



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:02 AM UTC

PDB ID : 8XUS / pdb_00008xus
EMDB ID : EMD-38682
Title : JN.1 Spike Trimer in complex with heparan sulfate
Authors : Yue, C.; Liu, P.
Deposited on : 2024-01-14
Resolution : 3.18 Å (reported)

This is a Full wwPDB EM 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/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:

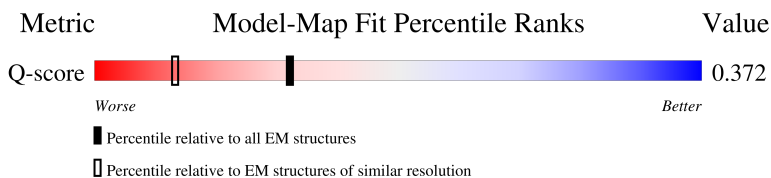
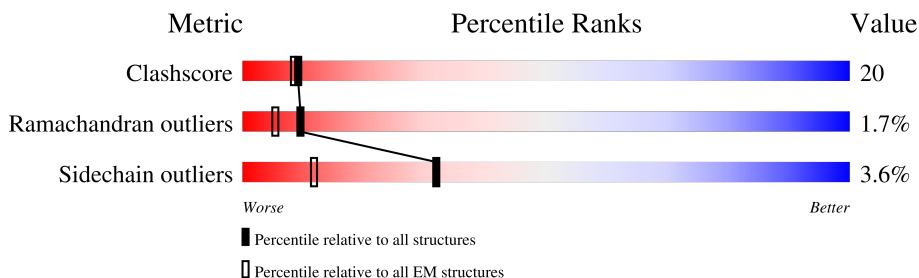
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1206	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">56%</div> <div style="text-align: right;">29%</div> <div style="text-align: right;">• 12%</div> </div>
1	B	1206	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">16%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">56%</div> <div style="text-align: right;">30%</div> <div style="text-align: right;">• 12%</div> </div>
1	C	1206	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">14%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">54%</div> <div style="text-align: right;">31%</div> <div style="text-align: right;">• 12%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25713 atoms, of which 0 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	1063	8314	5319	1383	1574	38	0	0
1	A	1063	8314	5319	1383	1574	38	0	0
1	B	1063	8314	5319	1383	1574	38	0	0

There are 222 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	16	MET	-	insertion	UNP P0DTC2
C	17	PRO	-	insertion	UNP P0DTC2
C	18	LEU	-	insertion	UNP P0DTC2
C	19	PHE	-	insertion	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	24	THR	ARG	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	455	SER	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	16	MET	-	insertion	UNP P0DTC2
A	17	PRO	-	insertion	UNP P0DTC2
A	18	LEU	-	insertion	UNP P0DTC2
A	19	PHE	-	insertion	UNP P0DTC2
A	22	ILE	THR	variant	UNP P0DTC2
A	24	THR	ARG	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	variant	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	455	SER	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	insertion	UNP P0DTC2
B	17	PRO	-	insertion	UNP P0DTC2
B	18	LEU	-	insertion	UNP P0DTC2
B	19	PHE	-	insertion	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	24	THR	ARG	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	455	SER	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2

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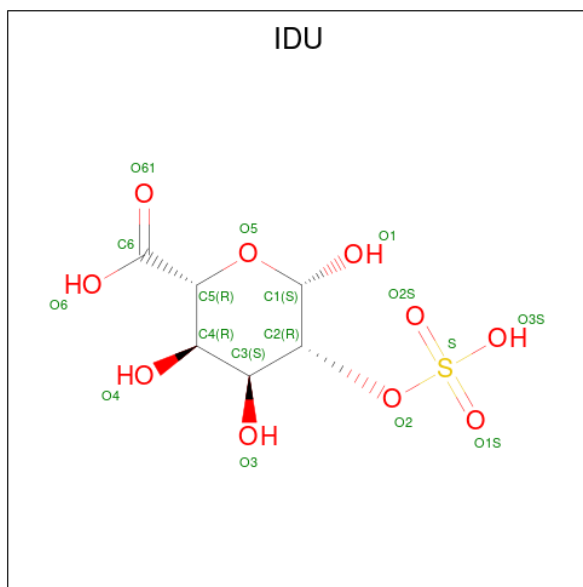
Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	

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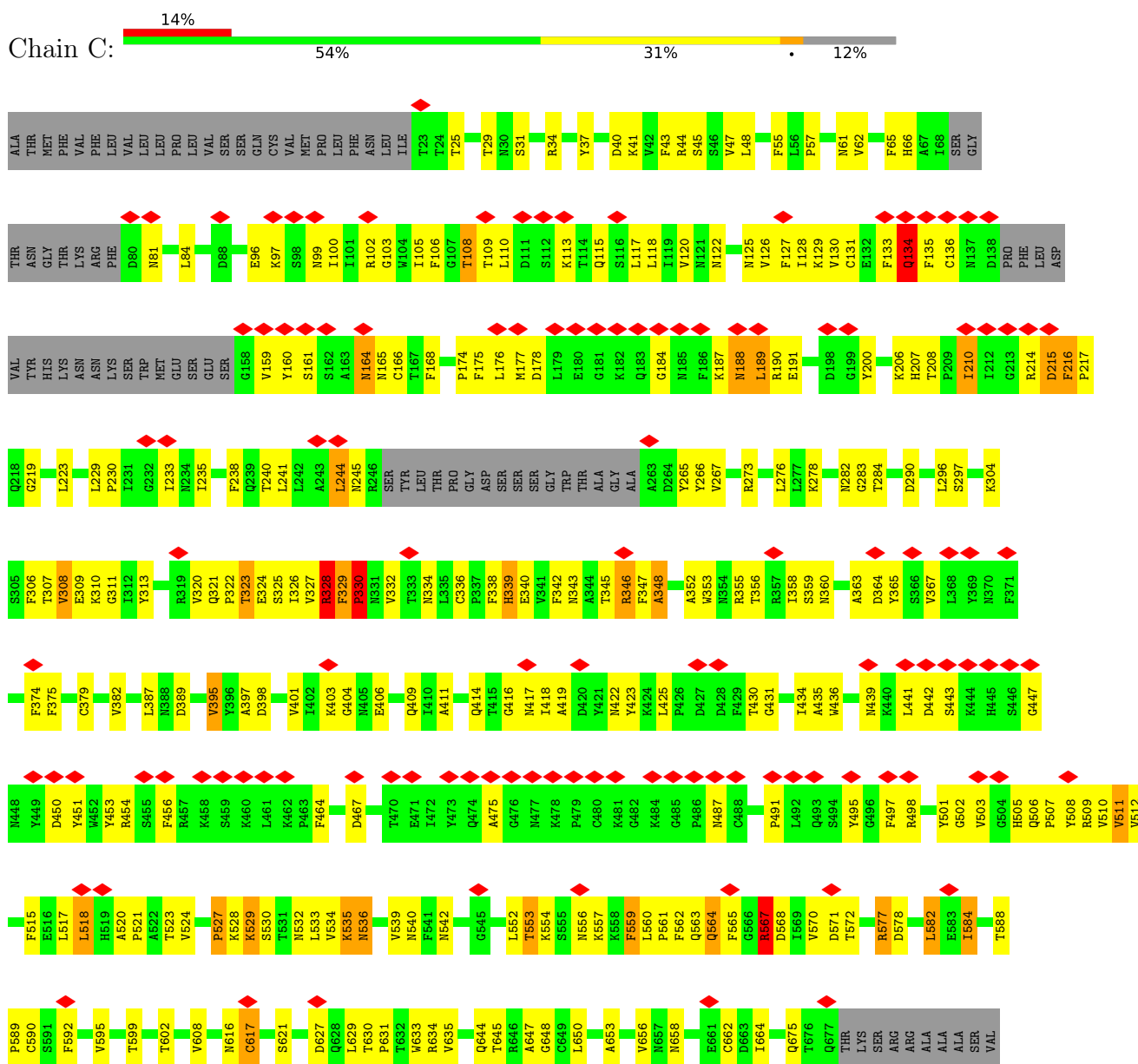


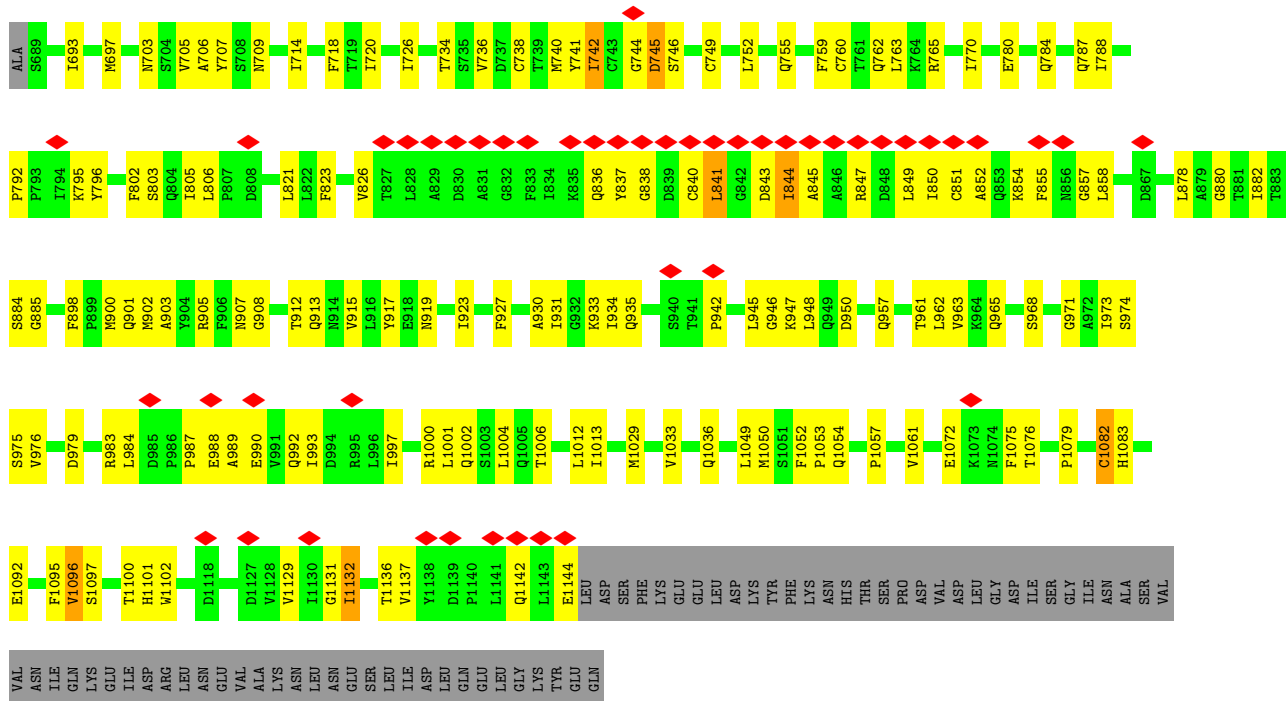
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
3	B	1	15	6	8	1	0

3 Residue-property plots

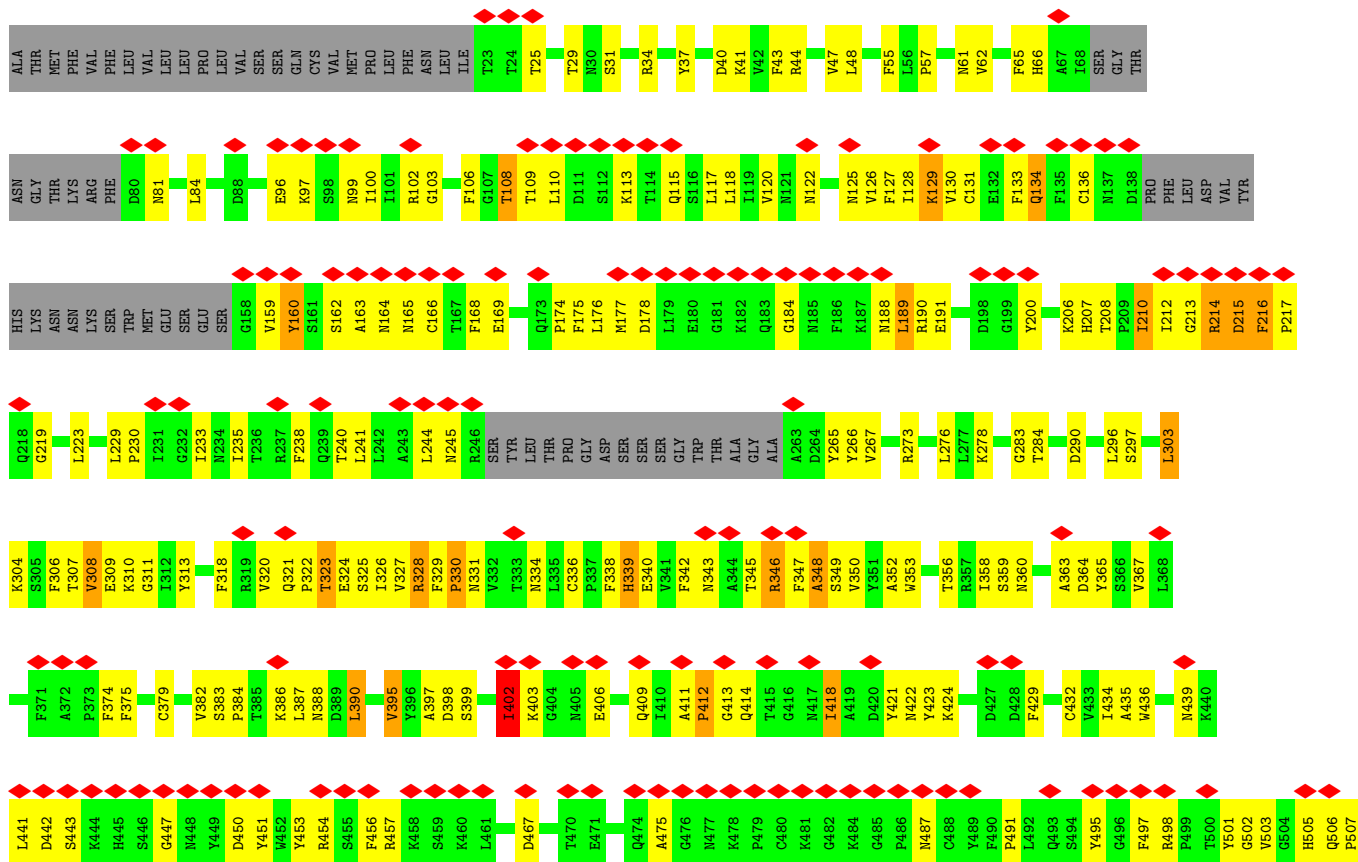
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

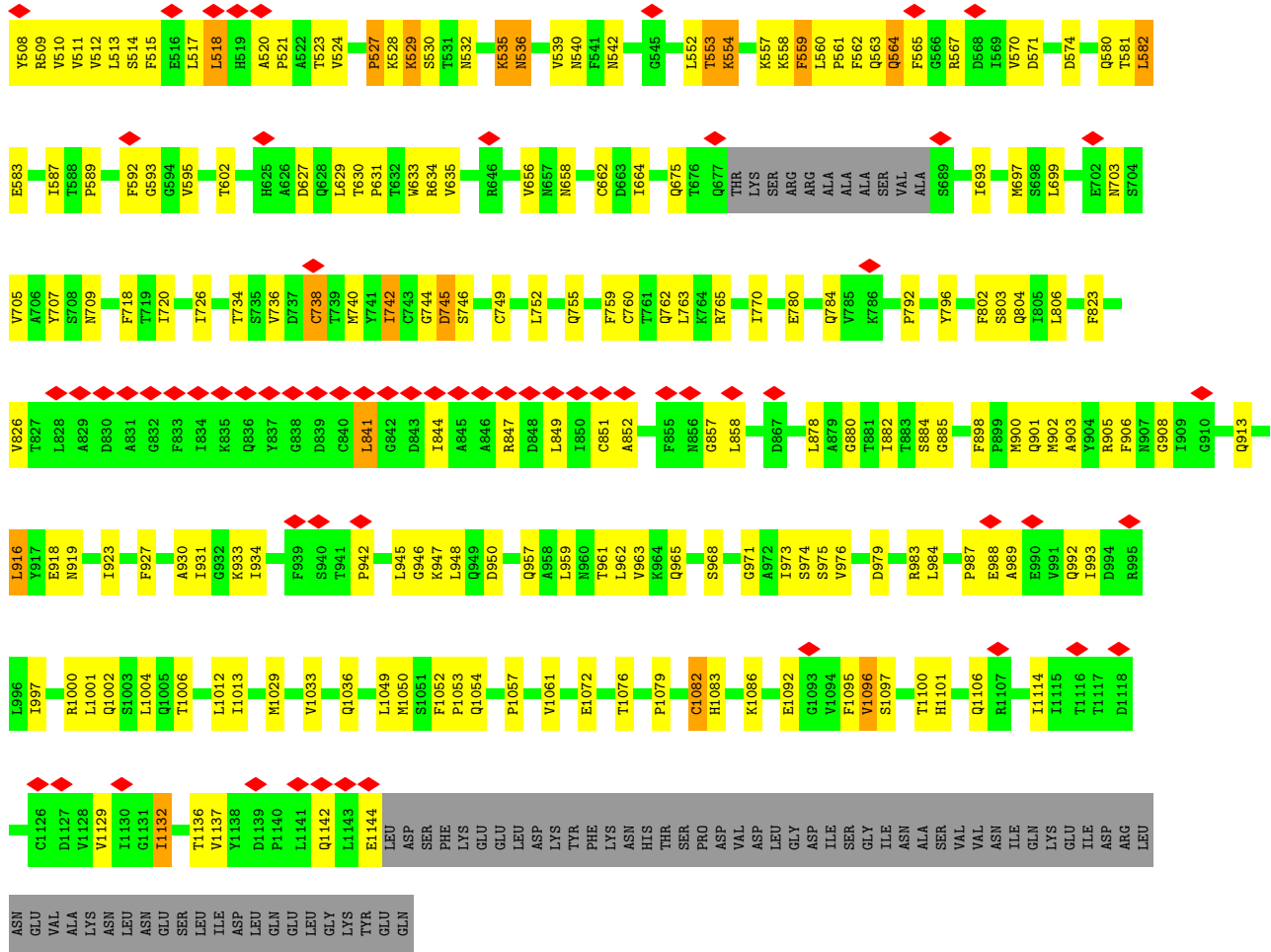
• Molecule 1: Spike glycoprotein



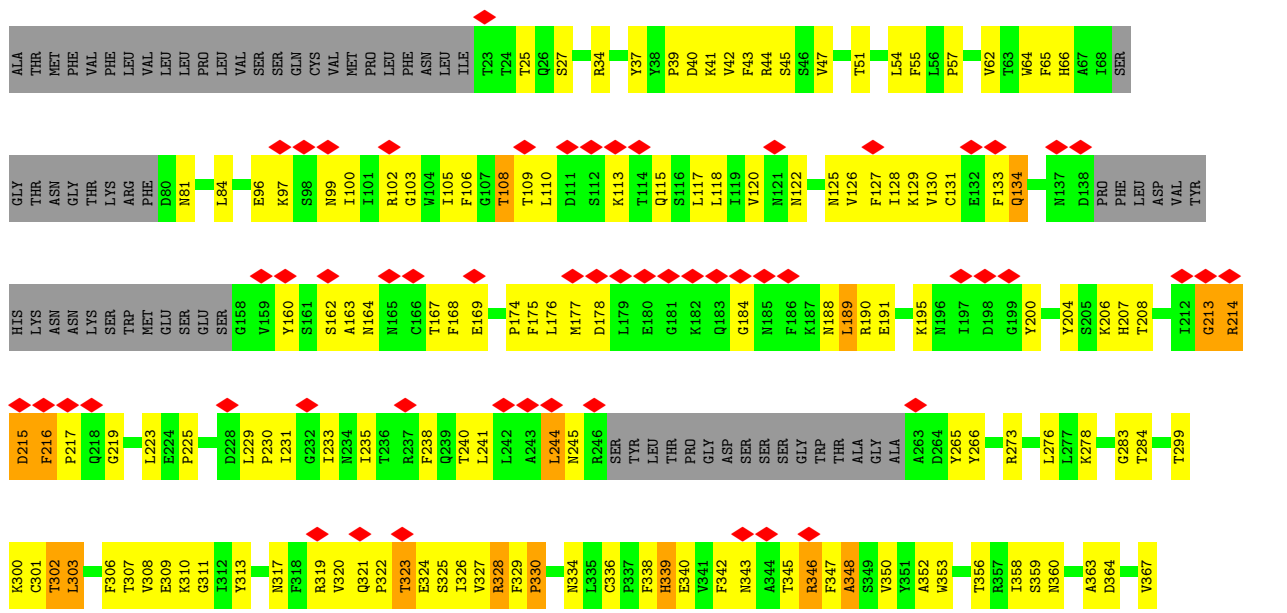


● Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



GLU	D1118	F906	F805	I693	Q580	V510	H445	L368
VAL	D1127	R907	R811	M697	T881	V511	S446	Y369
ALA	I1130	G908	L821	E702	L882	V512	G447	N370
LYS	G1131	T912	L822	V705	E583	L513	M448	F371
ASN	I1132	Q913	F823	A706	I584	L517	Y449	A372
ASN	T1136	Q914	V826	T707	L585	L518	D450	F375
GLU	Y1137	N915	F827	S708	T888	L519	Y451	A376
SER	E918	V916	L828	S709	P589	H519	W452	V382
LEU	Y1138	Q917	A829	N709	C590	A520	Y453	S383
LEU	D1139	N919	L829	T716	S591	A521	R454	P384
GLN	P1140	T923	A830	T717	F592	A522	S455	I385
LEU	L1141	F927	D830	N718	F593	G594	R457	K386
LEU	L1142	A930	A831	F718	G595	G594	K458	L387
GLY	Q1143	R931	G832	T719	V595	V524	S459	N388
TYR	L1144	I931	F833	I720	T599	P521	K460	D389
GLU	E1144	G832	I834	E725	T602	P527	L461	L390
LEU	ASP	K933	K835	I726	V608	K528	K467	V395
SER	SER	Q934	Q836	T734	V616	S530	I468	Y396
PHE	PHE	Q935	Q837	S735	N616	T531	S469	A397
LYS	LYS	Q935	Y837	V736	D627	N532	T470	D398
GLU	GLU	F939	G838	I736	Q628	K335	E471	S399
GLU	GLU	S940	D839	V736	L629	N536	I472	I402
LEU	LEU	T941	C840	S736	L829	V539	I473	K403
ASP	ASP	F942	C743	I736	T630	N540	Q474	G404
LYS	LYS	L841	C749	L752	L631	F541	A475	M405
TYR	TYR	D842	L752	Q755	T632	N542	G476	M406
PHE	PHE	L843	L752	F759	W633	G545	M477	A411
LYS	LYS	I844	L752	C760	R634	L546	K478	P412
ASN	ASN	A845	A846	T761	V635	L547	P479	G413
HIS	HIS	A846	A846	L762	V635	T547	C480	Q414
THR	THR	A847	A846	Q762	V635	G548	C481	T415
SER	SER	R847	A846	L763	V635	T547	K481	Q416
PRO	PRO	D848	A846	L764	V635	G548	G482	G416
ASP	ASP	L849	A846	R765	V635	F559	M484	M417
VAL	VAL	L849	A846	I770	V635	K558	P486	I418
ASP	ASP	T850	A846	E780	V635	F560	M487	A419
LEU	LEU	C851	A846	Q784	V635	L560	D420	D420
GLY	GLY	A852	A846	I788	V635	P561	Y421	Y421
ASP	ASP	F855	A846	Y789	V635	Q563	M422	Y423
ILE	ILE	L858	A846	Q784	V635	Q564	Y423	Y423
LYS	LYS	L878	A846	I788	V635	F565	K424	K424
SER	SER	A879	A846	Y788	V635	G566	D427	D427
SER	SER	G880	A846	Y789	V635	R567	D428	D428
VAL	VAL	T881	A846	P792	V635	V570	F429	F429
VAL	VAL	L882	A846	Y796	V635	D571	A435	A435
ASN	ASN	S883	A846	F802	V635	T572	W436	W436
ASN	ASN	C885	A846	F802	V635	A575	M437	M437
ILE	ILE	F888	A846	F802	V635	R576	S438	S438
GLN	GLN	F898	A846	F802	V635	R577	M439	M439
LYS	LYS	P899	A846	F802	V635	R577	K440	K440
GLU	GLU	N900	A846	F802	V635	R577	L441	L441
GLU	GLU	Q901	A846	F802	V635	R577	D442	D442
ASP	ASP	M902	A846	F802	V635	R577	S443	S443
ARG	ARG	A903	A846	F802	V635	R577	G504	G504
LEU	LEU	T904	A846	F802	V635	R577	H505	H505
ASN	ASN	R905	A846	F802	V635	R577	Q506	Q506
ASN	ASN		A846	F802	V635	R577	Y508	Y508
ASN	ASN		A846	F802	V635	R577	R509	R509

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.695	Depositor
Minimum map value	-1.681	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	310.80002, 310.80002, 310.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.036, 1.036, 1.036	Depositor

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, IDU

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	0.59	1/8514 (0.0%)	0.80	14/11588 (0.1%)
1	B	0.59	1/8514 (0.0%)	0.81	14/11588 (0.1%)
1	C	0.57	0/8514	0.79	16/11588 (0.1%)
All	All	0.58	2/25542 (0.0%)	0.80	44/34764 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	4
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	564	GLN	CA-C	5.13	1.54	1.52
1	A	564	GLN	CA-C	5.01	1.54	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	988	GLU	N-CA-C	-6.45	105.30	113.43
1	C	323	THR	O-C-N	6.16	129.40	122.32
1	B	323	THR	O-C-N	6.14	129.38	122.32
1	A	323	THR	O-C-N	6.14	129.38	122.32
1	A	1095	PHE	CA-C-N	-5.84	115.08	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1095	PHE	C-N-CA	-5.84	115.08	123.03
1	B	215	ASP	N-CA-C	5.83	118.28	110.35
1	C	1095	PHE	CA-C-N	-5.83	115.11	123.03
1	C	1095	PHE	C-N-CA	-5.83	115.11	123.03
1	C	215	ASP	N-CA-C	5.81	118.25	110.35
1	A	215	ASP	N-CA-C	5.81	118.25	110.35
1	B	1095	PHE	CA-C-N	-5.80	115.14	123.03
1	B	1095	PHE	C-N-CA	-5.80	115.14	123.03
1	A	1096	VAL	CA-C-O	-5.67	116.08	121.64
1	A	339	HIS	CA-C-N	-5.66	112.92	120.79
1	A	339	HIS	C-N-CA	-5.66	112.92	120.79
1	B	339	HIS	CA-C-N	-5.66	112.92	120.79
1	B	339	HIS	C-N-CA	-5.66	112.92	120.79
1	B	564	GLN	CA-C-O	-5.66	116.54	119.77
1	C	339	HIS	CA-C-N	-5.64	112.95	120.79
1	C	339	HIS	C-N-CA	-5.64	112.95	120.79
1	B	1096	VAL	CA-C-O	-5.64	116.11	121.64
1	C	564	GLN	CA-C-O	-5.64	116.56	119.77
1	C	1096	VAL	CA-C-O	-5.63	116.12	121.64
1	A	564	GLN	CA-C-O	-5.58	116.59	119.77
1	C	330	PRO	CA-C-N	-5.54	110.95	121.54
1	C	330	PRO	C-N-CA	-5.54	110.95	121.54
1	A	214	ARG	N-CA-C	5.54	115.87	108.23
1	B	214	ARG	N-CA-C	5.53	115.86	108.23
1	A	535	LYS	CA-C-O	-5.52	115.74	122.64
1	B	535	LYS	CA-C-O	-5.49	115.78	122.64
1	C	535	LYS	CA-C-O	-5.48	115.79	122.64
1	C	1102	TRP	CA-C-O	-5.33	115.52	121.81
1	C	1082	CYS	CB-CA-C	-5.11	102.73	111.41
1	A	841	LEU	N-CA-CB	-5.10	102.69	110.33
1	A	1082	CYS	CB-CA-C	-5.09	102.76	111.41
1	B	1082	CYS	CB-CA-C	-5.08	102.77	111.41
1	C	328	ARG	CB-CA-C	5.07	118.88	109.70
1	A	108	THR	CA-C-N	5.06	131.21	121.54
1	A	108	THR	C-N-CA	5.06	131.21	121.54
1	B	108	THR	CA-C-N	5.06	131.21	121.54
1	B	108	THR	C-N-CA	5.06	131.21	121.54
1	C	108	THR	CA-C-N	5.05	131.19	121.54
1	C	108	THR	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	A	346	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	328	ARG	Sidechain
1	B	346	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	346	ARG	Sidechain
1	C	567	ARG	Sidechain
1	C	577	ARG	Sidechain

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	8314	0	8094	396	0
1	B	8314	0	8094	380	0
1	C	8314	0	8094	417	0
2	A	252	0	234	6	0
2	B	252	0	234	5	0
2	C	252	0	234	10	0
3	B	15	0	4	1	0
All	All	25713	0	24988	1039	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 20.

All (1039) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:THR:CG2	1:C:517:LEU:HD12	1.63	1.26
1:C:503:VAL:CG2	1:A:505:HIS:CE1	2.20	1.25
1:C:759:PHE:HZ	1:A:1002:GLN:CG	1.49	1.24
1:A:503:VAL:CG2	1:B:505:HIS:CE1	2.21	1.23
1:A:759:PHE:HZ	1:B:1002:GLN:CG	1.56	1.17
1:C:1002:GLN:HG3	1:B:759:PHE:HZ	1.07	1.16
1:C:759:PHE:CZ	1:A:1002:GLN:HG3	1.80	1.16
1:C:503:VAL:HG21	1:A:505:HIS:CE1	1.78	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1002:GLN:HG3	1:B:759:PHE:CZ	1.81	1.15
1:C:430:THR:HG21	1:C:517:LEU:HD12	1.25	1.15
1:A:759:PHE:CZ	1:B:1002:GLN:HG3	1.82	1.14
1:C:505:HIS:CE1	1:B:503:VAL:CG2	2.29	1.14
1:C:503:VAL:HG21	1:A:505:HIS:HE1	1.00	1.13
1:C:505:HIS:HE1	1:B:503:VAL:HG21	1.06	1.13
1:A:759:PHE:HZ	1:B:1002:GLN:HG3	1.05	1.13
1:A:503:VAL:HG21	1:B:505:HIS:CE1	1.78	1.13
1:A:841:LEU:HB2	1:B:553:THR:HG21	1.22	1.12
1:C:1002:GLN:CG	1:B:759:PHE:HZ	1.63	1.12
1:C:326:ILE:HD11	1:C:534:VAL:HG23	1.19	1.11
1:C:759:PHE:HZ	1:A:1002:GLN:HG3	1.02	1.11
1:C:755:GLN:OE1	1:A:971:GLY:HA2	1.51	1.10
1:C:553:THR:HG21	1:B:841:LEU:HB2	1.13	1.09
1:C:759:PHE:CZ	1:A:1002:GLN:CG	2.33	1.09
1:A:503:VAL:HG21	1:B:505:HIS:HE1	0.97	1.09
1:C:971:GLY:HA2	1:B:755:GLN:OE1	1.51	1.08
1:A:759:PHE:CZ	1:B:1002:GLN:CG	2.38	1.07
1:A:755:GLN:OE1	1:B:971:GLY:HA2	1.54	1.07
1:C:983:ARG:CD	1:A:517:LEU:HD13	1.85	1.06
1:C:505:HIS:HE1	1:B:503:VAL:CG2	1.65	1.06
1:A:503:VAL:CG2	1:B:505:HIS:HE1	1.64	1.06
1:A:841:LEU:HB2	1:B:553:THR:CG2	1.88	1.03
1:C:505:HIS:CE1	1:B:503:VAL:HG21	1.92	1.03
1:A:903:ALA:HB1	1:A:913:GLN:HB3	1.42	1.02
1:C:1083:HIS:ND1	1:C:1137:VAL:HG22	1.74	1.02
1:B:1083:HIS:ND1	1:B:1137:VAL:HG22	1.74	1.02
1:C:553:THR:CG2	1:B:841:LEU:HB2	1.90	1.02
1:C:1002:GLN:CG	1:B:759:PHE:CZ	2.40	1.02
1:A:1083:HIS:ND1	1:A:1137:VAL:HG22	1.74	1.01
1:A:983:ARG:CD	1:B:517:LEU:HD13	1.90	1.00
1:C:1083:HIS:CG	1:C:1137:VAL:HG22	1.97	1.00
1:B:1083:HIS:CG	1:B:1137:VAL:HG22	1.97	0.99
1:C:503:VAL:CG2	1:A:505:HIS:HE1	1.64	0.99
1:A:1083:HIS:CG	1:A:1137:VAL:HG22	1.97	0.98
1:C:326:ILE:HD13	1:C:533:LEU:HA	1.47	0.95
1:C:983:ARG:HD3	1:A:517:LEU:HD13	1.45	0.95
1:C:841:LEU:HB2	1:A:553:THR:HG21	1.48	0.94
1:A:983:ARG:HD3	1:B:517:LEU:HD13	1.50	0.93
1:C:382:VAL:HG11	1:C:387:LEU:HD13	1.50	0.92
1:A:503:VAL:HG23	1:B:505:HIS:CE1	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:HIS:CE1	1:B:503:VAL:HG23	2.04	0.89
1:C:62:VAL:HG11	1:C:216:PHE:HE2	1.36	0.88
1:A:62:VAL:HG11	1:A:216:PHE:HE2	1.36	0.88
1:B:300:LYS:HG2	1:B:308:VAL:HG23	1.55	0.87
1:B:559:PHE:HB2	1:B:584:ILE:HD11	1.56	0.87
1:C:503:VAL:HG23	1:A:505:HIS:CE1	2.07	0.87
1:B:322:PRO:HG2	1:B:540:ASN:HD21	1.40	0.86
1:C:326:ILE:HD11	1:C:534:VAL:CG2	2.06	0.86
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.06	0.86
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.58	0.85
1:C:553:THR:HG21	1:B:841:LEU:CB	2.02	0.85
1:A:841:LEU:CB	1:B:553:THR:HG21	2.04	0.85
1:A:322:PRO:HG2	1:A:540:ASN:HD21	1.40	0.85
1:C:322:PRO:HG2	1:C:540:ASN:HD21	1.40	0.85
1:A:326:ILE:HD12	1:A:532:ASN:O	1.76	0.84
1:B:326:ILE:CG2	1:B:532:ASN:O	2.26	0.84
1:B:326:ILE:HD12	1:B:532:ASN:O	1.76	0.84
1:B:557:LYS:HD3	1:B:559:PHE:HE1	1.43	0.83
1:C:1082:CYS:HB2	1:C:1132:ILE:HG13	1.58	0.83
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.61	0.83
1:A:326:ILE:CG2	1:A:532:ASN:O	2.26	0.83
1:C:759:PHE:CZ	1:A:1002:GLN:HG2	2.14	0.82
1:B:326:ILE:HG23	1:B:532:ASN:O	1.80	0.82
1:C:983:ARG:HD2	1:A:517:LEU:HD13	1.60	0.81
1:A:983:ARG:HD2	1:B:517:LEU:HD13	1.63	0.81
1:A:326:ILE:HG23	1:A:532:ASN:O	1.80	0.81
1:B:325:SER:HA	1:B:539:VAL:HG13	1.63	0.81
1:B:1082:CYS:HB2	1:B:1132:ILE:HG13	1.61	0.81
1:A:325:SER:HA	1:A:539:VAL:HG13	1.63	0.81
1:C:326:ILE:HD13	1:C:533:LEU:CA	2.11	0.80
1:C:325:SER:HA	1:C:539:VAL:HG13	1.63	0.80
1:A:1082:CYS:HB2	1:A:1132:ILE:HG13	1.62	0.80
1:C:838:GLY:HA3	2:A:1309:NAG:H81	1.62	0.79
1:B:1083:HIS:ND1	1:B:1137:VAL:CG2	2.46	0.79
1:C:328:ARG:HG3	1:C:530:SER:HB2	1.66	0.78
1:A:328:ARG:HG3	1:A:530:SER:HB2	1.65	0.78
1:B:328:ARG:HG3	1:B:530:SER:HB2	1.66	0.78
1:C:1083:HIS:ND1	1:C:1137:VAL:CG2	2.46	0.77
1:A:1083:HIS:ND1	1:A:1137:VAL:CG2	2.46	0.77
1:C:178:ASP:HA	1:C:188:ASN:HD21	1.49	0.77
1:A:503:VAL:HG23	1:B:505:HIS:NE2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.66	0.76
1:A:322:PRO:HG2	1:A:540:ASN:ND2	2.01	0.76
1:C:310:LYS:HG2	1:C:664:ILE:HD11	1.68	0.76
1:C:802:PHE:H	2:C:1313:NAG:H82	1.49	0.76
1:C:322:PRO:HG2	1:C:540:ASN:ND2	2.01	0.76
1:A:310:LYS:HG2	1:A:664:ILE:HD11	1.68	0.76
1:C:417:ASN:O	1:C:422:ASN:ND2	2.20	0.75
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.68	0.75
1:B:322:PRO:HG2	1:B:540:ASN:ND2	2.01	0.75
1:C:788:ILE:HD11	1:A:699:LEU:HB2	1.67	0.75
1:A:62:VAL:HG11	1:A:216:PHE:CE2	2.21	0.75
1:C:503:VAL:HG23	1:A:505:HIS:NE2	2.02	0.75
1:C:707:TYR:HD1	1:B:792:PRO:HG3	1.52	0.75
1:C:62:VAL:HG11	1:C:216:PHE:CE2	2.21	0.75
2:C:1311:NAG:H62	1:B:796:TYR:CD2	2.22	0.75
1:A:37:TYR:HA	1:A:223:LEU:HB2	1.69	0.74
1:A:759:PHE:CZ	1:B:1002:GLN:HG2	2.22	0.73
1:A:43:PHE:HA	1:B:563:GLN:OE1	1.88	0.73
1:A:557:LYS:HD3	1:A:559:PHE:HE1	1.52	0.73
1:C:983:ARG:HD2	1:A:517:LEU:CD1	2.18	0.73
1:C:430:THR:HG22	1:C:517:LEU:HD12	1.64	0.73
1:C:365:TYR:CE2	1:C:387:LEU:HG	2.24	0.73
1:B:577:ARG:HG2	1:B:584:ILE:HG12	1.71	0.73
1:C:430:THR:CG2	1:C:517:LEU:CD1	2.57	0.72
1:C:326:ILE:CD1	1:C:533:LEU:C	2.62	0.72
1:C:330:PRO:HG2	1:C:332:VAL:HG22	1.71	0.72
1:C:375:PHE:CD1	1:C:508:TYR:OH	2.42	0.72
1:C:503:VAL:CB	1:A:505:HIS:CE1	2.72	0.72
1:C:983:ARG:CD	1:A:517:LEU:CD1	2.67	0.72
1:B:65:PHE:HB2	1:B:265:TYR:HB3	1.72	0.71
1:A:65:PHE:HB2	1:A:265:TYR:HB3	1.72	0.71
1:C:65:PHE:HB2	1:C:265:TYR:HB3	1.72	0.71
1:C:971:GLY:CA	1:B:755:GLN:OE1	2.36	0.71
1:B:44:ARG:HB3	1:B:47:VAL:HG11	1.72	0.71
1:C:1083:HIS:CE1	1:C:1137:VAL:HG22	2.26	0.71
1:A:852:ALA:HB1	1:B:570:VAL:HG22	1.72	0.71
1:A:106:PHE:HD1	1:A:235:ILE:HD13	1.56	0.71
1:B:1083:HIS:CE1	1:B:1137:VAL:HG22	2.26	0.71
1:A:503:VAL:CG2	1:B:505:HIS:NE2	2.53	0.71
1:C:44:ARG:HB3	1:C:47:VAL:HG11	1.72	0.70
1:A:1083:HIS:CE1	1:A:1137:VAL:HG22	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:OE1	1:B:100:ILE:N	2.24	0.70
1:C:43:PHE:HA	1:A:563:GLN:OE1	1.91	0.70
1:C:96:GLU:OE1	1:C:100:ILE:N	2.24	0.70
1:A:44:ARG:HB3	1:A:47:VAL:HG11	1.72	0.70
1:C:503:VAL:CG2	1:A:505:HIS:NE2	2.53	0.70
1:C:987:PRO:HD2	1:C:988:GLU:OE2	1.92	0.70
1:A:96:GLU:OE1	1:A:100:ILE:N	2.24	0.70
1:B:106:PHE:HD1	1:B:235:ILE:HD13	1.56	0.70
1:C:903:ALA:HB1	1:C:913:GLN:HB3	1.72	0.70
1:C:106:PHE:HD1	1:C:235:ILE:HD13	1.56	0.69
1:C:326:ILE:CD1	1:C:534:VAL:HG23	2.11	0.69
1:C:505:HIS:NE2	1:B:503:VAL:HG23	2.08	0.69
1:A:987:PRO:HD2	1:A:988:GLU:OE2	1.92	0.69
1:B:327:VAL:HG11	1:B:528:LYS:CE	2.23	0.69
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.75	0.69
1:C:326:ILE:HD11	1:C:533:LEU:C	2.18	0.69
1:B:903:ALA:HB1	1:B:913:GLN:HB3	1.75	0.69
1:C:229:LEU:HD23	1:C:229:LEU:H	1.58	0.68
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.75	0.68
1:C:454:ARG:NH1	1:C:467:ASP:O	2.27	0.68
1:A:43:PHE:CA	1:B:563:GLN:OE1	2.42	0.68
1:B:128:ILE:HD11	1:B:175:PHE:HZ	1.59	0.68
1:C:456:PHE:HB2	1:C:491:PRO:HA	1.75	0.68
1:C:1129:VAL:HG13	1:B:917:TYR:HB3	1.76	0.68
1:C:326:ILE:CD1	1:C:534:VAL:N	2.57	0.68
1:A:454:ARG:NH1	1:A:467:ASP:O	2.27	0.68
1:A:456:PHE:HB2	1:A:491:PRO:HA	1.75	0.68
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.75	0.68
1:A:983:ARG:HD2	1:B:517:LEU:CD1	2.24	0.68
1:A:327:VAL:HG11	1:A:528:LYS:CE	2.23	0.67
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.77	0.67
1:B:456:PHE:HB2	1:B:491:PRO:HA	1.75	0.67
1:A:229:LEU:HD23	1:A:229:LEU:H	1.58	0.67
1:C:327:VAL:HG11	1:C:528:LYS:CE	2.23	0.67
1:A:350:VAL:HG21	1:A:418:ILE:HG23	1.74	0.67
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.77	0.67
1:B:129:LYS:HD2	1:B:160:TYR:CE2	2.30	0.67
1:B:454:ARG:NH1	1:B:467:ASP:O	2.27	0.67
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.77	0.67
1:C:852:ALA:HB1	1:A:570:VAL:HG22	1.77	0.66
1:A:852:ALA:HB1	1:B:570:VAL:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLN:HE21	1:B:233:ILE:HB	1.61	0.65
1:B:327:VAL:HG11	1:B:528:LYS:HE3	1.78	0.65
1:B:375:PHE:CD1	1:B:508:TYR:OH	2.41	0.65
1:A:379:CYS:HA	1:A:432:CYS:HA	1.79	0.65
1:C:564:GLN:O	1:C:565:PHE:C	2.40	0.65
1:A:327:VAL:HG11	1:A:528:LYS:HE3	1.78	0.65
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.30	0.65
1:A:375:PHE:CD1	1:A:508:TYR:OH	2.41	0.65
1:C:115:GLN:HE21	1:C:233:ILE:HB	1.61	0.65
1:C:327:VAL:HG11	1:C:528:LYS:HE3	1.78	0.65
1:C:128:ILE:HD11	1:C:175:PHE:HZ	1.62	0.65
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.30	0.65
1:C:174:PRO:HG2	1:C:177:MET:HE1	1.80	0.64
1:C:503:VAL:HB	1:A:505:HIS:CE1	2.32	0.64
1:A:128:ILE:HD11	1:A:175:PHE:HZ	1.62	0.64
1:A:796:TYR:CD2	2:B:1311:NAG:H62	2.33	0.64
1:C:206:LYS:HB3	1:C:223:LEU:HD13	1.80	0.64
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.30	0.64
1:B:564:GLN:O	1:B:565:PHE:C	2.40	0.64
1:C:406:GLU:OE1	1:C:406:GLU:N	2.30	0.64
1:A:564:GLN:O	1:A:565:PHE:C	2.40	0.64
1:C:557:LYS:HG3	1:B:844:ILE:O	1.98	0.64
1:C:917:TYR:HB3	1:A:1129:VAL:HG13	1.80	0.64
1:A:174:PRO:HG2	1:A:177:MET:HE1	1.80	0.64
1:C:326:ILE:CG2	1:C:532:ASN:O	2.45	0.64
1:A:983:ARG:CD	1:B:517:LEU:CD1	2.74	0.64
1:A:200:TYR:HA	1:A:230:PRO:HA	1.80	0.64
1:C:759:PHE:CE2	1:A:1002:GLN:HG2	2.33	0.64
1:C:1079:PRO:HB3	1:B:917:TYR:CE1	2.33	0.64
1:A:118:LEU:HD11	1:A:159:VAL:HB	1.80	0.64
1:C:311:GLY:HA2	1:C:664:ILE:HD12	1.81	0.63
1:A:303:LEU:HD21	1:A:308:VAL:HG12	1.79	0.63
1:B:174:PRO:HG2	1:B:177:MET:HE1	1.80	0.63
1:C:200:TYR:HA	1:C:230:PRO:HA	1.80	0.63
1:C:852:ALA:HB1	1:A:570:VAL:CG2	2.28	0.63
1:A:503:VAL:CB	1:B:505:HIS:CE1	2.80	0.63
1:C:787:GLN:OE1	1:A:703:ASN:ND2	2.29	0.63
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.81	0.63
1:B:311:GLY:HA2	1:B:664:ILE:HD12	1.81	0.63
1:A:792:PRO:HG3	1:B:707:TYR:HD1	1.64	0.63
1:C:556:ASN:H	1:B:844:ILE:HG23	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.81	0.63
1:B:39:PRO:HG3	1:B:55:PHE:HZ	1.64	0.63
1:C:788:ILE:CD1	1:A:699:LEU:HB2	2.28	0.63
1:B:134:GLN:HG2	1:B:162:SER:HB2	1.80	0.63
1:C:1079:PRO:HA	1:B:900:MET:HE2	1.81	0.62
1:B:300:LYS:HG2	1:B:308:VAL:CG2	2.29	0.62
1:C:796:TYR:CD2	2:A:1311:NAG:H62	2.34	0.62
1:A:398:ASP:HB2	1:A:512:VAL:HG12	1.81	0.62
1:C:821:LEU:HD11	1:C:935:GLN:HG3	1.82	0.62
1:C:136:CYS:HB2	1:C:159:VAL:HA	1.81	0.62
1:B:1100:THR:HB	2:B:1315:NAG:HN2	1.64	0.62
1:A:311:GLY:HA2	1:A:664:ILE:HD12	1.81	0.62
1:C:189:LEU:HD23	1:C:210:ILE:HA	1.81	0.62
1:A:441:LEU:HD22	1:A:509:ARG:HH12	1.65	0.62
1:A:1100:THR:HB	2:A:1315:NAG:HN2	1.65	0.62
1:C:917:TYR:CE1	1:A:1079:PRO:HB3	2.35	0.62
1:B:326:ILE:HG21	1:B:532:ASN:O	2.00	0.61
1:C:1002:GLN:HG2	1:B:759:PHE:CE2	2.34	0.61
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.28	0.61
1:C:276:LEU:HD11	1:C:304:LYS:HA	1.81	0.61
1:A:276:LEU:HD11	1:A:304:LYS:HA	1.82	0.61
1:B:441:LEU:HD22	1:B:509:ARG:HH12	1.65	0.61
1:C:215:ASP:O	1:C:216:PHE:C	2.44	0.61
1:C:1013:ILE:HD13	1:B:1012:LEU:HB3	1.83	0.61
1:B:323:THR:OG1	1:B:324:GLU:N	2.34	0.61
1:C:441:LEU:HD22	1:C:509:ARG:HH12	1.65	0.60
1:C:1002:GLN:HG2	1:B:759:PHE:CZ	2.32	0.60
1:A:759:PHE:CE2	1:B:1002:GLN:HG2	2.35	0.60
1:C:326:ILE:HG23	1:C:532:ASN:O	2.01	0.60
1:C:557:LYS:HD3	1:C:559:PHE:HE1	1.65	0.60
1:C:645:THR:HG23	1:C:647:ALA:H	1.65	0.60
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.34	0.60
1:A:356:THR:OG1	1:A:397:ALA:HB3	2.02	0.60
1:B:215:ASP:O	1:B:216:PHE:C	2.44	0.60
1:A:215:ASP:O	1:A:216:PHE:C	2.44	0.60
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.36	0.60
1:A:513:LEU:HG	1:A:515:PHE:CE1	2.37	0.60
1:C:1002:GLN:CG	1:B:759:PHE:CE2	2.84	0.60
1:A:318:PHE:CE1	1:A:593:GLY:HA3	2.37	0.60
1:B:350:VAL:HG21	1:B:418:ILE:HG23	1.84	0.60
1:C:282:ASN:OD1	1:A:558:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:THR:C	1:A:583:GLU:H	2.10	0.59
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.84	0.59
1:A:567:ARG:HD3	1:A:571:ASP:HA	1.84	0.59
1:A:900:MET:HE2	1:B:1079:PRO:HA	1.83	0.59
1:A:213:GLY:O	1:A:214:ARG:HG3	2.02	0.59
1:C:627:ASP:HA	1:C:634:ARG:HH22	1.68	0.59
1:A:513:LEU:HG	1:A:515:PHE:HE1	1.67	0.59
1:A:206:LYS:HB3	1:A:223:LEU:HD13	1.83	0.59
1:C:359:SER:HA	1:C:524:VAL:HG23	1.85	0.59
1:C:841:LEU:CB	1:A:553:THR:HG21	2.29	0.59
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.28	0.59
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.38	0.59
1:C:323:THR:OG1	1:C:324:GLU:N	2.34	0.59
1:A:323:THR:OG1	1:A:324:GLU:N	2.34	0.59
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.34	0.59
1:B:326:ILE:H	1:B:539:VAL:HG11	1.68	0.59
1:B:356:THR:OG1	1:B:397:ALA:HB3	2.03	0.58
1:B:213:GLY:O	1:B:214:ARG:HG3	2.02	0.58
1:B:334:ASN:ND2	1:B:360:ASN:O	2.35	0.58
1:B:567:ARG:HD3	1:B:571:ASP:HA	1.84	0.58
1:A:326:ILE:H	1:A:539:VAL:HG11	1.68	0.58
1:A:382:VAL:HG23	1:A:517:LEU:HD11	1.84	0.58
1:C:334:ASN:ND2	1:C:360:ASN:O	2.35	0.58
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.28	0.58
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.84	0.58
1:C:792:PRO:HG3	1:A:707:TYR:HD1	1.68	0.58
1:C:844:ILE:O	1:A:557:LYS:HG3	2.03	0.58
1:C:976:VAL:HG12	1:C:979:ASP:H	1.69	0.58
1:A:326:ILE:HG21	1:A:532:ASN:O	2.00	0.58
1:A:976:VAL:HG12	1:A:979:ASP:H	1.69	0.58
1:B:81:ASN:ND2	1:B:240:THR:O	2.25	0.58
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.39	0.58
1:C:326:ILE:H	1:C:539:VAL:HG11	1.68	0.58
1:C:592:PHE:CG	1:B:740:MET:HE3	2.39	0.58
1:B:62:VAL:HG11	1:B:216:PHE:HE2	1.68	0.58
1:C:742:ILE:HG23	1:C:1000:ARG:HB2	1.86	0.58
1:A:1142:GLN:N	1:A:1142:GLN:OE1	2.36	0.58
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.85	0.58
1:C:336:CYS:HB2	1:C:338:PHE:CE2	2.39	0.57
1:B:976:VAL:HG12	1:B:979:ASP:H	1.69	0.57
1:A:965:GLN:O	1:A:968:SER:OG	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CB	1:B:563:GLN:OE1	2.53	0.57
1:A:847:ARG:HB2	1:A:851:CYS:CB	2.34	0.57
1:A:102:ARG:HH21	1:A:122:ASN:CA	2.18	0.57
1:B:382:VAL:HG23	1:B:517:LEU:HD11	1.86	0.57
1:C:447:GLY:HA2	1:C:498:ARG:HG2	1.87	0.57
1:C:805:ILE:HB	1:C:878:LEU:HD21	1.85	0.57
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.36	0.57
1:A:1012:LEU:HB3	1:B:1013:ILE:HD13	1.86	0.57
1:B:108:THR:C	1:B:110:LEU:H	2.13	0.57
1:B:965:GLN:O	1:B:968:SER:OG	2.22	0.57
1:A:336:CYS:HB2	1:A:338:PHE:CE2	2.39	0.56
1:A:557:LYS:HD3	1:A:559:PHE:CE1	2.36	0.56
1:A:1144:GLU:N	1:A:1144:GLU:OE2	2.38	0.56
1:B:1142:GLN:N	1:B:1142:GLN:OE1	2.36	0.56
1:C:847:ARG:HB2	1:C:851:CYS:HB2	1.85	0.56
1:A:81:ASN:ND2	1:A:240:THR:O	2.25	0.56
1:A:136:CYS:HB2	1:A:159:VAL:HA	1.86	0.56
1:A:213:GLY:O	1:A:214:ARG:CG	2.54	0.56
1:A:447:GLY:HA2	1:A:498:ARG:HG2	1.87	0.56
1:B:1144:GLU:OE2	1:B:1144:GLU:N	2.38	0.56
1:A:322:PRO:CG	1:A:540:ASN:HD21	2.16	0.56
1:A:108:THR:C	1:A:110:LEU:H	2.13	0.56
1:B:39:PRO:HG2	1:B:51:THR:HG21	1.87	0.56
1:C:505:HIS:NE2	1:B:503:VAL:CG2	2.68	0.56
1:A:334:ASN:ND2	1:A:360:ASN:O	2.35	0.56
1:B:102:ARG:HH21	1:B:122:ASN:CA	2.18	0.56
1:B:447:GLY:HA2	1:B:498:ARG:HG2	1.87	0.56
1:C:43:PHE:CA	1:A:563:GLN:OE1	2.53	0.56
1:B:336:CYS:HB2	1:B:338:PHE:CE2	2.39	0.56
1:C:503:VAL:HB	1:A:505:HIS:NE2	2.20	0.56
1:C:736:VAL:HG22	1:C:858:LEU:HD22	1.87	0.56
1:C:1144:GLU:N	1:C:1144:GLU:OE2	2.38	0.56
1:B:429:PHE:HE1	1:B:514:SER:HB2	1.71	0.56
1:C:102:ARG:HH21	1:C:122:ASN:CA	2.18	0.56
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.87	0.56
1:B:359:SER:HA	1:B:524:VAL:HG23	1.87	0.56
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.72	0.55
1:C:1002:GLN:NE2	1:B:759:PHE:CZ	2.74	0.55
1:A:359:SER:HA	1:A:524:VAL:HG23	1.87	0.55
1:C:102:ARG:HH21	1:C:122:ASN:HA	1.71	0.55
1:C:563:GLN:OE1	1:B:43:PHE:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLY:O	1:B:214:ARG:CG	2.54	0.55
1:C:836:GLN:HG2	1:C:840:CYS:SG	2.47	0.55
1:C:852:ALA:CB	1:A:570:VAL:HG22	2.36	0.55
1:A:384:PRO:HA	1:A:387:LEU:HB2	1.87	0.55
1:B:847:ARG:HB2	1:B:851:CYS:HB2	1.88	0.55
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.34	0.55
1:C:102:ARG:HH12	1:C:176:LEU:HD12	1.72	0.55
1:C:358:ILE:HB	1:C:395:VAL:HB	1.89	0.55
1:C:130:VAL:HG23	1:C:168:PHE:HB3	1.87	0.55
1:C:836:GLN:O	1:C:837:TYR:C	2.50	0.55
1:A:102:ARG:HH12	1:A:176:LEU:HD12	1.72	0.55
1:A:453:TYR:CD1	1:A:495:TYR:HD1	2.24	0.55
1:C:178:ASP:N	1:C:178:ASP:OD1	2.39	0.55
1:A:852:ALA:CB	1:B:570:VAL:HG22	2.36	0.55
1:B:453:TYR:CD1	1:B:495:TYR:HD1	2.24	0.55
1:B:581:THR:C	1:B:583:GLU:H	2.14	0.55
1:C:41:LYS:O	1:A:563:GLN:HA	2.07	0.55
1:A:178:ASP:N	1:A:178:ASP:OD1	2.39	0.55
1:B:102:ARG:HH12	1:B:176:LEU:HD12	1.72	0.55
1:C:187:LYS:O	1:C:188:ASN:C	2.50	0.54
1:A:189:LEU:HG	1:A:208:THR:O	2.07	0.54
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.88	0.54
1:A:102:ARG:HH21	1:A:122:ASN:HA	1.71	0.54
1:A:880:GLY:O	1:A:884:SER:OG	2.23	0.54
1:B:570:VAL:HG23	1:B:570:VAL:O	2.08	0.54
1:C:37:TYR:HA	1:C:223:LEU:HB2	1.88	0.54
1:C:326:ILE:HD11	1:C:534:VAL:N	2.21	0.54
1:C:707:TYR:CD1	1:B:792:PRO:HG3	2.39	0.54
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.90	0.54
1:A:326:ILE:H	1:A:539:VAL:CG1	2.21	0.54
1:A:403:LYS:HD2	1:A:505:HIS:HA	1.89	0.54
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.90	0.54
1:C:1012:LEU:HB3	1:A:1013:ILE:HD13	1.88	0.54
1:A:570:VAL:O	1:A:570:VAL:HG23	2.08	0.54
1:B:975:SER:O	1:B:975:SER:OG	2.25	0.54
1:C:505:HIS:CE1	1:B:503:VAL:CB	2.91	0.54
1:A:43:PHE:HB2	1:B:563:GLN:OE1	2.08	0.54
1:A:503:VAL:HB	1:B:505:HIS:CE1	2.43	0.54
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.36	0.54
1:C:418:ILE:H	1:C:418:ILE:HD12	1.72	0.54
1:B:736:VAL:HG22	1:B:858:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:ILE:HD12	1:C:923:ILE:HD11	1.90	0.54
1:A:742:ILE:HG23	1:A:1000:ARG:HB2	1.88	0.54
1:B:102:ARG:HH21	1:B:122:ASN:HA	1.71	0.54
1:B:475:ALA:HB3	1:B:487:ASN:HB3	1.90	0.54
1:C:62:VAL:CG1	1:C:216:PHE:HE2	2.15	0.54
1:C:453:TYR:CD1	1:C:495:TYR:HD1	2.24	0.54
1:C:898:PHE:CZ	1:C:1050:MET:HE1	2.43	0.54
1:A:560:LEU:O	1:A:562:PHE:N	2.41	0.54
1:B:326:ILE:H	1:B:539:VAL:CG1	2.21	0.54
1:C:326:ILE:H	1:C:539:VAL:CG1	2.21	0.54
1:C:965:GLN:O	1:C:968:SER:OG	2.22	0.54
1:C:1100:THR:HB	2:C:1315:NAG:HN2	1.73	0.54
1:A:752:LEU:HD12	1:A:993:ILE:HG21	1.90	0.54
1:C:108:THR:C	1:C:110:LEU:H	2.13	0.53
1:C:560:LEU:O	1:C:562:PHE:N	2.41	0.53
1:C:975:SER:O	1:C:975:SER:OG	2.25	0.53
1:C:1002:GLN:NE2	1:B:759:PHE:HZ	2.05	0.53
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.90	0.53
1:A:759:PHE:CE2	1:B:1002:GLN:CG	2.90	0.53
1:B:559:PHE:HB2	1:B:584:ILE:CD1	2.35	0.53
1:C:326:ILE:HD13	1:C:533:LEU:C	2.31	0.53
1:C:475:ALA:HB3	1:C:487:ASN:HB3	1.90	0.53
1:C:971:GLY:HA2	1:B:755:GLN:CD	2.31	0.53
1:C:1002:GLN:HE21	1:B:759:PHE:HZ	1.55	0.53
1:A:117:LEU:HD12	1:A:118:LEU:N	2.24	0.53
1:A:429:PHE:HE1	1:A:514:SER:HB2	1.74	0.53
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.90	0.53
1:B:200:TYR:HA	1:B:230:PRO:HA	1.91	0.53
1:B:560:LEU:O	1:B:562:PHE:N	2.41	0.53
1:B:720:ILE:HD12	1:B:923:ILE:HD11	1.90	0.53
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.90	0.53
1:C:375:PHE:CG	1:C:508:TYR:CZ	2.97	0.53
1:C:880:GLY:O	1:C:884:SER:OG	2.23	0.53
1:A:62:VAL:CG1	1:A:216:PHE:HE2	2.15	0.53
1:B:556:ASN:O	1:B:557:LYS:C	2.51	0.53
1:B:752:LEU:HD12	1:B:993:ILE:HG21	1.90	0.53
1:C:403:LYS:HG2	1:C:505:HIS:HA	1.90	0.53
1:A:129:LYS:HD3	1:A:133:PHE:CZ	2.43	0.53
1:A:975:SER:O	1:A:975:SER:OG	2.25	0.53
1:B:129:LYS:HA	1:B:168:PHE:O	2.09	0.53
1:B:439:ASN:O	1:B:443:SER:OG	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:LEU:HD12	1:B:948:LEU:HD12	1.90	0.53
1:C:957:GLN:OE1	1:B:765:ARG:HD3	2.08	0.53
1:A:898:PHE:CZ	1:A:1050:MET:HE1	2.43	0.53
1:B:178:ASP:OD1	1:B:178:ASP:N	2.39	0.53
1:C:765:ARG:HD3	1:A:957:GLN:OE1	2.08	0.53
1:B:847:ARG:HB2	1:B:851:CYS:CB	2.39	0.53
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.90	0.53
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.90	0.53
1:B:375:PHE:CG	1:B:508:TYR:CZ	2.97	0.53
1:B:898:PHE:CZ	1:B:1050:MET:HE1	2.43	0.53
1:C:858:LEU:HD12	1:C:963:VAL:HG12	1.91	0.53
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.44	0.53
1:A:720:ILE:HD12	1:A:923:ILE:HD11	1.90	0.53
1:B:353:TRP:H	1:B:353:TRP:CD1	2.27	0.53
1:B:880:GLY:O	1:B:884:SER:OG	2.23	0.53
1:C:752:LEU:HD12	1:C:993:ILE:HG21	1.90	0.52
1:B:403:LYS:HD2	1:B:505:HIS:HA	1.90	0.52
1:A:858:LEU:HD12	1:A:963:VAL:HG12	1.91	0.52
1:B:420:ASP:HB3	1:B:460:LYS:HD2	1.91	0.52
1:B:1083:HIS:HB2	1:B:1137:VAL:HG13	1.91	0.52
1:C:993:ILE:O	1:C:997:ILE:HG12	2.10	0.52
1:B:752:LEU:HD12	1:B:993:ILE:CG2	2.40	0.52
1:B:858:LEU:HD12	1:B:963:VAL:HG12	1.91	0.52
1:B:993:ILE:O	1:B:997:ILE:HG12	2.10	0.52
1:C:133:PHE:CD2	1:C:160:TYR:HA	2.45	0.52
1:C:191:GLU:HB2	1:C:223:LEU:HD11	1.91	0.52
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.91	0.52
1:A:520:ALA:O	1:A:521:PRO:C	2.53	0.52
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.91	0.52
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.92	0.52
1:B:213:GLY:C	1:B:214:ARG:HG3	2.35	0.52
1:C:803:SER:HB3	2:C:1313:NAG:HN2	1.74	0.52
1:C:1002:GLN:CD	1:B:759:PHE:HZ	2.15	0.52
1:A:375:PHE:CG	1:A:508:TYR:CZ	2.97	0.52
1:A:475:ALA:HB3	1:A:487:ASN:HB3	1.90	0.52
1:B:912:THR:O	1:B:915:VAL:HG12	2.10	0.52
1:B:559:PHE:CB	1:B:584:ILE:HD11	2.36	0.52
1:B:397:ALA:HA	1:B:512:VAL:O	2.09	0.52
1:C:117:LEU:HD12	1:C:118:LEU:N	2.24	0.52
1:C:755:GLN:OE1	1:A:971:GLY:CA	2.41	0.52
1:A:755:GLN:OE1	1:B:971:GLY:CA	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:PHE:O	1:B:217:PRO:C	2.52	0.52
1:A:213:GLY:C	1:A:214:ARG:HG3	2.34	0.52
1:A:752:LEU:HD12	1:A:993:ILE:CG2	2.40	0.52
1:C:1083:HIS:HB2	1:C:1137:VAL:HG13	1.91	0.51
1:B:229:LEU:H	1:B:229:LEU:HD23	1.75	0.51
1:B:364:ASP:OD1	1:B:364:ASP:N	2.43	0.51
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.92	0.51
1:A:115:GLN:HE21	1:A:233:ILE:HB	1.76	0.51
1:A:353:TRP:CD1	1:A:353:TRP:H	2.27	0.51
1:A:993:ILE:O	1:A:997:ILE:HG12	2.10	0.51
1:A:216:PHE:O	1:A:217:PRO:C	2.52	0.51
1:A:759:PHE:HZ	1:B:1002:GLN:CD	2.17	0.51
1:C:847:ARG:HB2	1:C:851:CYS:CB	2.41	0.51
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.34	0.51
1:A:1083:HIS:HB2	1:A:1137:VAL:HG13	1.91	0.51
1:B:347:PHE:HD2	1:B:399:SER:HB2	1.75	0.51
1:C:752:LEU:HD12	1:C:993:ILE:CG2	2.40	0.51
1:C:912:THR:O	1:C:915:VAL:HG12	2.11	0.51
1:B:931:ILE:O	1:B:934:ILE:HG22	2.09	0.51
1:C:755:GLN:CD	1:A:971:GLY:HA2	2.30	0.51
1:A:307:THR:HA	1:A:602:THR:HG21	1.93	0.51
1:B:322:PRO:CG	1:B:540:ASN:ND2	2.74	0.51
1:C:364:ASP:OD1	1:C:364:ASP:N	2.43	0.51
1:C:854:LYS:HE2	1:A:592:PHE:CD2	2.46	0.51
1:C:1006:THR:HG21	1:B:762:GLN:OE1	2.10	0.51
1:B:631:PRO:HB3	1:B:633:TRP:CZ2	2.45	0.51
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.43	0.51
1:B:805:ILE:HB	1:B:878:LEU:HD21	1.93	0.51
1:C:898:PHE:HZ	1:C:1050:MET:HE1	1.76	0.51
1:A:31:SER:HB3	1:A:62:VAL:CG2	2.41	0.50
1:B:559:PHE:HD2	1:B:577:ARG:HD2	1.77	0.50
1:C:631:PRO:HB3	1:C:633:TRP:CZ2	2.46	0.50
1:C:759:PHE:CE2	1:A:1002:GLN:CG	2.90	0.50
1:B:382:VAL:CG2	1:B:517:LEU:HD11	2.41	0.50
1:B:557:LYS:HD3	1:B:559:PHE:CE1	2.34	0.50
1:C:276:LEU:CD1	1:C:304:LYS:HA	2.42	0.50
1:C:854:LYS:HE2	1:A:592:PHE:HD2	1.75	0.50
1:A:387:LEU:HD11	1:A:515:PHE:CE2	2.47	0.50
1:C:563:GLN:OE1	1:B:43:PHE:CA	2.60	0.50
1:C:675:GLN:HG3	1:C:693:ILE:HD11	1.94	0.50
1:A:177:MET:H	1:A:207:HIS:CE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ARG:HD3	1:B:957:GLN:OE1	2.11	0.50
1:B:162:SER:O	1:B:163:ALA:C	2.54	0.50
1:B:189:LEU:HG	1:B:208:THR:O	2.12	0.50
1:C:353:TRP:CD1	1:C:353:TRP:H	2.27	0.50
1:B:27:SER:O	1:B:64:TRP:N	2.45	0.50
1:A:290:ASP:O	1:A:297:SER:HB3	2.12	0.50
1:B:520:ALA:O	1:B:521:PRO:C	2.53	0.50
1:C:403:LYS:HB3	1:C:406:GLU:OE1	2.12	0.50
1:B:113:LYS:HD2	1:B:113:LYS:O	2.12	0.50
1:B:317:ASN:HB2	1:B:592:PHE:CE1	2.46	0.50
1:C:31:SER:HB3	1:C:62:VAL:CG2	2.41	0.50
1:C:759:PHE:HZ	1:A:1002:GLN:CD	2.16	0.50
1:C:762:GLN:OE1	1:A:1006:THR:HG21	2.12	0.50
1:A:382:VAL:CG2	1:A:517:LEU:HD11	2.41	0.50
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.12	0.50
1:B:215:ASP:HB2	1:B:266:TYR:OH	2.12	0.50
1:C:503:VAL:CB	1:A:505:HIS:NE2	2.75	0.49
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.12	0.49
1:A:364:ASP:OD1	1:A:364:ASP:N	2.43	0.49
1:A:762:GLN:OE1	1:B:1006:THR:HG21	2.12	0.49
1:C:177:MET:H	1:C:207:HIS:CE1	2.30	0.49
1:C:215:ASP:HB2	1:C:266:TYR:OH	2.12	0.49
1:C:290:ASP:O	1:C:297:SER:HB3	2.11	0.49
1:A:360:ASN:H	1:A:523:THR:HB	1.78	0.49
1:B:675:GLN:HG3	1:B:693:ILE:HD11	1.94	0.49
1:C:113:LYS:HD2	1:C:113:LYS:O	2.12	0.49
1:C:1079:PRO:CA	1:B:900:MET:HE2	2.41	0.49
1:A:276:LEU:CD1	1:A:304:LYS:HA	2.42	0.49
1:A:322:PRO:CG	1:A:540:ASN:ND2	2.74	0.49
1:C:946:GLY:O	1:C:950:ASP:HB2	2.13	0.49
1:A:44:ARG:HB3	1:A:47:VAL:CG1	2.41	0.49
1:B:384:PRO:HA	1:B:387:LEU:HB2	1.94	0.49
1:B:821:LEU:HD11	1:B:935:GLN:HG3	1.94	0.49
1:C:570:VAL:HG23	1:C:572:THR:HG23	1.94	0.49
1:A:113:LYS:HD2	1:A:113:LYS:O	2.12	0.49
1:A:631:PRO:HB3	1:A:633:TRP:CZ2	2.47	0.49
1:A:844:ILE:O	1:B:557:LYS:HG3	2.12	0.49
1:A:898:PHE:HZ	1:A:1050:MET:HE1	1.76	0.49
1:B:131:CYS:SG	1:B:163:ALA:O	2.71	0.49
1:B:946:GLY:O	1:B:950:ASP:HB2	2.13	0.49
1:C:131:CYS:HB3	1:C:133:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:O	1:B:563:GLN:HA	2.12	0.49
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.53	0.49
1:C:189:LEU:HG	1:C:208:THR:O	2.12	0.49
1:A:191:GLU:HB2	1:A:223:LEU:HD11	1.93	0.49
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.48	0.49
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.93	0.49
1:A:902:MET:SD	1:A:1050:MET:HE2	2.53	0.49
1:C:520:ALA:O	1:C:521:PRO:C	2.53	0.49
1:C:360:ASN:H	1:C:523:THR:HB	1.77	0.49
1:A:131:CYS:HB3	1:A:133:PHE:CE2	2.48	0.49
1:A:946:GLY:O	1:A:950:ASP:HB2	2.13	0.49
1:B:177:MET:H	1:B:207:HIS:CE1	2.30	0.49
1:C:44:ARG:HB3	1:C:47:VAL:CG1	2.41	0.48
1:C:307:THR:HA	1:C:602:THR:HG21	1.95	0.48
1:A:497:PHE:HA	1:A:501:TYR:HE2	1.78	0.48
1:A:675:GLN:HG3	1:A:693:ILE:HD11	1.94	0.48
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.48	0.48
1:B:360:ASN:H	1:B:523:THR:HB	1.77	0.48
1:B:588:THR:HG23	1:B:589:PRO:HD2	1.95	0.48
1:C:578:ASP:O	1:C:582:LEU:N	2.45	0.48
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.53	0.48
1:A:740:MET:HG3	1:B:592:PHE:CZ	2.48	0.48
1:A:973:ILE:HG22	1:A:992:GLN:HG3	1.95	0.48
1:B:927:PHE:HZ	1:B:1052:PHE:HE2	1.60	0.48
1:C:568:ASP:HA	1:B:846:ALA:HB1	1.95	0.48
1:C:588:THR:OG1	1:B:841:LEU:HB3	2.13	0.48
1:C:588:THR:HG22	1:C:589:PRO:O	2.13	0.48
1:A:296:LEU:HD11	1:A:308:VAL:HG21	1.95	0.48
1:B:126:VAL:HG11	1:B:175:PHE:CE1	2.49	0.48
1:B:214:ARG:O	1:B:217:PRO:HG3	2.13	0.48
1:B:555:SER:HB3	1:B:584:ILE:HG22	1.95	0.48
1:C:216:PHE:O	1:C:217:PRO:C	2.52	0.48
1:C:705:VAL:C	1:C:707:TYR:H	2.21	0.48
1:C:760:CYS:HA	1:C:763:LEU:HG	1.96	0.48
1:A:215:ASP:HB2	1:A:266:TYR:OH	2.12	0.48
1:A:374:PHE:CZ	1:A:434:ILE:HG23	2.48	0.48
1:A:927:PHE:HZ	1:A:1052:PHE:HE2	1.61	0.48
1:A:1106:GLN:OE1	1:A:1106:GLN:N	2.47	0.48
1:B:497:PHE:HA	1:B:501:TYR:HE2	1.78	0.48
1:C:214:ARG:O	1:C:217:PRO:HG3	2.13	0.48
1:B:339:HIS:O	1:B:340:GLU:C	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:CYS:HA	1:B:763:LEU:HG	1.95	0.48
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.12	0.48
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.95	0.48
1:A:106:PHE:CD1	1:A:235:ILE:HG21	2.49	0.48
1:A:802:PHE:O	1:A:804:GLN:N	2.47	0.48
1:C:431:GLY:HA2	1:C:515:PHE:HD2	1.77	0.48
1:B:44:ARG:HB3	1:B:47:VAL:CG1	2.41	0.48
1:B:106:PHE:CD1	1:B:235:ILE:HG21	2.49	0.48
1:B:191:GLU:HB2	1:B:223:LEU:HD11	1.95	0.48
1:C:126:VAL:HG11	1:C:175:PHE:CE1	2.49	0.48
1:A:331:ASN:HB3	1:A:580:GLN:HG2	1.94	0.48
1:B:322:PRO:CG	1:B:540:ASN:HD21	2.16	0.48
1:B:902:MET:SD	1:B:1050:MET:HE2	2.53	0.48
1:C:131:CYS:HA	1:C:166:CYS:HA	1.96	0.48
1:C:744:GLY:O	1:C:745:ASP:C	2.57	0.48
1:A:126:VAL:HG11	1:A:175:PHE:CE1	2.49	0.48
1:A:339:HIS:O	1:A:340:GLU:C	2.53	0.48
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.53	0.48
1:B:898:PHE:HZ	1:B:1050:MET:HE1	1.76	0.48
1:B:973:ILE:HG22	1:B:992:GLN:HG3	1.95	0.48
1:C:81:ASN:ND2	1:C:240:THR:O	2.25	0.48
1:C:296:LEU:HD11	1:C:308:VAL:HG21	1.95	0.48
1:C:497:PHE:HA	1:C:501:TYR:HE2	1.78	0.48
1:C:843:ASP:O	1:C:845:ALA:N	2.47	0.48
1:C:902:MET:SD	1:C:1050:MET:HE2	2.53	0.48
1:C:439:ASN:O	1:C:443:SER:OG	2.25	0.47
1:B:878:LEU:HD13	1:B:1053:PRO:HD2	1.96	0.47
1:C:31:SER:HB3	1:C:62:VAL:HG21	1.96	0.47
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.48	0.47
1:A:439:ASN:O	1:A:443:SER:OG	2.25	0.47
1:C:106:PHE:HB3	1:C:235:ILE:HG23	1.97	0.47
1:C:557:LYS:HB3	1:C:559:PHE:HD1	1.79	0.47
1:C:973:ILE:HG22	1:C:992:GLN:HG3	1.95	0.47
1:A:760:CYS:HA	1:A:763:LEU:HG	1.96	0.47
1:B:726:ILE:HG23	1:B:1061:VAL:HG22	1.96	0.47
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.96	0.47
1:C:927:PHE:HZ	1:C:1052:PHE:HE2	1.60	0.47
1:A:726:ILE:HG23	1:A:1061:VAL:HG22	1.96	0.47
1:B:342:PHE:CZ	1:B:511:VAL:HG21	2.49	0.47
1:C:84:LEU:HB2	1:C:238:PHE:HD2	1.79	0.47
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:HIS:CD2	2:A:1315:NAG:H3	2.49	0.47
1:B:84:LEU:HB2	1:B:238:PHE:HD2	1.79	0.47
1:B:383:SER:HB3	1:B:386:LYS:HG2	1.95	0.47
1:C:322:PRO:CG	1:C:540:ASN:HD21	2.16	0.47
1:C:726:ILE:HG23	1:C:1061:VAL:HG22	1.96	0.47
1:C:850:ILE:O	1:C:854:LYS:HG2	2.15	0.47
1:C:931:ILE:O	1:C:934:ILE:HG22	2.15	0.47
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.96	0.47
1:C:106:PHE:CD1	1:C:235:ILE:HG21	2.49	0.47
1:C:356:THR:OG1	1:C:397:ALA:HB3	2.15	0.47
1:A:744:GLY:O	1:A:745:ASP:C	2.57	0.47
1:A:931:ILE:O	1:A:934:ILE:HG22	2.15	0.47
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.47
1:B:206:LYS:HB3	1:B:223:LEU:HD13	1.97	0.47
1:B:1132:ILE:HD12	1:B:1132:ILE:HA	1.78	0.47
1:C:339:HIS:O	1:C:340:GLU:C	2.53	0.47
1:C:823:PHE:CD1	1:C:1057:PRO:HG3	2.50	0.47
1:A:106:PHE:HB3	1:A:235:ILE:HG23	1.97	0.47
1:A:214:ARG:O	1:A:217:PRO:HG3	2.13	0.47
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.50	0.47
1:C:177:MET:HB2	1:C:207:HIS:ND1	2.30	0.47
1:C:322:PRO:CG	1:C:540:ASN:ND2	2.74	0.47
1:C:577:ARG:HG2	1:C:584:ILE:HD13	1.97	0.47
1:C:631:PRO:HA	1:C:633:TRP:CZ3	2.50	0.47
1:C:741:TYR:CD2	1:C:1004:LEU:HD22	2.50	0.47
1:A:31:SER:HB3	1:A:62:VAL:HG21	1.96	0.47
1:A:627:ASP:HA	1:A:634:ARG:HH22	1.80	0.47
1:A:823:PHE:CD1	1:A:1057:PRO:HG3	2.50	0.47
1:B:823:PHE:CD1	1:B:1057:PRO:HG3	2.50	0.47
1:A:878:LEU:HD13	1:A:1053:PRO:HD2	1.96	0.46
1:C:175:PHE:CD1	1:C:175:PHE:N	2.82	0.46
1:C:355:ARG:NE	1:C:398:ASP:OD2	2.48	0.46
1:C:742:ILE:HG22	1:C:997:ILE:CD1	2.45	0.46
1:C:983:ARG:HD3	1:A:517:LEU:CD1	2.30	0.46
1:C:1132:ILE:HA	1:C:1132:ILE:HD12	1.77	0.46
1:B:204:TYR:CE2	1:B:225:PRO:HG3	2.50	0.46
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.97	0.46
1:C:25:THR:HG23	1:C:66:HIS:HB2	1.98	0.46
1:C:878:LEU:HD13	1:C:1053:PRO:HD2	1.96	0.46
1:C:900:MET:HE2	1:A:1079:PRO:HA	1.95	0.46
1:A:84:LEU:HB2	1:A:238:PHE:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PHE:HD2	1:A:629:LEU:HD11	1.81	0.46
1:B:103:GLY:HA3	1:B:120:VAL:HA	1.96	0.46
1:B:559:PHE:CD1	1:B:584:ILE:HD13	2.50	0.46
1:B:718:PHE:HE1	1:B:919:ASN:ND2	2.14	0.46
1:A:718:PHE:HE1	1:A:919:ASN:ND2	2.14	0.46
1:B:177:MET:HB2	1:B:207:HIS:ND1	2.31	0.46
1:C:176:LEU:HD22	1:C:190:ARG:HD2	1.98	0.46
1:C:645:THR:HG23	1:C:647:ALA:N	2.31	0.46
1:C:650:LEU:HD23	1:C:653:ALA:HB3	1.98	0.46
1:B:129:LYS:HE2	1:B:169:GLU:HG3	1.98	0.46
1:B:307:THR:HA	1:B:602:THR:HG21	1.96	0.46
1:C:563:GLN:HA	1:B:41:LYS:O	2.16	0.46
1:B:25:THR:HG23	1:B:66:HIS:HB2	1.98	0.46
1:B:454:ARG:HH22	1:B:467:ASP:HB3	1.81	0.46
1:A:133:PHE:CD2	1:A:160:TYR:HA	2.51	0.46
1:A:581:THR:C	1:A:583:GLU:N	2.74	0.46
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.81	0.46
1:C:1083:HIS:CE1	1:C:1137:VAL:CG2	2.96	0.46
1:A:175:PHE:CD1	1:A:175:PHE:N	2.82	0.46
1:A:347:PHE:HD2	1:A:399:SER:HB2	1.81	0.46
1:B:627:ASP:HA	1:B:634:ARG:HH22	1.80	0.46
1:B:1092:GLU:N	1:B:1092:GLU:OE2	2.49	0.46
1:C:763:LEU:HD13	1:C:1004:LEU:HG	1.98	0.46
1:A:342:PHE:CE2	1:A:436:TRP:CZ3	3.04	0.46
1:C:454:ARG:HH22	1:C:467:ASP:HB3	1.81	0.46
1:C:718:PHE:HE1	1:C:919:ASN:ND2	2.14	0.46
1:A:25:THR:HG23	1:A:66:HIS:HB2	1.98	0.46
1:A:177:MET:HB2	1:A:207:HIS:ND1	2.31	0.46
1:A:439:ASN:OD1	1:A:507:PRO:HD2	2.17	0.46
1:A:631:PRO:HA	1:A:633:TRP:CZ3	2.50	0.46
1:B:575:ALA:HA	1:B:585:LEU:O	2.16	0.46
1:C:423:TYR:OH	1:C:464:PHE:HE1	1.98	0.45
1:A:40:ASP:CG	1:A:41:LYS:H	2.24	0.45
1:A:454:ARG:HH22	1:A:467:ASP:HB3	1.81	0.45
1:B:528:LYS:O	1:B:529:LYS:HB3	2.16	0.45
1:C:105:ILE:HD13	1:C:159:VAL:HG11	1.98	0.45
1:C:439:ASN:OD1	1:C:507:PRO:HD2	2.17	0.45
1:C:528:LYS:O	1:C:529:LYS:HB3	2.16	0.45
1:C:617:CYS:O	1:C:621:SER:N	2.40	0.45
1:A:759:PHE:CZ	1:B:1002:GLN:NE2	2.84	0.45
1:A:1092:GLU:OE2	1:A:1092:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASP:CG	1:B:41:LYS:H	2.24	0.45
1:B:106:PHE:HB3	1:B:235:ILE:HG23	1.97	0.45
1:B:631:PRO:HA	1:B:633:TRP:CZ3	2.51	0.45
1:B:763:LEU:HD13	1:B:1004:LEU:HG	1.98	0.45
1:B:1101:HIS:CD2	2:B:1315:NAG:H3	2.51	0.45
1:C:644:GLN:NE2	1:C:648:GLY:O	2.49	0.45
1:A:528:LYS:O	1:A:529:LYS:HB3	2.16	0.45
1:A:763:LEU:HD13	1:A:1004:LEU:HG	1.98	0.45
1:B:106:PHE:CE2	1:B:238:PHE:HD1	2.34	0.45
1:B:878:LEU:O	1:B:882:ILE:HG12	2.17	0.45
1:C:164:ASN:HB2	2:C:1302:NAG:HN2	1.81	0.45
1:A:1101:HIS:CG	2:A:1315:NAG:H5	2.52	0.45
1:B:327:VAL:HG11	1:B:528:LYS:CG	2.47	0.45
1:C:343:ASN:OD1	1:C:343:ASN:N	2.50	0.45
1:C:1092:GLU:OE2	1:C:1092:GLU:N	2.49	0.45
1:A:176:LEU:HD22	1:A:190:ARG:HD2	1.98	0.45
1:B:705:VAL:HG12	1:B:707:TYR:H	1.82	0.45
1:A:131:CYS:HA	1:A:166:CYS:HA	1.99	0.45
1:A:210:ILE:H	1:A:210:ILE:HG13	1.56	0.45
1:A:501:TYR:HB3	1:A:505:HIS:HB2	1.98	0.45
1:A:742:ILE:HD13	1:A:1001:LEU:HD13	1.99	0.45
1:B:363:ALA:O	1:B:527:PRO:HD3	2.17	0.45
1:B:878:LEU:HD12	1:B:878:LEU:HA	1.75	0.45
1:C:505:HIS:CE1	1:B:503:VAL:HB	2.52	0.45
1:C:742:ILE:HG22	1:C:997:ILE:HD12	1.99	0.45
1:A:303:LEU:H	1:A:303:LEU:HG	1.67	0.45
1:A:857:GLY:C	1:A:858:LEU:HD23	2.42	0.45
1:B:97:LYS:HE2	1:B:184:GLY:HA3	1.99	0.45
1:B:342:PHE:CE2	1:B:436:TRP:CZ3	3.04	0.45
1:A:188:ASN:OD1	1:A:188:ASN:N	2.50	0.45
1:A:343:ASN:N	1:A:343:ASN:OD1	2.50	0.45
1:A:390:LEU:HD13	1:A:390:LEU:HA	1.83	0.45
1:A:503:VAL:HB	1:B:505:HIS:NE2	2.31	0.45
1:B:343:ASN:OD1	1:B:343:ASN:N	2.50	0.45
1:C:41:LYS:HB3	1:A:562:PHE:O	2.17	0.45
1:C:97:LYS:HE2	1:C:184:GLY:HA3	1.98	0.45
1:C:125:ASN:HB2	2:C:1301:NAG:H62	1.99	0.45
1:C:321:GLN:NE2	1:C:630:THR:OG1	2.49	0.45
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.98	0.45
1:C:741:TYR:CE2	1:C:1004:LEU:HB2	2.51	0.45
1:C:878:LEU:O	1:C:882:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HD3	1:A:133:PHE:HZ	1.82	0.45
1:A:327:VAL:HG11	1:A:528:LYS:CG	2.47	0.45
1:A:705:VAL:HG12	1:A:707:TYR:H	1.82	0.45
1:A:744:GLY:O	1:A:746:SER:N	2.50	0.45
1:A:759:PHE:HZ	1:B:1002:GLN:NE2	2.15	0.45
1:C:106:PHE:CE2	1:C:238:PHE:HD1	2.34	0.45
1:C:278:LYS:HB2	1:C:306:PHE:CE1	2.52	0.45
1:C:363:ALA:O	1:C:527:PRO:HD3	2.17	0.45
1:A:106:PHE:CE2	1:A:238:PHE:HD1	2.34	0.45
1:A:363:ALA:O	1:A:527:PRO:HD3	2.17	0.45
1:B:175:PHE:CD1	1:B:175:PHE:N	2.82	0.45
1:C:40:ASP:CG	1:C:41:LYS:H	2.24	0.44
1:C:342:PHE:CE2	1:C:436:TRP:CZ3	3.04	0.44
1:C:1013:ILE:CD1	1:B:1012:LEU:HD13	2.47	0.44
1:A:340:GLU:C	1:A:342:PHE:N	2.75	0.44
1:B:176:LEU:HD22	1:B:190:ARG:HD2	1.98	0.44
1:C:907:ASN:HB2	1:C:913:GLN:HG2	1.99	0.44
1:B:276:LEU:HD22	1:B:301:CYS:HA	1.99	0.44
1:C:44:ARG:O	1:C:283:GLY:HA2	2.18	0.44
1:C:326:ILE:HG12	1:C:532:ASN:O	2.18	0.44
1:A:321:GLN:NE2	1:A:630:THR:OG1	2.49	0.44
1:B:501:TYR:HB3	1:B:505:HIS:HB2	1.98	0.44
1:C:327:VAL:HG11	1:C:528:LYS:CG	2.47	0.44
1:C:577:ARG:O	1:C:578:ASP:C	2.60	0.44
1:C:780:GLU:O	1:C:784:GLN:NE2	2.49	0.44
1:C:858:LEU:HD13	1:C:962:LEU:HD13	2.00	0.44
1:A:348:ALA:HB1	1:A:352:ALA:O	2.18	0.44
1:B:450:ASP:OD1	1:B:450:ASP:N	2.50	0.44
1:C:244:LEU:HD23	1:C:244:LEU:HA	1.87	0.44
1:C:567:ARG:HB3	1:C:568:ASP:H	1.67	0.44
1:A:103:GLY:C	1:A:241:LEU:HG	2.43	0.44
1:A:278:LYS:HB2	1:A:306:PHE:CE1	2.52	0.44
1:A:309:GLU:HG2	1:A:313:TYR:OH	2.18	0.44
1:B:34:ARG:NH2	1:B:217:PRO:O	2.51	0.44
1:B:656:VAL:C	1:B:658:ASN:H	2.26	0.44
1:A:97:LYS:HE2	1:A:184:GLY:HA3	1.98	0.44
1:A:402:ILE:HD11	1:A:510:VAL:HG21	2.00	0.44
1:B:340:GLU:C	1:B:342:PHE:N	2.75	0.44
1:C:1002:GLN:HG3	1:B:759:PHE:CE2	2.44	0.44
1:A:125:ASN:HB2	2:A:1301:NAG:H62	1.99	0.44
1:A:742:ILE:HG22	1:A:997:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ALA:HA	1:A:933:LYS:HG2	2.00	0.44
1:B:125:ASN:HB2	2:B:1301:NAG:H62	1.99	0.44
1:B:439:ASN:OD1	1:B:507:PRO:HD2	2.17	0.44
1:B:1101:HIS:CG	2:B:1315:NAG:H5	2.53	0.44
1:C:930:ALA:HA	1:C:933:LYS:HG2	2.00	0.44
1:A:878:LEU:O	1:A:882:ILE:HG12	2.17	0.44
1:B:348:ALA:HB1	1:B:352:ALA:O	2.18	0.44
1:C:348:ALA:HB1	1:C:352:ALA:O	2.18	0.44
1:B:195:LYS:HE2	1:B:195:LYS:HB2	1.79	0.44
1:B:358:ILE:HB	1:B:395:VAL:HB	2.00	0.44
1:B:930:ALA:HA	1:B:933:LYS:HG2	2.00	0.44
1:C:103:GLY:C	1:C:241:LEU:HG	2.43	0.43
1:C:322:PRO:CB	1:C:540:ASN:ND2	2.81	0.43
1:C:450:ASP:N	1:C:450:ASP:OD1	2.51	0.43
1:C:562:PHE:O	1:B:41:LYS:HD3	2.17	0.43
1:A:44:ARG:O	1:A:283:GLY:HA2	2.18	0.43
1:A:581:THR:O	1:A:583:GLU:N	2.50	0.43
1:A:792:PRO:HG3	1:B:707:TYR:CD1	2.50	0.43
1:B:419:ALA:HA	1:B:423:TYR:O	2.18	0.43
1:C:34:ARG:NH2	1:C:217:PRO:O	2.51	0.43
1:C:656:VAL:C	1:C:658:ASN:H	2.26	0.43
1:C:1001:LEU:HD12	1:C:1001:LEU:HA	1.77	0.43
1:A:806:LEU:HD23	1:A:878:LEU:HD23	1.99	0.43
1:A:413:GLY:HA2	1:A:424:LYS:HD2	1.98	0.43
1:A:857:GLY:O	1:A:858:LEU:HD23	2.18	0.43
3:B:1317:IDU:O1S	3:B:1317:IDU:O3	2.22	0.43
1:C:567:ARG:HG2	1:C:571:ASP:C	2.44	0.43
1:A:454:ARG:HH12	1:A:467:ASP:HB3	1.84	0.43
1:A:900:MET:HE2	1:B:1079:PRO:CA	2.47	0.43
1:B:885:GLY:HA2	1:B:901:GLN:CD	2.43	0.43
1:C:401:VAL:HG21	1:C:451:TYR:CE2	2.54	0.43
1:B:97:LYS:O	1:B:97:LYS:NZ	2.52	0.43
1:B:103:GLY:C	1:B:241:LEU:HG	2.43	0.43
1:B:322:PRO:CB	1:B:540:ASN:ND2	2.81	0.43
1:B:358:ILE:HG22	1:B:524:VAL:HG21	2.00	0.43
1:C:309:GLU:HG2	1:C:313:TYR:OH	2.18	0.43
1:C:742:ILE:HD13	1:C:1001:LEU:HD13	2.00	0.43
1:A:108:THR:O	1:A:110:LEU:N	2.50	0.43
1:A:212:ILE:HG13	1:A:212:ILE:O	2.18	0.43
1:A:858:LEU:HD13	1:A:962:LEU:HD13	2.00	0.43
1:A:947:LYS:HE3	1:A:947:LYS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HG22	1:C:524:VAL:HG21	2.00	0.43
1:C:557:LYS:CD	1:C:559:PHE:HE1	2.32	0.43
1:C:885:GLY:HA2	1:C:901:GLN:CD	2.43	0.43
1:A:755:GLN:CD	1:B:971:GLY:HA2	2.34	0.43
1:A:908:GLY:HA3	1:A:1036:GLN:HE22	1.84	0.43
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.51	0.43
1:B:278:LYS:HB2	1:B:306:PHE:CE1	2.52	0.43
1:B:789:TYR:CE2	1:B:888:PHE:HD2	2.36	0.43
1:C:34:ARG:NH2	1:C:219:GLY:O	2.52	0.43
1:C:382:VAL:HG22	1:C:517:LEU:HD11	2.01	0.43
1:A:164:ASN:O	1:A:166:CYS:N	2.52	0.43
1:B:418:ILE:O	1:B:422:ASN:HB2	2.19	0.43
1:B:454:ARG:HH12	1:B:467:ASP:HB3	1.84	0.43
1:C:118:LEU:HD11	1:C:159:VAL:HB	2.00	0.43
1:C:411:ALA:C	1:C:425:LEU:HD12	2.43	0.43
2:C:1311:NAG:H62	1:B:796:TYR:CG	2.54	0.43
1:A:841:LEU:HB3	1:B:588:THR:OG1	2.19	0.43
1:A:1083:HIS:CE1	1:A:1137:VAL:CG2	2.96	0.43
1:B:44:ARG:O	1:B:283:GLY:HA2	2.18	0.43
1:B:908:GLY:HA3	1:B:1036:GLN:HE22	1.84	0.43
1:C:1029:MET:O	1:C:1033:VAL:HB	2.19	0.43
1:A:322:PRO:CB	1:A:540:ASN:ND2	2.81	0.43
1:A:742:ILE:HG22	1:A:997:ILE:HD12	1.99	0.43
1:A:802:PHE:C	1:A:804:GLN:N	2.77	0.43
1:C:134:GLN:HE21	1:C:135:PHE:H	1.67	0.42
1:A:34:ARG:NH2	1:A:217:PRO:O	2.51	0.42
1:A:34:ARG:NH2	1:A:219:GLY:O	2.52	0.42
1:A:320:VAL:HG22	1:A:629:LEU:HD12	2.01	0.42
1:A:340:GLU:O	1:A:342:PHE:N	2.52	0.42
1:B:303:LEU:H	1:B:303:LEU:HG	1.73	0.42
1:B:375:PHE:CG	1:B:508:TYR:OH	2.68	0.42
1:B:388:ASN:HB3	1:B:527:PRO:HD2	2.00	0.42
1:C:327:VAL:HG13	1:C:542:ASN:HB3	2.01	0.42
1:C:434:ILE:HB	1:C:511:VAL:HG22	2.01	0.42
1:C:744:GLY:O	1:C:746:SER:N	2.52	0.42
1:A:130:VAL:HG23	1:A:168:PHE:HB3	2.00	0.42
1:A:503:VAL:CB	1:B:505:HIS:NE2	2.82	0.42
1:A:656:VAL:C	1:A:658:ASN:H	2.26	0.42
1:A:847:ARG:HB2	1:A:851:CYS:HB3	2.00	0.42
1:A:885:GLY:HA2	1:A:901:GLN:CD	2.43	0.42
1:B:299:THR:O	1:B:302:THR:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLU:HG2	1:B:313:TYR:OH	2.19	0.42
1:B:340:GLU:O	1:B:342:PHE:N	2.52	0.42
1:C:62:VAL:HG13	1:C:267:VAL:O	2.20	0.42
1:C:759:PHE:CZ	1:A:1002:GLN:NE2	2.86	0.42
1:C:843:ASP:CG	1:C:847:ARG:HA	2.45	0.42
1:C:908:GLY:HA3	1:C:1036:GLN:HE22	1.84	0.42
1:A:99:ASN:HD21	1:A:102:ARG:HH11	1.68	0.42
1:A:423:TYR:OH	1:A:512:VAL:HG11	2.19	0.42
1:A:780:GLU:O	1:A:784:GLN:NE2	2.49	0.42
1:A:984:LEU:HB3	1:A:989:ALA:HB2	2.02	0.42
1:B:34:ARG:NH2	1:B:219:GLY:O	2.52	0.42
1:B:387:LEU:HD11	1:B:515:PHE:CE2	2.55	0.42
1:B:1029:MET:O	1:B:1033:VAL:HB	2.19	0.42
1:C:97:LYS:O	1:C:97:LYS:NZ	2.52	0.42
1:C:454:ARG:HH12	1:C:467:ASP:HB3	1.84	0.42
1:A:802:PHE:C	1:A:804:GLN:H	2.27	0.42
1:A:847:ARG:HB2	1:A:851:CYS:HB2	2.00	0.42
1:A:878:LEU:HA	1:A:878:LEU:HD12	1.75	0.42
1:B:858:LEU:HD13	1:B:962:LEU:HD13	2.00	0.42
1:C:99:ASN:HD21	1:C:102:ARG:HH11	1.68	0.42
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.53	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.73	0.42
1:A:326:ILE:CD1	1:A:532:ASN:O	2.59	0.42
1:A:1114:ILE:HD13	1:A:1114:ILE:HA	1.93	0.42
1:B:320:VAL:HG22	1:B:629:LEU:HD12	2.02	0.42
1:A:574:ASP:O	1:A:587:ILE:N	2.50	0.42
1:A:983:ARG:HD3	1:B:517:LEU:CD1	2.37	0.42
1:B:364:ASP:O	1:B:367:VAL:HG12	2.20	0.42
1:C:340:GLU:C	1:C:342:PHE:N	2.75	0.42
1:C:379:CYS:HB3	1:C:382:VAL:O	2.19	0.42
1:C:403:LYS:N	1:C:495:TYR:OH	2.51	0.42
1:C:409:GLN:CD	1:C:416:GLY:HA3	2.45	0.42
1:A:358:ILE:HB	1:A:395:VAL:HB	2.02	0.42
1:C:1101:HIS:CD2	2:C:1315:NAG:H3	2.54	0.42
1:C:532:ASN:CG	1:C:533:LEU:H	2.28	0.42
1:C:984:LEU:HB3	1:C:989:ALA:HB2	2.02	0.42
1:A:738:CYS:O	1:A:742:ILE:HG13	2.19	0.42
1:A:878:LEU:HD11	1:A:1052:PHE:HB3	2.02	0.42
1:B:327:VAL:HG13	1:B:542:ASN:HB3	2.01	0.42
1:B:375:PHE:CG	1:B:508:TYR:CE1	3.08	0.42
1:B:502:GLY:O	1:B:506:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ALA:HA	1:C:423:TYR:O	2.19	0.42
1:A:129:LYS:HB3	1:A:169:GLU:HG3	2.01	0.42
1:A:387:LEU:HD11	1:A:515:PHE:CZ	2.55	0.42
1:B:559:PHE:CG	1:B:584:ILE:CD1	3.03	0.42
1:B:984:LEU:HB3	1:B:989:ALA:HB2	2.02	0.42
1:C:187:LYS:H	1:C:210:ILE:CG1	2.33	0.41
1:C:340:GLU:O	1:C:342:PHE:N	2.52	0.41
1:C:347:PHE:CE1	1:C:509:ARG:NH1	2.88	0.41
1:C:527:PRO:O	1:C:528:LYS:HB3	2.20	0.41
1:C:567:ARG:HE	1:B:42:VAL:HG11	1.85	0.41
1:C:616:ASN:HA	1:C:644:GLN:HE22	1.85	0.41
1:C:742:ILE:CD1	1:C:1001:LEU:HD13	2.49	0.41
1:A:62:VAL:HG13	1:A:267:VAL:O	2.20	0.41
1:A:97:LYS:O	1:A:97:LYS:NZ	2.52	0.41
1:A:130:VAL:CG1	1:A:233:ILE:HD13	2.50	0.41
1:A:318:PHE:CD2	1:A:629:LEU:HD11	2.55	0.41
1:A:375:PHE:CG	1:A:508:TYR:OH	2.68	0.41
1:B:878:LEU:HD11	1:B:1052:PHE:HB3	2.02	0.41
1:C:320:VAL:HG22	1:C:629:LEU:HD12	2.02	0.41
1:C:740:MET:HG2	1:C:857:GLY:HA3	2.01	0.41
1:C:806:LEU:HD21	1:C:882:ILE:HD11	2.02	0.41
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	2.02	0.41
1:C:974:SER:OG	1:C:975:SER:N	2.53	0.41
1:A:1029:MET:O	1:A:1033:VAL:HB	2.19	0.41
1:B:99:ASN:HD21	1:B:102:ARG:HH11	1.68	0.41
1:B:974:SER:OG	1:B:975:SER:N	2.53	0.41
1:C:502:GLY:O	1:C:506:GLN:HG2	2.20	0.41
1:C:703:ASN:HB2	1:B:787:GLN:HB3	2.02	0.41
1:C:1101:HIS:HB2	2:C:1315:NAG:H5	2.02	0.41
1:A:327:VAL:HG13	1:A:542:ASN:HB3	2.01	0.41
1:A:347:PHE:CE1	1:A:509:ARG:NH1	2.88	0.41
1:A:450:ASP:OD1	1:A:450:ASP:N	2.50	0.41
1:B:108:THR:O	1:B:110:LEU:N	2.50	0.41
1:B:527:PRO:O	1:B:528:LYS:HB3	2.20	0.41
1:B:581:THR:O	1:B:583:GLU:N	2.53	0.41
1:C:216:PHE:C	1:C:217:PRO:O	2.63	0.41
1:B:322:PRO:HB2	1:B:540:ASN:ND2	2.36	0.41
1:B:347:PHE:CE1	1:B:509:ARG:NH1	2.88	0.41
1:C:629:LEU:HD23	1:C:631:PRO:HG2	2.03	0.41
1:B:402:ILE:HD11	1:B:510:VAL:HG21	2.01	0.41
1:B:629:LEU:HD23	1:B:631:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:LEU:HA	1:C:878:LEU:HD12	1.75	0.41
1:A:388:ASN:HB3	1:A:527:PRO:HD2	2.02	0.41
1:B:105:ILE:C	1:B:106:PHE:HD2	2.29	0.41
1:B:328:ARG:HE	1:B:580:GLN:CD	2.29	0.41
1:C:105:ILE:C	1:C:106:PHE:HD2	2.29	0.41
1:C:322:PRO:HB2	1:C:540:ASN:ND2	2.36	0.41
1:A:502:GLY:O	1:A:506:GLN:HG2	2.20	0.41
1:A:518:LEU:HD12	1:A:518:LEU:HA	1.83	0.41
1:A:697:MET:H	1:A:697:MET:HG2	1.72	0.41
1:A:974:SER:OG	1:A:975:SER:N	2.53	0.41
1:A:1001:LEU:HD12	1:A:1001:LEU:HA	1.77	0.41
1:C:375:PHE:CG	1:C:508:TYR:CE1	3.08	0.41
1:C:588:THR:HG23	1:C:589:PRO:HD2	2.03	0.41
1:C:947:LYS:HE3	1:C:947:LYS:HB2	1.83	0.41
1:A:134:GLN:HG2	1:A:162:SER:HB2	2.02	0.41
1:A:345:THR:OG1	1:A:346:ARG:N	2.54	0.41
1:A:375:PHE:CG	1:A:508:TYR:CE1	3.08	0.41
1:A:1012:LEU:HB3	1:B:1013:ILE:CD1	2.51	0.41
1:B:390:LEU:HA	1:B:390:LEU:HD13	1.87	0.41
1:B:411:ALA:HB3	1:B:414:GLN:CG	2.49	0.41
1:B:780:GLU:O	1:B:784:GLN:NE2	2.49	0.41
1:C:120:VAL:HG13	1:C:127:PHE:HB3	2.02	0.41
1:C:364:ASP:O	1:C:367:VAL:HG12	2.20	0.41
1:C:435:ALA:HB2	1:C:510:VAL:HG22	2.03	0.41
1:C:759:PHE:HZ	1:A:1002:GLN:NE2	2.19	0.41
1:C:795:LYS:HB3	2:C:1313:NAG:H83	2.03	0.41
1:C:1012:LEU:HB3	1:A:1013:ILE:CD1	2.50	0.41
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.54	0.41
1:A:120:VAL:HG13	1:A:127:PHE:HB3	2.02	0.41
1:A:364:ASP:O	1:A:367:VAL:HG12	2.20	0.41
1:A:383:SER:HB3	1:A:386:LYS:HG2	2.02	0.41
1:A:435:ALA:HB2	1:A:510:VAL:HG22	2.03	0.41
1:A:961:THR:O	1:A:965:GLN:HG2	2.21	0.41
1:B:131:CYS:HB3	1:B:133:PHE:CZ	2.56	0.41
1:B:321:GLN:NE2	1:B:630:THR:OG1	2.49	0.41
1:B:435:ALA:HB2	1:B:510:VAL:HG22	2.03	0.41
1:B:581:THR:C	1:B:583:GLU:N	2.77	0.41
1:B:802:PHE:HB3	1:B:805:ILE:HG12	2.02	0.41
1:B:961:THR:O	1:B:965:GLN:HG2	2.21	0.41
1:B:1083:HIS:CE1	1:B:1137:VAL:CG2	2.96	0.41
1:C:535:LYS:O	1:C:536:ASN:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:ILE:HB	1:C:1075:PHE:CE2	2.56	0.41
1:C:961:THR:O	1:C:965:GLN:HG2	2.21	0.41
1:A:365:TYR:CE2	1:A:387:LEU:HG	2.56	0.41
1:A:406:GLU:HA	1:A:409:GLN:HB3	2.03	0.41
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.03	0.41
1:B:188:ASN:OD1	1:B:188:ASN:N	2.50	0.41
1:C:345:THR:OG1	1:C:346:ARG:N	2.54	0.40
1:A:535:LYS:O	1:A:536:ASN:CB	2.69	0.40
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.82	0.40
1:C:1029:MET:HE2	1:C:1053:PRO:HB3	2.03	0.40
1:C:1079:PRO:HD2	1:C:1131:GLY:O	2.22	0.40
1:A:358:ILE:HG22	1:A:524:VAL:HG21	2.02	0.40
1:A:913:GLN:H	1:A:913:GLN:HG3	1.74	0.40
1:B:345:THR:OG1	1:B:346:ARG:N	2.54	0.40
1:B:420:ASP:O	1:B:461:LEU:HB2	2.20	0.40
1:B:1029:MET:HE2	1:B:1053:PRO:HB3	2.03	0.40
1:C:168:PHE:CZ	1:C:229:LEU:HB2	2.57	0.40
1:C:176:LEU:C	1:C:177:MET:HE2	2.46	0.40
1:C:411:ALA:HB3	1:C:414:GLN:CG	2.51	0.40
1:C:599:THR:HB	1:C:608:VAL:HG12	2.04	0.40
1:A:959:LEU:O	1:A:963:VAL:HG13	2.22	0.40
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.88	0.40
1:B:231:ILE:HG22	1:B:233:ILE:HG23	2.03	0.40
1:B:599:THR:HB	1:B:608:VAL:HG12	2.04	0.40
1:C:48:LEU:HA	1:C:48:LEU:HD23	1.73	0.40
1:C:374:PHE:CZ	1:C:434:ILE:HG23	2.56	0.40
1:C:375:PHE:CD2	1:C:508:TYR:CZ	3.09	0.40
1:A:206:LYS:HB3	1:A:223:LEU:CD1	2.51	0.40
1:A:349:SER:OG	1:A:451:TYR:HA	2.22	0.40
1:A:527:PRO:O	1:A:528:LYS:HB3	2.20	0.40
1:A:554:LYS:NZ	1:A:554:LYS:HA	2.36	0.40
1:A:806:LEU:HD21	1:A:882:ILE:HD11	2.02	0.40
1:B:110:LEU:HD13	1:B:110:LEU:HA	1.94	0.40
1:B:326:ILE:CD1	1:B:532:ASN:O	2.59	0.40
1:B:375:PHE:CD2	1:B:508:TYR:CZ	3.09	0.40
1:B:437:ASN:OD1	1:B:439:ASN:ND2	2.54	0.40
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.86	0.40
1:C:25:THR:O	1:C:65:PHE:HA	2.21	0.40
1:C:518:LEU:HD12	1:C:518:LEU:HA	1.83	0.40
1:C:806:LEU:HD23	1:C:878:LEU:HD23	2.03	0.40
1:C:855:PHE:HD1	1:A:589:PRO:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:GLU:O	1:C:993:ILE:HG22	2.22	0.40
1:B:25:THR:O	1:B:65:PHE:HA	2.21	0.40
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.87	0.40
1:B:716:THR:HA	1:B:1110:TYR:HB3	2.04	0.40
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.54	0.40
1:B:1083:HIS:CD2	1:B:1137:VAL:H	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1053/1206 (87%)	944 (90%)	91 (9%)	18 (2%)	7	32
1	B	1053/1206 (87%)	944 (90%)	92 (9%)	17 (2%)	7	34
1	C	1053/1206 (87%)	942 (90%)	91 (9%)	20 (2%)	6	30
All	All	3159/3618 (87%)	2830 (90%)	274 (9%)	55 (2%)	9	32

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	329	PHE
1	C	348	ALA
1	C	527	PRO
1	C	536	ASN
1	C	745	ASP
1	A	348	ALA
1	A	527	PRO
1	A	536	ASN
1	A	745	ASP
1	B	348	ALA
1	B	527	PRO

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Mol	Chain	Res	Type
1	B	536	ASN
1	C	109	THR
1	C	559	PHE
1	C	590	CYS
1	A	109	THR
1	A	559	PHE
1	A	803	SER
1	B	109	THR
1	B	213	GLY
1	B	590	CYS
1	C	161	SER
1	C	165	ASN
1	C	188	ASN
1	C	244	LEU
1	C	518	LEU
1	A	165	ASN
1	A	244	LEU
1	A	518	LEU
1	B	244	LEU
1	B	518	LEU
1	B	593	GLY
1	C	529	LYS
1	C	561	PRO
1	A	529	LYS
1	A	561	PRO
1	A	582	LEU
1	B	529	LYS
1	B	557	LYS
1	B	561	PRO
1	C	330	PRO
1	C	706	ALA
1	A	402	ILE
1	B	402	ILE
1	B	582	LEU
1	C	134	GLN
1	C	844	ILE
1	A	163	ALA
1	A	330	PRO
1	B	164	ASN
1	A	412	PRO
1	B	330	PRO
1	C	942	PRO

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Mol	Chain	Res	Type
1	A	942	PRO
1	B	942	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	925/1054 (88%)	891 (96%)	34 (4%)	30 59
1	B	925/1054 (88%)	895 (97%)	30 (3%)	34 62
1	C	925/1054 (88%)	890 (96%)	35 (4%)	29 59
All	All	2775/3162 (88%)	2676 (96%)	99 (4%)	32 60

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	THR
1	C	45	SER
1	C	55	PHE
1	C	61	ASN
1	C	129	LYS
1	C	134	GLN
1	C	164	ASN
1	C	189	LEU
1	C	210	ILE
1	C	216	PHE
1	C	245	ASN
1	C	284	THR
1	C	308	VAL
1	C	389	ASP
1	C	395	VAL
1	C	511	VAL
1	C	512	VAL
1	C	552	LEU
1	C	553	THR
1	C	554	LYS

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Mol	Chain	Res	Type
1	C	567	ARG
1	C	582	LEU
1	C	584	ILE
1	C	595	VAL
1	C	617	CYS
1	C	635	VAL
1	C	709	ASN
1	C	734	THR
1	C	738	CYS
1	C	742	ILE
1	C	841	LEU
1	C	849	LEU
1	C	1096	VAL
1	C	1132	ILE
1	C	1136	THR
1	A	29	THR
1	A	55	PHE
1	A	61	ASN
1	A	129	LYS
1	A	134	GLN
1	A	160	TYR
1	A	189	LEU
1	A	210	ILE
1	A	216	PHE
1	A	245	ASN
1	A	284	THR
1	A	303	LEU
1	A	308	VAL
1	A	390	LEU
1	A	395	VAL
1	A	402	ILE
1	A	418	ILE
1	A	511	VAL
1	A	552	LEU
1	A	553	THR
1	A	554	LYS
1	A	582	LEU
1	A	595	VAL
1	A	635	VAL
1	A	709	ASN
1	A	734	THR
1	A	738	CYS

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Mol	Chain	Res	Type
1	A	742	ILE
1	A	849	LEU
1	A	916	LEU
1	A	918	GLU
1	A	1096	VAL
1	A	1132	ILE
1	A	1136	THR
1	B	45	SER
1	B	54	LEU
1	B	127	PHE
1	B	134	GLN
1	B	167	THR
1	B	189	LEU
1	B	216	PHE
1	B	245	ASN
1	B	284	THR
1	B	302	THR
1	B	303	LEU
1	B	390	LEU
1	B	395	VAL
1	B	552	LEU
1	B	553	THR
1	B	554	LYS
1	B	557	LYS
1	B	572	THR
1	B	582	LEU
1	B	588	THR
1	B	595	VAL
1	B	616	ASN
1	B	635	VAL
1	B	709	ASN
1	B	734	THR
1	B	788	ILE
1	B	983	ARG
1	B	1096	VAL
1	B	1132	ILE
1	B	1136	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	66	HIS

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Mol	Chain	Res	Type
1	C	99	ASN
1	C	188	ASN
1	C	207	HIS
1	C	271	GLN
1	C	394	ASN
1	C	439	ASN
1	C	505	HIS
1	C	540	ASN
1	C	556	ASN
1	C	804	GLN
1	C	914	ASN
1	C	965	GLN
1	C	978	ASN
1	C	1119	ASN
1	A	66	HIS
1	A	99	ASN
1	A	164	ASN
1	A	207	HIS
1	A	271	GLN
1	A	439	ASN
1	A	540	ASN
1	A	804	GLN
1	A	965	GLN
1	A	978	ASN
1	A	1011	GLN
1	A	1058	HIS
1	A	1119	ASN
1	B	99	ASN
1	B	207	HIS
1	B	540	ASN
1	B	556	ASN
1	B	914	ASN
1	B	965	GLN
1	B	1011	GLN
1	B	1036	GLN
1	B	1058	HIS
1	B	1119	ASN

5.3.3 RNA

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](#)

55 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
2	NAG	B	1304	1	14,14,15	0.38	0	17,19,21	0.56	0
2	NAG	A	1302	1	14,14,15	0.36	0	17,19,21	1.02	1 (5%)
2	NAG	A	1311	1	14,14,15	0.37	0	17,19,21	0.56	0
2	NAG	C	1302	1	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
2	NAG	B	1303	1	14,14,15	0.39	0	17,19,21	0.78	1 (5%)
2	NAG	B	1316	1	14,14,15	0.39	0	17,19,21	0.67	0
2	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.80	0
2	NAG	A	1317	1	14,14,15	0.41	0	17,19,21	0.75	0
2	NAG	B	1306	1	14,14,15	0.40	0	17,19,21	0.74	0
2	NAG	C	1308	1	14,14,15	0.39	0	17,19,21	0.72	0
2	NAG	C	1317	1	14,14,15	0.39	0	17,19,21	0.75	0
2	NAG	A	1316	1	14,14,15	0.39	0	17,19,21	0.67	0
2	NAG	B	1309	1	14,14,15	0.39	0	17,19,21	0.40	0
2	NAG	C	1301	1	14,14,15	0.39	0	17,19,21	0.81	0
2	NAG	C	1312	1	14,14,15	0.39	0	17,19,21	0.75	0
2	NAG	B	1307	1	14,14,15	0.39	0	17,19,21	0.76	1 (5%)
2	NAG	B	1318	1	14,14,15	0.38	0	17,19,21	0.51	0
2	NAG	B	1312	1	14,14,15	0.40	0	17,19,21	0.75	0
2	NAG	A	1310	1	14,14,15	0.38	0	17,19,21	0.64	0
2	NAG	A	1305	1	14,14,15	0.41	0	17,19,21	0.72	1 (5%)
2	NAG	A	1309	1	14,14,15	0.39	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1305	1	14,14,15	0.42	0	17,19,21	0.73	1 (5%)
2	NAG	A	1306	1	14,14,15	0.41	0	17,19,21	0.74	0
2	NAG	B	1319	1	14,14,15	0.38	0	17,19,21	0.48	0
2	NAG	C	1306	1	14,14,15	0.39	0	17,19,21	0.37	0
2	NAG	C	1303	1	14,14,15	0.39	0	17,19,21	0.78	1 (5%)
2	NAG	B	1305	1	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
2	NAG	B	1315	1	14,14,15	0.39	0	17,19,21	0.42	0
2	NAG	B	1302	1	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
2	NAG	C	1311	1	14,14,15	0.38	0	17,19,21	0.56	0
2	NAG	B	1314	1	14,14,15	0.39	0	17,19,21	0.39	0
2	NAG	C	1314	1	14,14,15	0.40	0	17,19,21	0.38	0
2	NAG	A	1304	1	14,14,15	0.35	0	17,19,21	0.56	0
2	NAG	A	1314	1	14,14,15	0.41	0	17,19,21	0.47	0
2	NAG	B	1301	1	14,14,15	0.37	0	17,19,21	0.81	0
2	NAG	B	1311	1	14,14,15	0.37	0	17,19,21	0.56	0
3	IDU	B	1317	-	15,15,17	0.91	1 (6%)	14,22,26	1.14	1 (7%)
2	NAG	A	1303	1	14,14,15	0.39	0	17,19,21	0.78	1 (5%)
2	NAG	C	1304	1	14,14,15	0.37	0	17,19,21	0.56	0
2	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.72	0
2	NAG	C	1313	1	14,14,15	0.38	0	17,19,21	0.47	0
2	NAG	B	1313	1	14,14,15	0.41	0	17,19,21	0.76	0
2	NAG	B	1308	1	14,14,15	0.40	0	17,19,21	0.71	0
2	NAG	A	1307	1	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
2	NAG	C	1316	1	14,14,15	0.39	0	17,19,21	0.67	0
2	NAG	A	1315	1	14,14,15	0.40	0	17,19,21	0.40	0
2	NAG	A	1312	1	14,14,15	0.39	0	17,19,21	0.75	0
2	NAG	A	1318	1	14,14,15	0.38	0	17,19,21	0.51	0
2	NAG	C	1315	1	14,14,15	0.41	0	17,19,21	0.44	0
2	NAG	A	1313	1	14,14,15	0.40	0	17,19,21	0.75	0
2	NAG	C	1318	1	14,14,15	0.37	0	17,19,21	0.50	0
2	NAG	B	1310	1	14,14,15	0.38	0	17,19,21	0.65	0
2	NAG	C	1310	1	14,14,15	0.38	0	17,19,21	0.64	0
2	NAG	C	1309	1	14,14,15	0.40	0	17,19,21	0.38	0
2	NAG	C	1307	1	14,14,15	0.39	0	17,19,21	0.76	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
2	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1317	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1317	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1319	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1315	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
3	IDU	B	1317	-	-	3/9/22/29	1/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1315	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1315	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1317	IDU	O6-C6	-3.00	1.21	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1302	NAG	C2-N2-C7	3.75	127.92	122.90
2	C	1302	NAG	C2-N2-C7	2.76	126.60	122.90
3	B	1317	IDU	O6-C6-C5	2.71	119.77	112.71
2	C	1307	NAG	C1-O5-C5	2.31	115.28	112.19
2	A	1307	NAG	C1-O5-C5	2.30	115.27	112.19
2	B	1307	NAG	C1-O5-C5	2.28	115.25	112.19
2	B	1302	NAG	C2-N2-C7	2.26	125.93	122.90
2	B	1305	NAG	C1-O5-C5	2.21	115.15	112.19
2	C	1305	NAG	C1-O5-C5	2.18	115.11	112.19
2	A	1305	NAG	C1-O5-C5	2.16	115.09	112.19
2	B	1303	NAG	C1-C2-N2	2.04	113.65	110.43
2	C	1303	NAG	C1-C2-N2	2.03	113.63	110.43
2	A	1303	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1317	IDU	C3-C2-O2-S
3	B	1317	IDU	O5-C5-C6-O61

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Mol	Chain	Res	Type	Atoms
2	C	1315	NAG	C8-C7-N2-C2
2	C	1315	NAG	O7-C7-N2-C2
2	A	1315	NAG	C8-C7-N2-C2
2	A	1315	NAG	O7-C7-N2-C2
2	B	1315	NAG	C8-C7-N2-C2
2	B	1315	NAG	O7-C7-N2-C2
2	B	1309	NAG	O5-C5-C6-O6
2	C	1309	NAG	O5-C5-C6-O6
2	C	1315	NAG	O5-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	A	1315	NAG	O5-C5-C6-O6
2	B	1315	NAG	O5-C5-C6-O6
2	C	1302	NAG	C3-C2-N2-C7
2	A	1302	NAG	C3-C2-N2-C7
2	B	1302	NAG	C3-C2-N2-C7
3	B	1317	IDU	O5-C5-C6-O6
2	C	1312	NAG	C1-C2-N2-C7
2	C	1317	NAG	C1-C2-N2-C7
2	A	1302	NAG	C1-C2-N2-C7
2	A	1312	NAG	C1-C2-N2-C7
2	A	1313	NAG	C1-C2-N2-C7
2	A	1317	NAG	C1-C2-N2-C7
2	B	1312	NAG	C1-C2-N2-C7
2	B	1313	NAG	C1-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1317	IDU	C1-C2-C3-C4-C5-O5

13 monomers are involved in 22 short contacts:

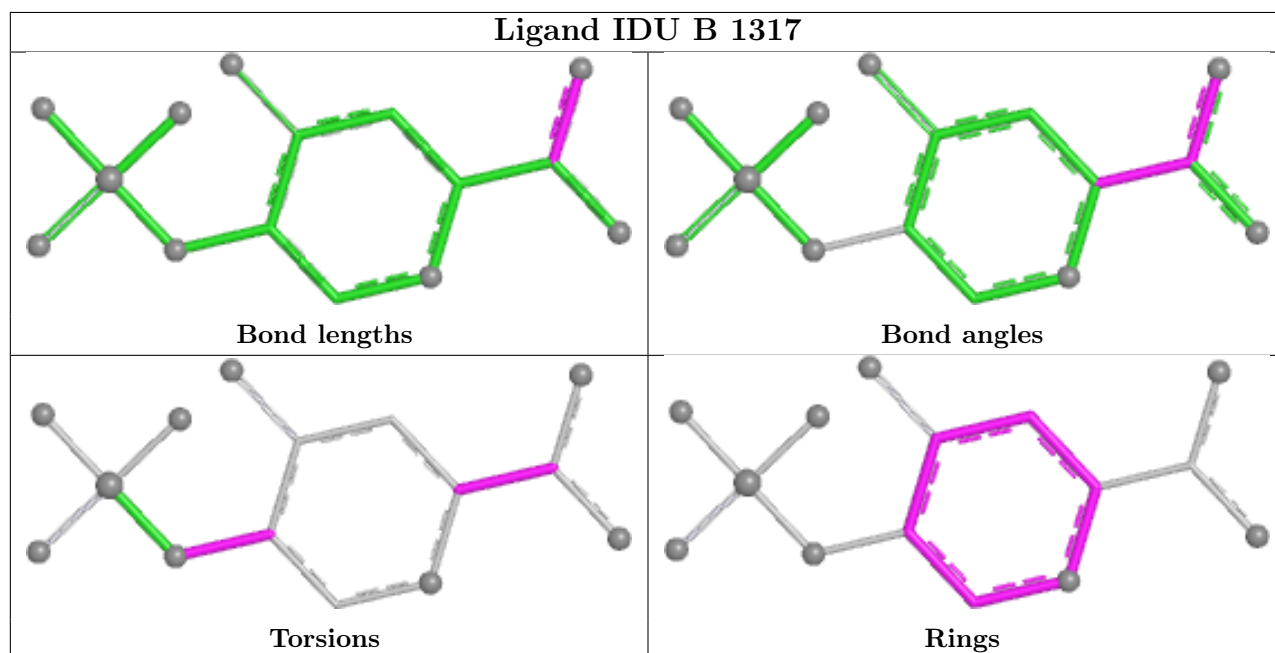
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1311	NAG	1	0
2	C	1302	NAG	1	0
2	A	1301	NAG	1	0
2	C	1301	NAG	1	0
2	A	1309	NAG	1	0
2	B	1315	NAG	3	0
2	C	1311	NAG	2	0
2	B	1301	NAG	1	0
2	B	1311	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1317	IDU	1	0
2	C	1313	NAG	3	0
2	A	1315	NAG	3	0
2	C	1315	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

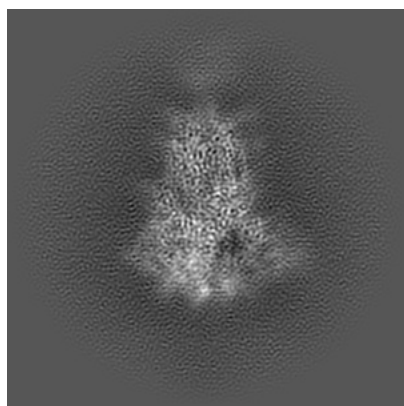
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38682. These allow visual inspection of the internal detail of the map and identification of artifacts.

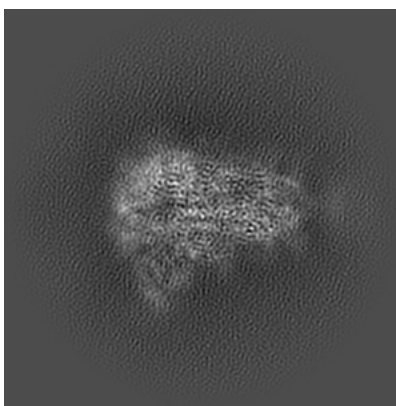
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

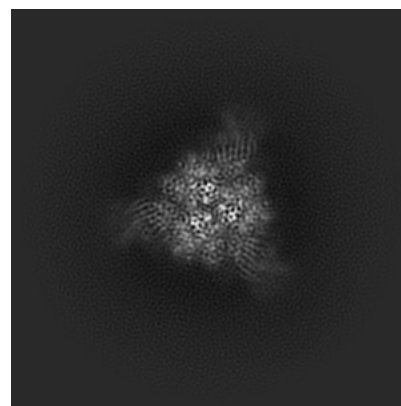
6.1.1 Primary map



X

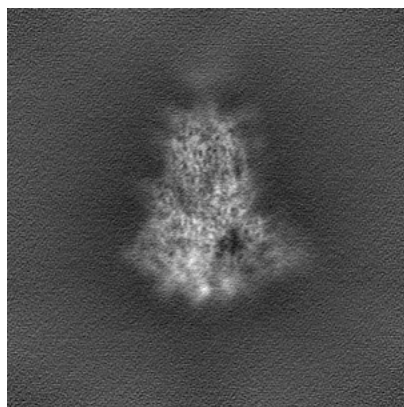


Y

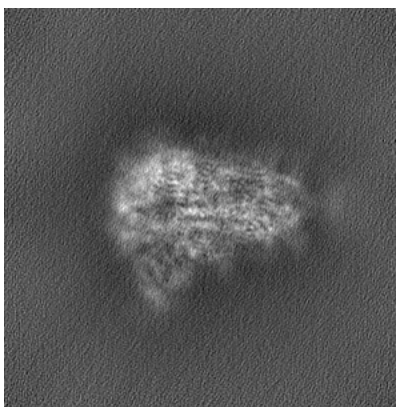


Z

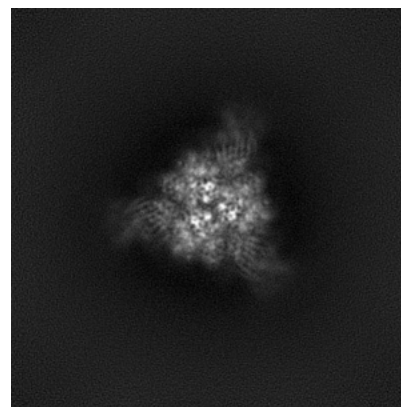
6.1.2 Raw map



X



Y

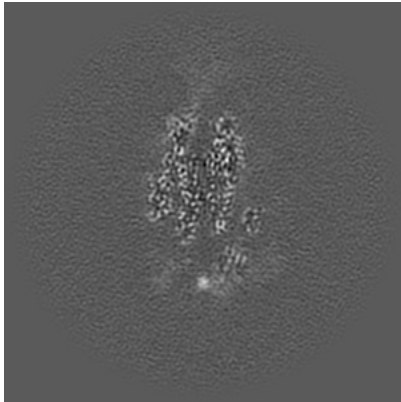


Z

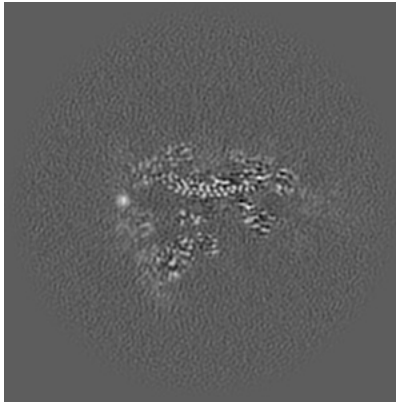
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

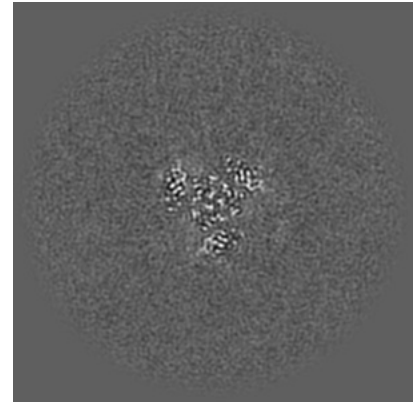
6.2.1 Primary map



X Index: 150

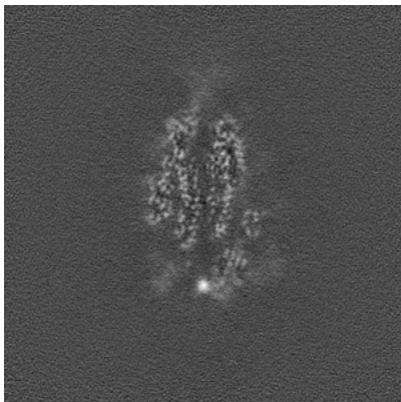


Y Index: 150

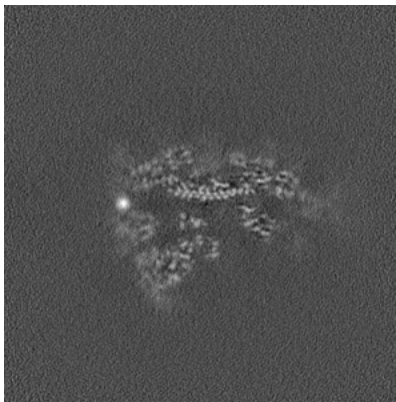


Z Index: 150

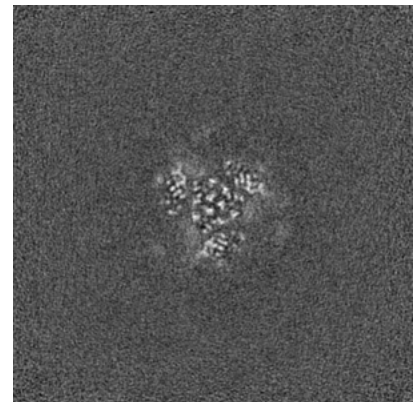
6.2.2 Raw map



X Index: 150



Y Index: 150

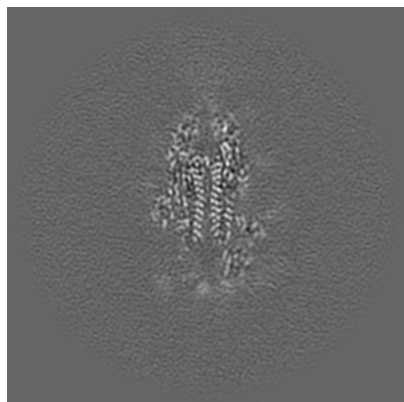


Z Index: 150

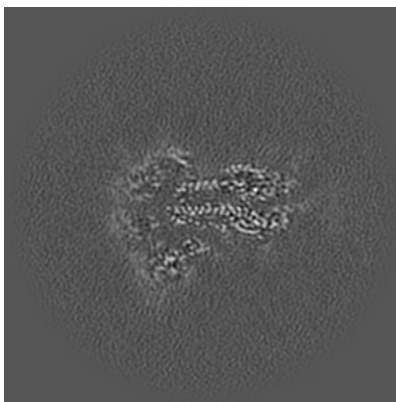
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

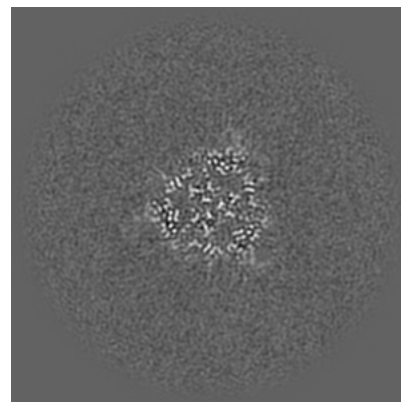
6.3.1 Primary map



X Index: 146

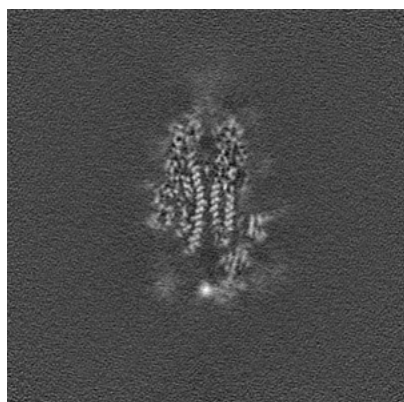


Y Index: 143

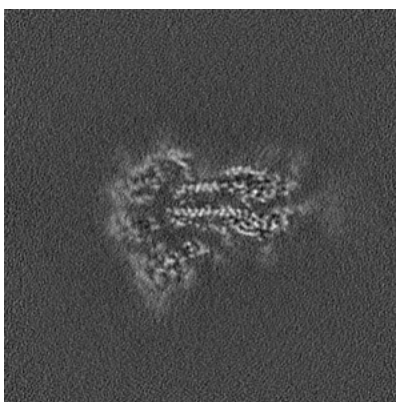


Z Index: 139

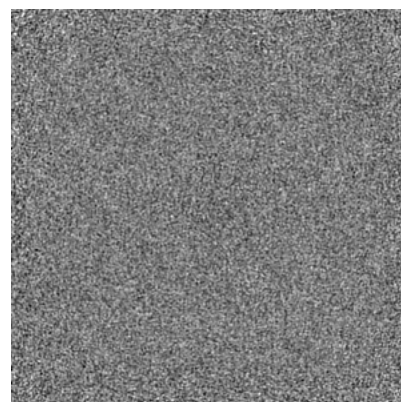
6.3.2 Raw map



X Index: 148



Y Index: 143

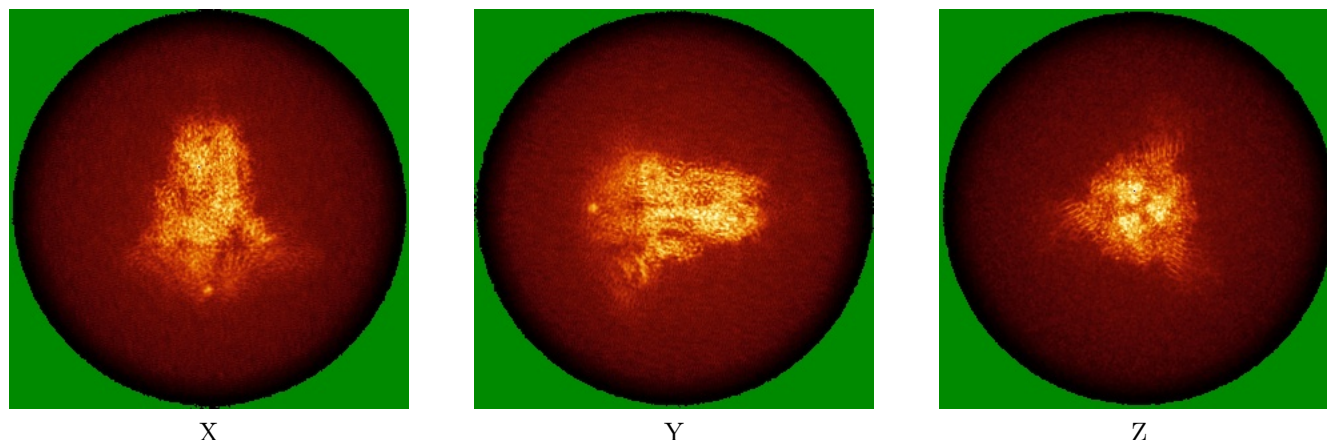


Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map

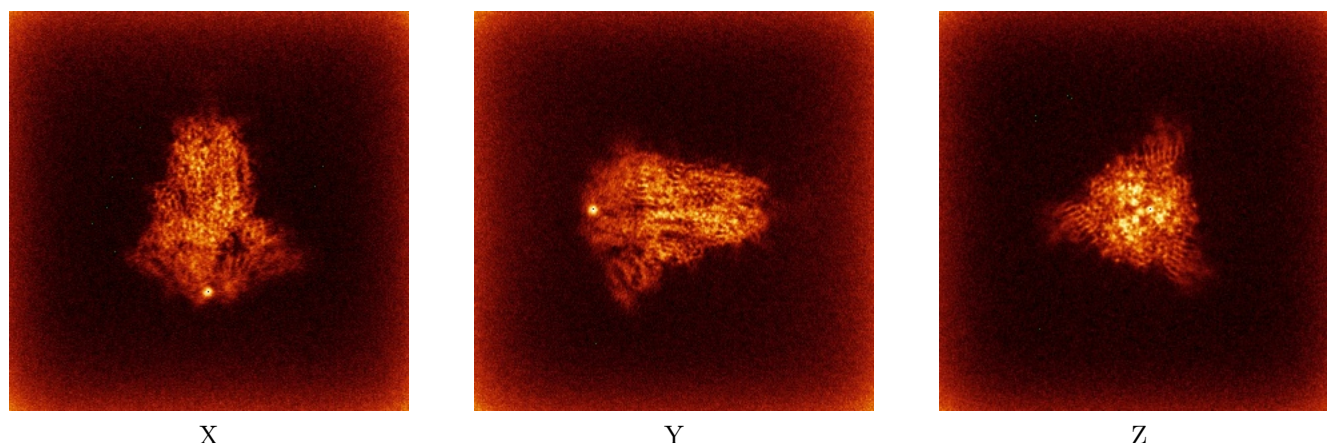


X

Y

Z

6.4.2 Raw map



X

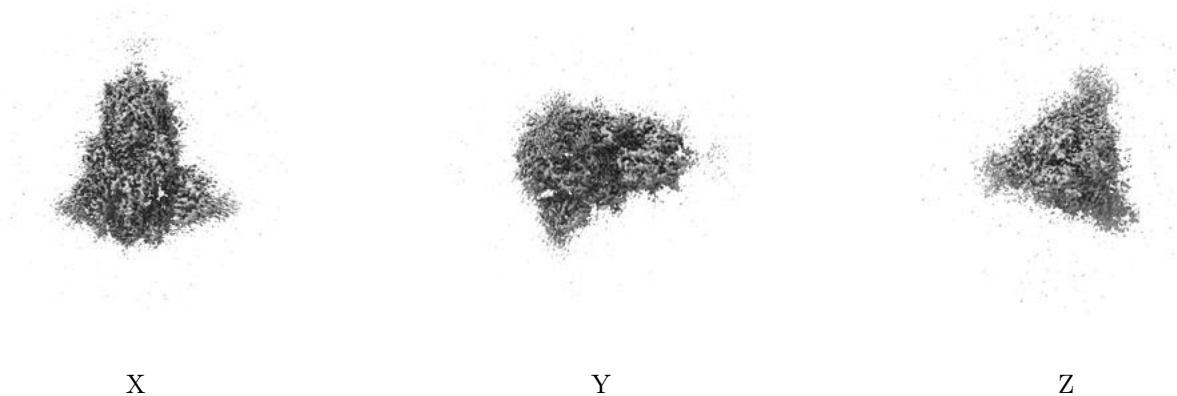
Y

Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

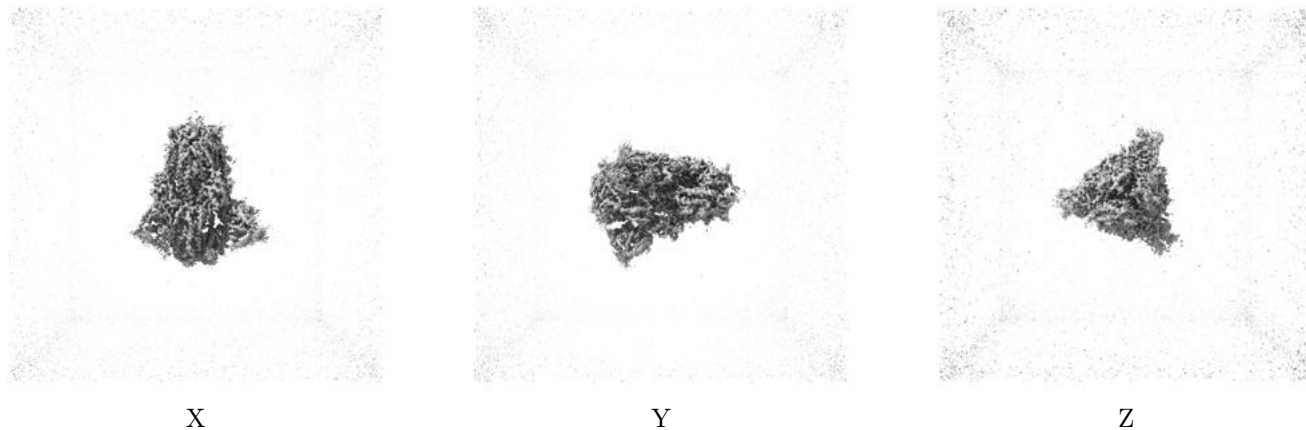
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

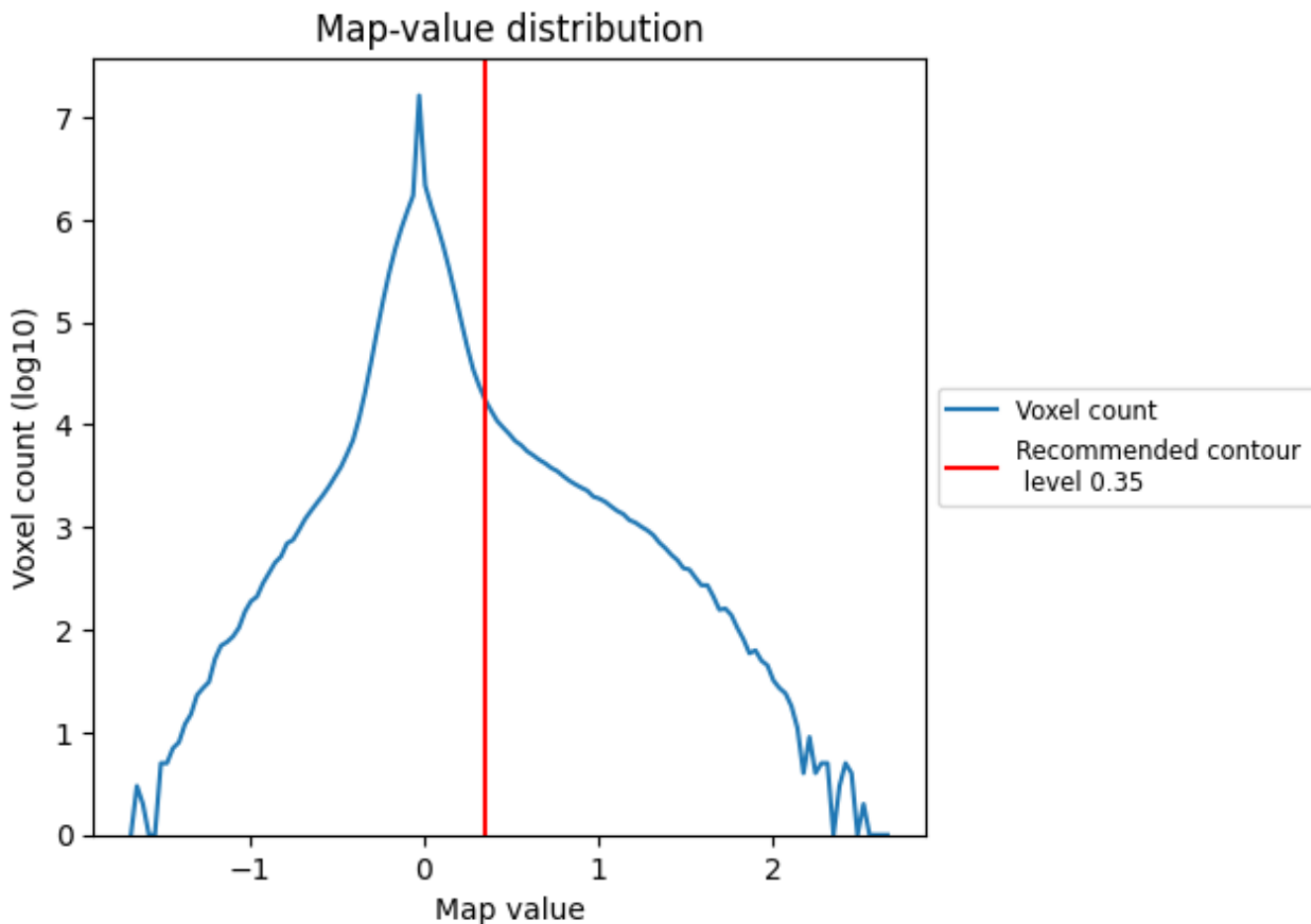
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

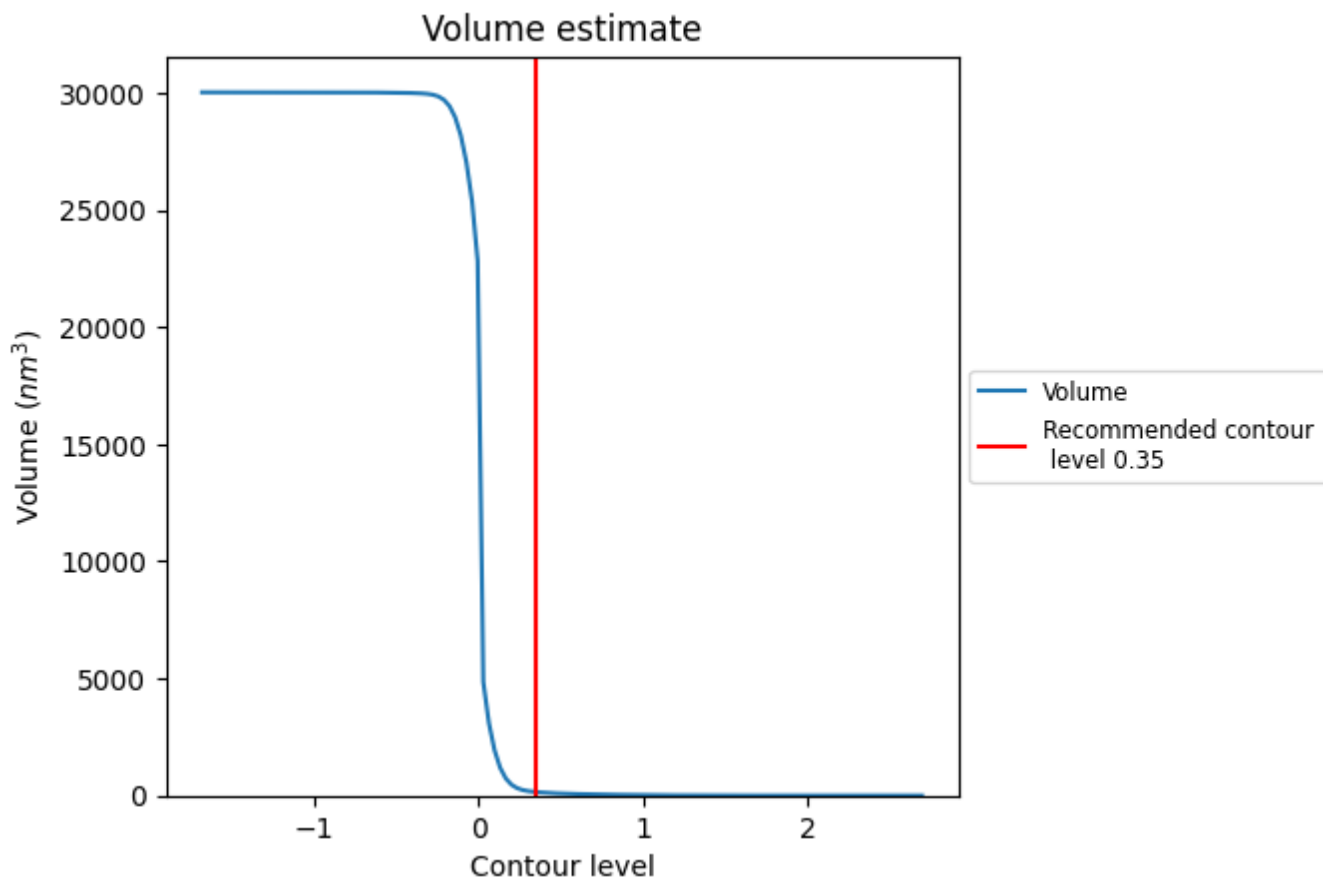
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

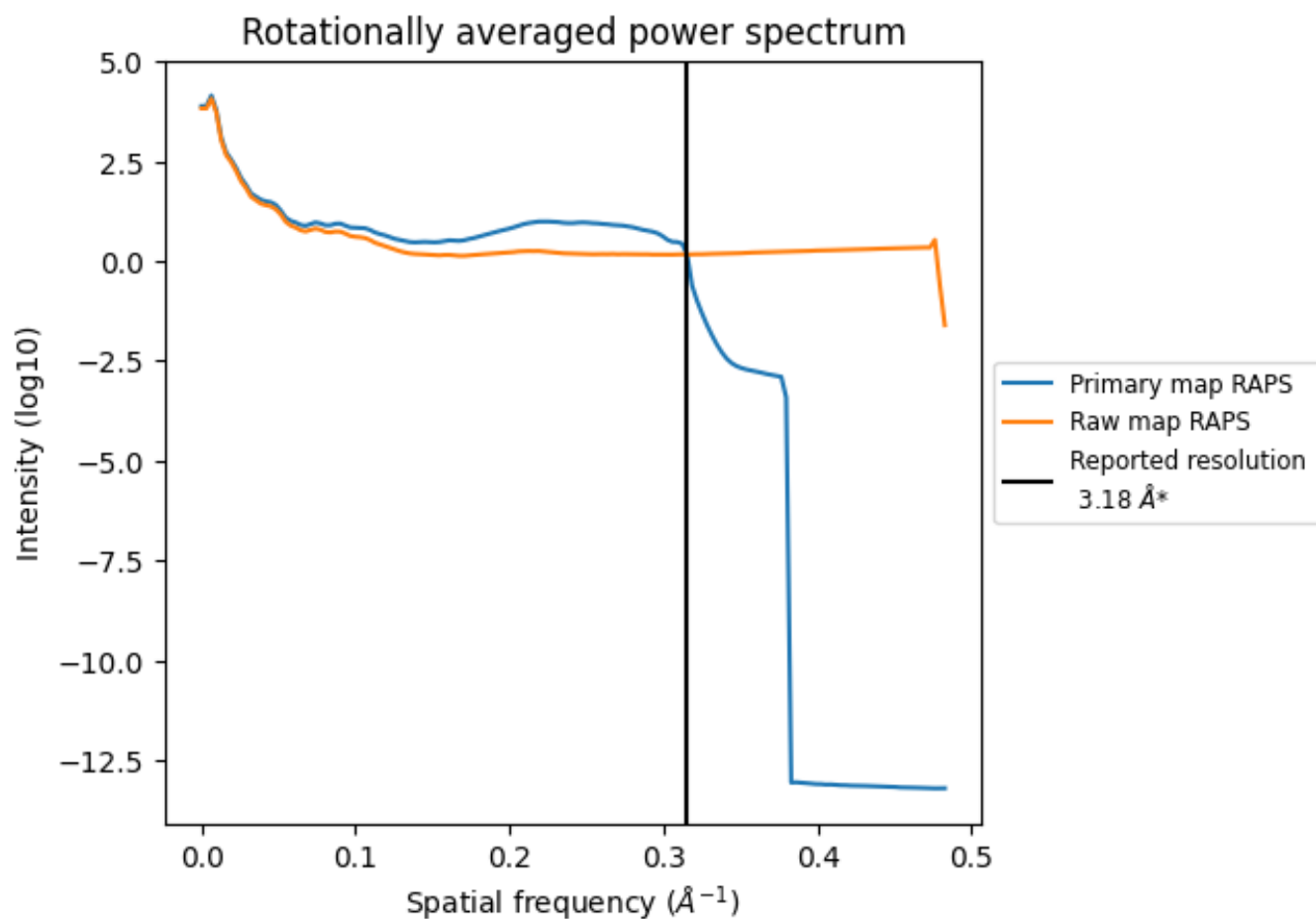
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 136 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

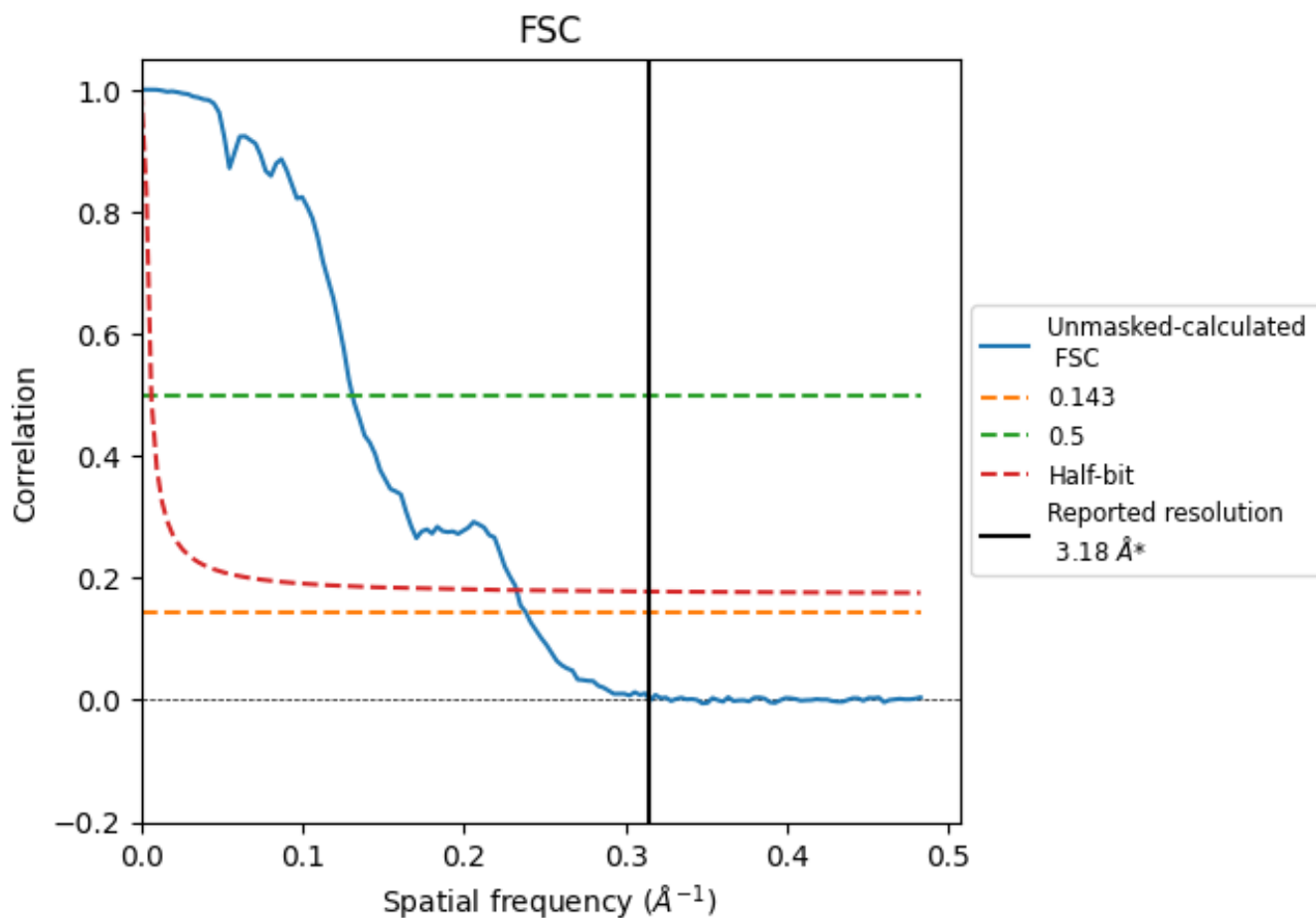


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.65	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.18 by more than 10 %

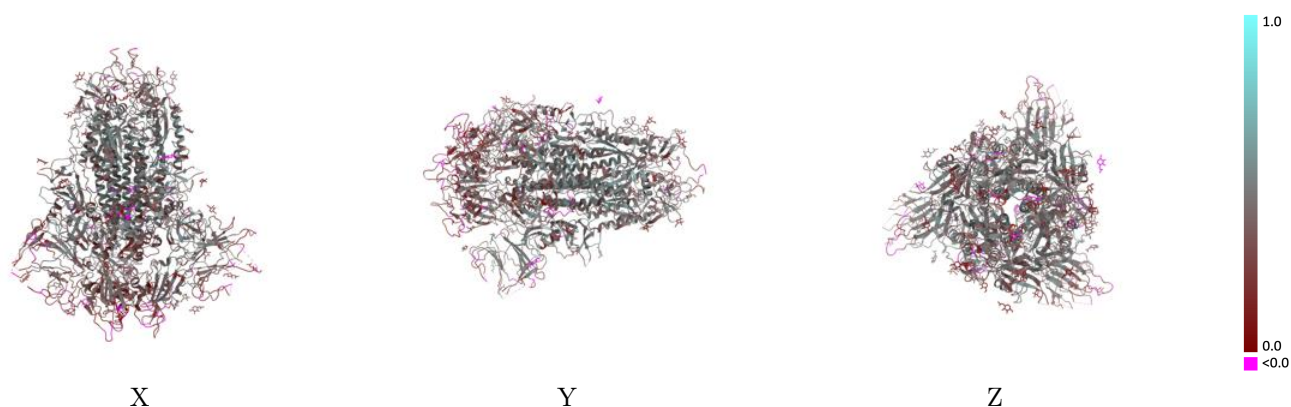
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38682 and PDB model 8XUS. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

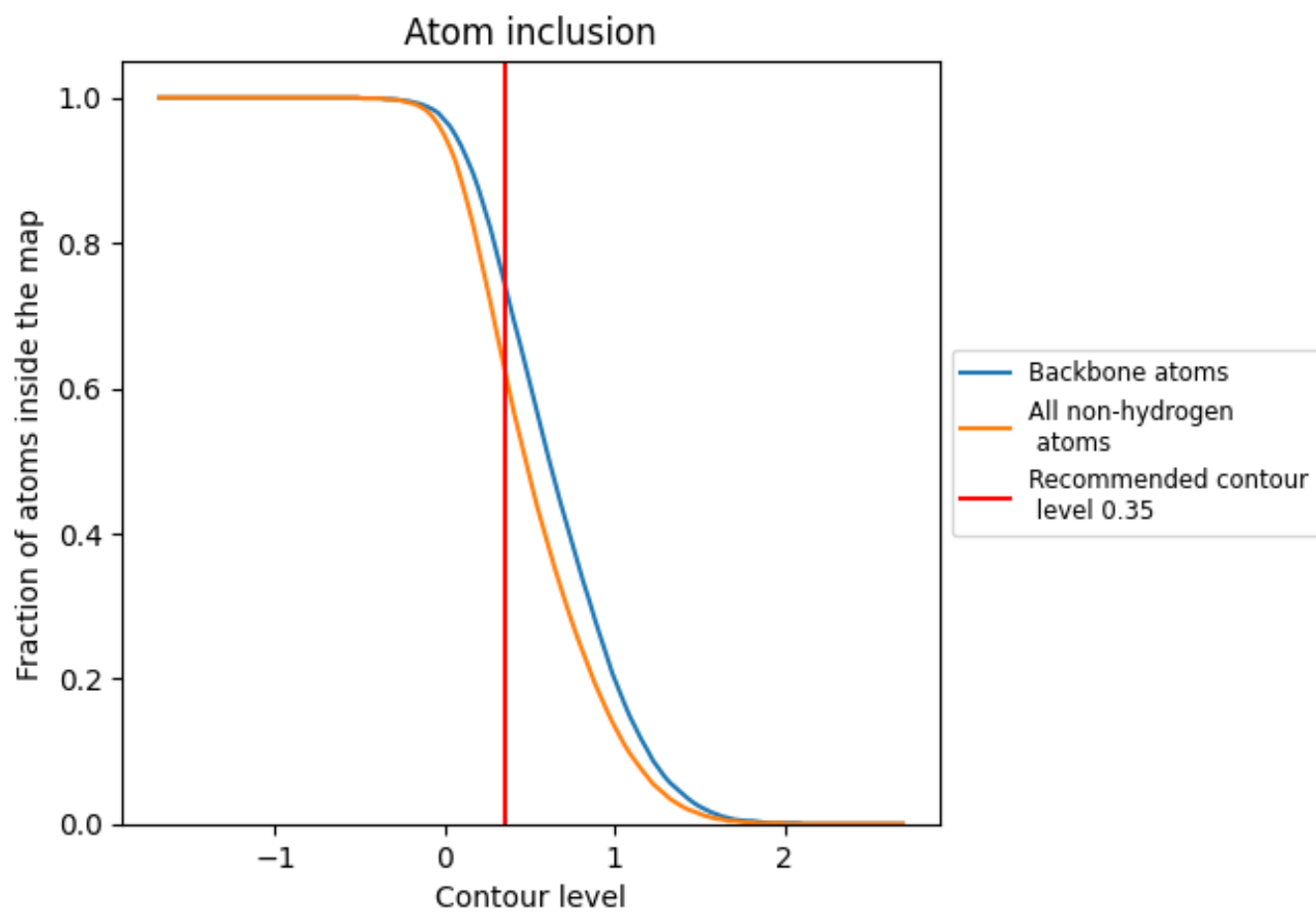


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.









9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6270	 0.3720
A	 0.6200	 0.3680
B	 0.6170	 0.3660
C	 0.6440	 0.3820

