ASN:OD1	2.14	0.47
1:B:579:TYR:O	1:B:582:VAL:HG22	2.15	0.47
1:F:836:LEU:HD23	1:F:836:LEU:C	2.40	0.47
1:B:678:GLY:O	1:B:712:ASN:ND2	2.48	0.47
1:A:638:LEU:HD11	1:A:654:LEU:HD11	1.97	0.47
1:A:668:GLU:HA	1:A:672:MET:SD	2.54	0.47
1:A:738:PHE:CD2	1:A:742:LEU:HD22	2.49	0.47
1:C:734:ILE:HG21	1:C:744:LEU:HD11	1.97	0.47
1:G:704:LEU:HD11	1:G:716:TYR:CD1	2.50	0.47
1:E:859:LEU:O	1:E:860:GLN:CB	2.63	0.47
1:G:745:LEU:HD23	1:G:746:GLU:CG	2.39	0.47
1:G:808:VAL:HG22	1:G:813:PHE:CD1	2.50	0.47
1:E:669:THR:CG2	1:E:670:ALA:N	2.78	0.47
1:F:744:LEU:HD23	1:F:855:TYR:CD2	2.50	0.47
1:G:594:LEU:HD13	1:G:625:ALA:HA	1.96	0.47
1:C:815:LEU:N	1:C:815:LEU:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:579:TYR:CZ	1:D:583:LYS:HE2	2.50	0.47
1:G:789:PHE:CD1	1:G:794:VAL:HG12	2.49	0.47
1:A:744:LEU:CD2	1:A:855:TYR:HD2	2.28	0.46
1:A:809:LEU:HD23	1:A:810:ASN:ND2	2.30	0.46
1:D:683:VAL:HG21	1:D:715:VAL:HG13	1.96	0.46
1:B:578:ASP:HB3	1:B:581:THR:HB	1.98	0.46
1:A:650:VAL:O	1:A:654:LEU:HD13	2.15	0.46
1:C:726:LEU:O	1:C:729:VAL:HG12	2.16	0.46
1:E:594:LEU:H	1:E:594:LEU:HD12	1.81	0.46
1:A:672:MET:HE2	1:A:706:PHE:CE2	2.51	0.46
1:C:756:LEU:HD13	1:C:756:LEU:O	2.16	0.46
1:H:612:GLY:HA2	1:H:649:THR:HG21	1.96	0.46
1:B:568:ASN:OD1	1:B:569:VAL:N	2.48	0.46
1:B:782:LEU:HD23	1:B:782:LEU:C	2.41	0.46
1:D:565:ILE:HA	1:F:837:PHE:HE2	1.80	0.46
1:D:602:MET:HE2	1:D:631:GLN:NE2	2.27	0.46
1:D:612:GLY:HA2	1:D:649:THR:HG21	1.98	0.46
1:G:790:LEU:HD12	1:G:790:LEU:N	2.30	0.46
1:H:578:ASP:HB3	1:H:581:THR:HG22	1.97	0.46
1:H:744:LEU:CD2	1:H:855:TYR:HD2	2.29	0.46
1:H:756:LEU:HD13	1:H:756:LEU:O	2.16	0.46
1:B:734:ILE:HD13	1:B:744:LEU:HD11	1.98	0.46
1:A:636:THR:HG22	1:A:639:ILE:HG12	1.98	0.46
1:D:617:LEU:O	1:D:621:ILE:HG12	2.16	0.46
1:E:617:LEU:O	1:E:621:ILE:HG12	2.16	0.46
1:B:647:LEU:C	1:B:647:LEU:HD23	2.40	0.45
1:B:683:VAL:HG21	1:B:715:VAL:HG13	1.99	0.45
1:C:795:ILE:HD12	1:C:795:ILE:C	2.41	0.45
1:F:762:PHE:O	1:F:837:PHE:HD1	1.99	0.45
1:H:734:ILE:HD13	1:H:744:LEU:HD11	1.97	0.45
1:C:704:LEU:HD11	1:C:716:TYR:CE1	2.51	0.45
1:F:782:LEU:C	1:F:782:LEU:HD23	2.41	0.45
1:G:836:LEU:HD23	1:G:837:PHE:N	2.31	0.45
1:H:628:ASN:ND2	1:H:659:PHE:H	2.14	0.45
1:B:756:LEU:HD13	1:B:756:LEU:O	2.16	0.45
1:D:615:ASP:N	1:D:615:ASP:OD1	2.49	0.45
1:E:726:LEU:O	1:E:729:VAL:HG12	2.16	0.45
1:E:859:LEU:HD12	1:E:859:LEU:N	2.31	0.45
1:A:582:VAL:HG21	1:A:616:LEU:HD22	1.97	0.45
1:G:738:PHE:CD2	1:G:742:LEU:HD22	2.51	0.45
1:G:756:LEU:HD13	1:G:756:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:738:PHE:CE2	1:C:742:LEU:HD22	2.49	0.45
1:E:669:THR:HG22	1:E:670:ALA:H	1.82	0.45
1:F:744:LEU:HD23	1:F:855:TYR:HD2	1.82	0.45
1:H:638:LEU:HD11	1:H:654:LEU:HD11	1.98	0.45
1:C:678:GLY:O	1:C:712:ASN:ND2	2.50	0.45
1:C:790:LEU:HD13	1:D:790:LEU:C	2.41	0.45
1:D:649:THR:HA	1:D:652:ILE:HG12	1.99	0.45
1:F:639:ILE:HG21	1:F:664:GLN:HE21	1.81	0.45
1:D:669:THR:CG2	1:D:670:ALA:N	2.80	0.45
1:F:841:THR:HG22	1:F:842:GLU:N	2.32	0.45
1:G:726:LEU:O	1:G:729:VAL:HG12	2.16	0.45
1:H:748:VAL:HB	1:H:854:ALA:O	2.17	0.45
1:E:602:MET:HA	1:E:606:MET:SD	2.56	0.45
1:E:801:PRO:HD3	1:F:737:TYR:CE1	2.52	0.45
1:F:836:LEU:HD21	1:F:838:ILE:HG13	1.99	0.44
1:B:808:VAL:HG22	1:B:813:PHE:HD1	1.80	0.44
1:B:836:LEU:HD23	1:B:837:PHE:N	2.33	0.44
1:A:734:ILE:HD12	1:A:744:LEU:HD21	1.99	0.44
1:C:836:LEU:HD23	1:C:836:LEU:C	2.42	0.44
1:F:636:THR:HG22	1:F:639:ILE:HG12	1.98	0.44
1:C:761:ASP:OD1	1:C:837:PHE:CE1	2.71	0.44
1:D:704:LEU:HD11	1:D:716:TYR:CD1	2.52	0.44
1:E:649:THR:HA	1:E:652:ILE:HG12	1.99	0.44
1:A:762:PHE:O	1:A:837:PHE:HD1	2.00	0.44
1:A:816:PRO:HB3	1:A:825:TYR:CE1	2.53	0.44
1:E:627:VAL:HG13	1:E:653:LEU:HD22	2.00	0.44
1:F:808:VAL:HG22	1:F:813:PHE:HD1	1.82	0.44
1:G:790:LEU:CD2	1:H:790:LEU:HB2	2.48	0.44
1:E:571:ARG:HD3	1:E:596:GLN:HE21	1.81	0.44
1:F:668:GLU:HA	1:F:672:MET:SD	2.57	0.44
1:G:738:PHE:O	1:G:741:ARG:HG2	2.18	0.44
1:A:568:ASN:OD1	1:A:569:VAL:N	2.51	0.44
1:C:798:LEU:CA	1:C:823:PHE:HD2	2.30	0.44
1:D:738:PHE:CE2	1:D:742:LEU:HD13	2.53	0.44
1:F:725:THR:HA	1:F:728:ARG:HG2	1.99	0.44
1:G:841:THR:HG22	1:G:842:GLU:N	2.33	0.44
1:D:803:SER:O	1:D:840:LEU:HA	2.17	0.44
1:F:704:LEU:HD11	1:F:716:TYR:CD1	2.53	0.44
1:C:823:PHE:CD1	1:C:823:PHE:N	2.85	0.44
1:F:771:PRO:HD2	1:F:856:ARG:NH2	2.32	0.44
1:A:699:HIS:ND1	1:F:845:SER:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:722:HIS:HE1	1:E:789:PHE:HE2	1.66	0.43
1:F:586:LEU:CD2	1:F:623:LYS:HD2	2.47	0.43
1:C:807:VAL:HG22	1:C:838:ILE:HG12	2.01	0.43
1:F:671:LEU:HD13	1:F:686:VAL:CG2	2.48	0.43
1:F:737:TYR:CD2	1:F:798:LEU:HB2	2.53	0.43
1:G:649:THR:HA	1:G:652:ILE:HG12	1.99	0.43
1:G:782:LEU:HD23	1:G:782:LEU:C	2.42	0.43
1:D:605:VAL:HG13	1:D:617:LEU:CD1	2.48	0.43
1:G:738:PHE:HD2	1:G:742:LEU:HB3	1.82	0.43
1:B:742:LEU:HG	1:B:857:VAL:HG22	2.00	0.43
1:D:856:ARG:C	1:D:857:VAL:HG23	2.44	0.43
1:A:638:LEU:HD11	1:A:654:LEU:CD1	2.48	0.43
1:A:737:TYR:CD2	1:A:798:LEU:HB2	2.53	0.43
1:A:738:PHE:CD2	1:A:742:LEU:HD13	2.54	0.43
1:A:836:LEU:HD23	1:A:837:PHE:N	2.34	0.43
1:E:749:PHE:HE1	1:E:854:ALA:CB	2.31	0.43
1:D:841:THR:HG22	1:D:842:GLU:N	2.34	0.43
1:H:678:GLY:O	1:H:712:ASN:OD1	2.37	0.43
1:C:802:CYS:SG	1:C:823:PHE:CE1	3.12	0.43
1:H:602:MET:HA	1:H:606:MET:HE3	2.01	0.43
1:A:802:CYS:SG	1:A:823:PHE:CE2	3.12	0.43
1:C:638:LEU:HD11	1:C:654:LEU:HD11	2.00	0.43
1:B:738:PHE:CD2	1:B:742:LEU:HD13	2.54	0.42
1:D:792:LYS:HG3	1:D:792:LYS:O	2.19	0.42
1:H:647:LEU:C	1:H:647:LEU:HD23	2.45	0.42
1:H:748:VAL:HG13	1:H:768:TYR:CD1	2.53	0.42
1:F:636:THR:CG2	1:F:639:ILE:HG12	2.49	0.42
1:B:636:THR:HG22	1:B:639:ILE:HG12	2.01	0.42
1:A:742:LEU:HG	1:A:857:VAL:HG22	2.00	0.42
1:E:647:LEU:HD11	1:E:685:LEU:CD1	2.48	0.42
1:H:571:ARG:HD3	1:H:604:LEU:CD2	2.49	0.42
1:D:726:LEU:O	1:D:729:VAL:HG12	2.19	0.42
1:B:704:LEU:HD11	1:B:716:TYR:CD1	2.54	0.42
1:B:744:LEU:CD2	1:B:855:TYR:HD2	2.32	0.42
1:B:807:VAL:HG22	1:B:838:ILE:HG12	2.01	0.42
1:D:792:LYS:O	1:D:792:LYS:CG	2.67	0.42
1:E:704:LEU:HD11	1:E:716:TYR:CE1	2.54	0.42
1:A:704:LEU:HD12	1:A:704:LEU:HA	1.84	0.42
1:D:816:PRO:HB3	1:D:825:TYR:CE1	2.54	0.42
1:F:744:LEU:CD2	1:F:855:TYR:CD2	3.02	0.42
1:G:671:LEU:HD12	1:G:703:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:671:LEU:CD1	1:G:703:ALA:HB1	2.50	0.42
1:D:602:MET:CG	1:D:606:MET:HG3	2.49	0.42
1:E:837:PHE:CD1	1:E:837:PHE:C	2.98	0.42
1:F:643:GLU:OE2	1:F:673:LYS:HD2	2.20	0.42
1:G:774:ILE:O	1:G:774:ILE:HG13	2.20	0.42
1:F:738:PHE:CD2	1:F:742:LEU:HD22	2.55	0.42
1:G:782:LEU:HD12	1:G:827:PHE:CE1	2.55	0.42
1:B:613:GLN:HB2	1:B:616:LEU:HD12	2.02	0.42
1:A:571:ARG:CD	1:A:604:LEU:HD21	2.49	0.42
1:C:590:GLU:OE1	1:C:592:TYR:OH	2.27	0.42
1:D:782:LEU:C	1:D:782:LEU:HD23	2.45	0.42
1:E:689:CYS:O	1:E:755:ARG:NH1	2.53	0.42
1:F:854:ALA:C	1:F:855:TYR:HD1	2.28	0.42
1:E:635:THR:HG23	1:E:639:ILE:HB	2.01	0.41
1:F:647:LEU:HD23	1:F:647:LEU:C	2.45	0.41
1:B:777:GLY:O	1:B:859:LEU:HD13	2.20	0.41
1:D:809:LEU:HD12	1:D:827:PHE:CD1	2.55	0.41
1:F:807:VAL:HG22	1:F:838:ILE:HG12	2.02	0.41
1:F:605:VAL:HG21	1:F:626:LYS:O	2.20	0.41
1:A:782:LEU:HD12	1:A:827:PHE:CE1	2.54	0.41
1:C:738:PHE:N	1:C:738:PHE:CD1	2.88	0.41
1:E:582:VAL:O	1:E:586:LEU:HD13	2.21	0.41
1:F:612:GLY:HA2	1:F:649:THR:HG21	2.02	0.41
1:F:639:ILE:HG21	1:F:664:GLN:NE2	2.36	0.41
1:F:652:ILE:HG13	1:F:653:LEU:N	2.34	0.41
1:H:575:LYS:HD3	1:H:607:LEU:HD22	2.01	0.41
1:C:569:VAL:HG23	1:C:570:LEU:N	2.36	0.41
1:H:713:VAL:HG13	1:H:714:LEU:HD22	2.02	0.41
1:A:747:PRO:HA	1:A:855:TYR:CD1	2.55	0.41
1:F:742:LEU:CD2	1:F:857:VAL:HG21	2.47	0.41
1:H:728:ARG:NH2	1:H:732:GLU:OE2	2.54	0.41
1:H:756:LEU:HD13	1:H:756:LEU:C	2.46	0.41
1:A:808:VAL:HG22	1:A:813:PHE:CD1	2.56	0.41
1:C:647:LEU:HD23	1:C:647:LEU:C	2.46	0.41
1:F:704:LEU:HD11	1:F:716:TYR:CE1	2.55	0.41
1:G:636:THR:HG22	1:G:639:ILE:HG12	2.03	0.41
1:G:737:TYR:CE1	1:H:801:PRO:HD3	2.56	0.41
1:G:837:PHE:CD1	1:G:837:PHE:C	2.99	0.41
1:C:649:THR:HA	1:C:652:ILE:HG12	2.03	0.41
1:C:683:VAL:HG21	1:C:715:VAL:HG13	2.01	0.41
1:D:600:SER:O	1:D:632:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:MET:HG3	1:D:631:GLN:HE21	1.85	0.41
1:D:722:HIS:HA	1:D:792:LYS:NZ	2.36	0.41
1:F:726:LEU:O	1:F:729:VAL:HG12	2.21	0.41
1:G:617:LEU:HB3	1:G:652:ILE:HD12	2.03	0.41
1:H:684:ARG:HA	1:H:687:ILE:HG12	2.03	0.41
1:A:602:MET:HA	1:A:606:MET:SD	2.61	0.41
1:C:579:TYR:O	1:C:582:VAL:HG22	2.21	0.41
1:C:803:SER:O	1:C:840:LEU:HA	2.20	0.41
1:H:712:ASN:C	1:H:712:ASN:HD22	2.29	0.41
1:A:677:ARG:O	1:A:677:ARG:HG2	2.21	0.40
1:D:579:TYR:HA	1:D:616:LEU:HD21	2.04	0.40
1:E:669:THR:H	1:E:672:MET:HG3	1.86	0.40
1:E:749:PHE:CE1	1:E:854:ALA:HB3	2.55	0.40
1:H:728:ARG:HG3	1:H:729:VAL:N	2.36	0.40
1:H:782:LEU:HD12	1:H:827:PHE:CE1	2.56	0.40
1:F:590:GLU:HG2	1:F:592:TYR:CZ	2.56	0.40
1:F:799:CYS:HA	1:F:823:PHE:CE2	2.56	0.40
1:A:738:PHE:HD2	1:A:742:LEU:HD22	1.86	0.40
1:C:568:ASN:O	1:C:568:ASN:ND2	2.49	0.40
1:C:841:THR:HG22	1:C:842:GLU:N	2.35	0.40
1:E:836:LEU:CD2	1:E:838:ILE:HG13	2.51	0.40
1:F:574:VAL:HG21	1:F:604:LEU:HD22	2.03	0.40
1:G:784:ILE:CD1	1:G:804:VAL:HG21	2.51	0.40
1:H:782:LEU:HD23	1:H:782:LEU:C	2.46	0.40
1:A:800:GLY:O	1:A:823:PHE:HZ	2.03	0.40
1:D:638:LEU:C	1:D:638:LEU:HD23	2.47	0.40
1:F:616:LEU:O	1:F:620:LEU:HD13	2.21	0.40
1:C:782:LEU:HD23	1:C:782:LEU:C	2.45	0.40
1:C:836:LEU:HD21	1:C:838:ILE:HG13	2.03	0.40
1:F:635:THR:HG23	1:F:639:ILE:HB	2.04	0.40
1:F:837:PHE:CD1	1:F:838:ILE:N	2.89	0.40
1:G:738:PHE:HE2	1:G:742:LEU:HD13	1.86	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:F:677:ARG:NH1	1:H:577:GLY:O[4_445]	2.12	0.08
1:F:677:ARG:HH11	1:H:577:GLY:O[4_445]	1.57	0.03

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	296/336 (88%)	289 (98%)	7 (2%)	0	100	100
1	B	292/336 (87%)	284 (97%)	8 (3%)	0	100	100
1	C	292/336 (87%)	283 (97%)	9 (3%)	0	100	100
1	D	296/336 (88%)	293 (99%)	3 (1%)	0	100	100
1	E	294/336 (88%)	289 (98%)	5 (2%)	0	100	100
1	F	292/336 (87%)	287 (98%)	5 (2%)	0	100	100
1	G	293/336 (87%)	286 (98%)	7 (2%)	0	100	100
1	H	294/336 (88%)	286 (97%)	8 (3%)	0	100	100
All	All	2349/2688 (87%)	2297 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	237/283 (84%)	237 (100%)	0	100	100
1	B	232/283 (82%)	232 (100%)	0	100	100
1	C	228/283 (81%)	228 (100%)	0	100	100
1	D	243/283 (86%)	243 (100%)	0	100	100
1	E	231/283 (82%)	231 (100%)	0	100	100
1	F	234/283 (83%)	234 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	236/283 (83%)	236 (100%)	0	100	100
1	H	232/283 (82%)	232 (100%)	0	100	100
All	All	1873/2264 (83%)	1873 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	613	GLN
1	B	664	GLN
1	B	722	HIS
1	A	628	ASN
1	A	631	GLN
1	A	786	HIS
1	A	788	ASN
1	C	694	ASN
1	C	722	HIS
1	C	810	ASN
1	D	631	GLN
1	D	664	GLN
1	D	694	ASN
1	E	694	ASN
1	E	722	HIS
1	E	822	HIS
1	F	664	GLN
1	F	705	HIS
1	F	722	HIS
1	G	694	ASN
1	H	664	GLN
1	H	694	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](#)

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	298/336 (88%)	0.10	8 (2%)	56	32	62, 113, 186, 237	0
1	B	294/336 (87%)	-0.04	4 (1%)	73	50	95, 143, 210, 243	0
1	C	294/336 (87%)	0.25	6 (2%)	65	41	97, 143, 216, 268	0
1	D	298/336 (88%)	-0.14	1 (0%)	90	79	61, 111, 183, 262	0
1	E	296/336 (88%)	0.25	11 (3%)	45	25	87, 145, 206, 266	0
1	F	294/336 (87%)	0.11	5 (1%)	69	45	81, 130, 208, 255	0
1	G	295/336 (87%)	-0.01	8 (2%)	56	32	98, 146, 232, 297	0
1	H	296/336 (88%)	0.05	5 (1%)	69	45	110, 159, 223, 311	0
All	All	2365/2688 (87%)	0.07	48 (2%)	65	41	61, 138, 213, 311	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	860	GLN	3.9
1	F	860	GLN	3.9
1	C	819	LEU	3.5
1	E	795	ILE	3.3
1	F	773	ASN	3.3
1	F	737	TYR	3.2
1	A	820	ASP	3.1
1	C	820	ASP	3.0
1	E	580	ILE	3.0
1	E	819	LEU	2.9
1	F	845	SER	2.9
1	G	820	ASP	2.8
1	H	716	TYR	2.8
1	E	739	GLU	2.7
1	E	793	GLU	2.7
1	F	621	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	808	VAL	2.6
1	G	742	LEU	2.6
1	H	773	ASN	2.6
1	G	738	PHE	2.6
1	E	845	SER	2.5
1	H	691	ALA	2.5
1	C	591	GLU	2.5
1	E	740	ALA	2.4
1	D	689	CYS	2.4
1	B	744	LEU	2.4
1	G	615	ASP	2.4
1	B	574	VAL	2.4
1	A	748	VAL	2.4
1	B	860	GLN	2.3
1	G	582	VAL	2.3
1	A	854	ALA	2.3
1	E	742	LEU	2.3
1	E	782	LEU	2.3
1	A	580	ILE	2.3
1	G	744	LEU	2.3
1	G	776	GLU	2.2
1	C	582	VAL	2.2
1	B	772	GLN	2.1
1	A	742	LEU	2.1
1	A	860	GLN	2.1
1	E	738	PHE	2.1
1	C	859	LEU	2.1
1	G	859	LEU	2.1
1	A	776	GLU	2.1
1	H	683	VAL	2.1
1	A	836	LEU	2.1
1	H	749	PHE	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.