



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 08:04 AM UTC

PDB ID : 9EM8 / pdb_00009em8
EMDB ID : EMD-19813
Title : Oligomeric structure of SynDLP in presence of GDP
Authors : Junglas, B.; Gewehr, L.; Schoennenbeck, P.; Schneider, D.; Sachse, C.
Deposited on : 2024-03-07
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

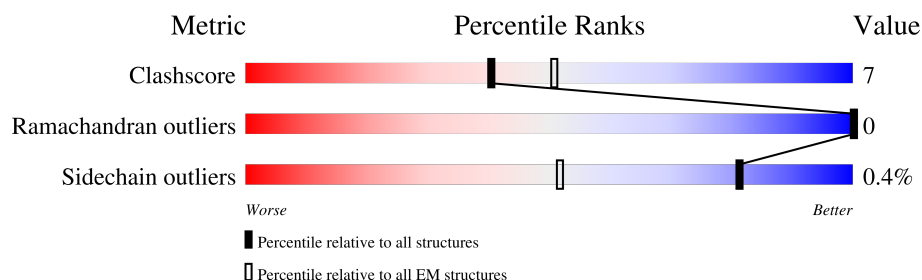
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	820	79% 17% .
1	B	820	80% 16% .
1	C	820	81% 15% .
1	D	820	80% 17% .
1	E	820	80% 17% .
1	F	820	79% 17% .
1	G	820	79% 17% .
1	H	820	80% 17% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 57040 atoms, of which 6168 are hydrogens and 0 are deuteriums.

In the tables below, 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 Slr0869 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		
1	B	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		
1	C	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		
1	D	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		
1	E	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		
1	F	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		
1	G	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		
1	H	792	Total	C	H	N	O	S	0	0
			7130	3993	771	1110	1236	20		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	813	LEU	-	expression tag	UNP P73765
A	814	GLU	-	expression tag	UNP P73765
A	815	HIS	-	expression tag	UNP P73765
A	816	HIS	-	expression tag	UNP P73765
A	817	HIS	-	expression tag	UNP P73765
A	818	HIS	-	expression tag	UNP P73765
A	819	HIS	-	expression tag	UNP P73765
A	820	HIS	-	expression tag	UNP P73765
B	813	LEU	-	expression tag	UNP P73765
B	814	GLU	-	expression tag	UNP P73765
B	815	HIS	-	expression tag	UNP P73765
B	816	HIS	-	expression tag	UNP P73765
B	817	HIS	-	expression tag	UNP P73765
B	818	HIS	-	expression tag	UNP P73765

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Chain	Residue	Modelled	Actual	Comment	Reference
B	819	HIS	-	expression tag	UNP P73765
B	820	HIS	-	expression tag	UNP P73765
C	813	LEU	-	expression tag	UNP P73765
C	814	GLU	-	expression tag	UNP P73765
C	815	HIS	-	expression tag	UNP P73765
C	816	HIS	-	expression tag	UNP P73765
C	817	HIS	-	expression tag	UNP P73765
C	818	HIS	-	expression tag	UNP P73765
C	819	HIS	-	expression tag	UNP P73765
C	820	HIS	-	expression tag	UNP P73765
D	813	LEU	-	expression tag	UNP P73765
D	814	GLU	-	expression tag	UNP P73765
D	815	HIS	-	expression tag	UNP P73765
D	816	HIS	-	expression tag	UNP P73765
D	817	HIS	-	expression tag	UNP P73765
D	818	HIS	-	expression tag	UNP P73765
D	819	HIS	-	expression tag	UNP P73765
D	820	HIS	-	expression tag	UNP P73765
E	813	LEU	-	expression tag	UNP P73765
E	814	GLU	-	expression tag	UNP P73765
E	815	HIS	-	expression tag	UNP P73765
E	816	HIS	-	expression tag	UNP P73765
E	817	HIS	-	expression tag	UNP P73765
E	818	HIS	-	expression tag	UNP P73765
E	819	HIS	-	expression tag	UNP P73765
E	820	HIS	-	expression tag	UNP P73765
F	813	LEU	-	expression tag	UNP P73765
F	814	GLU	-	expression tag	UNP P73765
F	815	HIS	-	expression tag	UNP P73765
F	816	HIS	-	expression tag	UNP P73765
F	817	HIS	-	expression tag	UNP P73765
F	818	HIS	-	expression tag	UNP P73765
F	819	HIS	-	expression tag	UNP P73765
F	820	HIS	-	expression tag	UNP P73765
G	813	LEU	-	expression tag	UNP P73765
G	814	GLU	-	expression tag	UNP P73765
G	815	HIS	-	expression tag	UNP P73765
G	816	HIS	-	expression tag	UNP P73765
G	817	HIS	-	expression tag	UNP P73765
G	818	HIS	-	expression tag	UNP P73765
G	819	HIS	-	expression tag	UNP P73765
G	820	HIS	-	expression tag	UNP P73765

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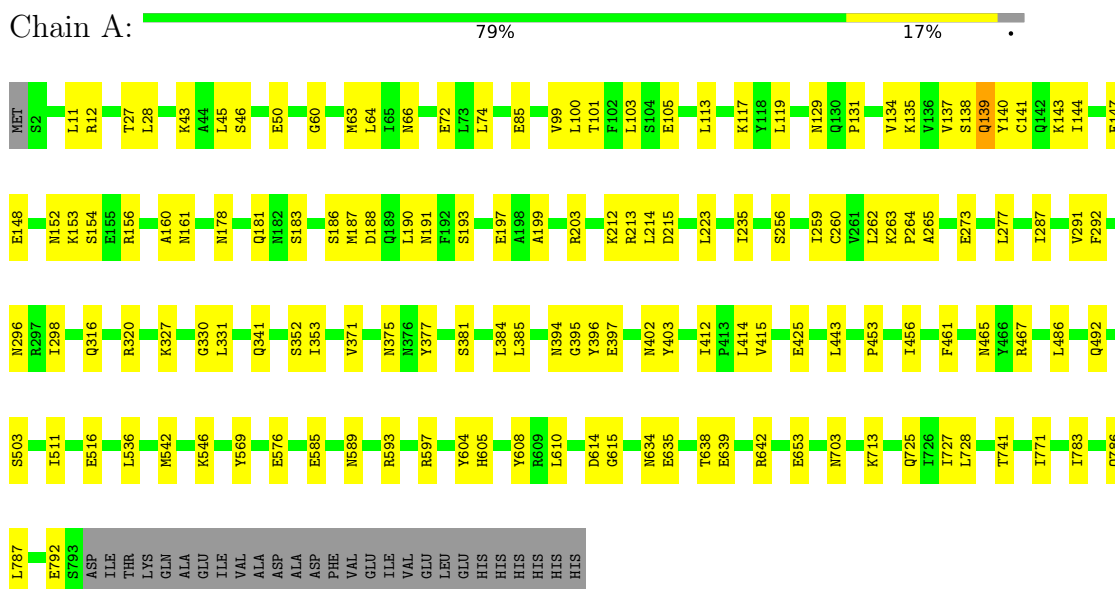
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Chain	Residue	Modelled	Actual	Comment	Reference
H	813	LEU	-	expression tag	UNP P73765
H	814	GLU	-	expression tag	UNP P73765
H	815	HIS	-	expression tag	UNP P73765
H	816	HIS	-	expression tag	UNP P73765
H	817	HIS	-	expression tag	UNP P73765
H	818	HIS	-	expression tag	UNP P73765
H	819	HIS	-	expression tag	UNP P73765
H	820	HIS	-	expression tag	UNP P73765

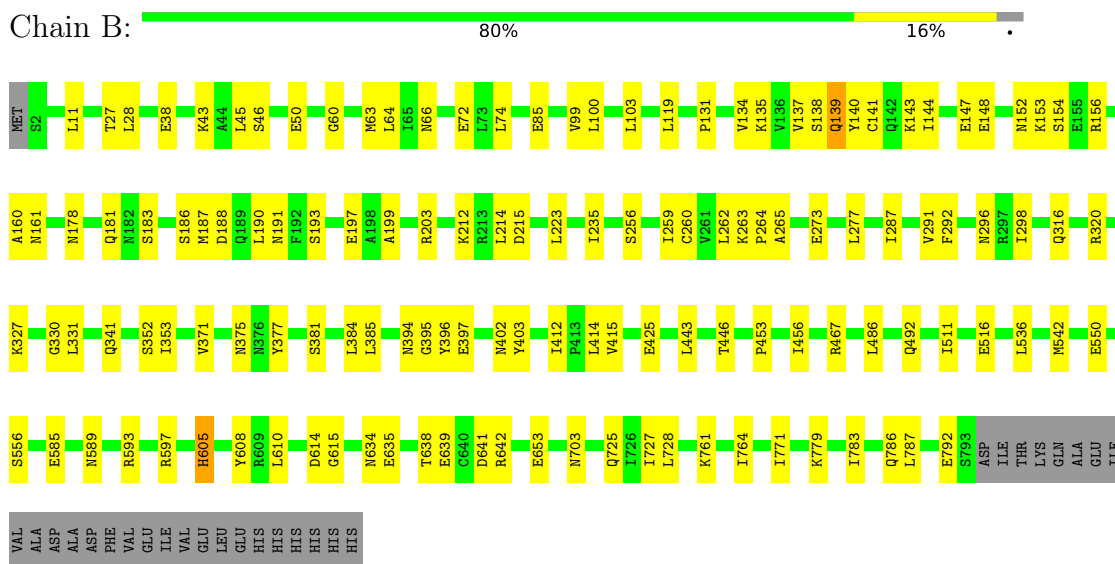
3 Residue-property plots [i](#)

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. 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. 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: Slr0869 protein

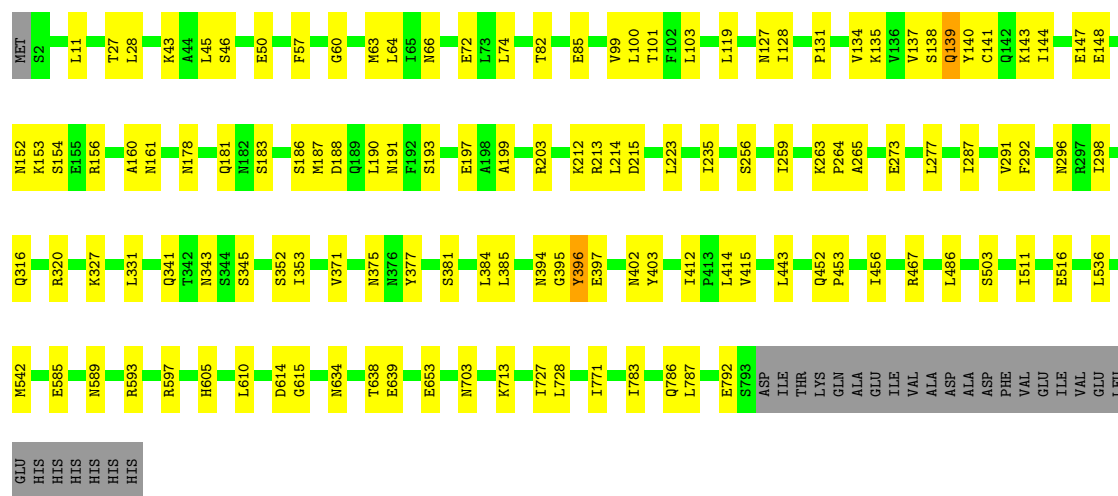


- Molecule 1: Slr0869 protein



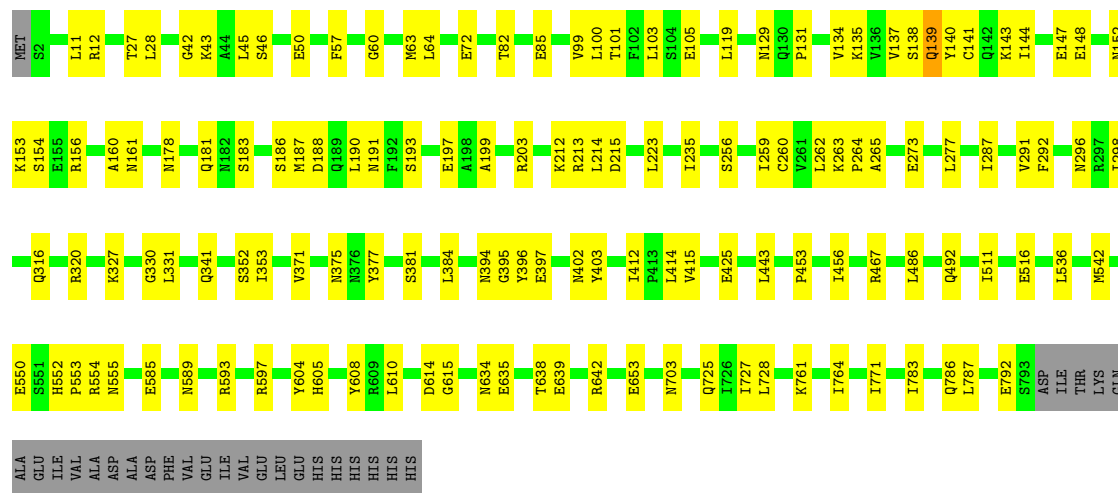
- Molecule 1: Slr0869 protein

Chain C:  81% 15%



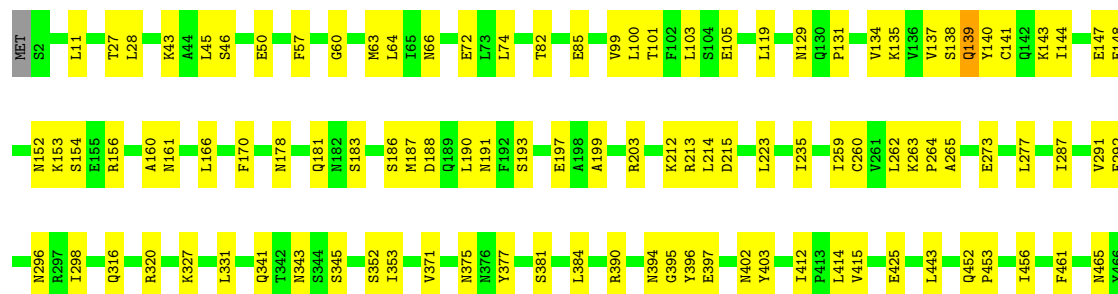
• Molecule 1: Slr0869 protein

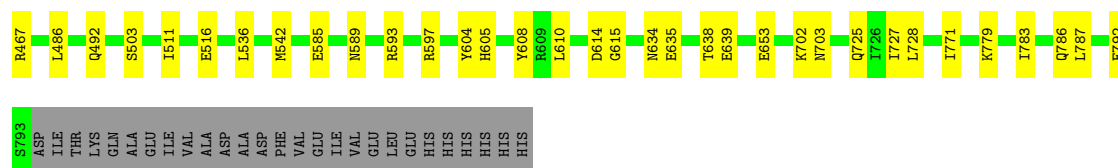
Chain D:  80% 17%



• Molecule 1: Slr0869 protein

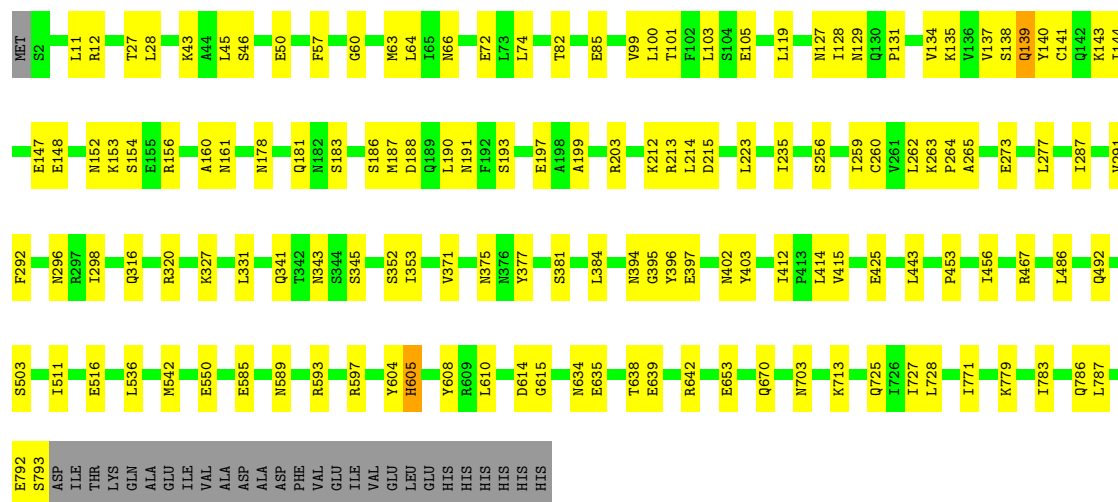
Chain E:  80% 17%





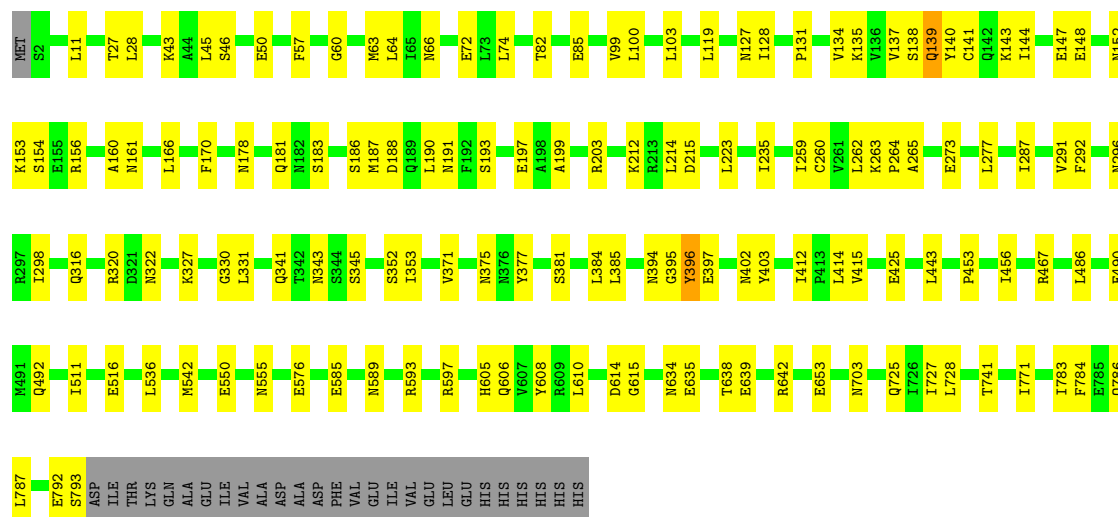
• Molecule 1: Slr0869 protein

Chain F: 79% 17% .



• Molecule 1: Slr0869 protein

Chain G: 79% 17% .



• Molecule 1: Slr0869 protein

Chain H: 80% 17% .

LYS	GLN	ALA	GLU	ILE	VAL	ALA	ASP	ALA	ASP	PHE	VAL	GLU	ILE	VAL	GLU	LEU	HIS	HIS	HIS	HIS	HIS	R297	E155																			
																						E516	R156																			
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101	F102	L103	L113	K117	Y118	L119	P131	V134	K135	V136	V137	S138	Q139	Y140	C141	I144	E148	M152	K153	S154
MET	S2	L11	R12	T27	L28	R29	S30	G42	K43	A44	L45	S46	E50	G60	M63	L64	E72	E85	R97	V98	L100	T101																				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	395948	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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	0.08	0/6459	0.21	0/8723
1	B	0.08	0/6459	0.21	0/8723
1	C	0.08	0/6459	0.21	0/8723
1	D	0.08	0/6459	0.21	0/8723
1	E	0.08	0/6459	0.21	0/8723
1	F	0.08	0/6459	0.21	0/8723
1	G	0.08	0/6459	0.21	0/8723
1	H	0.08	0/6459	0.21	0/8723
All	All	0.08	0/51672	0.21	0/69784

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	6359	771	6300	99	0
1	B	6359	771	6300	96	0
1	C	6359	771	6300	87	0
1	D	6359	771	6300	94	0
1	E	6359	771	6300	94	0
1	F	6359	771	6300	99	0
1	G	6359	771	6300	101	0
1	H	6359	771	6300	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50872	6168	50400	709	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 7.

All (709) 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:604:TYR:HH	1:F:608:TYR:HH	1.20	0.88
1:A:642:ARG:NH2	1:G:703:ASN:OD1	2.06	0.87
1:B:492:GLN:NE2	1:G:725:GLN:OE1	2.07	0.86
1:H:604:TYR:HH	1:H:608:TYR:HH	1.16	0.85
1:C:377:TYR:O	1:C:381:SER:OG	1.97	0.83
1:F:779:LYS:NZ	1:G:741:THR:OG1	2.11	0.82
1:B:377:TYR:O	1:B:381:SER:OG	1.97	0.82
1:D:377:TYR:O	1:D:381:SER:OG	1.97	0.82
1:F:377:TYR:O	1:F:381:SER:OG	1.97	0.81
1:H:377:TYR:O	1:H:381:SER:OG	1.97	0.81
1:A:377:TYR:O	1:A:381:SER:OG	1.97	0.81
1:E:377:TYR:O	1:E:381:SER:OG	1.97	0.81
1:E:787:LEU:HD21	1:F:608:TYR:CD2	2.16	0.81
1:G:377:TYR:O	1:G:381:SER:OG	1.97	0.80
1:B:608:TYR:CD2	1:C:787:LEU:HD21	2.15	0.80
1:F:604:TYR:OH	1:F:608:TYR:OH	2.01	0.79
1:D:604:TYR:OH	1:D:608:TYR:OH	2.01	0.79
1:A:604:TYR:HH	1:A:608:TYR:HH	1.14	0.79
1:E:604:TYR:HH	1:E:608:TYR:HH	1.20	0.79
1:E:452:GLN:OE1	1:F:605:HIS:NE2	2.18	0.77
1:B:725:GLN:OE1	1:G:492:GLN:NE2	2.18	0.76
1:G:385:LEU:O	1:H:12:ARG:NH2	2.20	0.73
1:H:193:SER:OG	1:H:197:GLU:OE1	2.07	0.73
1:A:703:ASN:OD1	1:G:642:ARG:NH2	2.23	0.72
1:F:193:SER:OG	1:F:197:GLU:OE1	2.07	0.72
1:D:604:TYR:HH	1:D:608:TYR:HH	1.32	0.71
1:B:193:SER:OG	1:B:197:GLU:OE1	2.07	0.71
1:D:193:SER:OG	1:D:197:GLU:OE1	2.07	0.71
1:A:152:ASN:OD1	1:A:161:ASN:ND2	2.24	0.71
1:C:152:ASN:OD1	1:C:161:ASN:ND2	2.24	0.70
1:C:193:SER:OG	1:C:197:GLU:OE1	2.07	0.70
1:H:152:ASN:OD1	1:H:161:ASN:ND2	2.24	0.70
1:E:585:GLU:O	1:E:589:ASN:ND2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASN:OD1	1:B:161:ASN:ND2	2.24	0.70
1:D:152:ASN:OD1	1:D:161:ASN:ND2	2.24	0.70
1:D:585:GLU:O	1:D:589:ASN:ND2	2.25	0.70
1:C:585:GLU:O	1:C:589:ASN:ND2	2.25	0.70
1:F:585:GLU:O	1:F:589:ASN:ND2	2.25	0.70
1:G:152:ASN:OD1	1:G:161:ASN:ND2	2.24	0.70
1:D:639:GLU:OE2	1:D:703:ASN:ND2	2.25	0.70
1:A:585:GLU:O	1:A:589:ASN:ND2	2.25	0.69
1:E:639:GLU:OE2	1:E:703:ASN:ND2	2.25	0.69
1:B:585:GLU:O	1:B:589:ASN:ND2	2.25	0.69
1:F:152:ASN:OD1	1:F:161:ASN:ND2	2.24	0.69
1:F:639:GLU:OE2	1:F:703:ASN:ND2	2.25	0.69
1:G:585:GLU:O	1:G:589:ASN:ND2	2.25	0.69
1:E:152:ASN:OD1	1:E:161:ASN:ND2	2.24	0.69
1:E:316:GLN:O	1:E:320:ARG:NH2	2.26	0.69
1:G:316:GLN:O	1:G:320:ARG:NH2	2.26	0.69
1:H:585:GLU:O	1:H:589:ASN:ND2	2.25	0.69
1:B:316:GLN:O	1:B:320:ARG:NH2	2.26	0.69
1:B:639:GLU:OE2	1:B:703:ASN:ND2	2.25	0.69
1:G:193:SER:OG	1:G:197:GLU:OE1	2.07	0.68
1:C:639:GLU:OE2	1:C:703:ASN:ND2	2.25	0.68
1:A:639:GLU:OE2	1:A:703:ASN:ND2	2.25	0.68
1:G:639:GLU:OE2	1:G:703:ASN:ND2	2.25	0.68
1:H:316:GLN:O	1:H:320:ARG:NH2	2.26	0.68
1:H:639:GLU:OE2	1:H:703:ASN:ND2	2.25	0.68
1:F:316:GLN:O	1:F:320:ARG:NH2	2.26	0.68
1:E:193:SER:OG	1:E:197:GLU:OE1	2.07	0.68
1:A:316:GLN:O	1:A:320:ARG:NH2	2.26	0.68
1:D:316:GLN:O	1:D:320:ARG:NH2	2.26	0.68
1:C:316:GLN:O	1:C:320:ARG:NH2	2.26	0.67
1:E:199:ALA:O	1:E:203:ARG:N	2.28	0.67
1:C:137:VAL:O	1:C:141:CYS:N	2.28	0.66
1:D:137:VAL:O	1:D:141:CYS:N	2.28	0.66
1:H:137:VAL:O	1:H:141:CYS:N	2.28	0.66
1:H:199:ALA:O	1:H:203:ARG:N	2.28	0.66
1:A:199:ALA:O	1:A:203:ARG:N	2.28	0.66
1:B:394:ASN:OD1	1:B:395:GLY:N	2.29	0.66
1:G:394:ASN:OD1	1:G:395:GLY:N	2.29	0.66
1:A:137:VAL:O	1:A:141:CYS:N	2.28	0.66
1:G:199:ALA:O	1:G:203:ARG:N	2.28	0.66
1:F:137:VAL:O	1:F:141:CYS:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ASN:OD1	1:C:395:GLY:N	2.29	0.66
1:D:199:ALA:O	1:D:203:ARG:N	2.28	0.66
1:D:394:ASN:OD1	1:D:395:GLY:N	2.29	0.66
1:F:199:ALA:O	1:F:203:ARG:N	2.28	0.66
1:G:137:VAL:O	1:G:141:CYS:N	2.28	0.66
1:B:199:ALA:O	1:B:203:ARG:N	2.28	0.65
1:B:137:VAL:O	1:B:141:CYS:N	2.28	0.65
1:C:199:ALA:O	1:C:203:ARG:N	2.28	0.65
1:E:394:ASN:OD1	1:E:395:GLY:N	2.29	0.65
1:H:394:ASN:OD1	1:H:395:GLY:N	2.29	0.65
1:F:394:ASN:OD1	1:F:395:GLY:N	2.29	0.65
1:A:193:SER:OG	1:A:197:GLU:OE1	2.07	0.65
1:A:394:ASN:OD1	1:A:395:GLY:N	2.29	0.65
1:E:137:VAL:O	1:E:141:CYS:N	2.28	0.65
1:A:713:LYS:NZ	1:D:555:ASN:O	2.30	0.64
1:A:148:GLU:OE2	1:A:156:ARG:NH1	2.31	0.64
1:A:786:GLN:N	1:A:786:GLN:OE1	2.31	0.64
1:B:786:GLN:OE1	1:B:786:GLN:N	2.31	0.64
1:C:148:GLU:OE2	1:C:156:ARG:NH1	2.31	0.64
1:D:786:GLN:OE1	1:D:786:GLN:N	2.31	0.63
1:F:148:GLU:OE2	1:F:156:ARG:NH1	2.31	0.63
1:G:148:GLU:OE2	1:G:156:ARG:NH1	2.31	0.63
1:H:786:GLN:N	1:H:786:GLN:OE1	2.31	0.63
1:H:148:GLU:OE2	1:H:156:ARG:NH1	2.31	0.63
1:C:786:GLN:N	1:C:786:GLN:OE1	2.31	0.63
1:G:786:GLN:OE1	1:G:786:GLN:N	2.31	0.63
1:F:786:GLN:N	1:F:786:GLN:OE1	2.31	0.63
1:D:148:GLU:OE2	1:D:156:ARG:NH1	2.31	0.63
1:E:148:GLU:OE2	1:E:156:ARG:NH1	2.31	0.63
1:A:45:LEU:O	1:A:46:SER:OG	2.15	0.62
1:A:725:GLN:OE1	1:F:492:GLN:NE2	2.32	0.62
1:E:397:GLU:O	1:E:402:ASN:ND2	2.33	0.62
1:E:786:GLN:N	1:E:786:GLN:OE1	2.31	0.62
1:H:397:GLU:O	1:H:402:ASN:ND2	2.33	0.62
1:B:148:GLU:OE2	1:B:156:ARG:NH1	2.31	0.62
1:A:385:LEU:O	1:D:12:ARG:NH2	2.25	0.62
1:C:397:GLU:O	1:C:402:ASN:ND2	2.33	0.62
1:A:397:GLU:O	1:A:402:ASN:ND2	2.33	0.62
1:D:397:GLU:O	1:D:402:ASN:ND2	2.33	0.62
1:F:397:GLU:O	1:F:402:ASN:ND2	2.33	0.62
1:G:397:GLU:O	1:G:402:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLU:O	1:B:402:ASN:ND2	2.33	0.62
1:E:503:SER:OG	1:F:550:GLU:OE1	2.16	0.62
1:G:178:ASN:OD1	1:G:183:SER:OG	2.11	0.62
1:H:604:TYR:OH	1:H:608:TYR:OH	2.01	0.61
1:B:45:LEU:O	1:B:46:SER:OG	2.15	0.61
1:G:131:PRO:O	1:G:135:LYS:N	2.33	0.61
1:H:187:MET:SD	1:H:188:ASP:N	2.74	0.61
1:D:187:MET:SD	1:D:188:ASP:N	2.74	0.61
1:C:187:MET:SD	1:C:188:ASP:N	2.74	0.61
1:A:187:MET:SD	1:A:188:ASP:N	2.74	0.61
1:H:72:GLU:O	1:H:203:ARG:NH1	2.34	0.61
1:G:72:GLU:O	1:G:203:ARG:NH1	2.34	0.60
1:B:131:PRO:O	1:B:135:LYS:N	2.33	0.60
1:E:187:MET:SD	1:E:188:ASP:N	2.74	0.60
1:B:187:MET:SD	1:B:188:ASP:N	2.74	0.60
1:F:72:GLU:O	1:F:203:ARG:NH1	2.34	0.60
1:G:187:MET:SD	1:G:188:ASP:N	2.74	0.60
1:A:503:SER:OG	1:D:550:GLU:OE1	2.18	0.60
1:E:72:GLU:O	1:E:203:ARG:NH1	2.34	0.60
1:F:187:MET:SD	1:F:188:ASP:N	2.74	0.60
1:D:72:GLU:O	1:D:203:ARG:NH1	2.34	0.60
1:D:131:PRO:O	1:D:135:LYS:N	2.33	0.59
1:A:72:GLU:O	1:A:203:ARG:NH1	2.34	0.59
1:C:43:LYS:O	1:C:443:LEU:HD21	2.03	0.59
1:A:713:LYS:NZ	1:D:552:HIS:O	2.34	0.59
1:F:131:PRO:O	1:F:135:LYS:N	2.33	0.59
1:B:140:TYR:O	1:B:144:ILE:N	2.36	0.59
1:F:43:LYS:O	1:F:443:LEU:HD21	2.03	0.59
1:C:72:GLU:O	1:C:203:ARG:NH1	2.34	0.59
1:G:43:LYS:O	1:G:443:LEU:HD21	2.03	0.59
1:C:45:LEU:O	1:C:46:SER:OG	2.15	0.58
1:B:72:GLU:O	1:B:203:ARG:NH1	2.34	0.58
1:E:178:ASN:OD1	1:E:183:SER:OG	2.11	0.58
1:H:45:LEU:O	1:H:46:SER:OG	2.15	0.58
1:H:43:LYS:O	1:H:443:LEU:HD21	2.03	0.58
1:H:131:PRO:O	1:H:135:LYS:N	2.33	0.58
1:B:43:LYS:O	1:B:443:LEU:HD21	2.03	0.58
1:G:140:TYR:O	1:G:144:ILE:N	2.36	0.58
1:D:43:LYS:O	1:D:443:LEU:HD21	2.03	0.58
1:A:43:LYS:O	1:A:443:LEU:HD21	2.03	0.58
1:G:45:LEU:O	1:G:46:SER:OG	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:ASN:HB3	1:H:30:SER:HB3	1.86	0.58
1:B:703:ASN:OD1	1:H:642:ARG:NH2	2.37	0.57
1:E:43:LYS:O	1:E:443:LEU:HD21	2.03	0.57
1:C:131:PRO:O	1:C:135:LYS:N	2.33	0.57
1:F:45:LEU:O	1:F:46:SER:OG	2.15	0.57
1:G:259:ILE:HD13	1:G:292:PHE:HB2	1.87	0.57
1:A:178:ASN:OD1	1:A:183:SER:OG	2.11	0.56
1:H:259:ILE:HD13	1:H:292:PHE:HB2	1.86	0.56
1:B:259:ILE:HD13	1:B:292:PHE:HB2	1.86	0.56
1:A:140:TYR:O	1:A:144:ILE:N	2.36	0.56
1:E:131:PRO:O	1:E:135:LYS:N	2.33	0.56
1:E:140:TYR:O	1:E:144:ILE:N	2.36	0.56
1:A:131:PRO:O	1:A:135:LYS:N	2.33	0.56
1:C:178:ASN:OD1	1:C:183:SER:OG	2.11	0.56
1:A:12:ARG:NH2	1:B:385:LEU:O	2.39	0.56
1:A:259:ILE:HD13	1:A:292:PHE:HB2	1.87	0.56
1:C:259:ILE:HD13	1:C:292:PHE:HB2	1.86	0.56
1:D:259:ILE:HD13	1:D:292:PHE:HB2	1.86	0.56
1:F:259:ILE:HD13	1:F:292:PHE:HB2	1.86	0.56
1:E:259:ILE:HD13	1:E:292:PHE:HB2	1.86	0.55
1:C:140:TYR:O	1:C:144:ILE:N	2.36	0.55
1:D:45:LEU:O	1:D:46:SER:OG	2.15	0.55
1:A:341:GLN:N	1:A:341:GLN:OE1	2.40	0.55
1:E:45:LEU:O	1:E:46:SER:OG	2.15	0.55
1:H:140:TYR:O	1:H:144:ILE:N	2.36	0.55
1:E:341:GLN:OE1	1:E:341:GLN:N	2.40	0.55
1:G:341:GLN:N	1:G:341:GLN:OE1	2.40	0.55
1:B:341:GLN:N	1:B:341:GLN:OE1	2.40	0.55
1:H:341:GLN:OE1	1:H:341:GLN:N	2.40	0.55
1:B:467:ARG:NH2	1:B:792:GLU:O	2.40	0.55
1:A:134:VAL:O	1:A:138:SER:OG	2.23	0.54
1:C:341:GLN:OE1	1:C:341:GLN:N	2.40	0.54
1:F:178:ASN:OD1	1:F:183:SER:OG	2.11	0.54
1:F:341:GLN:N	1:F:341:GLN:OE1	2.40	0.54
1:D:341:GLN:N	1:D:341:GLN:OE1	2.40	0.54
1:B:186:SER:HB2	1:C:396:TYR:CE2	2.43	0.54
1:H:178:ASN:OD1	1:H:183:SER:OG	2.11	0.54
1:F:467:ARG:NH2	1:F:792:GLU:O	2.40	0.54
1:D:516:GLU:OE1	1:D:516:GLU:N	2.40	0.54
1:F:516:GLU:OE1	1:F:516:GLU:N	2.40	0.54
1:H:139:GLN:N	1:H:139:GLN:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ASN:OD1	1:D:183:SER:OG	2.11	0.54
1:G:467:ARG:NH2	1:G:792:GLU:O	2.40	0.54
1:D:140:TYR:O	1:D:144:ILE:N	2.36	0.54
1:C:467:ARG:NH2	1:C:792:GLU:O	2.40	0.53
1:D:139:GLN:N	1:D:139:GLN:OE1	2.41	0.53
1:E:139:GLN:OE1	1:E:139:GLN:N	2.41	0.53
1:F:140:TYR:O	1:F:144:ILE:N	2.36	0.53
1:A:139:GLN:N	1:A:139:GLN:OE1	2.41	0.53
1:F:139:GLN:N	1:F:139:GLN:OE1	2.41	0.53
1:A:385:LEU:HD21	1:D:42:GLY:HA3	1.90	0.53
1:A:467:ARG:NH2	1:A:792:GLU:O	2.40	0.53
1:G:139:GLN:OE1	1:G:139:GLN:N	2.41	0.53
1:H:467:ARG:NH2	1:H:792:GLU:O	2.40	0.53
1:B:139:GLN:OE1	1:B:139:GLN:N	2.41	0.53
1:C:139:GLN:N	1:C:139:GLN:OE1	2.41	0.53
1:A:516:GLU:OE1	1:A:516:GLU:N	2.40	0.53
1:B:178:ASN:OD1	1:B:183:SER:OG	2.11	0.53
1:A:741:THR:OG1	1:B:779:LYS:NZ	2.42	0.53
1:D:467:ARG:NH2	1:D:792:GLU:O	2.40	0.53
1:E:604:TYR:OH	1:E:608:TYR:OH	2.01	0.53
1:G:385:LEU:HD11	1:H:42:GLY:HA3	1.91	0.52
1:C:516:GLU:OE1	1:C:516:GLU:N	2.40	0.52
1:D:298:ILE:HG21	1:D:327:LYS:HB3	1.92	0.52
1:B:186:SER:HB2	1:C:396:TYR:CZ	2.44	0.52
1:E:298:ILE:HG21	1:E:327:LYS:HB3	1.92	0.52
1:A:298:ILE:HG21	1:A:327:LYS:HB3	1.92	0.52
1:C:542:MET:HE2	1:C:542:MET:HA	1.92	0.52
1:E:516:GLU:OE1	1:E:516:GLU:N	2.40	0.52
1:F:298:ILE:HG21	1:F:327:LYS:HB3	1.92	0.52
1:G:298:ILE:HG21	1:G:327:LYS:HB3	1.92	0.52
1:F:503:SER:OG	1:G:550:GLU:OE1	2.25	0.52
1:G:542:MET:HE2	1:G:542:MET:HA	1.92	0.52
1:H:134:VAL:O	1:H:138:SER:N	2.41	0.52
1:H:516:GLU:OE1	1:H:516:GLU:N	2.40	0.52
1:H:542:MET:HE2	1:H:542:MET:HA	1.92	0.52
1:B:542:MET:HE2	1:B:542:MET:HA	1.92	0.52
1:D:542:MET:HA	1:D:542:MET:HE2	1.92	0.52
1:D:703:ASN:OD1	1:F:642:ARG:NH2	2.43	0.52
1:E:542:MET:HE2	1:E:542:MET:HA	1.92	0.52
1:H:50:GLU:OE2	1:H:256:SER:OG	2.22	0.52
1:B:516:GLU:OE1	1:B:516:GLU:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:LEU:CG	1:H:42:GLY:HA3	2.40	0.51
1:H:298:ILE:HG21	1:H:327:LYS:HB3	1.92	0.51
1:B:298:ILE:HG21	1:B:327:LYS:HB3	1.92	0.51
1:D:153:LYS:O	1:D:154:SER:OG	2.25	0.51
1:A:50:GLU:OE2	1:A:256:SER:OG	2.22	0.51
1:A:492:GLN:NE2	1:F:725:GLN:OE1	2.43	0.51
1:A:542:MET:HA	1:A:542:MET:HE2	1.92	0.51
1:E:153:LYS:O	1:E:154:SER:OG	2.25	0.51
1:E:467:ARG:NH2	1:E:792:GLU:O	2.40	0.51
1:B:641:ASP:OD2	1:H:710:ASN:ND2	2.44	0.51
1:E:371:VAL:O	1:E:375:ASN:ND2	2.44	0.51
1:G:396:TYR:CZ	1:H:97:ARG:HD2	2.46	0.51
1:C:298:ILE:HG21	1:C:327:LYS:HB3	1.92	0.50
1:D:134:VAL:O	1:D:138:SER:N	2.41	0.50
1:B:38:GLU:O	1:C:385:LEU:HD23	2.11	0.50
1:E:787:LEU:HD21	1:F:608:TYR:CG	2.46	0.50
1:E:134:VAL:O	1:E:138:SER:N	2.41	0.50
1:F:614:ASP:OD1	1:F:615:GLY:N	2.45	0.50
1:C:134:VAL:O	1:C:138:SER:OG	2.23	0.50
1:F:273:GLU:OE1	1:F:273:GLU:N	2.44	0.50
1:F:542:MET:HA	1:F:542:MET:HE2	1.92	0.50
1:A:134:VAL:O	1:A:138:SER:N	2.41	0.50
1:A:614:ASP:OD1	1:A:615:GLY:N	2.45	0.50
1:C:614:ASP:OD1	1:C:615:GLY:N	2.45	0.50
1:H:614:ASP:OD1	1:H:615:GLY:N	2.45	0.50
1:B:614:ASP:OD1	1:B:615:GLY:N	2.45	0.50
1:G:614:ASP:OD1	1:G:615:GLY:N	2.45	0.50
1:E:614:ASP:OD1	1:E:615:GLY:N	2.45	0.49
1:B:134:VAL:O	1:B:138:SER:N	2.41	0.49
1:E:787:LEU:HD21	1:F:608:TYR:HB3	1.94	0.49
1:F:787:LEU:HD11	1:G:608:TYR:HB3	1.93	0.49
1:B:181:GLN:OE1	1:B:181:GLN:N	2.41	0.49
1:D:614:ASP:OD1	1:D:615:GLY:N	2.45	0.49
1:F:263:LYS:O	1:F:265:ALA:N	2.46	0.49
1:G:273:GLU:OE1	1:G:273:GLU:N	2.44	0.49
1:A:60:GLY:O	1:A:64:LEU:HD23	2.13	0.49
1:A:187:MET:O	1:A:191:ASN:N	2.46	0.49
1:D:187:MET:O	1:D:191:ASN:N	2.46	0.49
1:D:653:GLU:OE1	1:D:653:GLU:N	2.42	0.49
1:B:263:LYS:O	1:B:265:ALA:N	2.46	0.49
1:D:263:LYS:O	1:D:265:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:GLN:OE1	1:E:492:GLN:NE2	2.46	0.49
1:E:60:GLY:O	1:E:64:LEU:HD23	2.13	0.49
1:F:134:VAL:O	1:F:138:SER:N	2.41	0.49
1:H:99:VAL:N	1:H:215:ASP:OD1	2.46	0.49
1:H:153:LYS:O	1:H:154:SER:OG	2.25	0.49
1:C:187:MET:O	1:C:191:ASN:N	2.46	0.49
1:F:181:GLN:OE1	1:F:181:GLN:N	2.41	0.49
1:F:187:MET:O	1:F:191:ASN:N	2.46	0.49
1:F:371:VAL:O	1:F:375:ASN:ND2	2.44	0.49
1:B:60:GLY:O	1:B:64:LEU:HD23	2.13	0.49
1:C:99:VAL:N	1:C:215:ASP:OD1	2.46	0.49
1:D:181:GLN:OE1	1:D:181:GLN:N	2.41	0.49
1:G:99:VAL:N	1:G:215:ASP:OD1	2.46	0.49
1:C:273:GLU:OE1	1:C:273:GLU:N	2.44	0.49
1:E:187:MET:O	1:E:191:ASN:N	2.46	0.49
1:F:99:VAL:N	1:F:215:ASP:OD1	2.46	0.49
1:G:371:VAL:O	1:G:375:ASN:ND2	2.44	0.49
1:H:273:GLU:OE1	1:H:273:GLU:N	2.44	0.49
1:A:371:VAL:O	1:A:375:ASN:ND2	2.45	0.49
1:B:187:MET:O	1:B:191:ASN:N	2.46	0.48
1:B:486:LEU:O	1:B:486:LEU:HD23	2.13	0.48
1:C:99:VAL:C	1:C:100:LEU:HD12	2.38	0.48
1:C:134:VAL:O	1:C:138:SER:N	2.41	0.48
1:C:486:LEU:HD23	1:C:486:LEU:O	2.13	0.48
1:E:263:LYS:O	1:E:265:ALA:N	2.46	0.48
1:G:99:VAL:C	1:G:100:LEU:HD12	2.38	0.48
1:H:187:MET:O	1:H:191:ASN:N	2.46	0.48
1:H:371:VAL:O	1:H:375:ASN:ND2	2.44	0.48
1:A:99:VAL:N	1:A:215:ASP:OD1	2.46	0.48
1:A:486:LEU:HD23	1:A:486:LEU:O	2.13	0.48
1:B:99:VAL:N	1:B:215:ASP:OD1	2.46	0.48
1:C:263:LYS:O	1:C:265:ALA:N	2.46	0.48
1:C:371:VAL:O	1:C:375:ASN:ND2	2.44	0.48
1:D:99:VAL:C	1:D:100:LEU:HD12	2.38	0.48
1:F:99:VAL:C	1:F:100:LEU:HD12	2.38	0.48
1:F:486:LEU:HD23	1:F:486:LEU:O	2.13	0.48
1:G:516:GLU:N	1:G:516:GLU:OE1	2.40	0.48
1:A:153:LYS:O	1:A:154:SER:OG	2.25	0.48
1:G:187:MET:O	1:G:191:ASN:N	2.46	0.48
1:D:11:LEU:C	1:D:11:LEU:HD23	2.38	0.48
1:G:486:LEU:O	1:G:486:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:VAL:C	1:H:100:LEU:HD12	2.38	0.48
1:A:99:VAL:C	1:A:100:LEU:HD12	2.38	0.48
1:C:60:GLY:O	1:C:64:LEU:HD23	2.13	0.48
1:C:153:LYS:O	1:C:154:SER:OG	2.25	0.48
1:D:99:VAL:N	1:D:215:ASP:OD1	2.46	0.48
1:D:486:LEU:HD23	1:D:486:LEU:O	2.13	0.48
1:E:99:VAL:N	1:E:215:ASP:OD1	2.46	0.48
1:G:11:LEU:C	1:G:11:LEU:HD23	2.39	0.48
1:G:263:LYS:O	1:G:265:ALA:N	2.46	0.48
1:H:11:LEU:HD23	1:H:11:LEU:C	2.39	0.48
1:H:263:LYS:O	1:H:265:ALA:N	2.46	0.48
1:B:608:TYR:HD2	1:C:787:LEU:HD21	1.74	0.48
1:A:263:LYS:O	1:A:265:ALA:N	2.46	0.48
1:B:11:LEU:C	1:B:11:LEU:HD23	2.39	0.48
1:B:99:VAL:C	1:B:100:LEU:HD12	2.38	0.48
1:D:371:VAL:O	1:D:375:ASN:ND2	2.44	0.48
1:E:486:LEU:O	1:E:486:LEU:HD23	2.13	0.48
1:H:486:LEU:HD23	1:H:486:LEU:O	2.13	0.48
1:D:60:GLY:O	1:D:64:LEU:HD23	2.13	0.48
1:G:134:VAL:O	1:G:138:SER:N	2.42	0.48
1:C:453:PRO:O	1:C:456:ILE:HG22	2.14	0.48
1:G:60:GLY:O	1:G:64:LEU:HD23	2.13	0.48
1:B:371:VAL:O	1:B:375:ASN:ND2	2.44	0.48
1:C:11:LEU:HD23	1:C:11:LEU:C	2.39	0.48
1:E:11:LEU:HD23	1:E:11:LEU:C	2.39	0.48
1:B:186:SER:OG	1:B:188:ASP:OD1	2.23	0.47
1:B:453:PRO:O	1:B:456:ILE:HG22	2.14	0.47
1:E:99:VAL:C	1:E:100:LEU:HD12	2.38	0.47
1:F:11:LEU:C	1:F:11:LEU:HD23	2.39	0.47
1:F:60:GLY:O	1:F:64:LEU:HD23	2.13	0.47
1:A:11:LEU:C	1:A:11:LEU:HD23	2.39	0.47
1:A:453:PRO:O	1:A:456:ILE:HG22	2.14	0.47
1:B:550:GLU:OE1	1:C:503:SER:OG	2.31	0.47
1:H:60:GLY:O	1:H:64:LEU:HD23	2.13	0.47
1:B:783:ILE:HG22	1:B:783:ILE:O	2.14	0.47
1:D:50:GLU:OE2	1:D:256:SER:OG	2.22	0.47
1:D:783:ILE:HG22	1:D:783:ILE:O	2.14	0.47
1:F:783:ILE:HG22	1:F:783:ILE:O	2.14	0.47
1:C:783:ILE:O	1:C:783:ILE:HG22	2.14	0.47
1:D:453:PRO:O	1:D:456:ILE:HG22	2.14	0.47
1:E:653:GLU:OE1	1:E:653:GLU:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:783:ILE:HG22	1:G:783:ILE:O	2.14	0.47
1:H:783:ILE:O	1:H:783:ILE:HG22	2.14	0.47
1:B:273:GLU:OE1	1:B:273:GLU:N	2.44	0.47
1:E:453:PRO:O	1:E:456:ILE:HG22	2.14	0.47
1:A:783:ILE:HG22	1:A:783:ILE:O	2.14	0.47
1:E:783:ILE:O	1:E:783:ILE:HG22	2.14	0.47
1:F:453:PRO:O	1:F:456:ILE:HG22	2.14	0.47
1:F:713:LYS:NZ	1:G:555:ASN:O	2.47	0.47
1:B:153:LYS:O	1:B:154:SER:OG	2.25	0.47
1:F:50:GLU:OE2	1:F:256:SER:OG	2.22	0.47
1:H:653:GLU:OE1	1:H:653:GLU:N	2.42	0.47
1:A:576:GLU:OE2	1:H:554:ARG:NH2	2.48	0.47
1:G:453:PRO:O	1:G:456:ILE:HG22	2.14	0.47
1:G:181:GLN:OE1	1:G:181:GLN:N	2.41	0.46
1:D:554:ARG:NH2	1:G:576:GLU:OE2	2.48	0.46
1:B:371:VAL:HG13	1:B:403:TYR:HB2	1.98	0.46
1:G:371:VAL:HG13	1:G:403:TYR:HB2	1.98	0.46
1:A:273:GLU:OE1	1:A:273:GLU:N	2.44	0.46
1:H:453:PRO:O	1:H:456:ILE:HG22	2.14	0.46
1:C:787:LEU:HD12	1:C:787:LEU:N	2.31	0.46
1:E:371:VAL:HG13	1:E:403:TYR:HB2	1.98	0.46
1:C:50:GLU:OE2	1:C:256:SER:OG	2.22	0.46
1:C:63:MET:HE1	1:C:331:LEU:HD13	1.98	0.46
1:D:787:LEU:N	1:D:787:LEU:HD12	2.31	0.46
1:E:702:LYS:HZ3	1:F:670:GLN:HB3	1.81	0.46
1:E:787:LEU:HD11	1:F:608:TYR:HB3	1.97	0.46
1:G:787:LEU:N	1:G:787:LEU:HD12	2.31	0.46
1:D:642:ARG:NH2	1:F:703:ASN:OD1	2.49	0.46
1:G:63:MET:HE1	1:G:331:LEU:HD13	1.98	0.46
1:A:181:GLN:OE1	1:A:181:GLN:N	2.41	0.46
1:A:593:ARG:O	1:A:597:ARG:NE	2.49	0.46
1:F:653:GLU:OE1	1:F:653:GLU:N	2.42	0.46
1:G:153:LYS:O	1:G:154:SER:OG	2.25	0.46
1:A:511:ILE:HG22	1:A:511:ILE:O	2.16	0.45
1:A:787:LEU:HD12	1:A:787:LEU:N	2.31	0.45
1:B:787:LEU:N	1:B:787:LEU:HD12	2.31	0.45
1:C:771:ILE:HD13	1:C:787:LEU:O	2.16	0.45
1:E:771:ILE:HD13	1:E:787:LEU:O	2.16	0.45
1:G:425:GLU:OE1	1:G:425:GLU:N	2.43	0.45
1:E:425:GLU:OE1	1:E:425:GLU:N	2.43	0.45
1:F:771:ILE:HD13	1:F:787:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:787:LEU:HD12	1:F:787:LEU:N	2.31	0.45
1:B:634:ASN:O	1:B:638:THR:HG23	2.17	0.45
1:C:371:VAL:HG13	1:C:403:TYR:HB2	1.98	0.45
1:E:511:ILE:O	1:E:511:ILE:HG22	2.16	0.45
1:F:634:ASN:O	1:F:638:THR:HG23	2.17	0.45
1:G:384:LEU:HD21	1:G:414:LEU:HD11	1.99	0.45
1:G:511:ILE:HG22	1:G:511:ILE:O	2.16	0.45
1:B:63:MET:HE1	1:B:331:LEU:HD13	1.98	0.45
1:B:384:LEU:HD21	1:B:414:LEU:HD11	1.99	0.45
1:D:63:MET:HE1	1:D:331:LEU:HD13	1.98	0.45
1:E:103:LEU:HD23	1:E:212:LYS:NZ	2.32	0.45
1:B:99:VAL:O	1:B:214:LEU:HD23	2.17	0.45
1:C:343:ASN:CG	1:C:345:SER:HG	2.18	0.45
1:C:511:ILE:HG22	1:C:511:ILE:O	2.16	0.45
1:E:63:MET:HE1	1:E:331:LEU:HD13	1.98	0.45
1:G:103:LEU:HD23	1:G:212:LYS:NZ	2.32	0.45
1:A:634:ASN:O	1:A:638:THR:HG23	2.17	0.45
1:B:103:LEU:HD23	1:B:212:LYS:NZ	2.32	0.45
1:C:634:ASN:O	1:C:638:THR:HG23	2.17	0.45
1:D:273:GLU:OE1	1:D:273:GLU:N	2.44	0.45
1:E:787:LEU:N	1:E:787:LEU:HD12	2.31	0.45
1:F:63:MET:HE1	1:F:331:LEU:HD13	1.98	0.45
1:G:134:VAL:O	1:G:138:SER:OG	2.23	0.45
1:A:63:MET:HE1	1:A:331:LEU:HD13	1.98	0.45
1:A:99:VAL:O	1:A:214:LEU:HD23	2.17	0.45
1:B:511:ILE:HG22	1:B:511:ILE:O	2.16	0.45
1:D:287:ILE:O	1:D:291:VAL:HG23	2.17	0.45
1:D:371:VAL:HG13	1:D:403:TYR:HB2	1.98	0.45
1:D:384:LEU:HD21	1:D:414:LEU:HD11	1.99	0.45
1:D:771:ILE:HD13	1:D:787:LEU:O	2.16	0.45
1:E:634:ASN:O	1:E:638:THR:HG23	2.17	0.45
1:F:371:VAL:HG13	1:F:403:TYR:HB2	1.98	0.45
1:G:99:VAL:O	1:G:214:LEU:HD23	2.17	0.45
1:A:103:LEU:HD23	1:A:212:LYS:NZ	2.32	0.45
1:B:771:ILE:HD13	1:B:787:LEU:O	2.16	0.45
1:D:99:VAL:O	1:D:214:LEU:HD23	2.17	0.45
1:D:492:GLN:NE2	1:E:725:GLN:OE1	2.50	0.45
1:D:511:ILE:HG22	1:D:511:ILE:O	2.16	0.45
1:G:771:ILE:HD13	1:G:787:LEU:O	2.16	0.45
1:G:787:LEU:HD23	1:H:612:GLY:O	2.17	0.45
1:H:634:ASN:O	1:H:638:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LYS:HE2	1:D:553:PRO:O	2.16	0.45
1:B:223:LEU:HD12	1:B:223:LEU:N	2.32	0.45
1:E:771:ILE:HD11	1:E:786:GLN:HB3	1.99	0.45
1:F:511:ILE:HG22	1:F:511:ILE:O	2.16	0.45
1:G:634:ASN:O	1:G:638:THR:HG23	2.17	0.45
1:H:371:VAL:HG13	1:H:403:TYR:HB2	1.98	0.45
1:B:642:ARG:NH2	1:H:703:ASN:OD1	2.50	0.45
1:F:593:ARG:O	1:F:597:ARG:NE	2.49	0.45
1:H:787:LEU:HD12	1:H:787:LEU:N	2.31	0.45
1:A:771:ILE:HD13	1:A:787:LEU:O	2.16	0.44
1:B:556:SER:HB2	1:C:713:LYS:HD3	1.98	0.44
1:B:593:ARG:O	1:B:597:ARG:NE	2.49	0.44
1:C:287:ILE:O	1:C:291:VAL:HG23	2.17	0.44
1:D:634:ASN:O	1:D:638:THR:HG23	2.17	0.44
1:E:101:THR:OG1	1:E:213:ARG:N	2.50	0.44
1:H:223:LEU:N	1:H:223:LEU:HD12	2.32	0.44
1:A:371:VAL:HG13	1:A:403:TYR:HB2	1.98	0.44
1:B:287:ILE:O	1:B:291:VAL:HG23	2.17	0.44
1:C:653:GLU:OE1	1:C:653:GLU:N	2.42	0.44
1:F:425:GLU:OE1	1:F:425:GLU:N	2.43	0.44
1:H:99:VAL:O	1:H:214:LEU:HD23	2.17	0.44
1:C:99:VAL:O	1:C:214:LEU:HD23	2.17	0.44
1:E:223:LEU:N	1:E:223:LEU:HD12	2.32	0.44
1:F:99:VAL:O	1:F:214:LEU:HD23	2.17	0.44
1:G:343:ASN:CG	1:G:345:SER:HG	2.21	0.44
1:H:384:LEU:HD21	1:H:414:LEU:HD11	1.99	0.44
1:B:605:HIS:NE2	1:C:452:GLN:OE1	2.50	0.44
1:E:99:VAL:O	1:E:214:LEU:HD23	2.17	0.44
1:E:384:LEU:HD21	1:E:414:LEU:HD11	1.99	0.44
1:F:635:GLU:O	1:F:638:THR:OG1	2.34	0.44
1:G:287:ILE:O	1:G:291:VAL:HG23	2.17	0.44
1:B:85:GLU:N	1:B:85:GLU:OE1	2.51	0.44
1:B:635:GLU:O	1:B:638:THR:OG1	2.34	0.44
1:C:143:LYS:O	1:C:147:GLU:N	2.41	0.44
1:C:181:GLN:OE1	1:C:181:GLN:N	2.41	0.44
1:D:771:ILE:HD11	1:D:786:GLN:HB3	1.99	0.44
1:E:287:ILE:O	1:E:291:VAL:HG23	2.17	0.44
1:G:223:LEU:N	1:G:223:LEU:HD12	2.32	0.44
1:H:63:MET:HE1	1:H:331:LEU:HD13	1.98	0.44
1:H:103:LEU:HD23	1:H:212:LYS:NZ	2.32	0.44
1:A:85:GLU:OE1	1:A:85:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:THR:HG23	1:C:28:LEU:HD22	2.00	0.44
1:C:384:LEU:HD21	1:C:414:LEU:HD11	1.99	0.44
1:C:593:ARG:O	1:C:597:ARG:NE	2.49	0.44
1:D:425:GLU:OE1	1:D:425:GLU:N	2.43	0.44
1:E:85:GLU:N	1:E:85:GLU:OE1	2.51	0.44
1:F:85:GLU:OE1	1:F:85:GLU:N	2.51	0.44
1:G:385:LEU:HG	1:H:42:GLY:HA3	2.00	0.44
1:H:263:LYS:N	1:H:264:PRO:CD	2.81	0.44
1:A:101:THR:OG1	1:A:213:ARG:N	2.50	0.44
1:A:287:ILE:O	1:A:291:VAL:HG23	2.17	0.44
1:A:384:LEU:HD21	1:A:414:LEU:HD11	1.99	0.44
1:B:771:ILE:HD11	1:B:786:GLN:HB3	1.99	0.44
1:C:85:GLU:N	1:C:85:GLU:OE1	2.51	0.44
1:C:263:LYS:N	1:C:264:PRO:CD	2.81	0.44
1:C:771:ILE:HD11	1:C:786:GLN:HB3	1.99	0.44
1:D:103:LEU:HD23	1:D:212:LYS:NZ	2.32	0.44
1:E:593:ARG:O	1:E:597:ARG:NE	2.49	0.44
1:F:103:LEU:HD23	1:F:212:LYS:NZ	2.32	0.44
1:F:223:LEU:HD12	1:F:223:LEU:N	2.32	0.44
1:G:85:GLU:N	1:G:85:GLU:OE1	2.51	0.44
1:G:653:GLU:OE1	1:G:653:GLU:N	2.42	0.44
1:H:85:GLU:N	1:H:85:GLU:OE1	2.51	0.44
1:H:511:ILE:HG22	1:H:511:ILE:O	2.16	0.44
1:H:771:ILE:HD13	1:H:787:LEU:O	2.16	0.44
1:A:223:LEU:N	1:A:223:LEU:HD12	2.32	0.44
1:A:425:GLU:OE1	1:A:425:GLU:N	2.43	0.44
1:A:771:ILE:HD11	1:A:786:GLN:HB3	1.99	0.44
1:B:263:LYS:N	1:B:264:PRO:CD	2.81	0.44
1:C:223:LEU:N	1:C:223:LEU:HD12	2.32	0.44
1:D:263:LYS:N	1:D:264:PRO:CD	2.81	0.44
1:E:779:LYS:HZ2	1:E:783:ILE:HD12	1.83	0.44
1:C:103:LEU:HD23	1:C:212:LYS:NZ	2.32	0.44
1:G:140:TYR:HE1	1:G:144:ILE:HD11	1.83	0.44
1:H:140:TYR:HE1	1:H:144:ILE:HD11	1.83	0.44
1:H:287:ILE:O	1:H:291:VAL:HG23	2.17	0.44
1:D:186:SER:O	1:D:190:LEU:N	2.51	0.43
1:D:223:LEU:HD12	1:D:223:LEU:N	2.32	0.43
1:F:153:LYS:O	1:F:154:SER:OG	2.25	0.43
1:F:412:ILE:O	1:F:415:VAL:N	2.51	0.43
1:A:140:TYR:HE1	1:A:144:ILE:HD11	1.83	0.43
1:A:263:LYS:N	1:A:264:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:GLU:O	1:A:638:THR:OG1	2.34	0.43
1:D:593:ARG:O	1:D:597:ARG:NE	2.49	0.43
1:F:140:TYR:HE1	1:F:144:ILE:HD11	1.83	0.43
1:F:143:LYS:O	1:F:147:GLU:N	2.41	0.43
1:G:263:LYS:N	1:G:264:PRO:CD	2.81	0.43
1:G:635:GLU:O	1:G:638:THR:OG1	2.34	0.43
1:H:425:GLU:OE1	1:H:425:GLU:N	2.43	0.43
1:A:186:SER:O	1:A:190:LEU:N	2.51	0.43
1:B:143:LYS:O	1:B:147:GLU:N	2.41	0.43
1:C:101:THR:OG1	1:C:213:ARG:N	2.50	0.43
1:D:85:GLU:OE1	1:D:85:GLU:N	2.51	0.43
1:E:140:TYR:HE1	1:E:144:ILE:HD11	1.83	0.43
1:E:143:LYS:O	1:E:147:GLU:N	2.41	0.43
1:E:263:LYS:N	1:E:264:PRO:CD	2.81	0.43
1:F:384:LEU:HD21	1:F:414:LEU:HD11	1.99	0.43
1:G:385:LEU:CD1	1:H:42:GLY:HA3	2.48	0.43
1:A:143:LYS:O	1:A:147:GLU:N	2.41	0.43
1:B:610:LEU:C	1:B:610:LEU:HD23	2.44	0.43
1:C:186:SER:O	1:C:190:LEU:N	2.51	0.43
1:E:186:SER:O	1:E:190:LEU:N	2.51	0.43
1:F:287:ILE:O	1:F:291:VAL:HG23	2.17	0.43
1:H:27:THR:HG23	1:H:28:LEU:HD22	2.00	0.43
1:H:771:ILE:HD11	1:H:786:GLN:HB3	1.99	0.43
1:A:461:PHE:O	1:A:465:ASN:ND2	2.48	0.43
1:B:50:GLU:OE2	1:B:256:SER:OG	2.22	0.43
1:E:27:THR:HG23	1:E:28:LEU:HD22	2.00	0.43
1:H:186:SER:O	1:H:190:LEU:N	2.51	0.43
1:B:27:THR:HG23	1:B:28:LEU:HD22	2.00	0.43
1:B:140:TYR:HE1	1:B:144:ILE:HD11	1.83	0.43
1:D:140:TYR:HE1	1:D:144:ILE:HD11	1.83	0.43
1:F:610:LEU:C	1:F:610:LEU:HD23	2.44	0.43
1:G:771:ILE:HD11	1:G:786:GLN:HB3	1.99	0.43
1:E:181:GLN:OE1	1:E:181:GLN:N	2.41	0.43
1:G:792:GLU:O	1:G:793:SER:OG	2.33	0.43
1:B:412:ILE:O	1:B:415:VAL:N	2.51	0.43
1:D:352:SER:O	1:D:353:ILE:HB	2.19	0.43
1:D:610:LEU:C	1:D:610:LEU:HD23	2.44	0.43
1:F:263:LYS:N	1:F:264:PRO:CD	2.81	0.43
1:G:352:SER:O	1:G:353:ILE:HB	2.19	0.43
1:G:593:ARG:O	1:G:597:ARG:NE	2.49	0.43
1:A:546:LYS:HD3	1:B:511:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LEU:C	1:A:610:LEU:HD23	2.44	0.43
1:E:352:SER:O	1:E:353:ILE:HB	2.19	0.43
1:F:27:THR:HG23	1:F:28:LEU:HD22	2.00	0.43
1:F:186:SER:O	1:F:190:LEU:N	2.51	0.43
1:F:352:SER:O	1:F:353:ILE:HB	2.19	0.43
1:H:461:PHE:O	1:H:465:ASN:ND2	2.48	0.43
1:F:792:GLU:O	1:F:793:SER:OG	2.33	0.43
1:A:352:SER:O	1:A:353:ILE:HB	2.19	0.42
1:A:653:GLU:OE1	1:A:653:GLU:N	2.42	0.42
1:E:412:ILE:O	1:E:415:VAL:N	2.52	0.42
1:H:635:GLU:O	1:H:638:THR:OG1	2.34	0.42
1:C:352:SER:O	1:C:353:ILE:HB	2.19	0.42
1:G:27:THR:HG23	1:G:28:LEU:HD22	2.00	0.42
1:A:27:THR:HG23	1:A:28:LEU:HD22	2.00	0.42
1:A:412:ILE:O	1:A:415:VAL:N	2.52	0.42
1:C:140:TYR:HE1	1:C:144:ILE:HD11	1.83	0.42
1:C:610:LEU:C	1:C:610:LEU:HD23	2.44	0.42
1:D:27:THR:HG23	1:D:28:LEU:HD22	2.00	0.42
1:E:273:GLU:OE1	1:E:273:GLU:N	2.44	0.42
1:G:186:SER:O	1:G:190:LEU:N	2.51	0.42
1:G:610:LEU:HD23	1:G:610:LEU:C	2.44	0.42
1:H:181:GLN:OE1	1:H:181:GLN:N	2.41	0.42
1:A:66:ASN:ND2	1:A:74:LEU:O	2.50	0.42
1:C:412:ILE:O	1:C:415:VAL:N	2.51	0.42
1:D:635:GLU:O	1:D:638:THR:OG1	2.34	0.42
1:F:105:GLU:OE2	1:F:129:ASN:ND2	2.50	0.42
1:H:352:SER:O	1:H:353:ILE:HB	2.19	0.42
1:B:186:SER:O	1:B:190:LEU:N	2.51	0.42
1:C:235:ILE:HD13	1:C:277:LEU:HD11	2.02	0.42
1:D:105:GLU:OE2	1:D:129:ASN:ND2	2.50	0.42
1:G:536:LEU:C	1:G:536:LEU:HD12	2.45	0.42
1:H:101:THR:HG1	1:H:213:ARG:H	1.67	0.42
1:H:412:ILE:O	1:H:415:VAL:N	2.51	0.42
1:B:536:LEU:C	1:B:536:LEU:HD12	2.45	0.42
1:F:771:ILE:HD11	1:F:786:GLN:HB3	1.99	0.42
1:H:610:LEU:C	1:H:610:LEU:HD23	2.44	0.42
1:A:113:LEU:O	1:A:117:LYS:N	2.50	0.42
1:B:235:ILE:HD13	1:B:277:LEU:HD11	2.02	0.42
1:D:235:ILE:HD13	1:D:277:LEU:HD11	2.02	0.42
1:G:66:ASN:ND2	1:G:74:LEU:O	2.50	0.42
1:A:235:ILE:HD13	1:A:277:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:610:LEU:HD23	1:E:610:LEU:C	2.44	0.42
1:C:66:ASN:ND2	1:C:74:LEU:O	2.50	0.42
1:D:536:LEU:C	1:D:536:LEU:HD12	2.45	0.42
1:B:64:LEU:HD21	1:B:296:ASN:CG	2.45	0.42
1:G:143:LYS:O	1:G:147:GLU:N	2.41	0.42
1:G:412:ILE:O	1:G:415:VAL:N	2.51	0.42
1:G:784:PHE:CE2	1:H:609:ARG:HD3	2.55	0.42
1:C:64:LEU:HD21	1:C:296:ASN:CG	2.45	0.41
1:D:101:THR:HG1	1:D:213:ARG:H	1.65	0.41
1:E:235:ILE:HD13	1:E:277:LEU:HD11	2.02	0.41
1:E:390:ARG:NH2	1:F:12:ARG:NH1	2.67	0.41
1:F:101:THR:OG1	1:F:213:ARG:N	2.50	0.41
1:H:166:LEU:O	1:H:170:PHE:N	2.44	0.41
1:B:352:SER:O	1:B:353:ILE:HB	2.19	0.41
1:D:143:LYS:O	1:D:147:GLU:N	2.41	0.41
1:F:64:LEU:HD21	1:F:296:ASN:CG	2.45	0.41
1:A:64:LEU:HD21	1:A:296:ASN:CG	2.45	0.41
1:C:536:LEU:HD12	1:C:536:LEU:C	2.45	0.41
1:H:101:THR:OG1	1:H:213:ARG:N	2.50	0.41
1:H:343:ASN:CG	1:H:345:SER:HG	2.24	0.41
1:E:343:ASN:CG	1:E:345:SER:HG	2.22	0.41
1:E:536:LEU:HD12	1:E:536:LEU:C	2.45	0.41
1:F:235:ILE:HD13	1:F:277:LEU:HD11	2.02	0.41
1:H:64:LEU:HD21	1:H:296:ASN:CG	2.45	0.41
1:D:101:THR:OG1	1:D:213:ARG:N	2.50	0.41
1:F:119:LEU:HD11	1:F:160:ALA:HA	2.03	0.41
1:G:456:ILE:CD1	1:H:608:TYR:CD2	3.03	0.41
1:B:186:SER:CB	1:C:396:TYR:CZ	3.03	0.41
1:B:653:GLU:OE1	1:B:653:GLU:N	2.42	0.41
1:E:64:LEU:HD21	1:E:296:ASN:CG	2.45	0.41
1:F:536:LEU:C	1:F:536:LEU:HD12	2.45	0.41
1:A:50:GLU:N	1:A:50:GLU:OE1	2.54	0.41
1:A:569:TYR:CE2	1:H:552:HIS:CE1	3.08	0.41
1:D:64:LEU:HD21	1:D:296:ASN:CG	2.45	0.41
1:E:105:GLU:OE2	1:E:129:ASN:ND2	2.50	0.41
1:E:727:ILE:HG23	1:E:728:LEU:N	2.36	0.41
1:H:727:ILE:HG23	1:H:728:LEU:N	2.36	0.41
1:E:166:LEU:O	1:E:170:PHE:N	2.44	0.41
1:F:343:ASN:CG	1:F:345:SER:HG	2.23	0.41
1:F:727:ILE:HG23	1:F:728:LEU:N	2.36	0.41
1:G:57:PHE:CE1	1:G:82:THR:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:ILE:HD13	1:G:277:LEU:HD11	2.02	0.41
1:B:727:ILE:HG23	1:B:728:LEU:N	2.36	0.41
1:C:50:GLU:N	1:C:50:GLU:OE1	2.54	0.41
1:D:412:ILE:O	1:D:415:VAL:N	2.51	0.41
1:E:50:GLU:OE1	1:E:50:GLU:N	2.54	0.41
1:E:101:THR:HG1	1:E:213:ARG:H	1.66	0.41
1:E:260:CYS:SG	1:E:262:LEU:HD21	2.61	0.41
1:E:635:GLU:O	1:E:638:THR:OG1	2.34	0.41
1:F:50:GLU:N	1:F:50:GLU:OE1	2.54	0.41
1:F:57:PHE:CE1	1:F:82:THR:HG22	2.56	0.41
1:H:50:GLU:OE1	1:H:50:GLU:N	2.54	0.41
1:H:235:ILE:HD13	1:H:277:LEU:HD11	2.02	0.41
1:H:536:LEU:HD12	1:H:536:LEU:C	2.45	0.41
1:H:593:ARG:O	1:H:597:ARG:NE	2.49	0.41
1:A:536:LEU:HD12	1:A:536:LEU:C	2.45	0.41
1:A:546:LYS:NZ	1:B:511:ILE:HG21	2.36	0.41
1:B:443:LEU:O	1:B:446:THR:OG1	2.39	0.41
1:C:119:LEU:HD11	1:C:160:ALA:HA	2.03	0.41
1:D:119:LEU:HD11	1:D:160:ALA:HA	2.03	0.41
1:H:260:CYS:SG	1:H:262:LEU:HD21	2.61	0.41
1:C:57:PHE:CE1	1:C:82:THR:HG22	2.56	0.40
1:C:127:ASN:OD1	1:C:128:ILE:N	2.55	0.40
1:D:57:PHE:CE1	1:D:82:THR:HG22	2.56	0.40
1:D:260:CYS:SG	1:D:262:LEU:HD21	2.61	0.40
1:G:50:GLU:OE1	1:G:50:GLU:N	2.54	0.40
1:G:64:LEU:HD22	1:G:330:GLY:HA3	2.04	0.40
1:A:119:LEU:HD11	1:A:160:ALA:HA	2.03	0.40
1:A:727:ILE:HG23	1:A:728:LEU:N	2.36	0.40
1:B:425:GLU:OE1	1:B:425:GLU:N	2.43	0.40
1:D:727:ILE:HG23	1:D:728:LEU:N	2.36	0.40
1:E:119:LEU:HD11	1:E:160:ALA:CA	2.51	0.40
1:E:461:PHE:O	1:E:465:ASN:ND2	2.48	0.40
1:F:127:ASN:OD1	1:F:128:ILE:N	2.55	0.40
1:G:64:LEU:HD21	1:G:296:ASN:CG	2.45	0.40
1:H:113:LEU:O	1:H:117:LYS:N	2.50	0.40
1:A:64:LEU:HD22	1:A:330:GLY:HA3	2.03	0.40
1:A:260:CYS:SG	1:A:262:LEU:HD21	2.61	0.40
1:A:792:GLU:OE1	1:A:792:GLU:N	2.46	0.40
1:B:66:ASN:ND2	1:B:74:LEU:O	2.50	0.40
1:B:260:CYS:SG	1:B:262:LEU:HD21	2.61	0.40
1:C:727:ILE:HG23	1:C:728:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LEU:HD11	1:D:160:ALA:CA	2.51	0.40
1:G:166:LEU:O	1:G:170:PHE:N	2.44	0.40
1:G:490:GLU:OE2	1:G:606:GLN:NE2	2.47	0.40
1:B:761:LYS:HD2	1:B:764:ILE:HD11	2.04	0.40
1:C:771:ILE:HD11	1:C:786:GLN:CB	2.52	0.40
1:D:50:GLU:N	1:D:50:GLU:OE1	2.54	0.40
1:E:57:PHE:CE1	1:E:82:THR:HG22	2.56	0.40
1:F:66:ASN:ND2	1:F:74:LEU:O	2.50	0.40
1:F:260:CYS:SG	1:F:262:LEU:HD21	2.61	0.40
1:G:119:LEU:HD11	1:G:160:ALA:CA	2.51	0.40
1:G:727:ILE:HG23	1:G:728:LEU:N	2.36	0.40
1:A:105:GLU:OE2	1:A:129:ASN:ND2	2.50	0.40
1:B:64:LEU:HD22	1:B:330:GLY:HA3	2.03	0.40
1:B:119:LEU:HD11	1:B:160:ALA:CA	2.51	0.40
1:D:64:LEU:HD22	1:D:330:GLY:HA3	2.03	0.40
1:D:761:LYS:HD2	1:D:764:ILE:HD11	2.04	0.40
1:E:66:ASN:ND2	1:E:74:LEU:O	2.50	0.40
1:G:127:ASN:OD1	1:G:128:ILE:N	2.55	0.40
1:G:260:CYS:SG	1:G:262:LEU:HD21	2.61	0.40
1:H:119:LEU:HD11	1:H:160:ALA:HA	2.03	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 PDB entries followed by that with respect to all EM entries.

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	790/820 (96%)	775 (98%)	15 (2%)	0	100	100
1	B	790/820 (96%)	776 (98%)	14 (2%)	0	100	100
1	C	790/820 (96%)	776 (98%)	14 (2%)	0	100	100
1	D	790/820 (96%)	776 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	790/820 (96%)	776 (98%)	14 (2%)	0	100	100
1	F	790/820 (96%)	775 (98%)	15 (2%)	0	100	100
1	G	790/820 (96%)	776 (98%)	14 (2%)	0	100	100
1	H	790/820 (96%)	776 (98%)	14 (2%)	0	100	100
All	All	6320/6560 (96%)	6206 (98%)	114 (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 PDB entries followed by that with respect to all EM entries.

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	689/714 (96%)	686 (100%)	3 (0%)	84	83
1	B	689/714 (96%)	686 (100%)	3 (0%)	84	83
1	C	689/714 (96%)	686 (100%)	3 (0%)	84	83
1	D	689/714 (96%)	686 (100%)	3 (0%)	84	83
1	E	689/714 (96%)	686 (100%)	3 (0%)	84	83
1	F	689/714 (96%)	686 (100%)	3 (0%)	84	83
1	G	689/714 (96%)	686 (100%)	3 (0%)	84	83
1	H	689/714 (96%)	686 (100%)	3 (0%)	84	83
All	All	5512/5712 (96%)	5488 (100%)	24 (0%)	81	83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	396	TYR
1	A	605	HIS
1	B	139	GLN
1	B	396	TYR
1	B	605	HIS

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Mol	Chain	Res	Type
1	C	139	GLN
1	C	396	TYR
1	C	605	HIS
1	D	139	GLN
1	D	396	TYR
1	D	605	HIS
1	E	139	GLN
1	E	396	TYR
1	E	605	HIS
1	F	139	GLN
1	F	396	TYR
1	F	605	HIS
1	G	139	GLN
1	G	396	TYR
1	G	605	HIS
1	H	139	GLN
1	H	396	TYR
1	H	605	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	152	ASN
1	A	161	ASN
1	A	322	ASN
1	A	460	GLN
1	A	492	GLN
1	A	505	GLN
1	A	552	HIS
1	A	670	GLN
1	B	87	HIS
1	B	152	ASN
1	B	161	ASN
1	B	207	ASN
1	B	460	GLN
1	B	492	GLN
1	B	505	GLN
1	B	634	ASN
1	B	670	GLN
1	C	17	GLN
1	C	87	HIS

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Mol	Chain	Res	Type
1	C	152	ASN
1	C	161	ASN
1	C	460	GLN
1	C	505	GLN
1	C	670	GLN
1	D	87	HIS
1	D	152	ASN
1	D	161	ASN
1	D	322	ASN
1	D	460	GLN
1	D	492	GLN
1	D	505	GLN
1	D	552	HIS
1	D	666	GLN
1	D	670	GLN
1	E	87	HIS
1	E	152	ASN
1	E	161	ASN
1	E	207	ASN
1	E	322	ASN
1	E	460	GLN
1	E	492	GLN
1	E	505	GLN
1	E	666	GLN
1	E	670	GLN
1	E	710	ASN
1	F	87	HIS
1	F	152	ASN
1	F	161	ASN
1	F	460	GLN
1	F	492	GLN
1	F	505	GLN
1	F	634	ASN
1	F	666	GLN
1	F	670	GLN
1	G	17	GLN
1	G	87	HIS
1	G	152	ASN
1	G	161	ASN
1	G	207	ASN
1	G	460	GLN
1	G	492	GLN

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Mol	Chain	Res	Type
1	G	505	GLN
1	G	634	ASN
1	G	670	GLN
1	H	17	GLN
1	H	87	HIS
1	H	152	ASN
1	H	161	ASN
1	H	207	ASN
1	H	322	ASN
1	H	369	GLN
1	H	460	GLN
1	H	492	GLN
1	H	505	GLN
1	H	552	HIS
1	H	670	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.