



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 01:01 AM EST

PDB ID : 6VXK
EMDB ID : EMD-21442
Title : Cryo-EM Structure of the full-length A39R/PlexinC1 complex
Authors : Kuo, Y.-C.; Chen, H.; Shang, G.; Uchikawa, E.; Tian, H.; Bai, X.; Zhang, X.
Deposited on : 2020-02-22
Resolution : 3.10 Å(reported)
Based on initial model : 3NVN

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

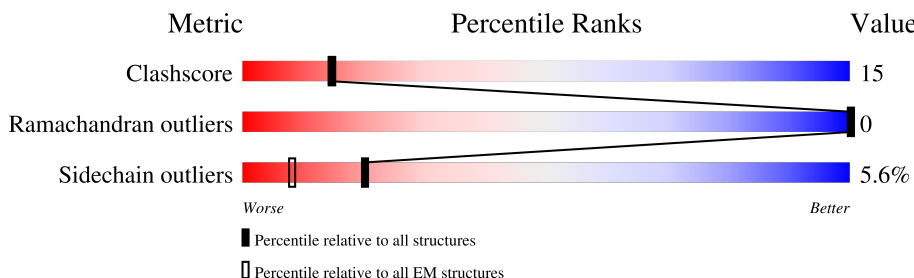
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	398	
1	C	398	
2	B	1545	
2	D	1545	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17418 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 Semaphorin-like protein 139.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			3022	1926	500	585	11		
1	C	380	Total	C	N	O	S	0	0
			3022	1926	500	585	11		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLU	-	expression tag	UNP Q8JL80
A	13	LEU	-	expression tag	UNP Q8JL80
A	14	GLU	-	expression tag	UNP Q8JL80
A	400	GLY	-	expression tag	UNP Q8JL80
A	401	THR	-	expression tag	UNP Q8JL80
A	402	HIS	-	expression tag	UNP Q8JL80
A	403	HIS	-	expression tag	UNP Q8JL80
A	404	HIS	-	expression tag	UNP Q8JL80
A	405	HIS	-	expression tag	UNP Q8JL80
A	406	HIS	-	expression tag	UNP Q8JL80
A	407	HIS	-	expression tag	UNP Q8JL80
A	408	HIS	-	expression tag	UNP Q8JL80
A	409	HIS	-	expression tag	UNP Q8JL80
C	12	GLU	-	expression tag	UNP Q8JL80
C	13	LEU	-	expression tag	UNP Q8JL80
C	14	GLU	-	expression tag	UNP Q8JL80
C	400	GLY	-	expression tag	UNP Q8JL80
C	401	THR	-	expression tag	UNP Q8JL80
C	402	HIS	-	expression tag	UNP Q8JL80
C	403	HIS	-	expression tag	UNP Q8JL80
C	404	HIS	-	expression tag	UNP Q8JL80
C	405	HIS	-	expression tag	UNP Q8JL80
C	406	HIS	-	expression tag	UNP Q8JL80
C	407	HIS	-	expression tag	UNP Q8JL80
C	408	HIS	-	expression tag	UNP Q8JL80
C	409	HIS	-	expression tag	UNP Q8JL80

- Molecule 2 is a protein called Plexin-C1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	747	Total	C	N	O	S	0	0
			5561	3496	971	1056	38		
2	D	747	Total	C	N	O	S	0	0
			5561	3496	971	1056	38		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1569	GLY	-	expression tag	UNP O60486
B	1570	THR	-	expression tag	UNP O60486
B	1571	SER	-	expression tag	UNP O60486
B	1572	SER	-	expression tag	UNP O60486
B	1573	GLY	-	expression tag	UNP O60486
B	1574	LEU	-	expression tag	UNP O60486
B	1575	GLU	-	expression tag	UNP O60486
B	1576	VAL	-	expression tag	UNP O60486
B	1577	LEU	-	expression tag	UNP O60486
B	1578	PHE	-	expression tag	UNP O60486
B	1579	GLN	-	expression tag	UNP O60486
D	1569	GLY	-	expression tag	UNP O60486
D	1570	THR	-	expression tag	UNP O60486
D	1571	SER	-	expression tag	UNP O60486
D	1572	SER	-	expression tag	UNP O60486
D	1573	GLY	-	expression tag	UNP O60486
D	1574	LEU	-	expression tag	UNP O60486
D	1575	GLU	-	expression tag	UNP O60486
D	1576	VAL	-	expression tag	UNP O60486
D	1577	LEU	-	expression tag	UNP O60486
D	1578	PHE	-	expression tag	UNP O60486
D	1579	GLN	-	expression tag	UNP O60486

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

Continued from previous page...

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



LYS	GLN	ASP	ARG	PHE	ARG	THR
LEU	LEU	ASP	LEU	ASP	SER	SER
LEU	LEU	LEU	PRO	ILE	ILE	ASP
HIS	PRO	PRO	LYS	LYS	TRP	GLU
VAL	LEU	LEU	THR	THR	LEU	TVR
LYS	SER	SER	PRO	PRO	PRO	SER
VAL	ASP	HIS	HIS	HIS	ASN	ASP
LEU	LEU	SER	ILE	SER	ASP	ASP
PHE	GLU	GLU	ASP	ASP	ARG	HIS
GLU	MET	GLY	ALA	GLY	CYS	CYS
ASP	GLU	LEU	CYS	LEU	PHE	HIS
LYS	GLU	GLU	LEU	LEU	LEU	LEU
LYS	LYS	PHE	SER	SER	ALA	ILE
LYS	LEU	LEU	VAL	VAL	ILE	LEU
CYS	THR	ILE	ILE	ILE	LYS	PRO
LYS	GLN	ALA	ALA	ALA	TVR	ASP
TRP	GLU	GLN	GLN	PHE	PHE	SER
MET	SER	PHE	ALA	ASP	PHE	GLU
GLY	LYS	ALA	MET	PHE	ASP	ALA
THR	THR	ASP	HIS	ASP	LEU	GLN
SER	SER	GLU	GLU	ALA	ASP	ASP
SER	ASN	ASN	ASN	PHE	ALA	VAL
GLY	LEU	GLU	GLU	SER	GLN	GLN
LEU	GLU	PHE	LEU	THR	ALA	GLY
GLU	VAL	ASN	ASN	THR	GLU	LYS
LEU	LEU	GLU	GLU	GLU	ASN	ARG
PHE	PHE	GLU	GLN	GLN	LYS	HIS
GLN	GLN	VAL	VAL	GLN	LYS	ARG
	ALA	LEU	LEU	GLY	ILE	GLY
	LEU	LEU	GLY	LYS	THR	LYS
	THR	TYR	THR	LYS	ASP	HIS
	GLU	ILE	ALA	ALA	PRO	LYS
	ILE	VAL	VAL	LEU	ASP	PHE
	LYS	LYS	LYS	LEU	VAL	LYS
	TYR	PHE	TYR	TYR	THR	TVR
	ASP	GLU	ASP	ALA	THR	LEU
	ILE	ILE	ILE	LYS	ASN	THR
	ASN	LEU	PRO	LEU	LEU	LYS
	THR	THR	TYR	THR	ARG	SER
	LYS	LYS	TYR	PHE	THR	THR
	LEU	LEU	GLY	TRP	VAL	LYS
	GLU	ARG	GLU	VAL	ALA	ILE
	GLU	GLU	VAL	VAL	ILE	HIS
	ARG	GLY	VAL	LYS	LEU	SER
	GLY	GLY	ARG	LYS	LEU	THR
	LEU	TYR	SER	THR	LYS	VAL
	LEU	LEU	LEU	ASN	ASN	LEU
	GLU	GLU	GLU	TYR	PRO	GLY
	GLU	GLU	GLU	LYS	GLN	LYS
	GLN	GLN	VAL	ILE	PHE	LEU
	THR	THR	THR	THR	VAL	PHE

- Molecule 2: Plexin-C1

Chain D:



L881	PHE	P811	W731	GLU	PHE	LYS	S422	ALA
L882	HIS	S812	D732	ASN	THR	THR	T423	ASP
L883	GLY	L733	LYS	LYS	ASN	TE20	P424	E37
L884	GLU	C734	GLY	GLY	CYS	V521	W425	
L885	SER	W735	ASN	ASN	SER	T522	P186	S42
L886	ASN	SER	ARG	ARG	LEU	H523	E43	Q44
L887	LYS	LYS	THR	THR	LEU	V524	T324	
L888	GLY	VAL	S743	ASN	LYS	LYS	T325	P188
L889	ARG	ARG	GLN	GLN	GLU	F527	T326	C194
L890	ALA	ALA	ALA	CYS	CYS	LYS	L328	S52
L891	LYS	L659	W750	PRO	PRO	ASN	C329	G56
L892	THR	T751	I751	ALA	ALA	LYS	T210	S61
L893	ILE	W822	A752	CYS	CYS	H531	P331	G62
L894	ARG	T823	L753	VAL	VAL	S532	T442	
L895	ASN	K824	F662	GLU	GLU	K533	K333	Y80
L896	ASN	K825	W754	THR	THR	V536	E446	C87
L897	GLN	L826	H755	GLY	GLY	K537	V447	T88
L898	ASP	C756	S757	CYS	CYS	ASN	R448	
L899	LEU	F760	K671	ALA	ALA	VAL	V452	V91
L900	THR	W611	V672	TRP	TRP	ASP	T349	A97
L901	THR	T611	L675	CYS	CYS	SER	A350	P99
L902	THR	T612	G676	LYS	LYS	SER	C455	R100
L903	THR	T613	K677	CYS	CYS	SER	W456	
L904	THR	T614	S678	ALA	ALA	ARG	K457	S104
L905	THR	W765	G678	ARG	ARG	E544	S352	T105
L906	THR	L766	N679	GLY	GLY	THR	H458	L110
L907	THR	S767	T683	CYS	CYS	THR	C461	P111
L908	THR	G768	G684	ILE	ILE	THR	L376	Y112
L909	THR	I772	F687	HIS	HIS	THR	L372	R113
L910	THR	T688	W688	PRO	PRO	ASN	P470	A117
L911	THR	G776	R683	PHE	PHE	ARG	W474	T125
L912	ALA	R777	A690	THR	THR	THR	C475	G126
L913	ASN	N778	S691	CYS	CYS	C556	C381	C134
L914	SER	W779	I693	ASP	ASP	T557	V384	R137
L915	SER	VAL	D780	THR	THR	C558	L478	L142
L916	GLU	GLU	W781	PRO	PRO	SER	Q479	N149
L917	GLU	GLU	L782	SER	SER	ILE	R480	V153
L918	VAL	VAL	D783	ASP	ASP	PRO	C481	S155
L919	ASP	ASP	W784	GLU	GLU	THR	T482	Q159
L920	ASP	ASP	L785	ARG	ARG	ALA	F483	V166
L921	THR	THR	L786	ASN	ASN	ALA	C487	R168
L922	THR	THR	W787	GLN	GLN	THR	D396	N172
L923	THR	THR	S701	GLU	GLU	LYS	V488	
L924	THR	THR	T702	GLU	GLU	LYS	L400	
L925	THR	THR	C703	CYS	CYS	ASP	K401	
L926	THR	THR	W707	VAL	VAL	VAL	V402	
L927	THR	THR	I708	VAL	VAL	SER	E491	
L928	THR	THR	Q709	ALA	ALA	VAL	N492	
L929	THR	THR	W710	VAL	VAL	VAL	L404	
L930	THR	THR	W719	GLU	GLU	VAL	G405	
L931	THR	THR	K720	LYS	LYS	VAL	E406	
L932	THR	THR	F721	THR	THR	THR	P507	
L933	THR	THR	S726	SER	SER	THR	L408	
L934	THR	THR	R727	GLY	GLY	THR	Q510	
L935	THR	THR	T728	GLY	GLY	THR	I511	
L936	THR	THR	E729	GLY	GLY	THR	ILE	
L937	THR	THR	K806	ARG	ARG	SER	P413	
L938	THR	THR	D876	PRO	PRO	SER	ARG	
L939	THR	THR	L877	LYS	LYS	SER	S911	
L940	THR	THR	E878	PHE	PHE	LYS	V415	
L941	THR	THR		THR	THR	GLY	E421	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	143750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	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

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	0.67	0/3093	0.53	0/4195
1	C	0.67	0/3093	0.53	0/4195
2	B	0.52	0/5663	0.52	1/7689 (0.0%)
2	D	0.52	0/5663	0.52	1/7689 (0.0%)
All	All	0.58	0/17512	0.53	2/23768 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	806	CYS	CA-CB-SG	6.76	126.17	114.00
2	B	806	CYS	CA-CB-SG	6.74	126.13	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	0	2956	88	0
1	C	3022	0	2956	86	0
2	B	5561	0	5301	167	0
2	D	5561	0	5301	174	0
3	A	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	112	0	104	4	0
3	C	14	0	13	0	0
3	D	112	0	104	4	0
All	All	17418	0	16748	511	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 15.

All (511) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:507:PRO:HA	2:D:524:VAL:O	1.45	1.14
2:B:507:PRO:HA	2:B:524:VAL:O	1.45	1.12
2:D:536:VAL:O	2:D:544:GLU:HA	1.62	0.99
2:B:536:VAL:O	2:B:544:GLU:HA	1.62	0.99
2:B:783:ASP:H	2:B:828:VAL:HG12	1.43	0.82
2:D:783:ASP:H	2:D:828:VAL:HG12	1.43	0.82
2:B:402:VAL:HG12	2:B:413:PRO:HB3	1.71	0.73
2:D:402:VAL:HG12	2:D:413:PRO:HB3	1.71	0.72
2:B:446:GLU:OE1	2:B:448:ARG:NH2	2.23	0.71
2:D:510:GLN:O	2:D:521:VAL:HA	1.91	0.71
2:B:510:GLN:O	2:B:521:VAL:HA	1.90	0.71
1:C:36:LEU:HB3	1:C:47:PHE:HB3	1.73	0.71
1:A:345:ILE:HD11	1:A:369:LEU:HD22	1.73	0.70
2:B:430:VAL:HG23	2:B:440:TYR:HB2	1.73	0.70
1:C:345:ILE:HD11	1:C:369:LEU:HD22	1.73	0.70
2:D:430:VAL:HG23	2:D:440:TYR:HB2	1.73	0.70
1:C:44:VAL:HG21	1:C:75:VAL:HG11	1.74	0.69
1:C:331:LYS:HB2	1:C:374:VAL:HG11	1.73	0.69
2:D:446:GLU:OE1	2:D:448:ARG:NH2	2.23	0.69
1:A:36:LEU:HB3	1:A:47:PHE:HB3	1.73	0.69
1:A:331:LYS:HB2	1:A:374:VAL:HG11	1.73	0.69
1:A:44:VAL:HG21	1:A:75:VAL:HG11	1.74	0.67
2:B:98:ARG:NH1	2:B:395:GLY:O	2.28	0.67
1:A:216:GLU:HB2	1:A:310:ILE:HD11	1.77	0.66
2:B:44:GLN:HE21	2:B:88:THR:HA	1.59	0.66
2:D:827:ARG:HH21	2:D:830:ASP:H	1.43	0.66
1:C:216:GLU:HB2	1:C:310:ILE:HD11	1.77	0.66
2:B:311:SER:HB2	2:B:326:THR:HG22	1.78	0.66
2:D:98:ARG:NH1	2:D:395:GLY:O	2.28	0.66
1:A:73:THR:O	1:A:73:THR:OG1	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:GLN:HE21	2:D:88:THR:HA	1.59	0.65
1:A:214:GLU:OE2	1:C:181:ARG:NH2	2.27	0.65
1:C:60:ASN:HD22	1:C:80:ASN:HB2	1.61	0.65
2:D:311:SER:HB2	2:D:326:THR:HG22	1.78	0.65
2:B:827:ARG:HH21	2:B:830:ASP:H	1.43	0.65
2:D:784:ASN:HD21	2:D:827:ARG:HH11	1.45	0.65
1:A:60:ASN:HD22	1:A:80:ASN:HB2	1.60	0.65
2:D:700:THR:HG22	2:D:702:THR:H	1.62	0.65
2:B:784:ASN:HD21	2:B:827:ARG:HH11	1.45	0.64
1:A:283:PRO:HB3	1:A:301:ILE:HD13	1.79	0.64
2:D:175:TRP:O	2:D:210:THR:OG1	2.12	0.64
1:A:369:LEU:HD23	1:A:382:ALA:HB2	1.79	0.64
1:C:369:LEU:HD23	1:C:382:ALA:HB2	1.79	0.64
2:B:700:THR:HG22	2:B:702:THR:H	1.63	0.64
1:C:283:PRO:HB3	1:C:301:ILE:HD13	1.79	0.64
1:C:127:GLU:HB3	2:D:350:ALA:HB1	1.80	0.64
1:A:116:GLU:HB2	1:A:138:PRO:HG2	1.79	0.63
2:D:766:ILE:N	2:D:841:ARG:O	2.25	0.63
1:C:116:GLU:HB2	1:C:138:PRO:HG2	1.79	0.63
2:B:205:ILE:HD12	2:B:223:LEU:HD23	1.80	0.63
1:C:48:SER:O	1:C:51:GLU:HB2	1.98	0.63
1:A:24:GLU:OE2	1:A:45:TYR:OH	2.16	0.63
2:D:726:SER:OG	2:D:727:ARG:N	2.32	0.63
1:A:48:SER:O	1:A:51:GLU:HB2	1.98	0.62
1:A:181:ARG:HD2	1:C:225:ARG:NH2	2.14	0.62
2:B:766:ILE:N	2:B:841:ARG:O	2.25	0.62
1:A:333:LYS:HE3	1:A:341:ARG:HH21	1.64	0.62
2:D:780:ASP:N	2:D:780:ASP:OD1	2.30	0.62
2:B:726:SER:OG	2:B:727:ARG:N	2.32	0.62
2:B:780:ASP:OD1	2:B:780:ASP:N	2.30	0.62
1:C:333:LYS:HE3	1:C:341:ARG:HH21	1.64	0.62
1:C:24:GLU:OE2	1:C:45:TYR:OH	2.16	0.62
1:C:236:ASP:OD2	1:C:338:ARG:NH2	2.32	0.62
2:D:104:SER:OG	2:D:105:PHE:N	2.32	0.61
2:D:205:ILE:HD12	2:D:223:LEU:HD23	1.80	0.61
2:D:442:THR:HG23	2:D:447:VAL:HG22	1.82	0.61
2:B:442:THR:HG23	2:B:447:VAL:HG22	1.82	0.61
1:C:247:SER:OG	1:C:251:LYS:O	2.18	0.61
1:A:236:ASP:OD2	1:A:338:ARG:NH2	2.32	0.61
2:D:227:GLU:OE1	2:D:227:GLU:N	2.33	0.61
2:B:475:CYS:O	2:B:479:GLN:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:HIS:ND1	2:D:324:THR:O	2.34	0.61
1:A:247:SER:OG	1:A:251:LYS:O	2.18	0.61
2:D:660:GLN:NE2	2:D:689:ARG:O	2.34	0.60
2:D:889:LEU:HA	2:D:909:ILE:HG12	1.83	0.60
2:B:660:GLN:NE2	2:B:689:ARG:O	2.34	0.60
2:D:324:THR:O	2:D:324:THR:OG1	2.19	0.60
2:B:104:SER:OG	2:B:105:PHE:N	2.32	0.60
2:B:175:TRP:O	2:B:210:THR:OG1	2.12	0.60
1:C:70:VAL:HG23	1:C:71:GLU:H	1.67	0.60
2:D:475:CYS:O	2:D:479:GLN:N	2.34	0.60
1:A:246:ASP:OD1	1:A:247:SER:N	2.34	0.60
1:C:246:ASP:OD1	1:C:247:SER:N	2.34	0.60
2:B:287:HIS:ND1	2:B:324:THR:O	2.34	0.60
1:C:73:THR:O	1:C:73:THR:OG1	2.14	0.59
2:D:789:HIS:O	2:D:793:GLY:N	2.36	0.59
2:B:889:LEU:HA	2:B:909:ILE:HG12	1.83	0.59
2:D:42:SER:OG	2:D:43:GLU:N	2.35	0.59
1:A:70:VAL:HG23	1:A:71:GLU:H	1.67	0.59
2:B:42:SER:OG	2:B:43:GLU:N	2.35	0.58
1:A:225:ARG:NH2	1:C:181:ARG:HD2	2.19	0.58
2:B:789:HIS:O	2:B:793:GLY:N	2.36	0.58
2:D:700:THR:OG1	2:D:729:GLU:OE2	2.16	0.58
1:A:309:ASP:OD1	1:A:310:ILE:N	2.35	0.58
2:B:227:GLU:OE1	2:B:227:GLU:N	2.33	0.58
1:A:60:ASN:OD1	1:A:60:ASN:N	2.38	0.57
2:B:324:THR:O	2:B:324:THR:OG1	2.19	0.57
1:C:309:ASP:OD1	1:C:310:ILE:N	2.35	0.57
2:B:172:ASN:OD1	2:B:172:ASN:N	2.36	0.57
2:D:172:ASN:OD1	2:D:172:ASN:N	2.36	0.57
1:A:266:PHE:HA	1:A:307:LEU:HD11	1.87	0.57
1:C:220:ASP:OD1	1:C:222:ARG:NH2	2.38	0.57
2:D:44:GLN:N	2:D:44:GLN:OE1	2.38	0.57
2:B:784:ASN:ND2	2:B:827:ARG:HH11	2.02	0.57
1:A:127:GLU:HB3	2:B:350:ALA:HB1	1.87	0.56
1:A:220:ASP:OD1	1:A:222:ARG:NH2	2.38	0.56
2:B:44:GLN:N	2:B:44:GLN:OE1	2.38	0.56
2:D:696:ILE:HB	2:D:734:CYS:SG	2.46	0.56
2:B:730:MET:HA	2:B:749:SER:HA	1.87	0.56
1:C:333:LYS:NZ	1:C:354:ASP:OD2	2.26	0.56
2:B:696:ILE:HB	2:B:734:CYS:SG	2.46	0.56
1:C:132:TRP:NE1	1:C:191:MET:SD	2.78	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:784:ASN:ND2	2:D:827:ARG:HH11	2.02	0.56
1:A:132:TRP:NE1	1:A:191:MET:SD	2.78	0.56
1:C:266:PHE:HA	1:C:307:LEU:HD11	1.87	0.55
2:B:326:THR:HG21	2:B:376:LEU:H	1.71	0.55
2:D:326:THR:HG21	2:D:376:LEU:H	1.71	0.55
2:B:766:ILE:HA	2:B:840:TYR:HB3	1.88	0.55
2:D:421:GLU:N	2:D:421:GLU:OE1	2.40	0.55
2:B:784:ASN:HD21	2:B:827:ARG:HD3	1.72	0.55
2:D:300:VAL:HG22	2:D:381:GLY:HA3	1.89	0.55
2:D:783:ASP:HB2	2:D:828:VAL:HA	1.89	0.55
2:D:785:LEU:HD11	2:D:824:VAL:HB	1.89	0.55
1:C:46:THR:OG1	1:C:53:ASN:O	2.24	0.55
2:D:730:MET:HA	2:D:749:SER:HA	1.88	0.55
2:B:783:ASP:HB2	2:B:828:VAL:HA	1.89	0.55
1:C:60:ASN:OD1	1:C:60:ASN:N	2.37	0.55
2:B:421:GLU:OE1	2:B:421:GLU:N	2.40	0.55
2:B:786:ILE:HG13	2:B:832:TYR:HE1	1.72	0.55
1:C:44:VAL:HG22	1:C:64:ILE:HG21	1.89	0.54
1:C:375:THR:OG1	1:C:376:SER:N	2.41	0.54
2:D:784:ASN:HD21	2:D:827:ARG:HD3	1.72	0.54
1:A:222:ARG:NH1	1:A:320:GLU:OE1	2.41	0.54
2:B:110:LEU:HD11	2:B:166:VAL:HG13	1.90	0.54
2:D:766:ILE:HA	2:D:840:TYR:HB3	1.88	0.54
2:D:786:ILE:HG13	2:D:832:TYR:HE1	1.72	0.54
2:B:660:GLN:OE1	2:B:660:GLN:N	2.39	0.54
2:D:52:SER:OG	2:D:56:GLY:O	2.25	0.54
2:D:110:LEU:HD11	2:D:166:VAL:HG13	1.90	0.54
2:D:820:THR:N	2:D:840:TYR:O	2.41	0.54
2:D:827:ARG:HA	2:D:831:THR:O	2.08	0.54
1:C:45:TYR:CE2	1:C:54:LYS:HB2	2.43	0.53
2:D:660:GLN:OE1	2:D:660:GLN:N	2.40	0.53
2:B:785:LEU:HD11	2:B:824:VAL:HB	1.89	0.53
2:D:403:ILE:HD13	2:D:470:PRO:HD3	1.90	0.53
2:B:300:VAL:HG22	2:B:381:GLY:HA3	1.89	0.53
2:B:573:ASN:HA	2:B:586:ARG:HA	1.90	0.53
2:D:573:ASN:HA	2:D:586:ARG:HA	1.90	0.53
1:C:222:ARG:NH1	1:C:320:GLU:OE1	2.41	0.53
1:A:44:VAL:HG22	1:A:64:ILE:HG21	1.89	0.53
2:B:403:ILE:HD13	2:B:470:PRO:HD3	1.90	0.53
1:A:375:THR:OG1	1:A:376:SER:N	2.41	0.53
2:B:820:THR:N	2:B:840:TYR:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD23	1:A:291:LYS:HB3	1.91	0.53
1:C:228:ILE:HD11	1:C:246:ASP:HB2	1.90	0.53
2:B:785:LEU:HD12	2:B:786:ILE:H	1.74	0.53
2:D:785:LEU:HD12	2:D:786:ILE:H	1.74	0.53
1:A:45:TYR:CE2	1:A:54:LYS:HB2	2.43	0.53
2:B:52:SER:OG	2:B:56:GLY:O	2.25	0.53
2:B:782:ILE:HD11	2:B:826:LEU:HD13	1.91	0.53
3:B:1608:NAG:H83	3:B:1608:NAG:H3	1.91	0.53
2:D:98:ARG:HH11	2:D:424:PRO:HB3	1.74	0.53
2:D:782:ILE:HD11	2:D:826:LEU:HD13	1.91	0.53
1:C:220:ASP:HB2	1:C:222:ARG:HE	1.73	0.52
2:B:492:ASN:OD1	2:B:492:ASN:N	2.42	0.52
2:B:536:VAL:O	2:B:544:GLU:CA	2.48	0.52
2:D:390:LEU:HB2	2:D:402:VAL:HG22	1.91	0.52
1:C:287:LEU:HD23	1:C:291:LYS:HB3	1.91	0.52
2:B:827:ARG:HA	2:B:831:THR:O	2.08	0.52
1:A:46:THR:OG1	1:A:53:ASN:O	2.24	0.52
1:A:220:ASP:HB2	1:A:222:ARG:HE	1.73	0.52
2:D:678:SER:OG	2:D:679:ASN:OD1	2.25	0.52
3:D:1604:NAG:O7	3:D:1604:NAG:O3	2.25	0.52
3:D:1608:NAG:H83	3:D:1608:NAG:H3	1.91	0.52
2:B:44:GLN:NE2	2:B:87:CYS:O	2.43	0.52
2:B:765:TRP:HZ3	2:B:930:GLY:HA3	1.75	0.52
2:D:44:GLN:NE2	2:D:87:CYS:O	2.43	0.52
2:D:675:LEU:HD12	2:D:753:LEU:HD21	1.92	0.52
2:D:824:VAL:HG23	2:D:835:CYS:HB2	1.92	0.52
1:A:228:ILE:HD11	1:A:246:ASP:HB2	1.90	0.52
2:B:870:PHE:HB2	2:B:872:ILE:HD11	1.92	0.52
2:D:492:ASN:OD1	2:D:492:ASN:N	2.42	0.52
2:D:870:PHE:HB2	2:D:872:ILE:HD11	1.92	0.52
2:B:98:ARG:HH11	2:B:424:PRO:HB3	1.74	0.52
2:B:268:ALA:HB3	2:B:274:LEU:HB3	1.91	0.51
2:D:761:PRO:HG2	2:D:772:ILE:HD13	1.92	0.51
1:A:27:ILE:HD13	1:A:63:TYR:HB3	1.92	0.51
2:B:824:VAL:HG23	2:B:835:CYS:HB2	1.92	0.51
1:C:19:LYS:HA	1:C:385:GLY:HA3	1.93	0.51
1:C:27:ILE:HD13	1:C:63:TYR:HB3	1.92	0.51
2:B:344:SER:HB2	2:B:349:THR:OG1	2.11	0.51
2:B:761:PRO:HG2	2:B:772:ILE:HD13	1.92	0.51
2:D:268:ALA:HB3	2:D:274:LEU:HB3	1.91	0.51
1:A:298:PHE:HA	1:A:301:ILE:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:700:THR:OG1	2:B:729:GLU:OE2	2.16	0.51
2:B:580:SER:HG	2:B:581:TRP:HD1	1.57	0.51
2:B:675:LEU:HD12	2:B:753:LEU:HD21	1.92	0.51
1:C:16:GLU:OE1	1:C:18:HIS:NE2	2.43	0.51
2:B:390:LEU:HB2	2:B:402:VAL:HG22	1.91	0.51
2:D:765:TRP:HZ3	2:D:930:GLY:HA3	1.75	0.51
2:D:872:ILE:HD12	2:D:872:ILE:H	1.75	0.51
2:B:694:THR:HG22	2:B:709:GLN:HE22	1.76	0.50
2:B:872:ILE:HD12	2:B:872:ILE:H	1.75	0.50
1:C:349:THR:OG1	1:C:364:GLN:OE1	2.29	0.50
1:A:16:GLU:OE1	1:A:18:HIS:NE2	2.43	0.50
2:D:344:SER:HB2	2:D:349:THR:OG1	2.11	0.50
1:C:79:ASN:OD1	1:C:84:LYS:HB3	2.11	0.50
1:C:298:PHE:HA	1:C:301:ILE:HG22	1.93	0.50
1:A:72:ASP:HB2	1:A:87:LYS:HD2	1.93	0.50
1:A:79:ASN:OD1	1:A:84:LYS:HB3	2.11	0.50
1:A:349:THR:OG1	1:A:364:GLN:OE1	2.29	0.50
1:C:72:ASP:HB2	1:C:87:LYS:HD2	1.93	0.50
1:A:19:LYS:HA	1:A:385:GLY:HA3	1.93	0.50
2:B:820:THR:O	2:B:840:TYR:N	2.41	0.50
2:D:91:VAL:HG22	2:D:105:PHE:HZ	1.77	0.50
2:D:871:ASN:HB3	3:D:1608:NAG:O5	2.11	0.50
2:B:802:VAL:HG22	2:B:803:ALA:H	1.77	0.49
1:C:236:ASP:OD1	1:C:236:ASP:N	2.43	0.49
2:D:755:HIS:CE1	2:D:777:ARG:HB2	2.47	0.49
2:D:802:VAL:HG22	2:D:803:ALA:H	1.77	0.49
2:B:678:SER:OG	2:B:679:ASN:OD1	2.25	0.49
2:D:694:THR:HG22	2:D:709:GLN:HE22	1.76	0.49
2:D:407:ASN:OD1	2:D:407:ASN:N	2.36	0.49
2:D:580:SER:HG	2:D:581:TRP:HD1	1.59	0.49
2:B:532:SER:OG	2:B:533:LYS:N	2.46	0.49
2:D:879:ILE:HA	2:D:926:ARG:O	2.12	0.49
1:A:218:ASP:OD1	1:A:218:ASP:N	2.45	0.49
2:B:871:ASN:HB3	3:B:1608:NAG:O5	2.11	0.49
2:B:764:THR:O	2:B:840:TYR:HA	2.13	0.49
1:C:224:TYR:OH	1:C:320:GLU:OE2	2.20	0.49
2:B:879:ILE:HA	2:B:926:ARG:O	2.12	0.49
1:A:60:ASN:ND2	1:A:80:ASN:HB2	2.28	0.49
2:B:755:HIS:CE1	2:B:777:ARG:HB2	2.47	0.48
2:D:764:THR:O	2:D:840:TYR:HA	2.13	0.48
1:A:236:ASP:N	1:A:236:ASP:OD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ASP:N	1:C:218:ASP:OD1	2.45	0.48
1:C:372:VAL:HG22	1:C:380:PHE:HD1	1.78	0.48
2:D:532:SER:OG	2:D:533:LYS:N	2.46	0.48
2:D:679:ASN:HB3	2:D:720:LYS:HE2	1.94	0.48
2:D:697:LEU:HA	2:D:732:ASP:O	2.13	0.48
2:B:697:LEU:HA	2:B:732:ASP:O	2.13	0.48
2:D:457:LYS:HE3	2:D:458:HIS:CE1	2.49	0.48
1:A:372:VAL:HG22	1:A:380:PHE:HD1	1.78	0.48
2:B:407:ASN:OD1	2:B:407:ASN:N	2.36	0.48
2:B:679:ASN:HB3	2:B:720:LYS:HE2	1.94	0.48
1:C:33:ASP:N	1:C:33:ASP:OD2	2.47	0.48
1:A:264:HIS:CE1	1:A:268:THR:HG21	2.49	0.48
2:B:874:LYS:HG2	2:B:889:LEU:HD22	1.96	0.48
1:C:264:HIS:CE1	1:C:268:THR:HG21	2.49	0.48
2:D:660:GLN:HE21	2:D:689:ARG:HB3	1.78	0.48
2:D:761:PRO:HD2	2:D:772:ILE:HG23	1.94	0.48
1:A:201:SER:OG	2:B:215:LEU:O	2.17	0.48
2:B:91:VAL:HG22	2:B:105:PHE:HZ	1.77	0.48
1:C:201:SER:OG	2:D:215:LEU:O	2.22	0.48
1:A:181:ARG:NH2	1:C:214:GLU:OE2	2.38	0.48
2:B:457:LYS:HE3	2:B:458:HIS:CE1	2.49	0.47
1:C:26:ILE:HD13	1:C:40:VAL:HG23	1.96	0.47
1:C:60:ASN:ND2	1:C:80:ASN:HB2	2.28	0.47
1:C:280:SER:OG	1:C:281:PRO:HD3	2.14	0.47
1:A:168:LYS:HE2	1:A:286:CYS:SG	2.55	0.47
1:A:280:SER:OG	1:A:281:PRO:HD3	2.14	0.47
2:B:761:PRO:HD2	2:B:772:ILE:HG23	1.94	0.47
3:B:1604:NAG:O7	3:B:1604:NAG:O3	2.25	0.47
2:D:536:VAL:O	2:D:544:GLU:CA	2.48	0.47
2:D:874:LYS:HG2	2:D:889:LEU:HD22	1.96	0.47
1:A:216:GLU:HG3	1:A:218:ASP:OD1	2.15	0.47
1:A:235:THR:OG1	1:A:238:ASP:O	2.20	0.47
2:B:765:TRP:O	2:B:768:GLY:N	2.45	0.47
1:C:68:ILE:HG21	1:C:111:ILE:HG12	1.96	0.47
1:A:26:ILE:HD13	1:A:40:VAL:HG23	1.96	0.47
1:A:37:TYR:CE1	1:A:46:THR:HG22	2.50	0.47
2:B:324:THR:HB	2:B:372:ILE:HG21	1.97	0.47
2:B:676:GLY:O	2:B:829:GLN:HG3	2.15	0.47
2:B:660:GLN:HE21	2:B:689:ARG:HB3	1.78	0.47
2:B:536:VAL:HG12	2:B:574:VAL:HG13	1.96	0.47
1:C:37:TYR:CE1	1:C:46:THR:HG22	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LYS:HE2	1:C:286:CYS:SG	2.55	0.47
2:D:671:LYS:NZ	2:D:780:ASP:OD2	2.48	0.47
2:D:676:GLY:O	2:D:829:GLN:HG3	2.15	0.47
2:D:765:TRP:O	2:D:768:GLY:N	2.45	0.47
2:B:99:PRO:HG2	2:B:314:ALA:HB3	1.97	0.47
2:B:580:SER:OG	2:B:581:TRP:HD1	1.98	0.47
2:B:671:LYS:NZ	2:B:780:ASP:OD2	2.48	0.47
2:B:98:ARG:NH2	2:B:318:GLN:OE1	2.46	0.47
2:B:475:CYS:O	2:B:479:GLN:CA	2.63	0.46
2:D:99:PRO:HG2	2:D:314:ALA:HB3	1.97	0.46
2:D:426:PHE:HB3	2:D:442:THR:HB	1.97	0.46
2:D:580:SER:OG	2:D:581:TRP:HD1	1.98	0.46
1:C:216:GLU:HG3	1:C:218:ASP:OD1	2.15	0.46
2:B:841:ARG:HB2	2:B:870:PHE:CZ	2.51	0.46
2:D:475:CYS:O	2:D:479:GLN:CA	2.63	0.46
2:D:841:ARG:HB2	2:D:870:PHE:CZ	2.51	0.46
1:A:33:ASP:OD2	1:A:33:ASP:N	2.47	0.46
2:B:108:LEU:HD23	2:B:108:LEU:HA	1.66	0.46
1:A:68:ILE:HG21	1:A:111:ILE:HG12	1.96	0.46
2:D:324:THR:HB	2:D:372:ILE:HG21	1.97	0.46
2:D:153:VAL:HG21	2:D:215:LEU:HD12	1.98	0.46
2:D:536:VAL:HG12	2:D:574:VAL:HG13	1.96	0.46
2:B:426:PHE:HB3	2:B:442:THR:HB	1.97	0.46
1:C:40:VAL:HG12	1:C:43:ALA:O	2.16	0.46
1:A:40:VAL:HG12	1:A:43:ALA:O	2.16	0.46
2:B:787:ILE:HG22	2:B:822:VAL:HG21	1.98	0.46
1:C:15:ILE:HA	1:C:388:VAL:O	2.16	0.45
2:D:751:ILE:HD13	2:D:751:ILE:HA	1.85	0.45
2:B:236:ASP:OD1	2:B:237:ALA:N	2.47	0.45
2:B:248:TYR:OH	2:B:278:GLN:NE2	2.49	0.45
2:D:446:GLU:HB2	2:D:448:ARG:HH21	1.82	0.45
1:C:349:THR:HG23	1:C:363:ALA:O	2.17	0.45
2:D:827:ARG:NH2	2:D:830:ASP:H	2.13	0.45
1:A:15:ILE:HA	1:A:388:VAL:O	2.16	0.45
2:B:287:HIS:CG	2:B:288:PRO:HD2	2.52	0.45
1:C:372:VAL:HG22	1:C:380:PHE:CD1	2.52	0.45
2:D:797:VAL:HB	2:D:811:PRO:HG3	1.98	0.45
2:B:665:LYS:N	2:B:683:THR:O	2.50	0.45
2:B:850:ARG:HA	2:B:859:LEU:HA	1.99	0.45
1:C:216:GLU:O	1:C:313:PRO:HD3	2.17	0.45
2:B:153:VAL:HG21	2:B:215:LEU:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:SER:HB2	2:B:306:TRP:HZ2	1.82	0.45
2:D:406:GLU:HG2	2:D:407:ASN:N	2.32	0.45
2:D:820:THR:O	2:D:840:TYR:N	2.41	0.45
2:B:754:PRO:HB3	2:B:778:ASN:O	2.17	0.45
2:B:769:GLY:N	2:B:810:ALA:O	2.43	0.45
2:D:98:ARG:NH2	2:D:318:GLN:OE1	2.46	0.45
2:D:248:TYR:OH	2:D:278:GLN:NE2	2.49	0.45
2:D:297:SER:HB2	2:D:306:TRP:HZ2	1.82	0.45
1:A:188:ILE:HG22	1:A:213:VAL:HG23	1.99	0.45
1:A:216:GLU:O	1:A:313:PRO:HD3	2.17	0.45
2:B:446:GLU:HB2	2:B:448:ARG:HH21	1.82	0.45
2:D:850:ARG:HA	2:D:859:LEU:HA	1.99	0.45
2:D:874:LYS:HZ1	2:D:888:GLN:N	2.15	0.45
2:B:797:VAL:HB	2:B:811:PRO:HG3	1.98	0.44
1:A:239:THR:O	1:A:259:MET:HB2	2.17	0.44
2:B:406:GLU:HG2	2:B:407:ASN:N	2.32	0.44
1:C:179:THR:OG1	1:C:180:LYS:N	2.50	0.44
2:D:287:HIS:CG	2:D:288:PRO:HD2	2.52	0.44
2:D:754:PRO:HB3	2:D:778:ASN:O	2.17	0.44
2:B:735:ILE:O	2:B:743:SER:OG	2.31	0.44
1:A:349:THR:HG23	1:A:363:ALA:O	2.17	0.44
2:D:665:LYS:N	2:D:683:THR:O	2.50	0.44
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.66	0.44
1:A:372:VAL:HG22	1:A:380:PHE:CD1	2.52	0.44
2:B:225:LEU:HD11	2:B:232:LEU:HD22	1.99	0.44
2:B:874:LYS:HZ1	2:B:888:GLN:N	2.15	0.44
2:D:80:TYR:CD2	2:D:87:CYS:HB3	2.53	0.44
2:D:787:ILE:HG22	2:D:822:VAL:HG21	1.98	0.44
1:C:76:CYS:HA	1:C:85:CYS:HA	1.99	0.44
2:D:405:GLY:N	2:D:409:THR:O	2.41	0.44
2:D:735:ILE:O	2:D:743:SER:OG	2.31	0.44
2:B:482:THR:OG1	2:B:483:PHE:N	2.51	0.44
2:D:351:GLU:OE2	2:D:352:SER:OG	2.29	0.44
2:B:168:ARG:HD3	2:B:175:TRP:CZ2	2.53	0.44
2:B:874:LYS:HE2	2:B:874:LYS:HB3	1.74	0.44
1:C:239:THR:O	1:C:259:MET:HB2	2.17	0.44
2:D:225:LEU:HD11	2:D:232:LEU:HD22	1.99	0.44
1:C:188:ILE:HG22	1:C:213:VAL:HG23	1.99	0.43
2:D:827:ARG:O	2:D:827:ARG:HG3	2.18	0.43
2:D:187:GLU:N	2:D:188:PRO:HD3	2.33	0.43
2:B:187:GLU:N	2:B:188:PRO:HD3	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:482:THR:OG1	2:D:483:PHE:N	2.51	0.43
2:B:691:SER:OG	2:B:692:ASN:N	2.51	0.43
2:B:723:LEU:HA	2:B:724:PRO:HD3	1.89	0.43
2:D:176:TYR:CZ	2:D:271:THR:HG23	2.53	0.43
2:D:734:CYS:HB2	2:D:742:CYS:HB3	1.47	0.43
2:B:185:LEU:HA	2:B:185:LEU:HD23	1.67	0.43
1:A:19:LYS:HB3	1:A:19:LYS:HE2	1.80	0.43
2:B:80:TYR:CD2	2:B:87:CYS:HB3	2.53	0.43
2:B:176:TYR:CZ	2:B:271:THR:HG23	2.53	0.43
2:B:752:ALA:HB3	2:B:778:ASN:ND2	2.33	0.43
2:D:168:ARG:HD3	2:D:175:TRP:CZ2	2.53	0.43
2:D:248:TYR:CZ	2:D:263:SER:HB2	2.54	0.43
1:A:179:THR:OG1	1:A:180:LYS:N	2.50	0.43
2:D:687:PHE:CD2	2:D:719:MET:HG2	2.54	0.43
2:D:694:THR:HG22	2:D:709:GLN:NE2	2.34	0.43
2:B:254:THR:OG1	2:B:255:SER:N	2.52	0.43
2:B:248:TYR:CZ	2:B:263:SER:HB2	2.54	0.43
2:B:757:SER:OG	2:B:776:GLY:HA2	2.19	0.43
2:D:304:ASP:OD1	2:D:304:ASP:N	2.51	0.43
2:D:691:SER:OG	2:D:692:ASN:N	2.51	0.43
2:D:752:ALA:HB3	2:D:778:ASN:ND2	2.33	0.43
1:A:76:CYS:HA	1:A:85:CYS:HA	1.99	0.42
1:A:171:ILE:HG13	1:A:189:ALA:HB3	2.01	0.42
1:A:298:PHE:CE2	1:A:302:GLU:HG3	2.54	0.42
2:D:61:SER:OG	2:D:62:GLY:N	2.52	0.42
2:D:874:LYS:HE2	2:D:874:LYS:HB3	1.74	0.42
1:A:127:GLU:HG3	1:A:128:GLY:H	1.84	0.42
2:D:306:TRP:HB2	2:D:333:MET:SD	2.60	0.42
2:B:304:ASP:OD1	2:B:304:ASP:N	2.51	0.42
2:B:400:LEU:HB3	2:B:415:VAL:HA	2.01	0.42
2:D:231:SER:HG	2:D:253:TYR:HD2	1.65	0.42
2:D:254:THR:OG1	2:D:255:SER:N	2.52	0.42
2:D:328:LEU:HD22	2:D:392:LEU:HD21	2.02	0.42
2:D:786:ILE:HG13	2:D:832:TYR:CE1	2.53	0.42
1:A:67:SER:HB3	1:A:75:VAL:HG22	2.01	0.42
2:B:728:LYS:HE3	2:B:752:ALA:HB2	2.01	0.42
2:B:827:ARG:HG3	2:B:827:ARG:O	2.18	0.42
2:D:396:ASP:OD1	2:D:396:ASP:N	2.53	0.42
2:D:659:LEU:HD23	2:D:659:LEU:HA	1.88	0.42
2:B:126:GLY:HA2	2:B:134:CYS:HA	2.01	0.42
2:B:461:CYS:O	2:B:464:CYS:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:THR:HG22	2:B:709:GLN:NE2	2.34	0.42
1:C:31:LEU:HD11	1:C:375:THR:HG22	2.02	0.42
1:C:171:ILE:HG13	1:C:189:ALA:HB3	2.01	0.42
2:D:126:GLY:HA2	2:D:134:CYS:HA	2.01	0.42
2:D:665:LYS:H	2:D:684:GLY:HA2	1.85	0.42
2:D:690:ALA:HB3	2:D:693:ILE:HD11	2.02	0.42
2:B:753:LEU:HD23	2:B:753:LEU:HA	1.80	0.42
1:C:127:GLU:HG3	1:C:128:GLY:H	1.84	0.42
1:C:336:GLU:OE1	1:C:356:LYS:HD2	2.19	0.42
2:D:478:LEU:HG	2:D:480:ARG:HB2	2.01	0.42
2:D:757:SER:OG	2:D:776:GLY:HA2	2.19	0.42
1:A:68:ILE:HD13	1:A:111:ILE:HD11	2.02	0.42
1:A:152:LYS:HA	1:A:152:LYS:HD3	1.88	0.42
1:A:336:GLU:OE1	1:A:356:LYS:HD2	2.19	0.42
2:B:306:TRP:HB2	2:B:333:MET:SD	2.60	0.42
2:B:396:ASP:OD1	2:B:396:ASP:N	2.53	0.42
2:D:185:LEU:HA	2:D:185:LEU:HD23	1.67	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.79	0.42
1:A:100:GLY:HA3	1:A:135:PHE:CZ	2.55	0.42
2:B:61:SER:OG	2:B:62:GLY:N	2.52	0.42
2:D:236:ASP:OD1	2:D:237:ALA:N	2.47	0.42
2:D:384:VAL:HG13	2:D:470:PRO:HB2	2.00	0.42
2:B:328:LEU:HD22	2:B:392:LEU:HD21	2.02	0.42
2:B:687:PHE:CD2	2:B:719:MET:HG2	2.54	0.42
1:C:189:ALA:HA	1:C:211:LEU:O	2.19	0.42
1:C:298:PHE:CE2	1:C:302:GLU:HG3	2.54	0.42
2:D:227:GLU:H	2:D:227:GLU:CD	2.22	0.42
2:D:728:LYS:HE3	2:D:752:ALA:HB2	2.01	0.42
1:A:189:ALA:HA	1:A:211:LEU:O	2.19	0.42
2:B:384:VAL:HG13	2:B:470:PRO:HB2	2.00	0.42
1:A:37:TYR:CD1	1:A:46:THR:HG22	2.54	0.41
2:B:326:THR:HB	2:B:376:LEU:HB2	2.03	0.41
2:B:432:ASP:HA	2:B:433:PRO:HD3	1.90	0.41
2:B:478:LEU:HG	2:B:480:ARG:HB2	2.02	0.41
2:B:825:LYS:HE3	2:B:825:LYS:HB2	1.82	0.41
1:C:37:TYR:CD1	1:C:46:THR:HG22	2.54	0.41
2:D:825:LYS:HB2	2:D:825:LYS:HE3	1.82	0.41
2:B:97:ALA:HB3	2:B:100:ARG:HD2	2.01	0.41
2:B:339:ARG:NH1	2:B:362:ARG:O	2.53	0.41
1:C:67:SER:HB3	1:C:75:VAL:HG22	2.01	0.41
2:D:248:TYR:CE1	2:D:263:SER:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:339:ARG:NH1	2:D:362:ARG:O	2.53	0.41
2:D:400:LEU:HB3	2:D:415:VAL:HA	2.01	0.41
2:D:475:CYS:O	2:D:479:GLN:HA	2.20	0.41
2:D:662:PHE:HZ	2:D:689:ARG:O	2.04	0.41
2:B:475:CYS:O	2:B:479:GLN:HA	2.20	0.41
1:C:68:ILE:HD13	1:C:111:ILE:HD11	2.02	0.41
2:D:474:TRP:NE1	2:D:479:GLN:OE1	2.52	0.41
1:A:162:LYS:HE3	1:A:162:LYS:HB3	1.86	0.41
1:A:191:MET:HE2	1:A:210:PHE:CD2	2.56	0.41
2:D:142:LEU:HD23	2:D:142:LEU:HA	1.78	0.41
2:D:461:CYS:O	2:D:464:CYS:N	2.51	0.41
2:D:769:GLY:N	2:D:810:ALA:O	2.43	0.41
2:B:166:VAL:HA	2:B:176:TYR:O	2.21	0.41
2:B:710:VAL:HG22	2:B:721:PHE:CZ	2.55	0.41
1:A:31:LEU:HD11	1:A:375:THR:HG22	2.02	0.41
2:B:672:VAL:HG23	2:B:677:LYS:HB2	2.03	0.41
1:C:100:GLY:HA3	1:C:135:PHE:CZ	2.55	0.41
2:D:97:ALA:HB3	2:D:100:ARG:HD2	2.01	0.41
1:A:211:LEU:HG	1:A:301:ILE:HD11	2.03	0.41
1:A:287:LEU:HB3	1:A:291:LYS:HB2	2.03	0.41
2:B:159:GLN:OE1	2:B:159:GLN:N	2.48	0.41
2:B:662:PHE:HZ	2:B:689:ARG:O	2.04	0.41
2:B:690:ALA:HB3	2:B:693:ILE:HD11	2.02	0.41
2:B:764:THR:HG22	2:B:765:TRP:N	2.36	0.41
2:D:149:ASN:O	2:D:214:SER:HA	2.21	0.41
1:A:301:ILE:HD12	1:A:301:ILE:HA	1.80	0.41
2:B:406:GLU:HG2	2:B:407:ASN:H	1.85	0.41
2:D:166:VAL:HA	2:D:176:TYR:O	2.21	0.41
2:D:329:CYS:HB3	2:D:331:PHE:CE1	2.56	0.41
2:D:406:GLU:HG2	2:D:407:ASN:H	1.85	0.41
2:D:710:VAL:HG22	2:D:721:PHE:CZ	2.55	0.41
1:A:222:ARG:H	1:A:222:ARG:HG2	1.66	0.41
2:B:248:TYR:CE1	2:B:263:SER:HB2	2.55	0.41
2:B:255:SER:OG	3:B:1604:NAG:N2	2.54	0.41
2:B:329:CYS:HB3	2:B:331:PHE:CE1	2.56	0.41
2:B:734:CYS:HB2	2:B:742:CYS:HB3	1.47	0.41
2:B:751:ILE:HD13	2:B:751:ILE:HA	1.85	0.41
2:B:878:GLU:O	2:B:927:VAL:HA	2.21	0.41
1:C:87:LYS:HA	1:C:87:LYS:HD3	1.66	0.41
1:C:200:SER:O	1:C:204:SER:HB2	2.21	0.41
2:D:159:GLN:OE1	2:D:159:GLN:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:432:ASP:HA	2:D:433:PRO:HD3	1.90	0.41
2:D:878:GLU:O	2:D:927:VAL:HA	2.21	0.41
1:A:200:SER:O	1:A:204:SER:HB2	2.21	0.41
2:B:185:LEU:O	2:B:187:GLU:N	2.50	0.41
2:B:728:LYS:H	2:B:728:LYS:HG3	1.74	0.41
1:C:222:ARG:H	1:C:222:ARG:HG2	1.66	0.41
2:B:172:ASN:HD21	2:B:174:ARG:HE	1.69	0.40
1:C:211:LEU:HG	1:C:301:ILE:HD11	2.03	0.40
2:D:726:SER:HB3	2:D:750:TYR:CE2	2.56	0.40
2:D:779:PHE:HD1	2:D:779:PHE:HA	1.74	0.40
2:D:875:LYS:HE2	2:D:875:LYS:HB2	1.86	0.40
2:B:149:ASN:OD1	2:B:150:GLY:N	2.49	0.40
1:C:251:LYS:N	1:C:323:SER:HB3	2.37	0.40
2:D:326:THR:HB	2:D:376:LEU:HB2	2.02	0.40
2:B:665:LYS:H	2:B:684:GLY:HA2	1.85	0.40
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.79	0.40
1:C:61:ASN:ND2	1:C:80:ASN:HD22	2.18	0.40
1:C:162:LYS:NZ	1:C:165:THR:O	2.52	0.40
2:D:110:LEU:HA	2:D:111:PRO:HD3	1.86	0.40
2:B:413:PRO:HD2	2:B:703:CYS:SG	2.62	0.40
1:C:192:CYS:N	1:C:209:THR:OG1	2.45	0.40
1:C:287:LEU:HB3	1:C:291:LYS:HB2	2.03	0.40
2:D:391:PHE:CZ	2:D:452:VAL:HB	2.57	0.40
2:D:672:VAL:HG23	2:D:677:LYS:HB2	2.03	0.40
1:A:224:TYR:OH	1:A:320:GLU:OE2	2.20	0.40
1:A:272:GLY:HA2	1:A:308:ASP:HB2	2.03	0.40
2:B:498:ASP:OD1	2:B:500:SER:N	2.53	0.40
2:D:255:SER:OG	3:D:1604:NAG:N2	2.54	0.40
2:D:413:PRO:HD2	2:D:703:CYS:SG	2.62	0.40
2:D:696:ILE:HG12	2:D:707:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/398 (95%)	341 (90%)	37 (10%)	0	100	100
1	C	378/398 (95%)	342 (90%)	36 (10%)	0	100	100
2	B	721/1545 (47%)	642 (89%)	79 (11%)	0	100	100
2	D	721/1545 (47%)	642 (89%)	79 (11%)	0	100	100
All	All	2198/3886 (57%)	1967 (90%)	231 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/358 (95%)	320 (94%)	19 (6%)	17	46
1	C	339/358 (95%)	320 (94%)	19 (6%)	17	46
2	B	587/1370 (43%)	554 (94%)	33 (6%)	17	46
2	D	587/1370 (43%)	554 (94%)	33 (6%)	17	46
All	All	1852/3456 (54%)	1748 (94%)	104 (6%)	20	46

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	52	LEU
1	A	55	THR
1	A	67	SER
1	A	71	GLU
1	A	73	THR
1	A	74	LEU
1	A	78	THR
1	A	87	LYS
1	A	165	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	213	VAL
1	A	218	ASP
1	A	230	SER
1	A	237	ASN
1	A	244	PHE
1	A	256	THR
1	A	365	VAL
1	A	375	THR
1	A	379	LEU
2	B	42	SER
2	B	113	ARG
2	B	125	THR
2	B	137	ARG
2	B	155	SER
2	B	172	ASN
2	B	194	CYS
2	B	213	ARG
2	B	255	SER
2	B	311	SER
2	B	322	SER
2	B	324	THR
2	B	351	GLU
2	B	370	THR
2	B	409	THR
2	B	423	THR
2	B	430	VAL
2	B	446	GLU
2	B	455	CYS
2	B	487	CYS
2	B	506	CYS
2	B	522	THR
2	B	527	PHE
2	B	683	THR
2	B	756	CYS
2	B	760	PHE
2	B	765	TRP
2	B	801	CYS
2	B	806	CYS
2	B	822	VAL
2	B	827	ARG
2	B	881	LEU
2	B	929	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	49	ASN
1	C	52	LEU
1	C	55	THR
1	C	67	SER
1	C	71	GLU
1	C	73	THR
1	C	74	LEU
1	C	78	THR
1	C	87	LYS
1	C	165	THR
1	C	213	VAL
1	C	218	ASP
1	C	230	SER
1	C	237	ASN
1	C	244	PHE
1	C	256	THR
1	C	365	VAL
1	C	375	THR
1	C	379	LEU
2	D	42	SER
2	D	113	ARG
2	D	125	THR
2	D	137	ARG
2	D	155	SER
2	D	172	ASN
2	D	194	CYS
2	D	213	ARG
2	D	255	SER
2	D	311	SER
2	D	322	SER
2	D	324	THR
2	D	351	GLU
2	D	370	THR
2	D	409	THR
2	D	423	THR
2	D	430	VAL
2	D	446	GLU
2	D	455	CYS
2	D	487	CYS
2	D	506	CYS
2	D	522	THR
2	D	527	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	683	THR
2	D	756	CYS
2	D	760	PHE
2	D	765	TRP
2	D	801	CYS
2	D	806	CYS
2	D	822	VAL
2	D	827	ARG
2	D	881	LEU
2	D	929	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	80	ASN
1	A	264	HIS
1	A	295	HIS
2	B	67	GLN
2	B	218	GLN
2	B	278	GLN
2	B	353	HIS
2	B	458	HIS
2	B	670	GLN
2	B	718	HIS
2	B	784	ASN
2	B	794	ASN
2	B	829	GLN
1	C	59	ASN
1	C	80	ASN
1	C	264	HIS
1	C	295	HIS
2	D	67	GLN
2	D	218	GLN
2	D	278	GLN
2	D	353	HIS
2	D	458	HIS
2	D	670	GLN
2	D	718	HIS
2	D	784	ASN
2	D	794	ASN
2	D	829	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1601	2	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	B	1602	2	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	D	1602	2	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	D	1605	2	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	B	1606	2	14,14,15	0.36	0	17,19,21	0.58	0
3	NAG	B	1603	2	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	D	1607	2	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
3	NAG	B	1608	2	14,14,15	0.33	0	17,19,21	1.31	2 (11%)
3	NAG	A	501	1	14,14,15	0.15	0	17,19,21	0.57	0
3	NAG	B	1604	2	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	D	1603	2	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	D	1604	2	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	D	1601	2	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	D	1608	2	14,14,15	0.34	0	17,19,21	1.31	2 (11%)
3	NAG	B	1607	2	14,14,15	0.31	0	17,19,21	0.77	1 (5%)
3	NAG	C	501	1	14,14,15	0.14	0	17,19,21	0.56	0
3	NAG	D	1606	2	14,14,15	0.35	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1605	2	14,14,15	0.16	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1601	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1602	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1602	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1605	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1606	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1603	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1607	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1608	2	-	6/6/23/26	0/1/1/1
3	NAG	A	501	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1604	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1603	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1604	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1601	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1608	2	-	6/6/23/26	0/1/1/1
3	NAG	B	1607	2	-	2/6/23/26	0/1/1/1
3	NAG	C	501	1	-	3/6/23/26	0/1/1/1
3	NAG	D	1606	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1605	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1608	NAG	C2-N2-C7	4.52	128.96	122.90
3	D	1608	NAG	C2-N2-C7	4.52	128.96	122.90
3	D	1607	NAG	C1-O5-C5	2.46	115.48	112.19
3	B	1607	NAG	C1-O5-C5	2.44	115.45	112.19
3	B	1608	NAG	C1-C2-N2	2.13	113.80	110.43
3	D	1608	NAG	C1-C2-N2	2.13	113.80	110.43

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C4-C5-C6-O6
3	C	501	NAG	C4-C5-C6-O6
3	B	1601	NAG	C4-C5-C6-O6
3	D	1601	NAG	C4-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	C	501	NAG	O5-C5-C6-O6
3	B	1602	NAG	C4-C5-C6-O6
3	D	1602	NAG	C4-C5-C6-O6
3	B	1601	NAG	O5-C5-C6-O6
3	D	1601	NAG	O5-C5-C6-O6
3	B	1607	NAG	O5-C5-C6-O6
3	D	1607	NAG	O5-C5-C6-O6
3	B	1608	NAG	C4-C5-C6-O6
3	D	1608	NAG	C4-C5-C6-O6
3	B	1608	NAG	O5-C5-C6-O6
3	D	1608	NAG	O5-C5-C6-O6
3	B	1602	NAG	O5-C5-C6-O6
3	D	1602	NAG	O5-C5-C6-O6
3	B	1603	NAG	C4-C5-C6-O6
3	D	1603	NAG	C4-C5-C6-O6
3	B	1607	NAG	C4-C5-C6-O6
3	D	1607	NAG	C4-C5-C6-O6
3	B	1608	NAG	C8-C7-N2-C2
3	B	1608	NAG	O7-C7-N2-C2
3	D	1608	NAG	C8-C7-N2-C2
3	D	1608	NAG	O7-C7-N2-C2
3	B	1603	NAG	O5-C5-C6-O6
3	D	1603	NAG	O5-C5-C6-O6
3	B	1605	NAG	O5-C5-C6-O6
3	D	1605	NAG	O5-C5-C6-O6
3	B	1608	NAG	C1-C2-N2-C7
3	D	1608	NAG	C1-C2-N2-C7
3	B	1604	NAG	C3-C2-N2-C7
3	B	1608	NAG	C3-C2-N2-C7
3	D	1604	NAG	C3-C2-N2-C7
3	D	1608	NAG	C3-C2-N2-C7
3	A	501	NAG	C1-C2-N2-C7
3	C	501	NAG	C1-C2-N2-C7
3	B	1604	NAG	O5-C5-C6-O6
3	D	1604	NAG	O5-C5-C6-O6
3	B	1604	NAG	C4-C5-C6-O6
3	D	1604	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1608	NAG	2	0
3	B	1604	NAG	2	0
3	D	1604	NAG	2	0
3	D	1608	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

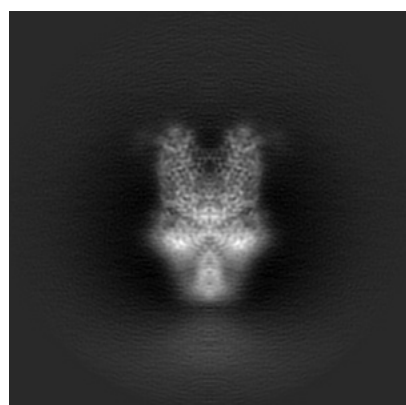
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21442. These allow visual inspection of the internal detail of the map and identification of artifacts.

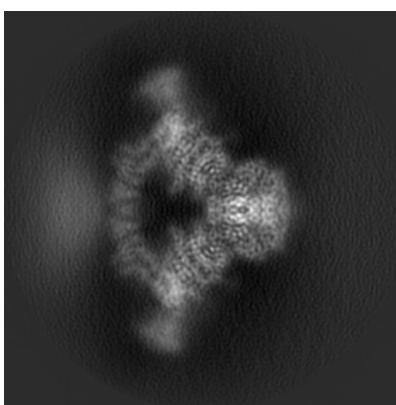
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

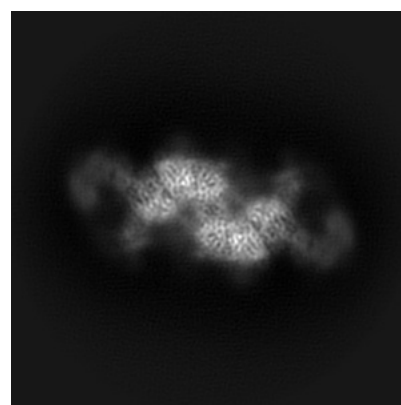
6.1.1 Primary map



X



Y

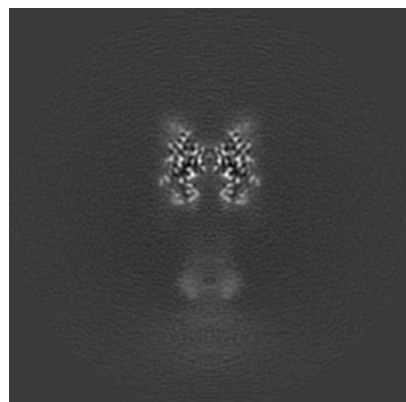


Z

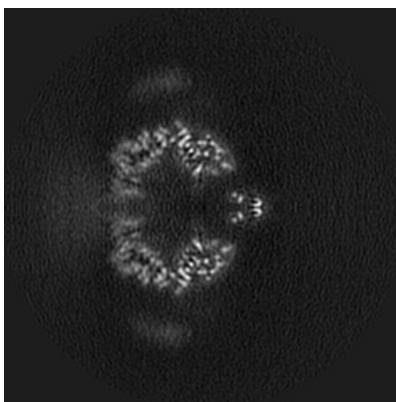
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

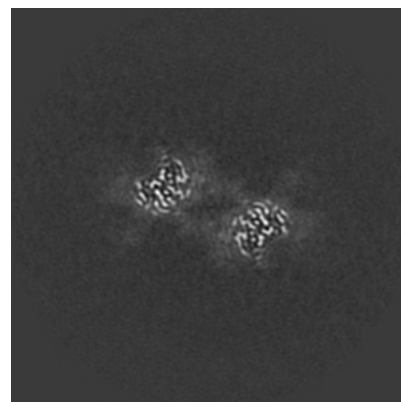
6.2.1 Primary map



X Index: 180



Y Index: 180

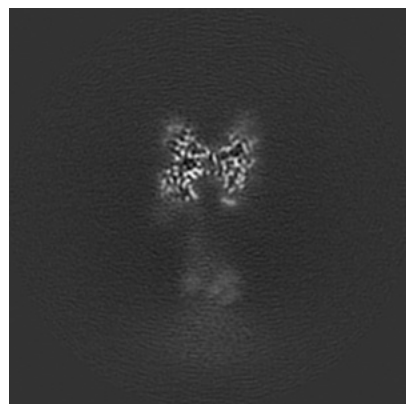


Z Index: 180

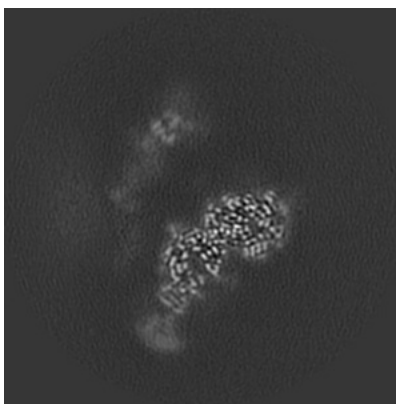
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

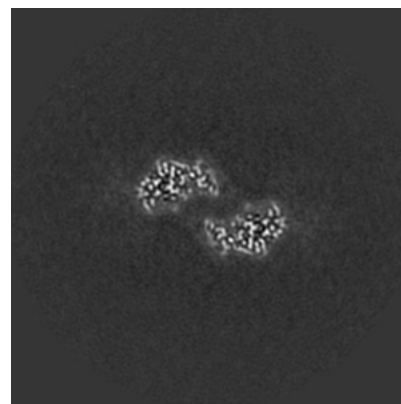
6.3.1 Primary map



X Index: 185



Y Index: 206

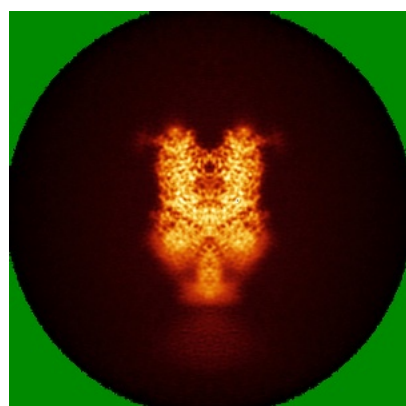


Z Index: 187

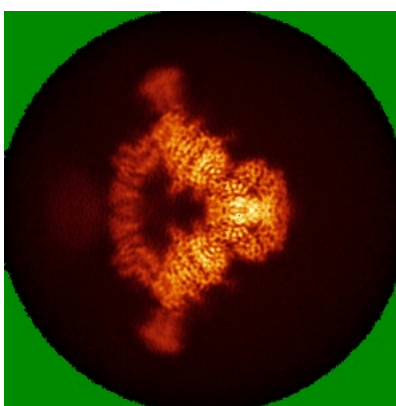
The images above show the largest variance slices of the map in three orthogonal directions.

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

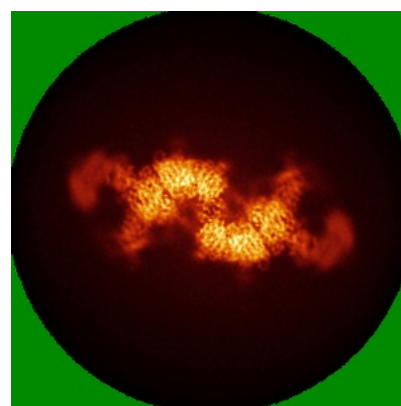
6.4.1 Primary map



X



Y

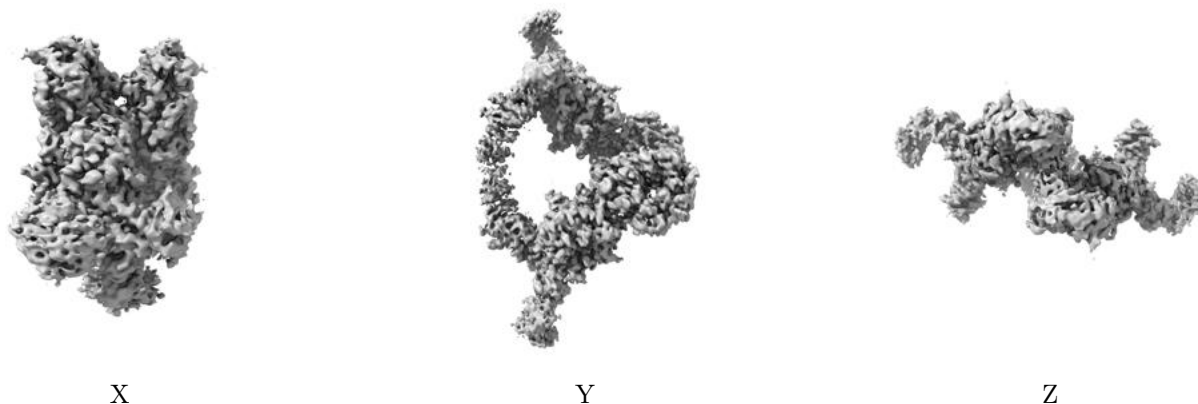


Z

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 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

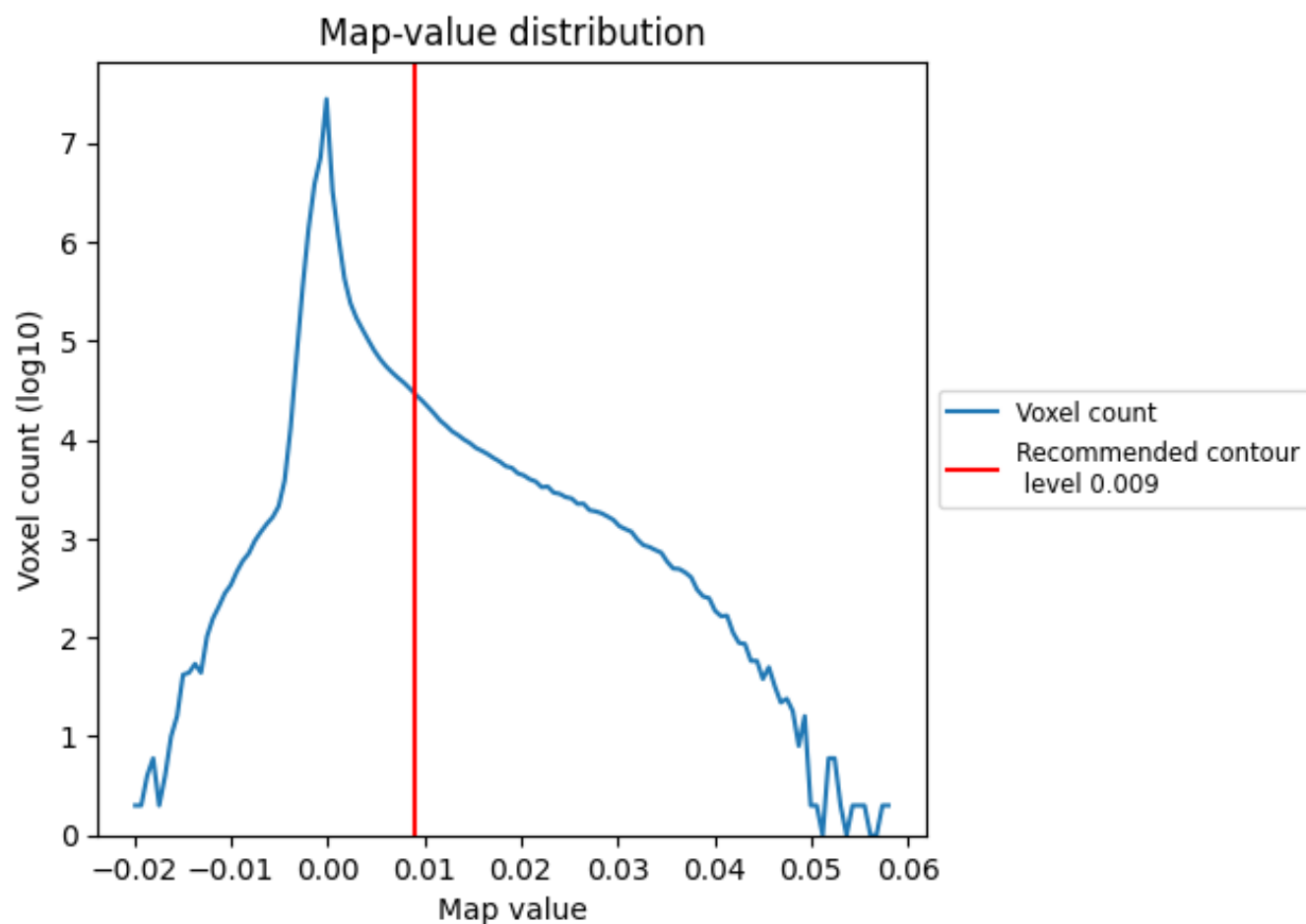
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

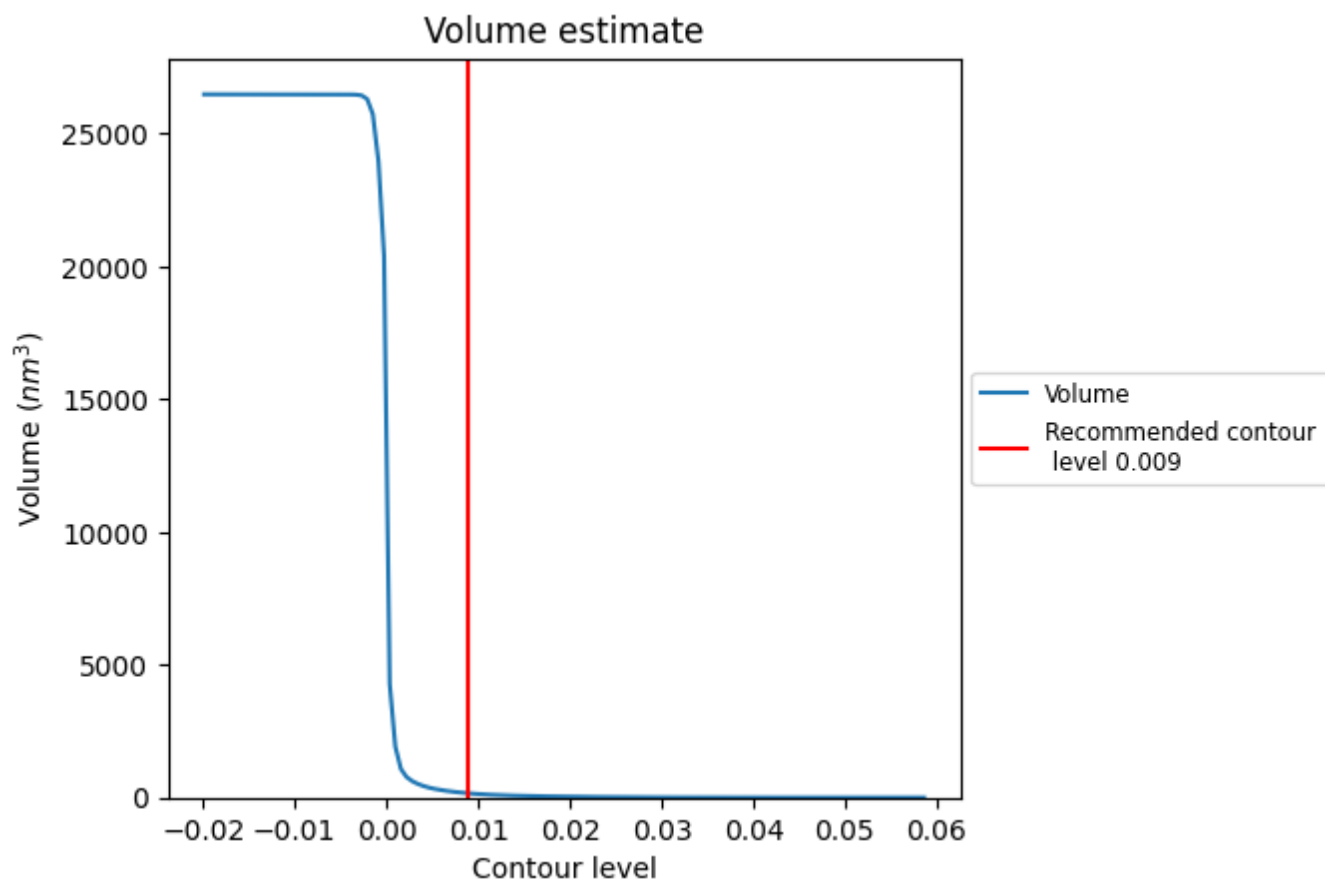
This section contains the results of statistical analysis of the map.

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.

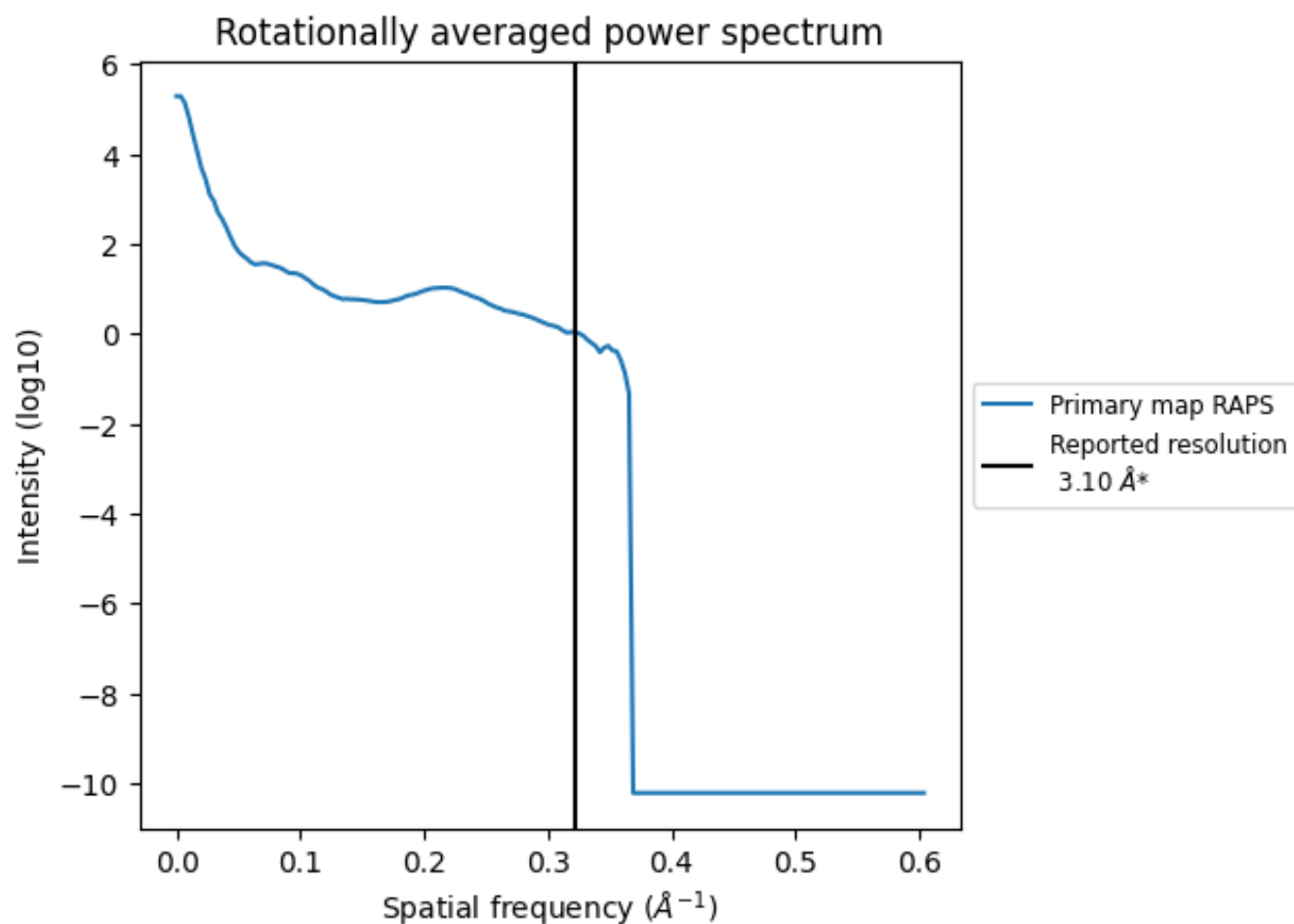
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm^3 ; this corresponds to an approximate mass of 143 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

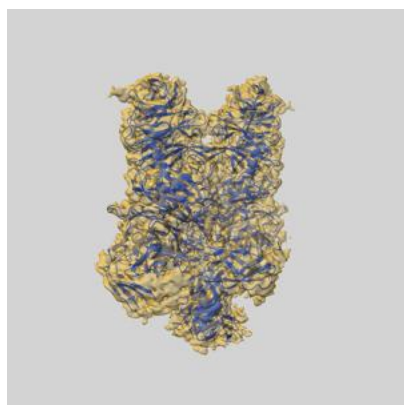
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

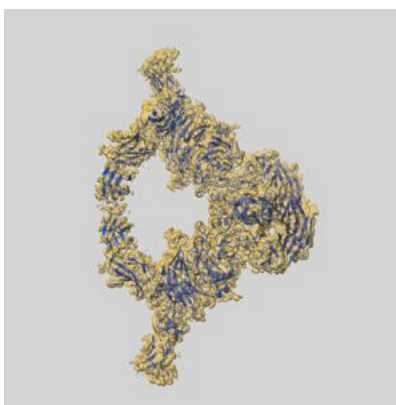
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21442 and PDB model 6VXK. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

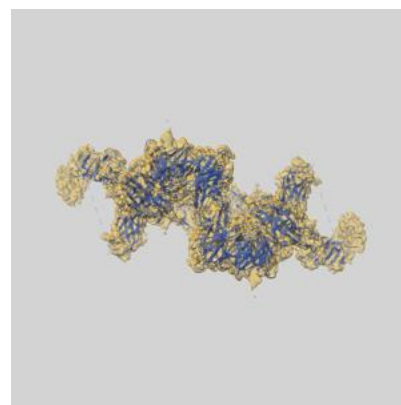
9.1 Map-model overlay [i](#)



X



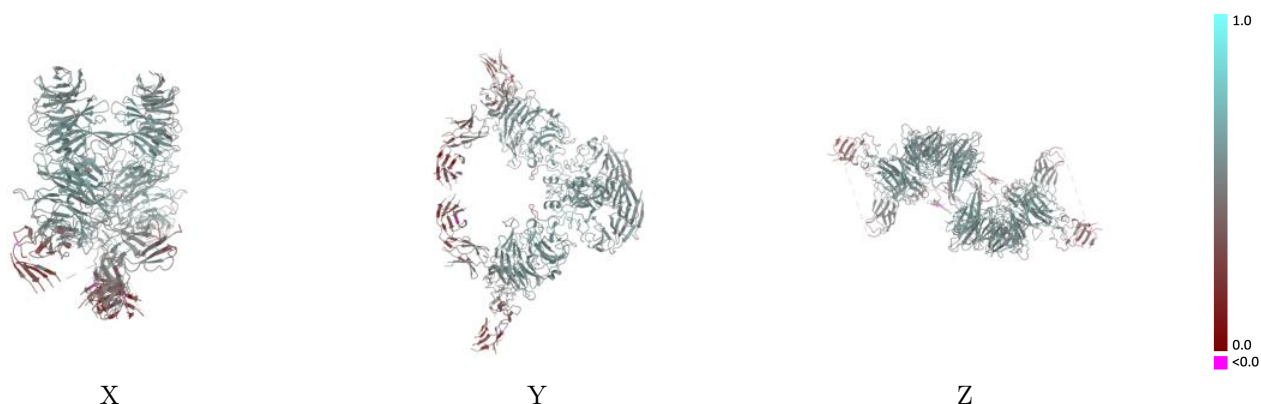
Y



Z

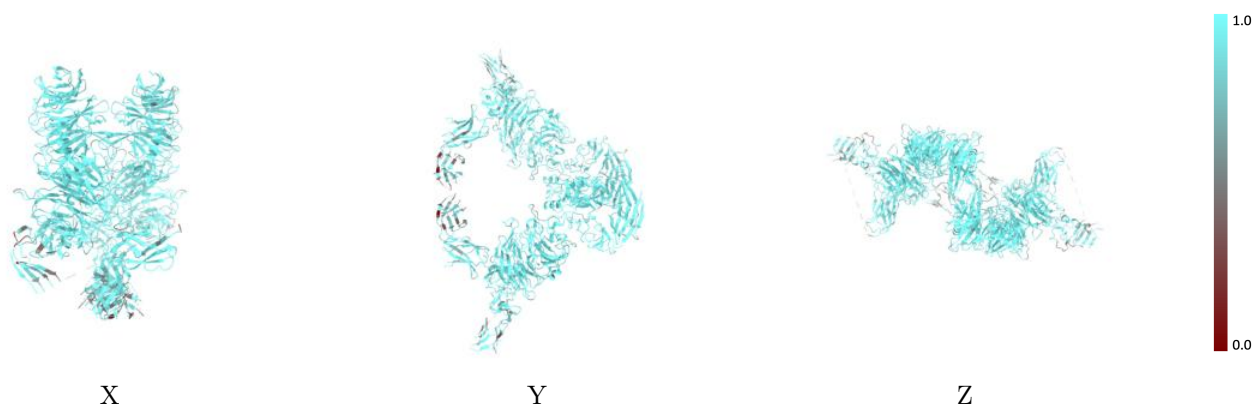
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



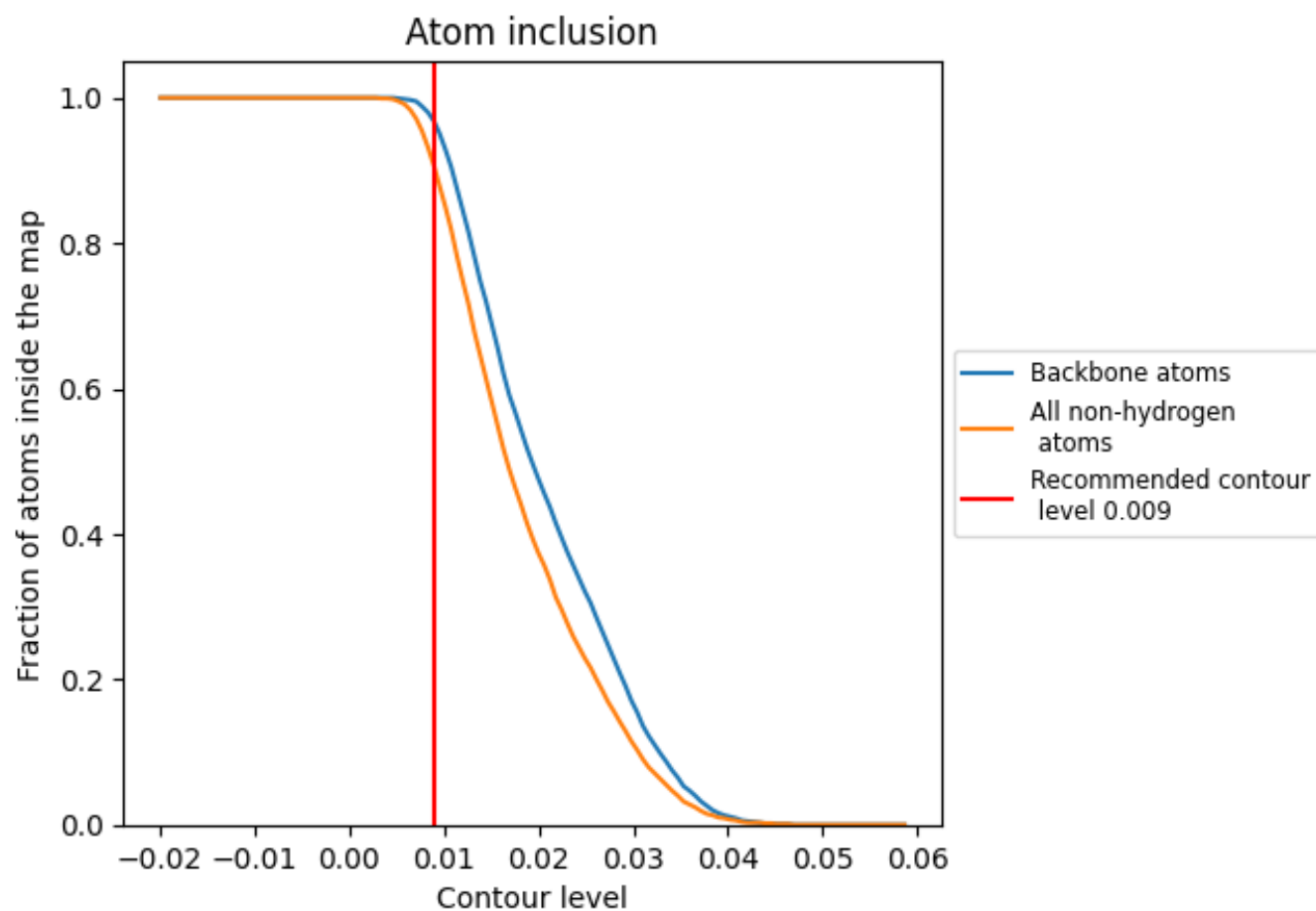
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9050	<div></div> 0.5120
A	<div></div> 0.9390	<div></div> 0.5510
B	<div></div> 0.8860	<div></div> 0.4920
C	<div></div> 0.9390	<div></div> 0.5500
D	<div></div> 0.8860	<div></div> 0.4910

