



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2022 – 02:17 PM EST

PDB ID : 7M0I
Title : Crystal structure of a human metapneumovirus subtype B2 trimeric fusion protein
Authors : Huang, J.; Mousa, J.J.
Deposited on : 2021-03-11
Resolution : 2.81 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.25
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.25

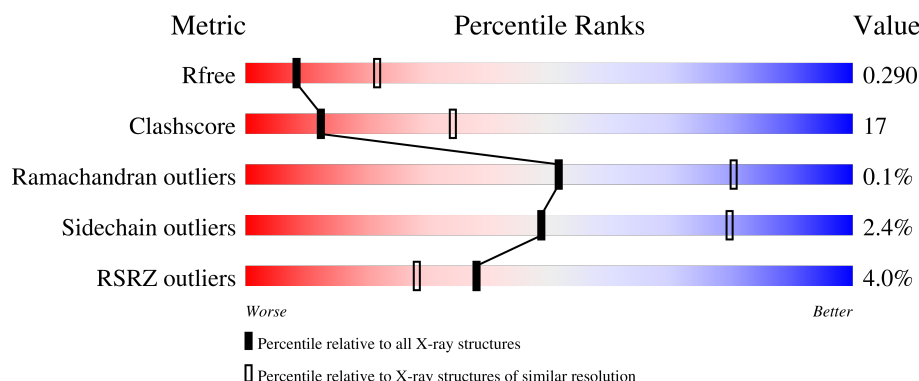
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	89	<div> <div>%</div> <div>54% 25% 21%</div> </div>
1	C	89	<div> <div>2%</div> <div>47% 31% 21%</div> </div>
1	E	89	<div> <div>%</div> <div>56% 21% 21%</div> </div>
1	G	89	<div> <div>%</div> <div>55% 20% 21%</div> </div>
1	I	89	<div> <div>58% 20% 21%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	89	
2	B	431	
2	D	431	
2	F	431	
2	H	431	
2	J	431	
2	L	431	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	201	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19556 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	70	Total	C	N	O	S	0	0	0
			544	341	84	117	2			
1	I	70	Total	C	N	O	S	0	0	0
			544	341	84	117	2			
1	K	70	Total	C	N	O	S	0	0	0
			536	335	82	117	2			
1	A	70	Total	C	N	O	S	0	0	0
			540	338	83	117	2			
1	C	70	Total	C	N	O	S	0	0	0
			544	341	84	117	2			
1	E	70	Total	C	N	O	S	0	0	0
			544	341	84	117	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	19	LEU	-	expression tag	UNP C6F474
G	20	LYS	-	expression tag	UNP C6F474
G	21	GLU	-	expression tag	UNP C6F474
G	22	SER	-	expression tag	UNP C6F474
G	102	LYS	-	expression tag	UNP C6F474
G	103	LYS	-	expression tag	UNP C6F474
G	104	ARG	-	expression tag	UNP C6F474
G	105	LYS	-	expression tag	UNP C6F474
G	106	ARG	-	expression tag	UNP C6F474
G	107	ARG	-	expression tag	UNP C6F474
I	19	LEU	-	expression tag	UNP C6F474
I	20	LYS	-	expression tag	UNP C6F474
I	21	GLU	-	expression tag	UNP C6F474
I	22	SER	-	expression tag	UNP C6F474
I	102	LYS	-	expression tag	UNP C6F474
I	103	LYS	-	expression tag	UNP C6F474
I	104	ARG	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
I	105	LYS	-	expression tag	UNP C6F474
I	106	ARG	-	expression tag	UNP C6F474
I	107	ARG	-	expression tag	UNP C6F474
K	19	LEU	-	expression tag	UNP C6F474
K	20	LYS	-	expression tag	UNP C6F474
K	21	GLU	-	expression tag	UNP C6F474
K	22	SER	-	expression tag	UNP C6F474
K	102	LYS	-	expression tag	UNP C6F474
K	103	LYS	-	expression tag	UNP C6F474
K	104	ARG	-	expression tag	UNP C6F474
K	105	LYS	-	expression tag	UNP C6F474
K	106	ARG	-	expression tag	UNP C6F474
K	107	ARG	-	expression tag	UNP C6F474
A	19	LEU	-	expression tag	UNP C6F474
A	20	LYS	-	expression tag	UNP C6F474
A	21	GLU	-	expression tag	UNP C6F474
A	22	SER	-	expression tag	UNP C6F474
A	102	LYS	-	expression tag	UNP C6F474
A	103	LYS	-	expression tag	UNP C6F474
A	104	ARG	-	expression tag	UNP C6F474
A	105	LYS	-	expression tag	UNP C6F474
A	106	ARG	-	expression tag	UNP C6F474
A	107	ARG	-	expression tag	UNP C6F474
C	19	LEU	-	expression tag	UNP C6F474
C	20	LYS	-	expression tag	UNP C6F474
C	21	GLU	-	expression tag	UNP C6F474
C	22	SER	-	expression tag	UNP C6F474
C	102	LYS	-	expression tag	UNP C6F474
C	103	LYS	-	expression tag	UNP C6F474
C	104	ARG	-	expression tag	UNP C6F474
C	105	LYS	-	expression tag	UNP C6F474
C	106	ARG	-	expression tag	UNP C6F474
C	107	ARG	-	expression tag	UNP C6F474
E	19	LEU	-	expression tag	UNP C6F474
E	20	LYS	-	expression tag	UNP C6F474
E	21	GLU	-	expression tag	UNP C6F474
E	22	SER	-	expression tag	UNP C6F474
E	102	LYS	-	expression tag	UNP C6F474
E	103	LYS	-	expression tag	UNP C6F474
E	104	ARG	-	expression tag	UNP C6F474
E	105	LYS	-	expression tag	UNP C6F474
E	106	ARG	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
E	107	ARG	-	expression tag	UNP C6F474

- Molecule 2 is a protein called Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	352	Total	C	N	O	S	0	0	0
			2677	1674	462	522	19			
2	J	352	Total	C	N	O	S	0	0	0
			2663	1664	458	522	19			
2	L	352	Total	C	N	O	S	0	0	0
			2677	1674	462	522	19			
2	B	351	Total	C	N	O	S	0	0	0
			2666	1667	460	520	19			
2	D	352	Total	C	N	O	S	0	0	0
			2668	1664	463	522	19			
2	F	351	Total	C	N	O	S	0	0	0
			2676	1673	464	520	19			

There are 318 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	490	SER	-	expression tag	UNP C6F474
H	491	GLY	-	expression tag	UNP C6F474
H	492	ARG	-	expression tag	UNP C6F474
H	493	GLU	-	expression tag	UNP C6F474
H	494	ASN	-	expression tag	UNP C6F474
H	495	LEU	-	expression tag	UNP C6F474
H	496	TYR	-	expression tag	UNP C6F474
H	497	PHE	-	expression tag	UNP C6F474
H	498	GLN	-	expression tag	UNP C6F474
H	499	GLY	-	expression tag	UNP C6F474
H	500	GLY	-	expression tag	UNP C6F474
H	501	GLY	-	expression tag	UNP C6F474
H	502	GLY	-	expression tag	UNP C6F474
H	503	GLY	-	expression tag	UNP C6F474
H	504	SER	-	expression tag	UNP C6F474
H	505	GLY	-	expression tag	UNP C6F474
H	506	TYR	-	expression tag	UNP C6F474
H	507	ILE	-	expression tag	UNP C6F474
H	508	PRO	-	expression tag	UNP C6F474
H	509	GLU	-	expression tag	UNP C6F474
H	510	ALA	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
H	511	PRO	-	expression tag	UNP C6F474
H	512	ARG	-	expression tag	UNP C6F474
H	513	ASP	-	expression tag	UNP C6F474
H	514	GLN	-	expression tag	UNP C6F474
H	515	ALA	-	expression tag	UNP C6F474
H	516	TYR	-	expression tag	UNP C6F474
H	517	VAL	-	expression tag	UNP C6F474
H	518	ARG	-	expression tag	UNP C6F474
H	519	LYS	-	expression tag	UNP C6F474
H	520	ASP	-	expression tag	UNP C6F474
H	521	GLY	-	expression tag	UNP C6F474
H	522	GLU	-	expression tag	UNP C6F474
H	523	TRP	-	expression tag	UNP C6F474
H	524	VAL	-	expression tag	UNP C6F474
H	525	LEU	-	expression tag	UNP C6F474
H	526	LEU	-	expression tag	UNP C6F474
H	527	SER	-	expression tag	UNP C6F474
H	528	THR	-	expression tag	UNP C6F474
H	529	PHE	-	expression tag	UNP C6F474
H	530	LEU	-	expression tag	UNP C6F474
H	531	GLY	-	expression tag	UNP C6F474
H	532	GLY	-	expression tag	UNP C6F474
H	533	THR	-	expression tag	UNP C6F474
H	534	GLU	-	expression tag	UNP C6F474
H	535	GLY	-	expression tag	UNP C6F474
H	536	ARG	-	expression tag	UNP C6F474
H	537	HIS	-	expression tag	UNP C6F474
H	538	HIS	-	expression tag	UNP C6F474
H	539	HIS	-	expression tag	UNP C6F474
H	540	HIS	-	expression tag	UNP C6F474
H	541	HIS	-	expression tag	UNP C6F474
H	542	HIS	-	expression tag	UNP C6F474
J	490	SER	-	expression tag	UNP C6F474
J	491	GLY	-	expression tag	UNP C6F474
J	492	ARG	-	expression tag	UNP C6F474
J	493	GLU	-	expression tag	UNP C6F474
J	494	ASN	-	expression tag	UNP C6F474
J	495	LEU	-	expression tag	UNP C6F474
J	496	TYR	-	expression tag	UNP C6F474
J	497	PHE	-	expression tag	UNP C6F474
J	498	GLN	-	expression tag	UNP C6F474
J	499	GLY	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
J	500	GLY	-	expression tag	UNP C6F474
J	501	GLY	-	expression tag	UNP C6F474
J	502	GLY	-	expression tag	UNP C6F474
J	503	GLY	-	expression tag	UNP C6F474
J	504	SER	-	expression tag	UNP C6F474
J	505	GLY	-	expression tag	UNP C6F474
J	506	TYR	-	expression tag	UNP C6F474
J	507	ILE	-	expression tag	UNP C6F474
J	508	PRO	-	expression tag	UNP C6F474
J	509	GLU	-	expression tag	UNP C6F474
J	510	ALA	-	expression tag	UNP C6F474
J	511	PRO	-	expression tag	UNP C6F474
J	512	ARG	-	expression tag	UNP C6F474
J	513	ASP	-	expression tag	UNP C6F474
J	514	GLN	-	expression tag	UNP C6F474
J	515	ALA	-	expression tag	UNP C6F474
J	516	TYR	-	expression tag	UNP C6F474
J	517	VAL	-	expression tag	UNP C6F474
J	518	ARG	-	expression tag	UNP C6F474
J	519	LYS	-	expression tag	UNP C6F474
J	520	ASP	-	expression tag	UNP C6F474
J	521	GLY	-	expression tag	UNP C6F474
J	522	GLU	-	expression tag	UNP C6F474
J	523	TRP	-	expression tag	UNP C6F474
J	524	VAL	-	expression tag	UNP C6F474
J	525	LEU	-	expression tag	UNP C6F474
J	526	LEU	-	expression tag	UNP C6F474
J	527	SER	-	expression tag	UNP C6F474
J	528	THR	-	expression tag	UNP C6F474
J	529	PHE	-	expression tag	UNP C6F474
J	530	LEU	-	expression tag	UNP C6F474
J	531	GLY	-	expression tag	UNP C6F474
J	532	GLY	-	expression tag	UNP C6F474
J	533	THR	-	expression tag	UNP C6F474
J	534	GLU	-	expression tag	UNP C6F474
J	535	GLY	-	expression tag	UNP C6F474
J	536	ARG	-	expression tag	UNP C6F474
J	537	HIS	-	expression tag	UNP C6F474
J	538	HIS	-	expression tag	UNP C6F474
J	539	HIS	-	expression tag	UNP C6F474
J	540	HIS	-	expression tag	UNP C6F474
J	541	HIS	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
J	542	HIS	-	expression tag	UNP C6F474
L	490	SER	-	expression tag	UNP C6F474
L	491	GLY	-	expression tag	UNP C6F474
L	492	ARG	-	expression tag	UNP C6F474
L	493	GLU	-	expression tag	UNP C6F474
L	494	ASN	-	expression tag	UNP C6F474
L	495	LEU	-	expression tag	UNP C6F474
L	496	TYR	-	expression tag	UNP C6F474
L	497	PHE	-	expression tag	UNP C6F474
L	498	GLN	-	expression tag	UNP C6F474
L	499	GLY	-	expression tag	UNP C6F474
L	500	GLY	-	expression tag	UNP C6F474
L	501	GLY	-	expression tag	UNP C6F474
L	502	GLY	-	expression tag	UNP C6F474
L	503	GLY	-	expression tag	UNP C6F474
L	504	SER	-	expression tag	UNP C6F474
L	505	GLY	-	expression tag	UNP C6F474
L	506	TYR	-	expression tag	UNP C6F474
L	507	ILE	-	expression tag	UNP C6F474
L	508	PRO	-	expression tag	UNP C6F474
L	509	GLU	-	expression tag	UNP C6F474
L	510	ALA	-	expression tag	UNP C6F474
L	511	PRO	-	expression tag	UNP C6F474
L	512	ARG	-	expression tag	UNP C6F474
L	513	ASP	-	expression tag	UNP C6F474
L	514	GLN	-	expression tag	UNP C6F474
L	515	ALA	-	expression tag	UNP C6F474
L	516	TYR	-	expression tag	UNP C6F474
L	517	VAL	-	expression tag	UNP C6F474
L	518	ARG	-	expression tag	UNP C6F474
L	519	LYS	-	expression tag	UNP C6F474
L	520	ASP	-	expression tag	UNP C6F474
L	521	GLY	-	expression tag	UNP C6F474
L	522	GLU	-	expression tag	UNP C6F474
L	523	TRP	-	expression tag	UNP C6F474
L	524	VAL	-	expression tag	UNP C6F474
L	525	LEU	-	expression tag	UNP C6F474
L	526	LEU	-	expression tag	UNP C6F474
L	527	SER	-	expression tag	UNP C6F474
L	528	THR	-	expression tag	UNP C6F474
L	529	PHE	-	expression tag	UNP C6F474
L	530	LEU	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
L	531	GLY	-	expression tag	UNP C6F474
L	532	GLY	-	expression tag	UNP C6F474
L	533	THR	-	expression tag	UNP C6F474
L	534	GLU	-	expression tag	UNP C6F474
L	535	GLY	-	expression tag	UNP C6F474
L	536	ARG	-	expression tag	UNP C6F474
L	537	HIS	-	expression tag	UNP C6F474
L	538	HIS	-	expression tag	UNP C6F474
L	539	HIS	-	expression tag	UNP C6F474
L	540	HIS	-	expression tag	UNP C6F474
L	541	HIS	-	expression tag	UNP C6F474
L	542	HIS	-	expression tag	UNP C6F474
B	490	SER	-	expression tag	UNP C6F474
B	491	GLY	-	expression tag	UNP C6F474
B	492	ARG	-	expression tag	UNP C6F474
B	493	GLU	-	expression tag	UNP C6F474
B	494	ASN	-	expression tag	UNP C6F474
B	495	LEU	-	expression tag	UNP C6F474
B	496	TYR	-	expression tag	UNP C6F474
B	497	PHE	-	expression tag	UNP C6F474
B	498	GLN	-	expression tag	UNP C6F474
B	499	GLY	-	expression tag	UNP C6F474
B	500	GLY	-	expression tag	UNP C6F474
B	501	GLY	-	expression tag	UNP C6F474
B	502	GLY	-	expression tag	UNP C6F474
B	503	GLY	-	expression tag	UNP C6F474
B	504	SER	-	expression tag	UNP C6F474
B	505	GLY	-	expression tag	UNP C6F474
B	506	TYR	-	expression tag	UNP C6F474
B	507	ILE	-	expression tag	UNP C6F474
B	508	PRO	-	expression tag	UNP C6F474
B	509	GLU	-	expression tag	UNP C6F474
B	510	ALA	-	expression tag	UNP C6F474
B	511	PRO	-	expression tag	UNP C6F474
B	512	ARG	-	expression tag	UNP C6F474
B	513	ASP	-	expression tag	UNP C6F474
B	514	GLN	-	expression tag	UNP C6F474
B	515	ALA	-	expression tag	UNP C6F474
B	516	TYR	-	expression tag	UNP C6F474
B	517	VAL	-	expression tag	UNP C6F474
B	518	ARG	-	expression tag	UNP C6F474
B	519	LYS	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
B	520	ASP	-	expression tag	UNP C6F474
B	521	GLY	-	expression tag	UNP C6F474
B	522	GLU	-	expression tag	UNP C6F474
B	523	TRP	-	expression tag	UNP C6F474
B	524	VAL	-	expression tag	UNP C6F474
B	525	LEU	-	expression tag	UNP C6F474
B	526	LEU	-	expression tag	UNP C6F474
B	527	SER	-	expression tag	UNP C6F474
B	528	THR	-	expression tag	UNP C6F474
B	529	PHE	-	expression tag	UNP C6F474
B	530	LEU	-	expression tag	UNP C6F474
B	531	GLY	-	expression tag	UNP C6F474
B	532	GLY	-	expression tag	UNP C6F474
B	533	THR	-	expression tag	UNP C6F474
B	534	GLU	-	expression tag	UNP C6F474
B	535	GLY	-	expression tag	UNP C6F474
B	536	ARG	-	expression tag	UNP C6F474
B	537	HIS	-	expression tag	UNP C6F474
B	538	HIS	-	expression tag	UNP C6F474
B	539	HIS	-	expression tag	UNP C6F474
B	540	HIS	-	expression tag	UNP C6F474
B	541	HIS	-	expression tag	UNP C6F474
B	542	HIS	-	expression tag	UNP C6F474
D	490	SER	-	expression tag	UNP C6F474
D	491	GLY	-	expression tag	UNP C6F474
D	492	ARG	-	expression tag	UNP C6F474
D	493	GLU	-	expression tag	UNP C6F474
D	494	ASN	-	expression tag	UNP C6F474
D	495	LEU	-	expression tag	UNP C6F474
D	496	TYR	-	expression tag	UNP C6F474
D	497	PHE	-	expression tag	UNP C6F474
D	498	GLN	-	expression tag	UNP C6F474
D	499	GLY	-	expression tag	UNP C6F474
D	500	GLY	-	expression tag	UNP C6F474
D	501	GLY	-	expression tag	UNP C6F474
D	502	GLY	-	expression tag	UNP C6F474
D	503	GLY	-	expression tag	UNP C6F474
D	504	SER	-	expression tag	UNP C6F474
D	505	GLY	-	expression tag	UNP C6F474
D	506	TYR	-	expression tag	UNP C6F474
D	507	ILE	-	expression tag	UNP C6F474
D	508	PRO	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
D	509	GLU	-	expression tag	UNP C6F474
D	510	ALA	-	expression tag	UNP C6F474
D	511	PRO	-	expression tag	UNP C6F474
D	512	ARG	-	expression tag	UNP C6F474
D	513	ASP	-	expression tag	UNP C6F474
D	514	GLN	-	expression tag	UNP C6F474
D	515	ALA	-	expression tag	UNP C6F474
D	516	TYR	-	expression tag	UNP C6F474
D	517	VAL	-	expression tag	UNP C6F474
D	518	ARG	-	expression tag	UNP C6F474
D	519	LYS	-	expression tag	UNP C6F474
D	520	ASP	-	expression tag	UNP C6F474
D	521	GLY	-	expression tag	UNP C6F474
D	522	GLU	-	expression tag	UNP C6F474
D	523	TRP	-	expression tag	UNP C6F474
D	524	VAL	-	expression tag	UNP C6F474
D	525	LEU	-	expression tag	UNP C6F474
D	526	LEU	-	expression tag	UNP C6F474
D	527	SER	-	expression tag	UNP C6F474
D	528	THR	-	expression tag	UNP C6F474
D	529	PHE	-	expression tag	UNP C6F474
D	530	LEU	-	expression tag	UNP C6F474
D	531	GLY	-	expression tag	UNP C6F474
D	532	GLY	-	expression tag	UNP C6F474
D	533	THR	-	expression tag	UNP C6F474
D	534	GLU	-	expression tag	UNP C6F474
D	535	GLY	-	expression tag	UNP C6F474
D	536	ARG	-	expression tag	UNP C6F474
D	537	HIS	-	expression tag	UNP C6F474
D	538	HIS	-	expression tag	UNP C6F474
D	539	HIS	-	expression tag	UNP C6F474
D	540	HIS	-	expression tag	UNP C6F474
D	541	HIS	-	expression tag	UNP C6F474
D	542	HIS	-	expression tag	UNP C6F474
F	490	SER	-	expression tag	UNP C6F474
F	491	GLY	-	expression tag	UNP C6F474
F	492	ARG	-	expression tag	UNP C6F474
F	493	GLU	-	expression tag	UNP C6F474
F	494	ASN	-	expression tag	UNP C6F474
F	495	LEU	-	expression tag	UNP C6F474
F	496	TYR	-	expression tag	UNP C6F474
F	497	PHE	-	expression tag	UNP C6F474

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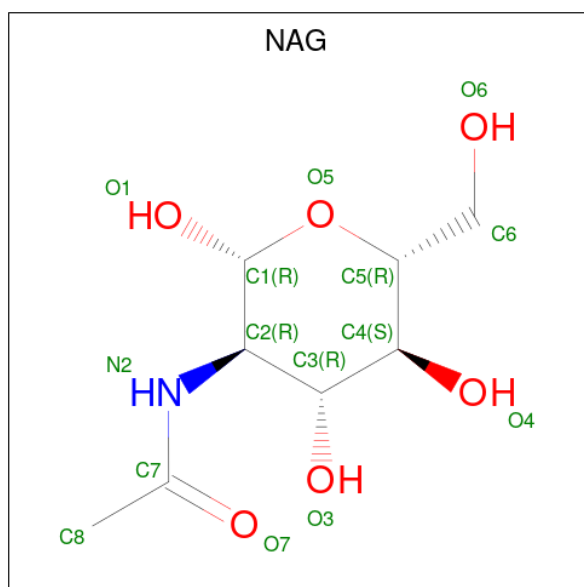
Chain	Residue	Modelled	Actual	Comment	Reference
F	498	GLN	-	expression tag	UNP C6F474
F	499	GLY	-	expression tag	UNP C6F474
F	500	GLY	-	expression tag	UNP C6F474
F	501	GLY	-	expression tag	UNP C6F474
F	502	GLY	-	expression tag	UNP C6F474
F	503	GLY	-	expression tag	UNP C6F474
F	504	SER	-	expression tag	UNP C6F474
F	505	GLY	-	expression tag	UNP C6F474
F	506	TYR	-	expression tag	UNP C6F474
F	507	ILE	-	expression tag	UNP C6F474
F	508	PRO	-	expression tag	UNP C6F474
F	509	GLU	-	expression tag	UNP C6F474
F	510	ALA	-	expression tag	UNP C6F474
F	511	PRO	-	expression tag	UNP C6F474
F	512	ARG	-	expression tag	UNP C6F474
F	513	ASP	-	expression tag	UNP C6F474
F	514	GLN	-	expression tag	UNP C6F474
F	515	ALA	-	expression tag	UNP C6F474
F	516	TYR	-	expression tag	UNP C6F474
F	517	VAL	-	expression tag	UNP C6F474
F	518	ARG	-	expression tag	UNP C6F474
F	519	LYS	-	expression tag	UNP C6F474
F	520	ASP	-	expression tag	UNP C6F474
F	521	GLY	-	expression tag	UNP C6F474
F	522	GLU	-	expression tag	UNP C6F474
F	523	TRP	-	expression tag	UNP C6F474
F	524	VAL	-	expression tag	UNP C6F474
F	525	LEU	-	expression tag	UNP C6F474
F	526	LEU	-	expression tag	UNP C6F474
F	527	SER	-	expression tag	UNP C6F474
F	528	THR	-	expression tag	UNP C6F474
F	529	PHE	-	expression tag	UNP C6F474
F	530	LEU	-	expression tag	UNP C6F474
F	531	GLY	-	expression tag	UNP C6F474
F	532	GLY	-	expression tag	UNP C6F474
F	533	THR	-	expression tag	UNP C6F474
F	534	GLU	-	expression tag	UNP C6F474
F	535	GLY	-	expression tag	UNP C6F474
F	536	ARG	-	expression tag	UNP C6F474
F	537	HIS	-	expression tag	UNP C6F474
F	538	HIS	-	expression tag	UNP C6F474
F	539	HIS	-	expression tag	UNP C6F474

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Chain	Residue	Modelled	Actual	Comment	Reference
F	540	HIS	-	expression tag	UNP C6F474
F	541	HIS	-	expression tag	UNP C6F474
F	542	HIS	-	expression tag	UNP C6F474

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

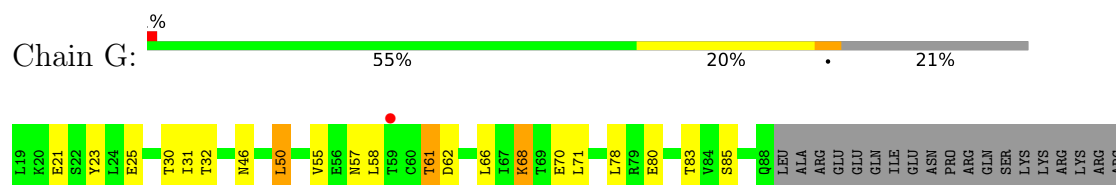
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		
4	I	2	Total	O	0	0
			2	2		
4	J	4	Total	O	0	0
			4	4		
4	L	6	Total	O	0	0
			6	6		
4	B	5	Total	O	0	0
			5	5		
4	C	2	Total	O	0	0
			2	2		
4	D	4	Total	O	0	0
			4	4		
4	F	1	Total	O	0	0
			1	1		

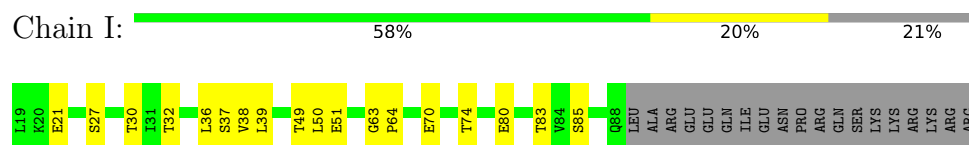
3 Residue-property plots [i](#)

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

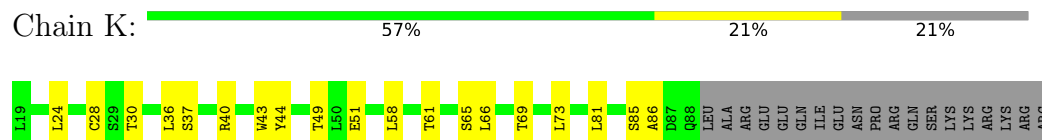
- Molecule 1: Fusion glycoprotein F2



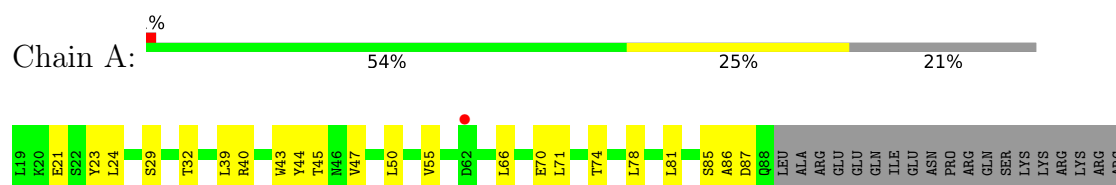
- Molecule 1: Fusion glycoprotein F2



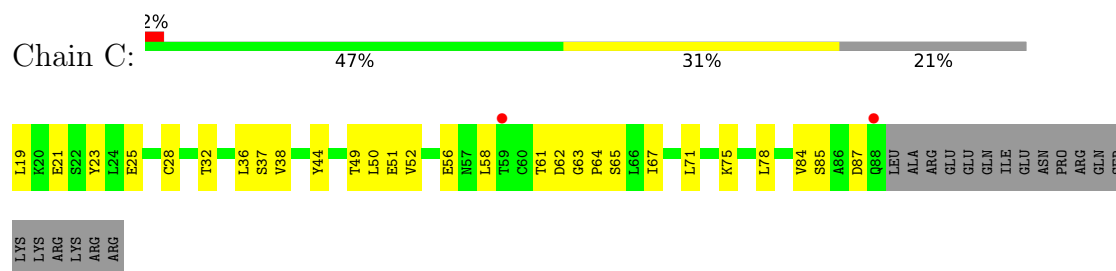
- Molecule 1: Fusion glycoprotein F2



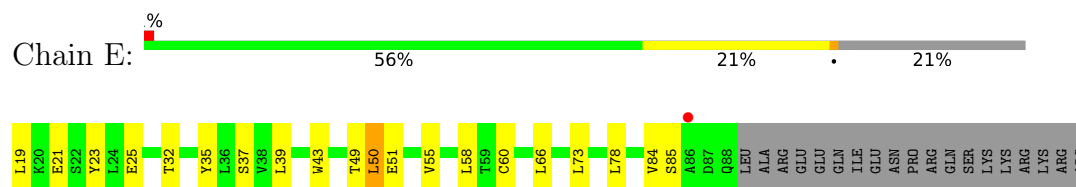
- Molecule 1: Fusion glycoprotein F2



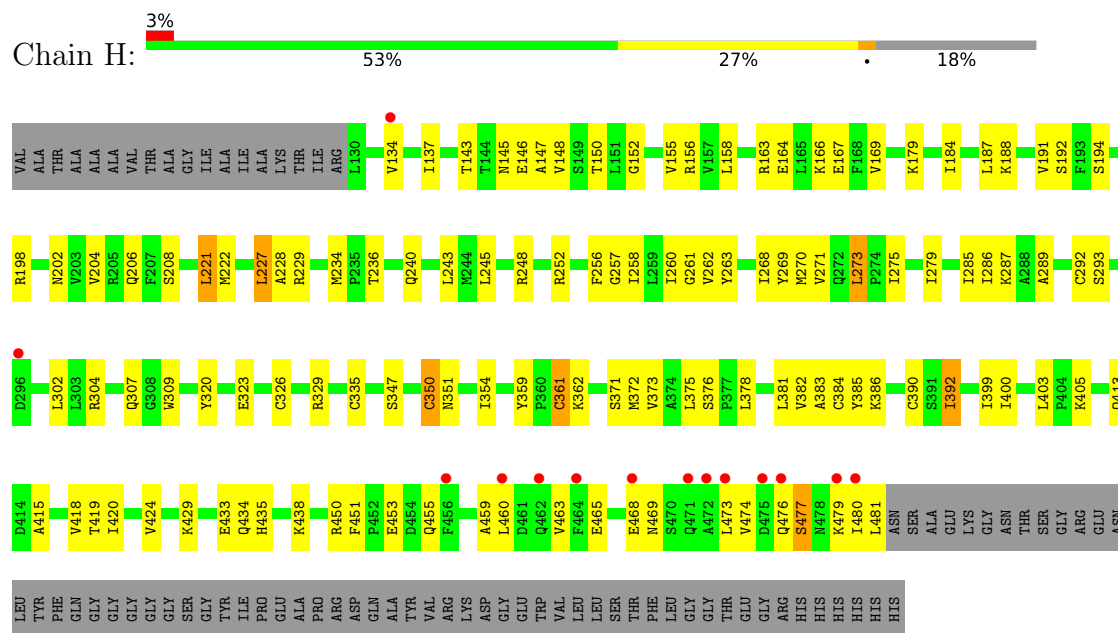
- Molecule 1: Fusion glycoprotein F2



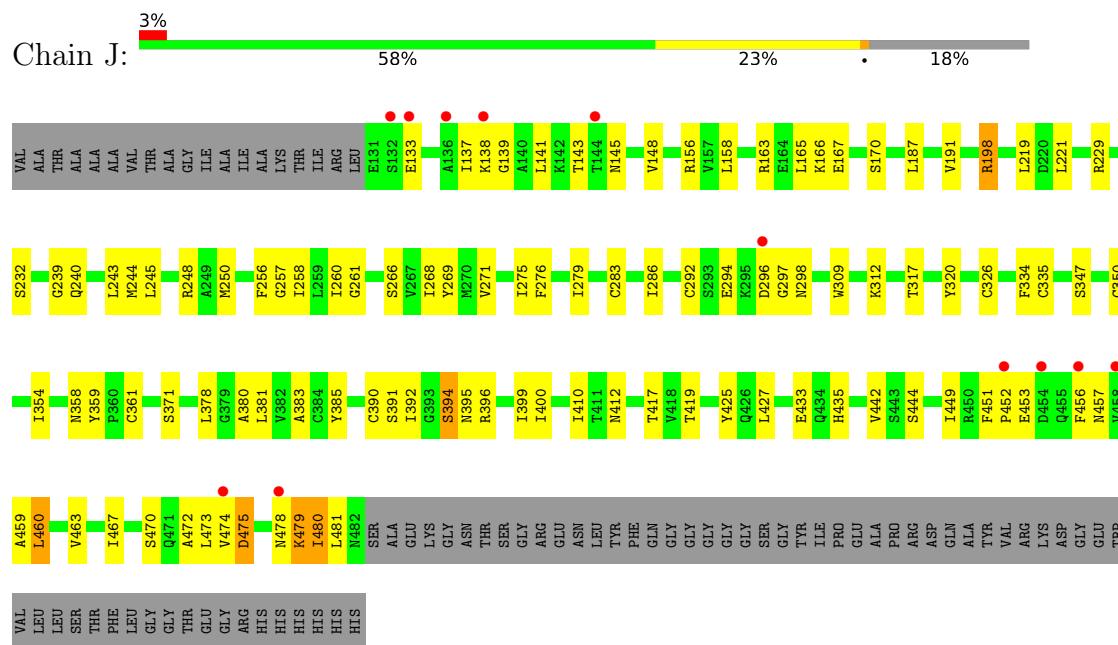
- Molecule 1: Fusion glycoprotein F2



- Molecule 2: Fusion glycoprotein F1



- Molecule 2: Fusion glycoprotein F1



- Molecule 2: Fusion glycoprotein F1

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	114.53Å 128.10Å 431.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.81 49.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	75.5 (49.69-2.81) 75.6 (49.69-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.254 , 0.291 0.254 , 0.290	Depositor DCC
R_{free} test set	5880 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	19556	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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](#)

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

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	0.61	0/546	0.90	0/743
1	C	0.63	0/550	0.94	1/747 (0.1%)
1	E	0.62	0/550	0.87	1/747 (0.1%)
1	G	0.75	0/550	0.96	1/747 (0.1%)
1	I	0.61	0/550	0.94	0/747
1	K	0.56	0/542	0.89	2/739 (0.3%)
2	B	0.64	1/2708 (0.0%)	0.92	5/3672 (0.1%)
2	D	0.57	1/2709 (0.0%)	0.85	3/3674 (0.1%)
2	F	0.61	0/2718	0.96	8/3683 (0.2%)
2	H	0.69	3/2719 (0.1%)	0.97	8/3687 (0.2%)
2	J	0.62	0/2705	0.89	3/3671 (0.1%)
2	L	0.64	2/2719 (0.1%)	0.87	2/3687 (0.1%)
All	All	0.63	7/19566 (0.0%)	0.91	34/26544 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	384	CYS	CB-SG	-7.99	1.68	1.82
2	H	273	LEU	C-N	7.12	1.47	1.34
2	L	384	CYS	CB-SG	-6.41	1.71	1.82
2	L	397	VAL	C-O	-5.79	1.12	1.23
2	H	390	CYS	CB-SG	-5.73	1.72	1.81
2	H	384	CYS	CB-SG	-5.58	1.72	1.81
2	D	233	TYR	C-N	-5.04	1.22	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	350	CYS	CA-CB-SG	-11.83	92.71	114.00
2	H	361	CYS	CA-CB-SG	-10.86	94.46	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	384	CYS	CA-CB-SG	-9.47	96.95	114.00
2	J	350	CYS	CA-CB-SG	-9.30	97.25	114.00
2	J	361	CYS	CA-CB-SG	-8.51	98.69	114.00
2	H	384	CYS	CA-CB-SG	-7.81	99.94	114.00
2	B	153	ASN	CB-CA-C	6.23	122.85	110.40
2	B	473	LEU	CA-CB-CG	6.22	129.61	115.30
2	H	221	LEU	CA-CB-CG	6.17	129.50	115.30
1	K	24	LEU	CA-CB-CG	6.06	129.25	115.30
2	D	151	LEU	CB-CG-CD1	-5.92	100.94	111.00
2	H	413	GLN	CA-CB-CG	5.78	126.11	113.40
2	H	375	LEU	CB-CG-CD2	-5.77	101.20	111.00
2	B	384	CYS	CA-CB-SG	-5.73	103.68	114.00
1	C	28	CYS	CA-CB-SG	-5.71	103.72	114.00
2	B	245	LEU	CA-CB-CG	-5.59	102.44	115.30
2	H	227	LEU	CA-CB-CG	-5.54	102.56	115.30
2	F	475	ASP	CB-CG-OD1	5.52	123.27	118.30
2	D	273	LEU	CB-CG-CD2	-5.51	101.62	111.00
1	E	50	LEU	CA-CB-CG	5.49	127.92	115.30
2	H	392	ILE	CG1-CB-CG2	5.46	123.40	111.40
2	L	280	ASP	C-N-CA	-5.41	108.17	121.70
1	K	28	CYS	CA-CB-SG	5.41	123.74	114.00
2	J	198	ARG	CA-CB-CG	-5.35	101.62	113.40
2	F	475	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	F	171	LYS	CA-CB-CG	-5.28	101.79	113.40
1	G	50	LEU	CA-CB-CG	-5.24	103.25	115.30
2	B	229	ARG	NE-CZ-NH1	-5.21	117.69	120.30
2	F	427	LEU	CB-CG-CD1	-5.21	102.15	111.00
2	F	153	ASN	CB-CA-C	5.12	120.65	110.40
2	F	471	GLN	CA-CB-CG	-5.03	102.33	113.40
2	D	336	ASP	CB-CG-OD1	5.02	122.82	118.30
2	F	151	LEU	CA-CB-CG	5.00	126.80	115.30
2	F	458	VAL	CG1-CB-CG2	-5.00	102.90	110.90

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	540	0	525	25	0
1	C	544	0	536	28	0
1	E	544	0	536	24	0
1	G	544	0	536	23	0
1	I	544	0	536	20	0
1	K	536	0	514	22	0
2	B	2666	0	2638	130	0
2	D	2668	0	2636	134	0
2	F	2676	0	2660	131	0
2	H	2677	0	2649	128	0
2	J	2663	0	2616	109	0
2	L	2677	0	2649	103	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	28	0	26	0	0
3	E	14	0	13	0	0
3	F	28	0	26	0	0
3	G	14	0	13	2	0
3	H	28	0	26	0	0
3	I	14	0	13	0	0
3	J	28	0	26	0	0
3	K	14	0	13	0	0
3	L	28	0	26	1	0
4	B	5	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	4	0
4	I	2	0	0	0	0
4	J	4	0	0	0	0
4	L	6	0	0	0	0
All	All	19556	0	19265	656	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 17.

All (656) 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)
2:H:350:CYS:SG	4:H:701:HOH:O	2.00	1.16
2:H:361:CYS:SG	4:H:701:HOH:O	2.08	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:393:GLY:C	2:F:417:THR:HG22	1.80	1.02
2:J:138:LYS:HE3	2:L:481:LEU:HB3	1.45	0.98
2:H:350:CYS:O	2:H:354:ILE:HD12	1.66	0.95
2:H:222:MET:HE2	2:H:273:LEU:HD21	1.49	0.93
1:G:30:THR:HG23	2:H:381:LEU:HD11	1.50	0.93
2:B:133:GLU:C	2:B:135:ASN:OD1	2.09	0.92
2:F:247:ASN:HD22	2:F:334:PHE:HZ	1.16	0.90
1:G:85:SER:HB3	2:H:261:GLY:HA2	1.54	0.88
2:H:463:VAL:HG21	2:J:158:LEU:HD13	1.58	0.85
2:J:243:LEU:HB3	2:J:279:ILE:HD13	1.58	0.84
2:B:158:LEU:HD13	2:F:463:VAL:HG11	1.60	0.84
2:D:139:GLY:O	2:D:143:THR:HG23	1.78	0.84
1:A:39:LEU:HB2	2:B:278:VAL:HB	1.59	0.83
2:H:350:CYS:O	2:H:354:ILE:CD1	2.26	0.83
2:H:361:CYS:CB	4:H:701:HOH:O	2.22	0.82
2:B:155:VAL:HG22	2:D:155:VAL:HG21	1.62	0.81
2:H:145:ASN:HB2	2:J:478:ASN:HD21	1.45	0.81
1:I:85:SER:HB3	2:J:261:GLY:HA2	1.62	0.81
2:J:453:GLU:HG2	2:J:457:ASN:OD1	1.80	0.81
2:H:361:CYS:HB2	4:H:701:HOH:O	1.79	0.80
2:H:145:ASN:HB2	2:J:478:ASN:ND2	1.97	0.79
2:F:153:ASN:HA	2:F:156:ARG:HG2	1.65	0.78
2:H:145:ASN:HA	2:H:148:VAL:HG22	1.66	0.78
2:H:184:ILE:HD11	2:L:184:ILE:HG13	1.66	0.77
2:B:250:MET:HG2	2:B:334:PHE:CD2	2.19	0.77
2:H:155:VAL:HG21	2:L:155:VAL:HG22	1.65	0.76
2:F:174:THR:HA	2:F:177:ILE:HG22	1.68	0.75
2:B:135:ASN:OD1	2:B:135:ASN:N	2.20	0.75
2:D:481:LEU:HD13	2:D:481:LEU:O	1.86	0.74
2:H:137:ILE:HA	2:L:481:LEU:HD21	1.70	0.74
2:B:144:THR:CG2	2:D:145:ASN:OD1	2.35	0.74
2:B:248:ARG:HA	2:B:251:VAL:HG22	1.69	0.74
2:D:166:LYS:HE3	2:D:167:GLU:HG3	1.67	0.73
1:A:40:ARG:NH1	2:B:337:THR:OG1	2.22	0.73
1:C:61:THR:HG21	1:C:65:SER:HB2	1.69	0.73
2:B:250:MET:HG2	2:B:334:PHE:CE2	2.23	0.73
2:J:481:LEU:N	2:J:481:LEU:HD23	2.03	0.72
2:B:144:THR:HG21	2:D:145:ASN:OD1	1.89	0.72
1:I:49:THR:HB	2:L:436:VAL:HG22	1.71	0.72
2:D:394:SER:OG	2:D:416:ASP:OD2	2.07	0.72
2:B:411:THR:HG22	2:B:413:GLN:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:SER:HA	2:D:471:GLN:HE22	1.56	0.70
2:L:418:VAL:HG23	2:L:427:LEU:HD11	1.73	0.69
2:J:245:LEU:HD22	2:J:248:ARG:HH21	1.57	0.69
2:D:460:LEU:HA	2:D:463:VAL:HG22	1.73	0.69
2:B:199:ARG:O	2:B:203:VAL:HG12	1.93	0.69
2:B:477:SER:OG	2:D:140:ALA:O	2.11	0.69
1:A:85:SER:HB3	2:B:261:GLY:HA2	1.72	0.69
1:E:50:LEU:HD23	2:F:269:TYR:HE1	1.58	0.69
2:F:462:GLN:HA	2:F:465:GLU:HG2	1.76	0.68
2:H:152:GLY:HA2	2:L:151:LEU:HD11	1.76	0.68
2:L:221:LEU:HD23	2:L:271:VAL:HG12	1.74	0.68
2:H:134:VAL:O	2:H:137:ILE:HG22	1.94	0.68
2:H:392:ILE:HG23	2:H:415:ALA:CB	2.24	0.67
2:B:438:LYS:HG3	1:E:51:GLU:HB3	1.74	0.67
2:H:229:ARG:HD2	2:J:433:GLU:OE1	1.95	0.67
1:K:49:THR:HG23	2:L:268:ILE:HG12	1.76	0.67
2:D:309:TRP:HB2	2:D:320:TYR:HB2	1.76	0.67
2:H:222:MET:CE	2:H:273:LEU:HD21	2.23	0.67
2:H:474:VAL:HG13	2:L:145:ASN:HB3	1.77	0.67
2:D:392:ILE:HD12	2:D:410:ILE:HD13	1.76	0.67
2:B:133:GLU:O	2:B:135:ASN:OD1	2.12	0.67
2:L:422:ASN:OD1	2:D:401:LYS:HD3	1.95	0.66
2:J:453:GLU:CG	2:J:457:ASN:OD1	2.43	0.66
1:A:50:LEU:HD12	2:B:203:VAL:HG11	1.78	0.66
1:G:31:ILE:HD12	2:H:351:ASN:HD22	1.60	0.66
2:H:480:ILE:HG23	2:H:481:LEU:HD12	1.77	0.66
2:L:134:VAL:O	2:L:137:ILE:HG13	1.96	0.66
2:F:170:SER:O	2:F:174:THR:OG1	2.12	0.66
2:H:260:ILE:HD11	2:H:270:MET:HB2	1.76	0.65
2:D:170:SER:O	2:D:174:THR:OG1	2.14	0.65
2:H:287:LYS:HA	2:H:307:GLN:HG2	1.79	0.65
2:H:477:SER:OG	2:L:145:ASN:ND2	2.29	0.65
2:H:221:LEU:HD21	2:H:257:GLY:HA3	1.78	0.64
2:L:392:ILE:HG21	2:L:410:ILE:HD13	1.78	0.64
2:B:137:ILE:HD12	2:B:137:ILE:O	1.97	0.64
2:B:477:SER:OG	2:D:140:ALA:CA	2.45	0.64
2:J:221:LEU:HG	2:J:269:TYR:CE1	2.33	0.64
2:L:256:PHE:HE1	2:L:258:ILE:HD11	1.64	0.63
1:K:51:GLU:HG2	2:L:266:SER:OG	1.97	0.63
2:B:137:ILE:HD12	2:B:137:ILE:C	2.17	0.63
2:D:433:GLU:HG2	2:D:434:GLN:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:234:MET:HE1	2:D:244:MET:SD	2.38	0.63
2:H:240:GLN:HG2	2:H:279:ILE:HG12	1.81	0.63
2:D:393:GLY:HA2	2:D:400:ILE:HG13	1.79	0.63
2:H:386:LYS:O	2:H:405:LYS:NZ	2.31	0.63
2:B:134:VAL:HA	2:B:137:ILE:CG2	2.29	0.63
2:J:138:LYS:CE	2:L:481:LEU:HB3	2.27	0.62
2:B:392:ILE:HD11	2:B:403:LEU:HD11	1.79	0.62
2:J:139:GLY:O	2:J:143:THR:HG23	1.99	0.62
2:J:358:ASN:OD1	2:L:367:ARG:NH2	2.32	0.62
2:H:145:ASN:CG	2:J:478:ASN:OD1	2.38	0.62
2:J:240:GLN:O	2:J:244:MET:HG3	1.98	0.62
2:B:134:VAL:HG11	2:D:134:VAL:HG11	1.82	0.62
2:H:245:LEU:O	2:H:248:ARG:HG3	1.99	0.62
2:D:390:CYS:HA	2:D:419:THR:O	1.99	0.62
2:H:450:ARG:HG2	2:H:451:PHE:H	1.64	0.61
2:H:163:ARG:HB2	2:J:460:LEU:HD11	1.80	0.61
2:H:392:ILE:HG23	2:H:415:ALA:HB2	1.82	0.61
2:B:454:ASP:O	2:B:458:VAL:HG23	2.00	0.61
2:F:346:GLN:O	2:F:349:GLU:HB2	2.00	0.61
1:K:36:LEU:HD23	2:L:280:ASP:OD1	2.00	0.61
2:D:411:THR:HG22	2:D:413:GLN:H	1.64	0.61
2:D:481:LEU:HD13	2:D:481:LEU:C	2.21	0.61
2:D:222:MET:HE1	2:D:227:LEU:HD13	1.83	0.60
2:D:256:PHE:HE1	2:D:258:ILE:HD11	1.66	0.60
1:C:44:TYR:CD2	2:D:234:MET:HG2	2.36	0.60
1:I:37:SER:HB3	2:J:283:CYS:SG	2.41	0.60
2:B:206:GLN:NE2	2:F:209:ASP:OD1	2.35	0.60
2:H:399:ILE:H	2:H:399:ILE:HD12	1.67	0.60
2:H:256:PHE:HE1	2:H:258:ILE:HD11	1.67	0.60
2:H:459:ALA:O	2:H:463:VAL:HG13	2.01	0.60
2:H:371:SER:HA	2:H:383:ALA:O	2.03	0.59
2:J:167:GLU:HA	2:J:170:SER:OG	2.01	0.59
2:B:213:ILE:HG13	2:B:258:ILE:HD13	1.83	0.59
2:B:476:GLN:O	2:B:480:ILE:HG13	2.02	0.59
2:L:134:VAL:HA	2:L:137:ILE:HG12	1.84	0.59
2:B:167:GLU:HB3	2:B:171:LYS:HE2	1.82	0.59
2:H:429:LYS:HG2	1:K:43:TRP:HB2	1.82	0.59
2:F:181:LYS:O	2:F:184:ILE:HG13	2.03	0.59
2:H:198:ARG:NH2	1:K:73:LEU:HD22	2.18	0.59
2:J:480:ILE:HG22	2:J:481:LEU:HD23	1.84	0.59
2:L:221:LEU:HD21	2:L:257:GLY:HA3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:OE2	2:D:198:ARG:NH2	2.36	0.59
2:B:133:GLU:CA	2:B:135:ASN:OD1	2.50	0.59
2:B:141:LEU:HB2	2:D:141:LEU:HD11	1.84	0.59
1:I:38:VAL:HG23	2:J:334:PHE:HA	1.85	0.59
2:L:130:LEU:HD12	2:L:130:LEU:O	2.03	0.58
2:L:392:ILE:HD12	2:L:415:ALA:HB2	1.85	0.58
1:G:55:VAL:HG12	2:J:442:VAL:HB	1.85	0.58
2:B:474:VAL:HG11	2:F:148:VAL:HG21	1.84	0.58
2:B:433:GLU:OE2	2:F:229:ARG:NH1	2.36	0.58
2:B:477:SER:OG	2:D:140:ALA:HA	2.02	0.58
1:G:21:GLU:OE1	2:H:376:SER:HB3	2.03	0.58
2:B:151:LEU:HD11	2:D:152:GLY:HA2	1.84	0.58
1:G:70:GLU:OE2	2:J:198:ARG:NH2	2.37	0.58
2:J:232:SER:O	2:D:396:ARG:NH2	2.37	0.58
2:B:467:ILE:HG12	2:F:156:ARG:HB3	1.86	0.58
2:F:200:PHE:O	2:F:204:VAL:HG23	2.04	0.58
2:H:465:GLU:OE2	2:H:468:GLU:HG2	2.04	0.58
2:J:243:LEU:HD11	2:D:413:GLN:OE1	2.04	0.58
1:E:39:LEU:HB2	2:F:278:VAL:HB	1.86	0.58
2:D:476:GLN:O	2:D:480:ILE:HG12	2.03	0.58
1:I:21:GLU:HB2	1:I:32:THR:HG23	1.86	0.57
2:J:166:LYS:CE	2:L:456:PHE:HB3	2.34	0.57
2:F:393:GLY:O	2:F:417:THR:HG22	2.03	0.57
1:I:27:SER:HB3	2:J:354:ILE:HG13	1.86	0.57
2:J:309:TRP:CD1	2:J:326:CYS:HB2	2.39	0.57
2:B:304:ARG:HA	2:B:363:VAL:HG12	1.84	0.57
2:D:174:THR:HA	2:D:177:ILE:HG22	1.87	0.57
2:B:144:THR:HG23	2:D:145:ASN:OD1	2.04	0.57
2:B:180:ASN:OD1	2:D:181:LYS:HG3	2.04	0.57
2:H:188:LYS:O	2:H:192:SER:OG	2.19	0.56
2:H:208:SER:HA	2:J:219:LEU:HD23	1.86	0.56
2:B:301:CYS:C	2:B:302:LEU:HD23	2.24	0.56
2:H:221:LEU:CD2	2:H:271:VAL:HG12	2.35	0.56
1:A:45:THR:HG22	2:B:272:GLN:HG3	1.87	0.56
2:D:132:SER:O	2:D:132:SER:OG	2.14	0.56
1:G:55:VAL:HG21	1:G:71:LEU:HD11	1.86	0.56
2:J:245:LEU:HD22	2:J:248:ARG:NH2	2.20	0.56
2:J:256:PHE:CE1	2:J:258:ILE:HD11	2.40	0.56
1:G:80:GLU:HG3	2:J:219:LEU:HD12	1.87	0.56
2:J:473:LEU:HB3	2:L:147:ALA:HB2	1.86	0.56
2:D:299:TYR:CE2	2:D:369:PRO:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:356:THR:HG22	2:F:358:ASN:H	1.71	0.56
1:E:43:TRP:CE3	2:F:272:GLN:HG2	2.40	0.56
2:B:156:ARG:HB2	2:D:467:ILE:HG21	1.87	0.56
2:B:157:VAL:HG23	2:F:463:VAL:HG23	1.88	0.56
1:K:86:ALA:HB3	2:L:260:ILE:HA	1.86	0.56
2:B:147:ALA:HB2	2:F:473:LEU:HB3	1.88	0.56
2:H:309:TRP:CD1	2:H:326:CYS:HB2	2.41	0.56
1:E:19:LEU:HD11	2:F:331:ASP:OD1	2.06	0.56
2:H:145:ASN:ND2	2:J:478:ASN:OD1	2.39	0.56
2:F:464:PHE:HA	2:F:467:ILE:HG12	1.87	0.55
1:K:30:THR:HG23	2:L:381:LEU:HD21	1.87	0.55
2:B:477:SER:OG	2:D:140:ALA:C	2.45	0.55
2:B:169:VAL:HG23	2:B:173:LEU:HD23	1.89	0.55
1:K:30:THR:CG2	2:L:381:LEU:HD11	2.37	0.55
2:J:239:GLY:O	2:J:243:LEU:HG	2.07	0.55
2:J:294:GLU:HG2	2:J:298:ASN:O	2.07	0.55
2:F:231:VAL:HA	2:F:234:MET:HG3	1.88	0.55
2:F:240:GLN:OE1	2:F:240:GLN:N	2.40	0.55
1:I:50:LEU:HD12	2:J:269:TYR:HE2	1.72	0.55
2:H:221:LEU:HD23	2:H:271:VAL:HG12	1.88	0.55
2:J:138:LYS:HG3	2:L:481:LEU:HD13	1.88	0.55
2:D:309:TRP:CD1	2:D:326:CYS:HB2	2.42	0.55
2:B:134:VAL:HA	2:B:137:ILE:HG23	1.87	0.55
2:B:221:LEU:HD21	2:B:257:GLY:HA3	1.88	0.55
2:B:388:VAL:O	2:B:405:LYS:NZ	2.40	0.55
2:H:158:LEU:HD13	2:L:463:VAL:HG11	1.89	0.55
1:G:21:GLU:HB3	2:H:378:LEU:HD12	1.89	0.54
2:B:147:ALA:O	2:B:150:THR:HG22	2.07	0.54
1:K:85:SER:CB	2:L:261:GLY:HA2	2.37	0.54
2:B:134:VAL:CG1	2:D:134:VAL:HG11	2.37	0.54
2:F:286:ILE:HD12	2:F:310:TYR:CD1	2.41	0.54
2:F:470:SER:O	2:F:474:VAL:HG13	2.08	0.54
2:L:309:TRP:HB2	2:L:320:TYR:HB2	1.90	0.54
2:B:473:LEU:HD23	2:D:147:ALA:N	2.23	0.54
1:C:85:SER:HB2	2:D:261:GLY:HA2	1.88	0.54
2:H:460:LEU:O	2:H:463:VAL:HG22	2.07	0.54
2:H:477:SER:HB2	2:J:143:THR:OG1	2.08	0.54
2:B:181:LYS:O	2:B:184:ILE:HG13	2.08	0.54
2:B:187:LEU:HD11	2:D:188:LYS:HG2	1.90	0.54
2:L:464:PHE:HA	2:L:467:ILE:HG22	1.90	0.54
2:H:147:ALA:O	2:H:150:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLU:HA	2:B:135:ASN:OD1	2.08	0.53
2:L:134:VAL:O	2:L:137:ILE:CG1	2.55	0.53
2:F:234:MET:CE	2:F:275:ILE:HG12	2.38	0.53
2:F:418:VAL:HG23	2:F:427:LEU:HD11	1.89	0.53
2:F:371:SER:HA	2:F:383:ALA:O	2.08	0.53
1:G:31:ILE:HD12	2:H:351:ASN:ND2	2.24	0.53
2:D:217:ILE:HG21	2:D:222:MET:HE2	1.91	0.53
2:H:392:ILE:HD11	2:H:403:LEU:HD21	1.91	0.53
2:L:318:VAL:HG23	2:L:320:TYR:CE1	2.44	0.53
2:H:286:ILE:HD11	2:H:351:ASN:ND2	2.24	0.53
2:B:463:VAL:HG23	2:D:157:VAL:HG12	1.91	0.53
2:F:237:SER:HB2	2:F:240:GLN:OE1	2.09	0.53
2:F:240:GLN:O	2:F:244:MET:HG3	2.09	0.53
2:J:145:ASN:HA	2:J:148:VAL:HG12	1.90	0.53
2:B:433:GLU:HG2	2:B:434:GLN:H	1.72	0.53
2:D:156:ARG:HB2	2:F:467:ILE:HD13	1.90	0.53
2:D:454:ASP:O	2:D:458:VAL:HG13	2.09	0.53
1:E:58:LEU:HD22	2:F:189:MET:HE1	1.91	0.53
2:B:473:LEU:HD21	2:D:146:GLU:HG2	1.91	0.52
2:F:286:ILE:CD1	2:F:310:TYR:CD1	2.92	0.52
2:H:145:ASN:HB2	2:J:478:ASN:CG	2.29	0.52
2:L:145:ASN:HA	2:L:148:VAL:HG22	1.91	0.52
2:H:228:ALA:HB2	2:H:248:ARG:HH21	1.74	0.52
2:F:247:ASN:ND2	2:F:334:PHE:HZ	1.95	0.52
1:C:51:GLU:HG3	2:F:438:LYS:HG3	1.90	0.52
1:A:81:LEU:HD22	2:B:204:VAL:HG13	1.91	0.52
2:D:456:PHE:HE2	2:F:165:LEU:HB2	1.74	0.52
2:J:394:SER:OG	2:J:395:ASN:N	2.41	0.52
2:B:302:LEU:HD23	2:B:302:LEU:N	2.24	0.52
2:B:392:ILE:CD1	2:B:418:VAL:HG22	2.39	0.52
2:D:137:ILE:HG23	2:D:137:ILE:O	2.09	0.52
1:I:70:GLU:OE1	2:L:198:ARG:NH2	2.43	0.52
2:F:210:ASN:HB2	2:F:213:ILE:O	2.10	0.52
1:I:51:GLU:HB2	2:L:438:LYS:HG3	1.92	0.51
2:B:248:ARG:O	2:B:251:VAL:HG22	2.10	0.51
2:L:170:SER:O	2:L:174:THR:OG1	2.20	0.51
2:F:453:GLU:HG2	2:F:457:ASN:OD1	2.11	0.51
1:G:55:VAL:CG2	1:G:71:LEU:HD11	2.41	0.51
2:H:438:LYS:HG3	1:K:51:GLU:HB2	1.92	0.51
2:D:456:PHE:CE2	2:F:165:LEU:HD13	2.46	0.51
2:J:472:ALA:HA	2:J:475:ASP:OD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ILE:HG13	2:B:258:ILE:CD1	2.41	0.51
2:D:253:ARG:HH21	2:D:329:ARG:HH21	1.58	0.51
2:J:221:LEU:HD21	2:J:257:GLY:HA3	1.92	0.51
2:B:151:LEU:HB2	2:F:470:SER:CB	2.40	0.51
2:F:395:ASN:OD1	2:F:426:GLN:NE2	2.36	0.51
1:I:38:VAL:HG21	2:J:334:PHE:CD2	2.45	0.51
2:L:346:GLN:OE1	2:L:346:GLN:N	2.43	0.51
1:A:21:GLU:CD	2:B:376:SER:HG	2.13	0.51
1:C:49:THR:HB	2:F:436:VAL:HG22	1.91	0.51
2:H:156:ARG:HA	2:J:467:ILE:HD13	1.93	0.51
2:H:350:CYS:O	2:H:354:ILE:HD11	2.10	0.51
2:J:166:LYS:HZ2	2:L:460:LEU:HD12	1.75	0.51
2:J:459:ALA:O	2:J:463:VAL:HG23	2.11	0.51
1:C:38:VAL:HG11	2:D:334:PHE:CE2	2.46	0.51
2:J:258:ILE:O	2:J:269:TYR:HB2	2.11	0.50
2:D:152:GLY:O	2:D:155:VAL:HG12	2.11	0.50
2:D:299:TYR:CD2	2:D:369:PRO:HB3	2.45	0.50
2:J:475:ASP:OD1	2:J:475:ASP:N	2.44	0.50
2:B:155:VAL:HG12	2:D:467:ILE:HD11	1.94	0.50
2:F:473:LEU:O	2:F:476:GLN:HB3	2.12	0.50
1:G:68:LYS:NZ	3:G:201:NAG:H83	2.27	0.50
1:G:80:GLU:O	1:G:83:THR:HG23	2.12	0.50
2:B:210:ASN:HB2	2:B:213:ILE:O	2.11	0.50
2:H:191:VAL:HG11	1:K:66:LEU:HD13	1.93	0.50
2:B:473:LEU:HB3	2:D:147:ALA:HB2	1.94	0.50
2:D:151:LEU:HD11	2:F:152:GLY:CA	2.41	0.50
2:F:396:ARG:HG2	2:F:397:VAL:N	2.26	0.50
2:F:417:THR:N	2:F:427:LEU:CD1	2.74	0.50
2:H:234:MET:HE1	2:H:275:ILE:HG12	1.93	0.50
2:F:213:ILE:HD12	2:F:258:ILE:CD1	2.42	0.50
2:H:137:ILE:HG13	2:L:481:LEU:HD11	1.94	0.50
2:H:164:GLU:HB3	2:L:456:PHE:CZ	2.46	0.50
2:H:309:TRP:HB2	2:H:320:TYR:HB2	1.94	0.50
2:H:145:ASN:OD1	2:L:144:THR:OG1	2.12	0.49
2:J:133:GLU:O	2:J:137:ILE:HG12	2.12	0.49
2:H:285:ILE:HB	2:H:309:TRP:CZ3	2.47	0.49
1:A:44:TYR:HB2	2:B:275:ILE:HD11	1.93	0.49
1:C:21:GLU:HB2	1:C:32:THR:HG23	1.93	0.49
2:D:481:LEU:HD23	2:F:140:ALA:CB	2.42	0.49
2:H:198:ARG:CZ	1:K:73:LEU:HD22	2.42	0.49
2:J:250:MET:HG3	2:J:334:PHE:CZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:390:CYS:HA	2:J:419:THR:O	2.12	0.49
2:H:419:THR:HG23	2:H:424:VAL:HG22	1.94	0.49
2:B:392:ILE:CG2	2:B:415:ALA:HB2	2.43	0.49
1:C:67:ILE:HD13	2:D:189:MET:C	2.33	0.49
1:K:85:SER:HB3	2:L:261:GLY:HA2	1.95	0.49
2:B:392:ILE:HG12	2:B:403:LEU:HG	1.95	0.49
1:E:49:THR:HG23	2:F:268:ILE:HG12	1.93	0.49
2:F:413:GLN:N	2:F:413:GLN:OE1	2.45	0.49
2:H:222:MET:HE3	2:H:227:LEU:HA	1.95	0.49
2:H:285:ILE:HB	2:H:309:TRP:CE3	2.48	0.49
1:A:39:LEU:HD12	2:B:278:VAL:HG11	1.95	0.49
2:F:256:PHE:CE1	2:F:258:ILE:HD11	2.47	0.49
1:A:70:GLU:O	1:A:74:THR:HG23	2.13	0.49
1:C:44:TYR:CG	2:D:234:MET:HG2	2.47	0.49
1:C:61:THR:OG1	1:C:62:ASP:N	2.46	0.49
1:C:87:ASP:OD1	2:D:263:TYR:OH	2.30	0.49
2:H:382:VAL:CG2	2:H:418:VAL:HG11	2.44	0.48
2:J:250:MET:HG3	2:J:334:PHE:CE1	2.48	0.48
1:A:43:TRP:HB2	2:D:429:LYS:HG2	1.96	0.48
2:B:284:TRP:NE1	2:B:310:TYR:HB2	2.27	0.48
2:D:136:ALA:C	2:D:138:LYS:H	2.17	0.48
2:J:165:LEU:HD11	2:L:169:VAL:HG21	1.95	0.48
2:J:292:CYS:HB2	2:J:385:TYR:CZ	2.49	0.48
2:L:390:CYS:HA	2:L:419:THR:O	2.13	0.48
1:C:19:LEU:HD11	2:D:331:ASP:OD1	2.13	0.48
2:D:166:LYS:HG2	2:F:456:PHE:CE1	2.48	0.48
2:L:411:THR:HG22	2:L:413:GLN:H	1.78	0.48
1:A:55:VAL:HG11	1:A:71:LEU:HD11	1.95	0.48
2:H:202:ASN:O	2:H:206:GLN:HG3	2.14	0.48
1:I:37:SER:HB2	1:I:39:LEU:CD1	2.43	0.48
2:J:479:LYS:N	2:J:479:LYS:HD3	2.28	0.48
2:D:230:ALA:O	2:D:234:MET:HG3	2.14	0.48
2:L:392:ILE:CG2	2:L:410:ILE:HD13	2.44	0.48
1:A:87:ASP:OD2	2:B:263:TYR:OH	2.31	0.48
2:B:133:GLU:C	2:B:135:ASN:H	2.15	0.48
2:B:474:VAL:HG11	2:F:148:VAL:CG2	2.43	0.48
2:D:463:VAL:HG11	2:F:158:LEU:HD13	1.95	0.48
1:E:35:TYR:HB2	2:F:283:CYS:HB2	1.96	0.48
2:L:179:LYS:HE2	2:L:183:ASP:OD2	2.13	0.48
1:C:56:GLU:OE1	2:F:444:SER:N	2.41	0.48
2:F:222:MET:HE1	2:F:273:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:287:LYS:NZ	2:H:323:GLU:OE2	2.40	0.48
2:H:392:ILE:CG2	2:H:415:ALA:HB2	2.43	0.48
2:H:248:ARG:O	2:H:252:ARG:HG3	2.14	0.48
2:J:187:LEU:CD2	2:L:187:LEU:HB3	2.44	0.48
2:J:240:GLN:HE22	2:J:279:ILE:HG22	1.78	0.48
2:J:378:LEU:HA	2:J:412:ASN:ND2	2.29	0.48
2:L:319:TYR:CZ	2:L:321:PRO:HA	2.49	0.48
2:B:152:GLY:HA2	2:F:151:LEU:HD21	1.95	0.48
2:B:306:ASP:O	2:B:310:TYR:OH	2.22	0.48
2:F:303:LEU:C	2:F:363:VAL:HG23	2.34	0.48
2:H:156:ARG:HB2	2:J:467:ILE:HG21	1.96	0.48
2:H:320:TYR:CE2	2:H:335:CYS:HB3	2.49	0.48
2:B:141:LEU:HB2	2:D:141:LEU:CD1	2.44	0.48
2:F:212:GLY:O	2:F:213:ILE:HD13	2.14	0.48
2:H:286:ILE:HD11	2:H:351:ASN:HD21	1.78	0.47
2:H:383:ALA:HB1	2:H:385:TYR:CE2	2.49	0.47
2:H:433:GLU:HG2	2:H:434:GLN:H	1.77	0.47
2:H:166:LYS:HD2	2:J:451:PHE:CE2	2.48	0.47
2:J:243:LEU:HD12	2:J:279:ILE:HG21	1.95	0.47
2:F:460:LEU:HD23	2:F:460:LEU:HA	1.62	0.47
2:J:166:LYS:HZ3	2:L:457:ASN:HA	1.79	0.47
2:B:161:ALA:HB1	2:F:456:PHE:CE2	2.49	0.47
1:C:85:SER:CB	2:D:261:GLY:HA2	2.44	0.47
2:D:469:ASN:O	2:D:473:LEU:HG	2.13	0.47
2:L:371:SER:HA	2:L:383:ALA:O	2.14	0.47
2:B:390:CYS:HA	2:B:419:THR:O	2.15	0.47
2:F:309:TRP:CZ3	2:F:333:VAL:HG11	2.48	0.47
2:J:371:SER:HA	2:J:383:ALA:O	2.14	0.47
2:L:221:LEU:CD2	2:L:257:GLY:HA3	2.44	0.47
1:C:52:VAL:HG23	2:D:265:SER:O	2.14	0.47
2:F:286:ILE:CD1	2:F:310:TYR:CE1	2.98	0.47
2:F:417:THR:N	2:F:427:LEU:HD13	2.30	0.47
2:H:292:CYS:HB2	2:H:385:TYR:CZ	2.50	0.47
2:H:304:ARG:NH2	2:H:351:ASN:OD1	2.44	0.47
2:H:309:TRP:NE1	2:H:326:CYS:HB2	2.30	0.47
2:H:362:LYS:HE2	2:H:362:LYS:HA	1.96	0.47
1:I:80:GLU:O	1:I:83:THR:HG23	2.14	0.47
1:E:19:LEU:N	1:E:19:LEU:HD12	2.30	0.47
2:F:393:GLY:CA	2:F:417:THR:HG22	2.43	0.47
2:H:166:LYS:HD3	2:J:456:PHE:CE1	2.50	0.47
2:J:187:LEU:HD21	2:L:187:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:456:PHE:HD1	2:J:457:ASN:ND2	2.13	0.47
2:H:137:ILE:CA	2:L:481:LEU:HD21	2.43	0.47
1:K:58:LEU:HD12	1:K:58:LEU:HA	1.73	0.47
2:B:148:VAL:HG11	2:F:148:VAL:HG12	1.95	0.47
2:L:455:GLN:O	2:L:458:VAL:HB	2.15	0.47
2:B:248:ARG:O	2:B:252:ARG:HG3	2.15	0.47
2:L:221:LEU:HG	2:L:269:TYR:CE1	2.50	0.46
1:A:47:VAL:HB	2:D:434:GLN:HG2	1.97	0.46
1:E:60:CYS:O	2:F:182:CYS:SG	2.73	0.46
2:F:393:GLY:HA2	2:F:400:ILE:HG23	1.97	0.46
2:F:450:ARG:HG2	2:F:451:PHE:N	2.30	0.46
2:H:194:SER:O	2:H:198:ARG:HG3	2.16	0.46
1:C:62:ASP:N	1:C:62:ASP:OD1	2.49	0.46
2:D:137:ILE:HD11	2:F:138:LYS:HG2	1.97	0.46
2:B:240:GLN:HB3	2:B:276:PHE:O	2.16	0.46
2:D:166:LYS:HA	2:D:169:VAL:HG22	1.96	0.46
2:H:145:ASN:CB	2:J:478:ASN:OD1	2.63	0.46
2:B:188:LYS:HG2	1:E:66:LEU:HD11	1.98	0.46
1:I:63:GLY:HA3	1:I:64:PRO:HD3	1.71	0.46
2:J:260:ILE:HB	2:J:268:ILE:HG22	1.96	0.46
1:I:30:THR:HG23	2:J:381:LEU:HD11	1.98	0.46
2:J:347:SER:HB3	2:J:359:TYR:CE2	2.50	0.46
2:J:470:SER:O	2:J:474:VAL:HG13	2.15	0.46
2:D:285:ILE:HB	2:D:309:TRP:CE3	2.51	0.46
1:K:37:SER:HB3	2:L:283:CYS:SG	2.56	0.46
2:D:156:ARG:O	2:D:160:THR:HG23	2.15	0.46
1:E:85:SER:HB2	2:F:261:GLY:HA2	1.97	0.46
2:F:417:THR:HA	2:F:427:LEU:HD12	1.97	0.46
2:J:245:LEU:HD23	2:J:245:LEU:HA	1.60	0.46
2:L:171:LYS:N	2:L:171:LYS:HD3	2.31	0.46
2:B:208:SER:HA	2:D:219:LEU:HD23	1.98	0.46
1:C:63:GLY:HA3	1:C:64:PRO:HD3	1.61	0.46
2:F:173:LEU:HD12	2:F:173:LEU:HA	1.83	0.46
2:F:309:TRP:HB2	2:F:320:TYR:HB2	1.98	0.46
2:F:317:THR:O	2:F:343:VAL:HG22	2.16	0.46
2:H:469:ASN:O	2:H:473:LEU:HG	2.16	0.46
1:K:30:THR:HG23	2:L:381:LEU:HD11	1.97	0.46
2:B:169:VAL:HG21	2:F:169:VAL:HG22	1.97	0.46
1:C:67:ILE:HD12	2:D:190:ALA:HA	1.97	0.46
2:F:231:VAL:HA	2:F:234:MET:SD	2.55	0.46
2:D:210:ASN:HB2	2:D:213:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:ILE:O	2:D:252:ARG:HD3	2.16	0.46
2:D:320:TYR:CE2	2:D:335:CYS:HB3	2.51	0.46
2:F:473:LEU:O	2:F:476:GLN:N	2.49	0.46
2:H:145:ASN:HB2	2:J:478:ASN:OD1	2.16	0.45
2:J:309:TRP:HB2	2:J:320:TYR:HB2	1.97	0.45
2:J:392:ILE:HG21	2:J:410:ILE:HD13	1.98	0.45
2:J:166:LYS:HD3	2:J:167:GLU:OE1	2.15	0.45
1:K:44:TYR:HB2	2:L:275:ILE:HD11	1.99	0.45
2:B:309:TRP:HB2	2:B:320:TYR:HB2	1.98	0.45
2:D:169:VAL:HG12	2:F:169:VAL:HG11	1.98	0.45
2:F:440:ARG:HA	2:F:441:PRO:HD3	1.85	0.45
2:B:221:LEU:O	2:B:269:TYR:OH	2.18	0.45
1:C:19:LEU:HD12	1:C:19:LEU:N	2.31	0.45
2:D:202:ASN:O	2:D:206:GLN:HG3	2.17	0.45
2:D:395:ASN:O	2:D:396:ARG:HG3	2.15	0.45
2:H:373:VAL:HG23	2:H:420:ILE:HD11	1.98	0.45
2:J:244:MET:HE1	2:J:275:ILE:HA	1.99	0.45
2:L:260:ILE:HB	2:L:268:ILE:O	2.16	0.45
2:D:194:SER:OG	2:D:198:ARG:NH1	2.49	0.45
2:F:158:LEU:O	2:F:162:VAL:HG13	2.16	0.45
2:H:392:ILE:O	2:H:400:ILE:HG12	2.16	0.45
2:B:383:ALA:HB1	2:B:385:TYR:CE2	2.52	0.45
2:B:442:VAL:HB	1:E:55:VAL:HG13	1.98	0.45
2:D:136:ALA:C	2:D:138:LYS:N	2.70	0.45
2:F:245:LEU:HD23	2:F:245:LEU:HA	1.50	0.45
1:G:57:ASN:HB2	3:G:201:NAG:O5	2.16	0.45
2:J:320:TYR:CE2	2:J:335:CYS:HB3	2.52	0.45
2:B:349:GLU:HB3	2:B:356:THR:HG21	1.98	0.45
1:E:23:TYR:HE1	2:F:381:LEU:HD21	1.81	0.45
1:E:32:THR:HG21	2:F:377:PRO:HG2	1.98	0.45
2:F:241:ILE:O	2:F:245:LEU:HB2	2.17	0.45
3:L:601:NAG:H3	3:L:601:NAG:H83	1.99	0.45
2:J:380:ALA:HB2	2:J:427:LEU:HD21	1.99	0.45
2:L:373:VAL:HG23	2:L:420:ILE:HD11	1.99	0.45
2:L:250:MET:HE2	2:L:334:PHE:CD2	2.52	0.45
2:B:295:LYS:O	2:B:298:ASN:HB2	2.17	0.45
1:C:78:LEU:HD21	2:D:200:PHE:CZ	2.52	0.45
2:D:221:LEU:HG	2:D:269:TYR:CE1	2.52	0.45
2:D:250:MET:HE1	2:D:254:LYS:HE2	2.00	0.45
1:G:21:GLU:HB2	1:G:32:THR:HG23	1.97	0.44
2:B:382:VAL:O	2:B:407:CYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:LEU:HD23	2:J:191:VAL:HG21	1.99	0.44
1:A:21:GLU:HB2	1:A:32:THR:HG23	1.99	0.44
2:F:194:SER:O	2:F:198:ARG:NH1	2.50	0.44
2:F:467:ILE:HG13	2:F:468:GLU:N	2.31	0.44
2:H:145:ASN:HA	2:H:148:VAL:CG2	2.44	0.44
1:K:65:SER:O	1:K:69:THR:HG23	2.17	0.44
2:J:229:ARG:O	2:J:232:SER:HB2	2.18	0.44
2:F:373:VAL:HG23	2:F:420:ILE:HD11	2.00	0.44
2:F:480:ILE:O	2:F:480:ILE:HG23	2.17	0.44
1:G:46:ASN:ND2	2:J:435:HIS:NE2	2.66	0.44
2:H:320:TYR:CD1	2:H:320:TYR:N	2.86	0.44
1:K:85:SER:HB2	2:L:261:GLY:HA2	1.99	0.44
2:D:326:CYS:HB3	2:D:333:VAL:CG1	2.48	0.44
2:D:393:GLY:HA2	2:D:400:ILE:CG1	2.47	0.44
1:E:73:LEU:HD23	1:E:73:LEU:HA	1.75	0.44
2:F:255:GLY:O	2:F:256:PHE:HB3	2.18	0.44
2:D:481:LEU:C	2:D:481:LEU:CD1	2.84	0.44
1:G:21:GLU:CB	2:H:378:LEU:HD12	2.47	0.44
2:L:240:GLN:HG2	2:L:279:ILE:HG12	1.99	0.44
1:A:78:LEU:HD11	2:B:200:PHE:HZ	1.83	0.44
1:C:37:SER:HB3	2:D:283:CYS:SG	2.57	0.44
2:F:180:ASN:O	2:F:184:ILE:HG23	2.18	0.44
2:F:245:LEU:O	2:F:248:ARG:HG3	2.18	0.44
2:F:417:THR:CA	2:F:427:LEU:CD1	2.95	0.44
2:H:260:ILE:HB	2:H:268:ILE:HG22	2.00	0.44
2:J:221:LEU:CD2	2:J:257:GLY:HA3	2.47	0.44
2:J:427:LEU:HA	2:J:427:LEU:HD23	1.60	0.44
2:B:474:VAL:HG13	2:D:147:ALA:CB	2.47	0.44
2:D:392:ILE:O	2:D:400:ILE:N	2.41	0.44
2:H:187:LEU:O	2:H:191:VAL:HG12	2.18	0.43
2:J:286:ILE:HD13	2:J:286:ILE:HA	1.81	0.43
2:L:227:LEU:HD23	2:L:248:ARG:HB3	2.00	0.43
2:L:227:LEU:O	2:L:231:VAL:HG23	2.17	0.43
1:C:84:VAL:HG12	2:F:249:ALA:HA	2.00	0.43
2:D:250:MET:HE3	2:D:254:LYS:HG3	2.00	0.43
2:H:152:GLY:O	2:H:155:VAL:HG12	2.17	0.43
2:J:187:LEU:HD11	2:L:188:LYS:HG3	2.00	0.43
2:J:296:ASP:OD1	2:J:296:ASP:N	2.49	0.43
2:L:219:LEU:HD13	2:L:219:LEU:HA	1.69	0.43
2:B:371:SER:HA	2:B:383:ALA:O	2.17	0.43
2:D:371:SER:HA	2:D:383:ALA:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:MET:HE3	2:D:372:MET:HB2	1.94	0.43
2:F:189:MET:HB2	2:F:189:MET:HE2	1.75	0.43
2:H:435:HIS:CD2	2:H:435:HIS:N	2.86	0.43
2:J:400:ILE:HD13	2:J:400:ILE:HG21	1.73	0.43
2:L:202:ASN:O	2:L:206:GLN:HG3	2.18	0.43
2:B:463:VAL:HG11	2:D:158:LEU:HD13	1.99	0.43
2:H:245:LEU:HD23	2:H:245:LEU:HA	1.83	0.43
2:L:398:GLY:HA3	2:D:399:ILE:N	2.33	0.43
2:D:244:MET:HB3	2:D:251:VAL:HG21	2.01	0.43
1:E:21:GLU:HB3	2:F:378:LEU:HD12	2.00	0.43
1:E:58:LEU:HB2	2:F:189:MET:CE	2.49	0.43
1:G:23:TYR:CZ	1:G:25:GLU:HA	2.54	0.43
2:H:147:ALA:HB2	2:L:473:LEU:CB	2.49	0.43
2:L:409:TYR:C	2:L:410:ILE:HG13	2.38	0.43
1:A:44:TYR:O	2:B:273:LEU:HB2	2.19	0.43
2:D:248:ARG:H	2:D:248:ARG:HG3	1.54	0.43
2:D:384:CYS:O	2:D:405:LYS:HA	2.18	0.43
2:D:456:PHE:CE2	2:F:165:LEU:HB2	2.53	0.43
2:F:234:MET:HE3	2:F:275:ILE:HG12	2.00	0.43
1:G:50:LEU:HA	1:G:50:LEU:HD23	1.55	0.43
2:B:149:SER:OG	2:D:471:GLN:OE1	2.15	0.43
1:E:78:LEU:HD11	2:F:200:PHE:HZ	1.82	0.43
2:F:221:LEU:HG	2:F:269:TYR:CE2	2.54	0.43
2:D:169:VAL:CG1	2:F:169:VAL:HG11	2.48	0.43
2:F:356:THR:HG22	2:F:358:ASN:N	2.32	0.43
2:J:243:LEU:HD23	2:J:243:LEU:N	2.34	0.43
1:A:21:GLU:HB3	2:B:378:LEU:HD12	2.01	0.43
1:C:32:THR:HG21	2:D:377:PRO:HB2	2.01	0.43
2:F:349:GLU:OE1	2:F:358:ASN:HB3	2.18	0.43
2:H:234:MET:CE	2:H:275:ILE:HG12	2.49	0.43
2:H:476:GLN:O	2:H:479:LYS:HB3	2.19	0.43
2:J:294:GLU:OE1	2:J:297:GLY:N	2.51	0.43
1:C:23:TYR:CE2	1:C:25:GLU:HG2	2.54	0.43
2:D:166:LYS:HG2	2:F:456:PHE:HE1	1.84	0.43
2:D:200:PHE:O	2:D:203:VAL:HG22	2.18	0.43
2:D:481:LEU:HD21	2:F:137:ILE:HG12	2.01	0.43
2:H:236:THR:HB	2:H:240:GLN:OE1	2.19	0.42
1:A:50:LEU:CD2	2:D:437:ILE:HB	2.49	0.42
1:A:66:LEU:HD21	2:D:191:VAL:HG11	2.00	0.42
2:B:199:ARG:NH2	2:B:226:GLU:OE1	2.44	0.42
2:B:249:ALA:HB2	1:E:84:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:SER:O	2:D:198:ARG:HG2	2.19	0.42
2:F:169:VAL:O	2:F:174:THR:HG23	2.19	0.42
2:D:317:THR:HB	2:D:343:VAL:HG23	2.01	0.42
2:F:213:ILE:HD12	2:F:258:ILE:HD13	2.00	0.42
1:G:66:LEU:HD22	2:J:191:VAL:HG12	2.01	0.42
2:J:221:LEU:HD23	2:J:271:VAL:HG12	2.00	0.42
2:B:253:ARG:NH1	2:F:213:ILE:HG12	2.34	0.42
2:B:471:GLN:O	2:B:474:VAL:HG23	2.19	0.42
2:F:174:THR:CA	2:F:177:ILE:HG22	2.42	0.42
2:H:382:VAL:HG22	2:H:418:VAL:HG11	2.01	0.42
2:J:417:THR:HA	2:J:425:TYR:O	2.20	0.42
2:L:219:LEU:HD13	2:L:252:ARG:CZ	2.49	0.42
1:I:37:SER:O	2:J:279:ILE:HG13	2.20	0.42
2:J:312:LYS:HG3	2:J:317:THR:HG22	2.02	0.42
1:K:61:THR:HG21	1:K:65:SER:HB3	2.01	0.42
2:B:219:LEU:HA	2:B:219:LEU:HD13	1.67	0.42
2:B:309:TRP:CD1	2:B:326:CYS:HB2	2.55	0.42
2:B:446:PHE:CE1	2:F:181:LYS:HB3	2.55	0.42
2:B:473:LEU:HD23	2:D:147:ALA:CA	2.49	0.42
2:F:471:GLN:O	2:F:471:GLN:HG2	2.19	0.42
2:H:166:LYS:NZ	2:H:167:GLU:OE2	2.52	0.42
1:K:40:ARG:HH21	2:L:337:THR:HB	1.84	0.42
2:H:169:VAL:HG11	2:L:169:VAL:HG12	2.01	0.42
2:H:260:ILE:H	2:H:269:TYR:HA	1.84	0.42
2:L:169:VAL:O	2:L:174:THR:HG23	2.19	0.42
2:B:157:VAL:HG23	2:F:463:VAL:CG2	2.49	0.42
1:C:36:LEU:HB2	2:D:332:HIS:ND1	2.34	0.42
1:A:24:LEU:HD13	1:A:29:SER:OG	2.20	0.42
2:D:169:VAL:O	2:D:174:THR:HG23	2.20	0.42
1:A:23:TYR:CD1	2:B:409:TYR:HB2	2.54	0.42
1:C:67:ILE:CD1	2:D:190:ALA:HA	2.50	0.42
2:F:417:THR:CA	2:F:427:LEU:HD12	2.50	0.42
1:I:70:GLU:O	1:I:74:THR:HG23	2.20	0.42
2:L:285:ILE:HB	2:L:309:TRP:CE3	2.55	0.42
2:D:263:TYR:HD2	2:D:268:ILE:HD13	1.84	0.42
1:G:78:LEU:HD21	2:H:204:VAL:HG21	2.02	0.41
2:H:481:LEU:HD22	2:L:142:LYS:HD3	2.02	0.41
2:L:199:ARG:NH2	2:L:226:GLU:OE1	2.51	0.41
2:B:265:SER:O	2:B:265:SER:OG	2.37	0.41
2:B:392:ILE:HD12	2:B:418:VAL:HG22	2.01	0.41
2:J:166:LYS:HE2	2:L:456:PHE:HB3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:236:THR:HB	2:L:240:GLN:OE1	2.20	0.41
2:B:250:MET:HE3	2:B:253:ARG:NH2	2.35	0.41
2:F:187:LEU:O	2:F:191:VAL:HG23	2.21	0.41
2:H:289:ALA:HA	2:H:372:MET:HE1	2.02	0.41
2:D:483:SER:HB3	2:F:133:GLU:OE2	2.21	0.41
2:H:146:GLU:O	2:H:146:GLU:HG2	2.20	0.41
2:L:224:ASP:OD1	2:L:248:ARG:HD3	2.20	0.41
2:L:235:PRO:O	2:L:236:THR:HG23	2.19	0.41
2:D:294:GLU:OE1	2:D:296:ASP:N	2.54	0.41
2:H:347:SER:HB3	2:H:359:TYR:CE2	2.55	0.41
1:I:85:SER:CB	2:J:261:GLY:HA2	2.43	0.41
2:J:243:LEU:HD12	2:J:279:ILE:CG2	2.50	0.41
2:J:244:MET:CE	2:J:276:PHE:H	2.32	0.41
2:J:449:ILE:HD12	2:J:449:ILE:HA	1.77	0.41
2:J:451:PHE:HA	2:J:452:PRO:HD3	1.97	0.41
2:J:472:ALA:HA	2:J:475:ASP:CG	2.40	0.41
2:B:309:TRP:NE1	2:B:326:CYS:HB2	2.35	0.41
2:D:313:ASN:O	2:D:316:SER:O	2.39	0.41
2:H:243:LEU:HA	2:H:243:LEU:HD12	1.76	0.41
1:I:36:LEU:HD23	1:I:36:LEU:HA	1.89	0.41
2:L:322:ASN:O	2:L:325:ASP:HB2	2.20	0.41
2:L:453:GLU:O	2:L:457:ASN:HB2	2.21	0.41
2:B:235:PRO:O	2:B:236:THR:HG23	2.21	0.41
2:D:301:CYS:O	2:D:365:THR:HA	2.21	0.41
1:G:30:THR:HG23	2:H:381:LEU:CD1	2.37	0.41
1:G:58:LEU:O	1:G:61:THR:HG23	2.21	0.41
2:H:194:SER:O	2:H:198:ARG:CG	2.68	0.41
1:I:83:THR:HG23	1:I:83:THR:H	1.58	0.41
2:J:141:LEU:HD13	2:L:141:LEU:HD12	2.03	0.41
2:L:187:LEU:O	2:L:191:VAL:HG13	2.21	0.41
2:L:460:LEU:HD23	2:L:460:LEU:HA	1.77	0.41
2:B:217:ILE:O	2:B:252:ARG:HD3	2.19	0.41
2:B:219:LEU:HD23	2:F:208:SER:HA	2.03	0.41
2:B:399:ILE:HG12	2:B:400:ILE:N	2.36	0.41
2:B:470:SER:HB2	2:D:147:ALA:O	2.21	0.41
1:C:50:LEU:HD23	1:C:50:LEU:HA	1.74	0.41
2:F:416:ASP:C	2:F:427:LEU:HD13	2.41	0.41
2:F:462:GLN:O	2:F:465:GLU:HG2	2.20	0.41
1:I:51:GLU:HG2	2:J:266:SER:OG	2.21	0.41
2:L:354:ILE:C	2:L:356:THR:H	2.24	0.41
2:D:240:GLN:HG2	2:D:279:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:LEU:HD12	2:D:381:LEU:HA	1.93	0.41
2:D:392:ILE:CD1	2:D:410:ILE:HD13	2.46	0.41
2:D:456:PHE:O	2:D:459:ALA:N	2.53	0.41
1:E:37:SER:HB3	2:F:283:CYS:SG	2.61	0.41
2:H:147:ALA:HB2	2:L:473:LEU:HB2	2.02	0.40
2:J:391:SER:HB2	2:J:399:ILE:HG13	2.02	0.40
2:B:433:GLU:CD	2:F:229:ARG:HH11	2.23	0.40
1:E:50:LEU:CD2	2:F:269:TYR:HE1	2.30	0.40
1:E:58:LEU:HB2	2:F:189:MET:HE1	2.02	0.40
2:F:287:LYS:HA	2:F:307:GLN:HG3	2.02	0.40
2:H:392:ILE:HG23	2:H:415:ALA:HB1	1.98	0.40
2:J:457:ASN:HD22	2:J:457:ASN:HA	1.67	0.40
1:K:81:LEU:HD11	2:L:207:PHE:HB3	2.03	0.40
1:A:55:VAL:CG1	1:A:71:LEU:HD11	2.51	0.40
2:B:392:ILE:HG23	2:B:415:ALA:CB	2.51	0.40
2:B:473:LEU:HD23	2:D:147:ALA:HA	2.02	0.40
2:B:474:VAL:HG13	2:D:147:ALA:HB3	2.02	0.40
1:C:58:LEU:HA	1:C:58:LEU:HD12	1.72	0.40
2:H:234:MET:HE1	2:H:275:ILE:HA	2.03	0.40
2:H:262:VAL:O	2:H:263:TYR:CG	2.75	0.40
2:L:156:ARG:O	2:L:160:THR:HG22	2.21	0.40
2:L:179:LYS:O	2:L:182:CYS:HB3	2.22	0.40
2:L:214:THR:O	2:L:256:PHE:HB2	2.20	0.40
2:L:318:VAL:HG23	2:L:320:TYR:HE1	1.84	0.40
2:B:173:LEU:HD11	2:D:174:THR:HG22	2.02	0.40
2:H:286:ILE:O	2:H:307:GLN:HA	2.22	0.40
2:H:451:PHE:O	2:H:453:GLU:N	2.53	0.40
2:L:130:LEU:O	2:L:130:LEU:CG	2.70	0.40
1:A:86:ALA:HB3	2:B:260:ILE:HA	2.04	0.40
2:B:376:SER:HB3	2:B:379:GLY:C	2.40	0.40
2:B:403:LEU:HA	2:B:403:LEU:HD23	1.80	0.40
2:D:460:LEU:O	2:D:463:VAL:HG22	2.21	0.40
1:E:23:TYR:CE1	2:F:381:LEU:HD21	2.57	0.40
2:H:143:THR:HB	2:L:476:GLN:HE21	1.87	0.40
2:L:138:LYS:HB3	2:L:138:LYS:HE3	1.63	0.40
2:L:247:ASN:ND2	2:L:334:PHE:HZ	2.20	0.40
2:B:446:PHE:HE1	2:F:181:LYS:HB3	1.86	0.40
2:F:286:ILE:HD13	2:F:310:TYR:CE1	2.56	0.40
2:F:464:PHE:O	2:F:467:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	68/89 (76%)	67 (98%)	1 (2%)	0	100	100
1	C	68/89 (76%)	66 (97%)	2 (3%)	0	100	100
1	E	68/89 (76%)	66 (97%)	2 (3%)	0	100	100
1	G	68/89 (76%)	66 (97%)	0	2 (3%)	4	15
1	I	68/89 (76%)	66 (97%)	2 (3%)	0	100	100
1	K	68/89 (76%)	68 (100%)	0	0	100	100
2	B	349/431 (81%)	336 (96%)	13 (4%)	0	100	100
2	D	350/431 (81%)	334 (95%)	16 (5%)	0	100	100
2	F	349/431 (81%)	342 (98%)	7 (2%)	0	100	100
2	H	350/431 (81%)	338 (97%)	12 (3%)	0	100	100
2	J	350/431 (81%)	338 (97%)	12 (3%)	0	100	100
2	L	350/431 (81%)	339 (97%)	11 (3%)	0	100	100
All	All	2506/3120 (80%)	2426 (97%)	78 (3%)	2 (0%)	51	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	61	THR
1	G	62	ASP

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	63/82 (77%)	63 (100%)	0	100	100
1	C	64/82 (78%)	62 (97%)	2 (3%)	40	72
1	E	64/82 (78%)	63 (98%)	1 (2%)	62	87
1	G	64/82 (78%)	63 (98%)	1 (2%)	62	87
1	I	64/82 (78%)	64 (100%)	0	100	100
1	K	62/82 (76%)	62 (100%)	0	100	100
2	B	297/357 (83%)	288 (97%)	9 (3%)	41	73
2	D	297/357 (83%)	289 (97%)	8 (3%)	44	77
2	F	299/357 (84%)	288 (96%)	11 (4%)	34	66
2	H	298/357 (84%)	292 (98%)	6 (2%)	55	83
2	J	295/357 (83%)	286 (97%)	9 (3%)	40	72
2	L	298/357 (84%)	293 (98%)	5 (2%)	60	86
All	All	2165/2634 (82%)	2113 (98%)	52 (2%)	49	80

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	68	LYS
2	H	179	LYS
2	H	293	SER
2	H	302	LEU
2	H	329	ARG
2	H	455	GLN
2	H	477	SER
2	J	156	ARG
2	J	163	ARG
2	J	394	SER
2	J	396	ARG
2	J	444	SER
2	J	460	LEU
2	J	475	ASP
2	J	479	LYS
2	J	480	ILE
2	L	132	SER
2	L	192	SER
2	L	348	ARG
2	L	394	SER
2	L	456	PHE
2	B	135	ASN

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Mol	Chain	Res	Type
2	B	137	ILE
2	B	138	LYS
2	B	163	ARG
2	B	295	LYS
2	B	435	HIS
2	B	470	SER
2	B	471	GLN
2	B	477	SER
1	C	71	LEU
1	C	75	LYS
2	D	137	ILE
2	D	141	LEU
2	D	156	ARG
2	D	166	LYS
2	D	192	SER
2	D	291	SER
2	D	389	SER
2	D	434	GLN
1	E	25	GLU
2	F	156	ARG
2	F	166	LYS
2	F	192	SER
2	F	265	SER
2	F	291	SER
2	F	293	SER
2	F	359	TYR
2	F	396	ARG
2	F	473	LEU
2	F	474	VAL
2	F	480	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	601	2	14,14,15	1.07	1 (7%)	17,19,21	0.99	1 (5%)
3	NAG	H	601	2	14,14,15	0.55	0	17,19,21	1.03	2 (11%)
3	NAG	E	201	1	14,14,15	1.47	2 (14%)	17,19,21	0.77	0
3	NAG	F	602	2	14,14,15	0.89	1 (7%)	17,19,21	0.72	1 (5%)
3	NAG	A	201	1	14,14,15	0.97	1 (7%)	17,19,21	1.29	2 (11%)
3	NAG	K	201	1	14,14,15	0.72	0	17,19,21	0.59	0
3	NAG	J	602	2	14,14,15	0.50	0	17,19,21	0.75	1 (5%)
3	NAG	B	601	2	14,14,15	1.04	1 (7%)	17,19,21	0.71	1 (5%)
3	NAG	D	602	2	14,14,15	1.82	1 (7%)	17,19,21	1.68	1 (5%)
3	NAG	F	601	2	14,14,15	0.79	1 (7%)	17,19,21	0.85	1 (5%)
3	NAG	C	201	1	14,14,15	0.82	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	D	601	2	14,14,15	0.73	1 (7%)	17,19,21	0.50	0
3	NAG	G	201	1	14,14,15	1.44	2 (14%)	17,19,21	0.86	0
3	NAG	L	602	2	14,14,15	1.14	1 (7%)	17,19,21	1.36	1 (5%)
3	NAG	L	601	2	14,14,15	0.48	0	17,19,21	1.52	3 (17%)
3	NAG	I	201	1	14,14,15	1.47	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	H	602	2	14,14,15	1.38	2 (14%)	17,19,21	0.62	0
3	NAG	B	602	2	14,14,15	0.68	1 (7%)	17,19,21	1.17	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	601	2	-	2/6/23/26	0/1/1/1
3	NAG	H	601	2	-	3/6/23/26	0/1/1/1
3	NAG	E	201	1	-	1/6/23/26	0/1/1/1
3	NAG	F	602	2	-	2/6/23/26	0/1/1/1
3	NAG	A	201	1	-	2/6/23/26	0/1/1/1
3	NAG	K	201	1	-	1/6/23/26	0/1/1/1
3	NAG	J	602	2	-	2/6/23/26	0/1/1/1
3	NAG	B	601	2	-	1/6/23/26	0/1/1/1
3	NAG	D	602	2	-	1/6/23/26	0/1/1/1
3	NAG	F	601	2	-	1/6/23/26	0/1/1/1
3	NAG	C	201	1	-	0/6/23/26	0/1/1/1
3	NAG	D	601	2	-	2/6/23/26	0/1/1/1
3	NAG	G	201	1	-	2/6/23/26	0/1/1/1
3	NAG	L	602	2	-	1/6/23/26	0/1/1/1
3	NAG	L	601	2	-	4/6/23/26	0/1/1/1
3	NAG	I	201	1	-	2/6/23/26	0/1/1/1
3	NAG	H	602	2	-	1/6/23/26	0/1/1/1
3	NAG	B	602	2	-	2/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NAG	O5-C1	6.64	1.54	1.43
3	I	201	NAG	O5-C1	5.34	1.52	1.43
3	E	201	NAG	O5-C1	4.96	1.51	1.43
3	G	201	NAG	O5-C1	4.52	1.50	1.43
3	H	602	NAG	O5-C1	4.09	1.50	1.43
3	L	602	NAG	O5-C1	4.06	1.50	1.43
3	B	601	NAG	O5-C1	3.72	1.49	1.43
3	J	601	NAG	C1-C2	3.64	1.57	1.52
3	F	602	NAG	O5-C1	3.03	1.48	1.43
3	H	602	NAG	C1-C2	2.94	1.56	1.52
3	A	201	NAG	O5-C1	-2.54	1.39	1.43
3	C	201	NAG	C1-C2	2.32	1.55	1.52
3	G	201	NAG	C1-C2	2.23	1.55	1.52
3	D	601	NAG	C1-C2	2.21	1.55	1.52
3	B	602	NAG	O5-C1	2.19	1.47	1.43
3	F	601	NAG	O5-C1	2.19	1.47	1.43
3	E	201	NAG	C1-C2	2.12	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	NAG	C1-O5-C5	6.47	120.96	112.19
3	L	602	NAG	C1-O5-C5	4.89	118.82	112.19
3	L	601	NAG	C2-N2-C7	4.40	129.17	122.90
3	B	602	NAG	C1-O5-C5	4.02	117.64	112.19
3	A	201	NAG	C1-O5-C5	-3.70	107.17	112.19
3	L	601	NAG	C1-O5-C5	2.88	116.09	112.19
3	A	201	NAG	C4-C3-C2	2.62	114.85	111.02
3	H	601	NAG	C1-O5-C5	2.59	115.71	112.19
3	J	602	NAG	C1-O5-C5	2.58	115.69	112.19
3	C	201	NAG	C1-O5-C5	2.57	115.67	112.19
3	J	601	NAG	C1-O5-C5	2.49	115.57	112.19
3	L	601	NAG	C1-C2-N2	2.45	114.68	110.49
3	F	602	NAG	C1-O5-C5	2.24	115.22	112.19
3	H	601	NAG	C2-N2-C7	2.12	125.93	122.90
3	B	601	NAG	C1-O5-C5	2.11	115.05	112.19
3	F	601	NAG	O5-C1-C2	-2.10	107.98	111.29
3	I	201	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	201	NAG	O5-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
3	A	201	NAG	O5-C5-C6-O6
3	F	602	NAG	O5-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6
3	F	602	NAG	C4-C5-C6-O6
3	I	201	NAG	C4-C5-C6-O6
3	D	601	NAG	O5-C5-C6-O6
3	A	201	NAG	C4-C5-C6-O6
3	J	602	NAG	O5-C5-C6-O6
3	D	601	NAG	C4-C5-C6-O6
3	G	201	NAG	C8-C7-N2-C2
3	G	201	NAG	O7-C7-N2-C2
3	L	601	NAG	C8-C7-N2-C2
3	L	601	NAG	O7-C7-N2-C2
3	H	601	NAG	O5-C5-C6-O6
3	J	602	NAG	C4-C5-C6-O6
3	K	201	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	E	201	NAG	O5-C5-C6-O6
3	D	602	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	H	602	NAG	O5-C5-C6-O6
3	H	601	NAG	C4-C5-C6-O6
3	J	601	NAG	C1-C2-N2-C7
3	L	602	NAG	C4-C5-C6-O6
3	H	601	NAG	C3-C2-N2-C7
3	J	601	NAG	C3-C2-N2-C7
3	L	601	NAG	C3-C2-N2-C7
3	F	601	NAG	C3-C2-N2-C7
3	L	601	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	201	NAG	2	0
3	L	601	NAG	1	0

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	70/89 (78%)	-0.06	1 (1%) 75 69	12, 27, 67, 96	0
1	C	70/89 (78%)	-0.06	2 (2%) 51 41	8, 31, 63, 75	0
1	E	70/89 (78%)	-0.12	1 (1%) 75 69	9, 28, 61, 75	0
1	G	70/89 (78%)	-0.17	1 (1%) 75 69	5, 25, 50, 62	0
1	I	70/89 (78%)	-0.22	0 100 100	7, 23, 47, 61	0
1	K	70/89 (78%)	-0.23	0 100 100	7, 22, 49, 65	0
2	B	351/431 (81%)	0.28	28 (7%) 12 7	10, 28, 109, 128	0
2	D	352/431 (81%)	0.18	22 (6%) 20 12	7, 29, 105, 126	0
2	F	351/431 (81%)	0.20	17 (4%) 30 21	8, 28, 106, 123	0
2	H	352/431 (81%)	0.10	14 (3%) 38 28	5, 26, 99, 114	0
2	J	352/431 (81%)	0.11	12 (3%) 45 35	6, 27, 101, 115	0
2	L	352/431 (81%)	0.03	3 (0%) 84 80	5, 30, 98, 111	0
All	All	2530/3120 (81%)	0.10	101 (3%) 38 28	5, 28, 102, 128	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	136	ALA	5.5
2	B	140	ALA	4.9
2	B	136	ALA	4.9
2	F	480	ILE	4.6
2	J	478	ASN	4.4
2	B	133	GLU	4.3
2	F	479	LYS	4.2
2	B	476	GLN	4.1
2	D	456	PHE	4.0
2	B	473	LEU	4.0
2	F	475	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	474	VAL	3.9
2	J	296	ASP	3.8
2	D	145	ASN	3.8
2	F	476	GLN	3.8
2	F	482	ASN	3.7
2	B	460	LEU	3.7
2	F	462	GLN	3.7
2	H	456	PHE	3.6
2	D	480	ILE	3.6
2	B	458	VAL	3.5
1	A	62	ASP	3.5
2	J	133	GLU	3.5
2	J	132	SER	3.4
2	L	141	LEU	3.3
2	D	141	LEU	3.3
2	B	464	PHE	3.3
2	B	480	ILE	3.3
2	B	481	LEU	3.3
2	B	477	SER	3.2
2	D	138	LYS	3.2
1	C	88	GLN	3.2
2	F	478	ASN	3.2
2	F	155	VAL	3.0
2	J	474	VAL	3.0
2	B	470	SER	3.0
2	B	462	GLN	3.0
2	J	458	VAL	3.0
2	B	459	ALA	3.0
2	D	358	ASN	3.0
2	F	481	LEU	2.9
2	J	136	ALA	2.9
2	B	145	ASN	2.9
2	B	137	ILE	2.9
2	H	471	GLN	2.9
2	D	479	LYS	2.8
2	F	473	LEU	2.8
2	B	468	GLU	2.8
2	F	138	LYS	2.8
2	B	139	GLY	2.8
2	D	133	GLU	2.8
2	D	135	ASN	2.8
2	H	464	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	296	ASP	2.8
2	F	146	GLU	2.7
2	H	462	GLN	2.7
2	L	455	GLN	2.7
2	D	137	ILE	2.7
2	D	298	ASN	2.7
2	H	460	LEU	2.7
2	B	453	GLU	2.6
2	H	475	ASP	2.6
2	J	138	LYS	2.6
2	J	456	PHE	2.5
2	B	482	ASN	2.5
2	F	456	PHE	2.5
2	J	452	PRO	2.5
2	D	151	LEU	2.5
2	F	148	VAL	2.5
1	C	59	THR	2.5
2	J	144	THR	2.5
1	G	59	THR	2.4
2	B	450	ARG	2.4
2	D	452	PRO	2.4
1	E	86	ALA	2.4
2	H	476	GLN	2.4
2	B	141	LEU	2.4
2	B	472	ALA	2.3
2	B	456	PHE	2.3
2	D	147	ALA	2.3
2	J	454	ASP	2.3
2	H	479	LYS	2.3
2	D	465	GLU	2.3
2	D	139	GLY	2.3
2	D	148	VAL	2.2
2	B	142	LYS	2.2
2	H	472	ALA	2.2
2	D	464	PHE	2.2
2	H	473	LEU	2.2
2	H	480	ILE	2.2
2	D	296	ASP	2.2
2	H	468	GLU	2.2
2	H	134	VAL	2.2
2	F	161	ALA	2.1
2	L	479	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	162	VAL	2.1
2	B	461	ASP	2.0
2	F	151	LEU	2.0
2	B	479	LYS	2.0
2	F	474	VAL	2.0
2	D	455	GLN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	H	602	14/15	0.64	0.33	55,77,85,88	0
3	NAG	G	201	14/15	0.67	0.45	64,85,94,103	0
3	NAG	A	201	14/15	0.68	0.34	46,81,94,96	0
3	NAG	B	602	14/15	0.72	0.26	43,63,74,75	0
3	NAG	J	601	14/15	0.73	0.37	73,84,89,89	0
3	NAG	C	201	14/15	0.75	0.29	57,75,87,89	0
3	NAG	H	601	14/15	0.78	0.24	52,74,81,86	0
3	NAG	F	602	14/15	0.78	0.24	35,64,83,85	0
3	NAG	L	602	14/15	0.79	0.30	39,58,62,65	0
3	NAG	D	602	14/15	0.82	0.24	35,61,76,80	0
3	NAG	E	201	14/15	0.84	0.28	48,61,68,69	0
3	NAG	I	201	14/15	0.85	0.18	37,59,63,63	0
3	NAG	L	601	14/15	0.85	0.24	56,74,89,103	0
3	NAG	D	601	14/15	0.85	0.16	69,82,89,91	0
3	NAG	J	602	14/15	0.86	0.22	52,59,67,69	0
3	NAG	K	201	14/15	0.89	0.27	48,62,69,72	0
3	NAG	B	601	14/15	0.90	0.16	66,73,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	F	601	14/15	0.91	0.21	63,71,75,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.