



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 03:29 PM UTC

PDB ID : 7QBA / pdb_00007qba
EMDB ID : EMD-13885
Title : CryoEM structure of the ABC transporter NosDFY complexed with nitrous oxide reductase NosZ
Authors : Zipfel, S.; Mueller, C.; Topitsch, A.; Lutz, M.; Zhang, L.; Einsle, O.
Deposited on : 2021-11-18
Resolution : 3.78 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:

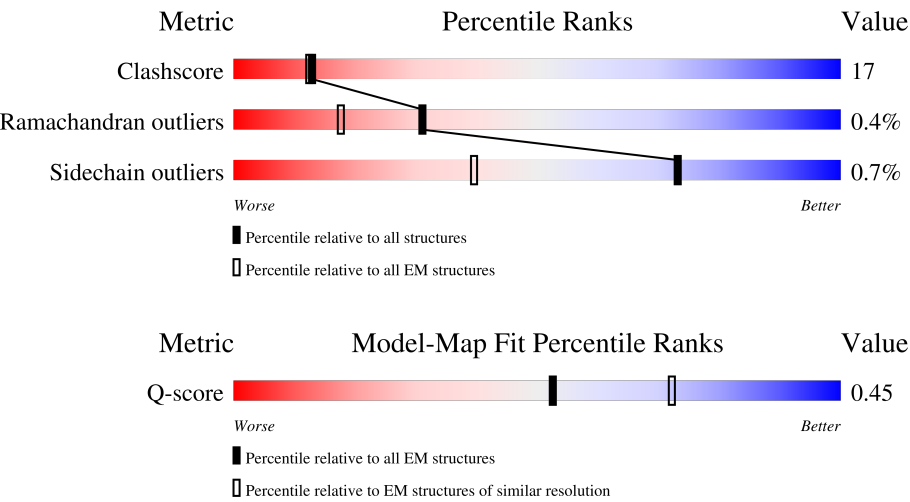
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.78 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.



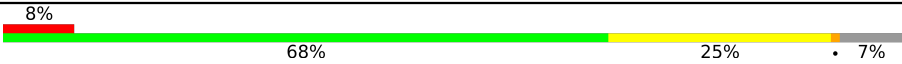
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10074 (3.28 - 4.27)

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	436	10% 52% 40% 8%
2	B	313	39% 62% 32% 5%
2	C	313	46% 59% 35% 5%
3	D	276	29% 60% 36% ••

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Mol	Chain	Length	Quality of chain
3	E	276	
4	H	646	
4	I	646	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20986 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 Probable ABC transporter binding protein NosD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	403	Total	C	N	O	S	0	0
			3149	1955	567	616	11		

- Molecule 2 is a protein called Probable ABC transporter ATP-binding protein NosF.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	0	0
			2295	1436	427	426	6		
2	C	298	Total	C	N	O	S	0	0
			2295	1436	427	426	6		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P19844
B	-3	HIS	-	expression tag	UNP P19844
B	-2	HIS	-	expression tag	UNP P19844
B	-1	HIS	-	expression tag	UNP P19844
B	0	HIS	-	expression tag	UNP P19844
B	1	HIS	-	expression tag	UNP P19844
B	154	GLN	GLU	conflict	UNP P19844
C	-4	HIS	-	expression tag	UNP P19844
C	-3	HIS	-	expression tag	UNP P19844
C	-2	HIS	-	expression tag	UNP P19844
C	-1	HIS	-	expression tag	UNP P19844
C	0	HIS	-	expression tag	UNP P19844
C	1	HIS	-	expression tag	UNP P19844
C	154	GLN	GLU	conflict	UNP P19844

- Molecule 3 is a protein called Probable ABC transporter permease protein NosY.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	275	Total	C	N	O	S	0	0
			2073	1393	328	345	7		
3	E	258	Total	C	N	O	S	0	0
			1966	1330	311	320	5		

- Molecule 4 is a protein called Nitrous-oxide reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	581	Total	C	N	O	S	2	0
			4575	2893	787	863	32		
4	I	581	Total	C	N	O	S	0	0
			4567	2888	787	860	32		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	639	TRP	-	expression tag	UNP P19573
H	640	SER	-	expression tag	UNP P19573
H	641	HIS	-	expression tag	UNP P19573
H	642	PRO	-	expression tag	UNP P19573
H	643	GLN	-	expression tag	UNP P19573
H	644	PHE	-	expression tag	UNP P19573
H	645	GLU	-	expression tag	UNP P19573
H	646	LYS	-	expression tag	UNP P19573
I	639	TRP	-	expression tag	UNP P19573
I	640	SER	-	expression tag	UNP P19573
I	641	HIS	-	expression tag	UNP P19573
I	642	PRO	-	expression tag	UNP P19573
I	643	GLN	-	expression tag	UNP P19573
I	644	PHE	-	expression tag	UNP P19573
I	645	GLU	-	expression tag	UNP P19573
I	646	LYS	-	expression tag	UNP P19573

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃)

ATP

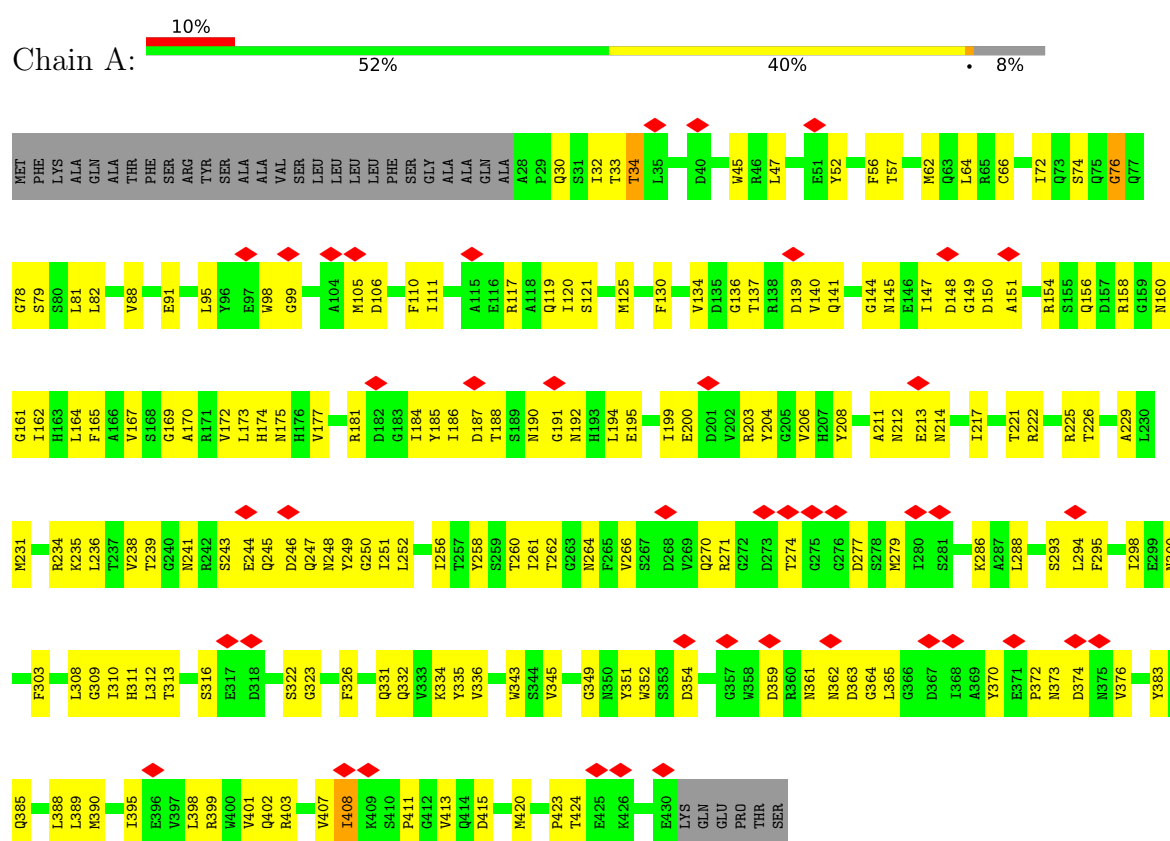
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total 31	C 10	N 5	O 13	P 3	0
6	C	1	Total 31	C 10	N 5	O 13	P 3	0

- | Chain | Residues | Atoms | | AltConf |
|-------|----------|------------|---------|---------|
| H | 1 | Total
1 | Ca
1 | 0 |
| I | 1 | Total
1 | Ca
1 | 0 |

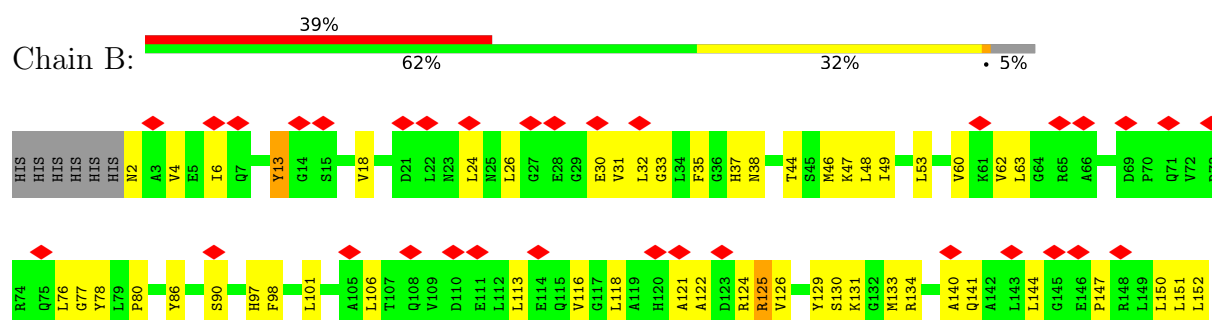
3 Residue-property plots

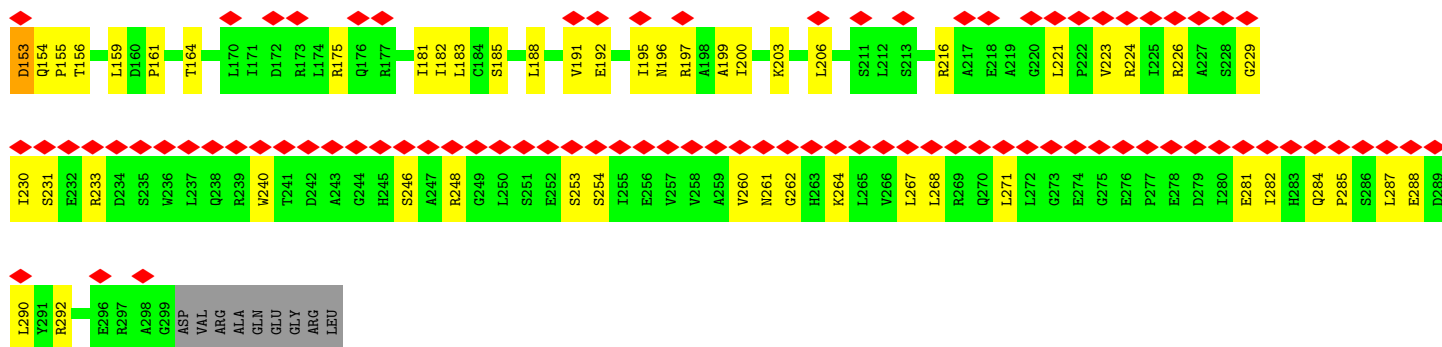
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Probable ABC transporter binding protein NosD



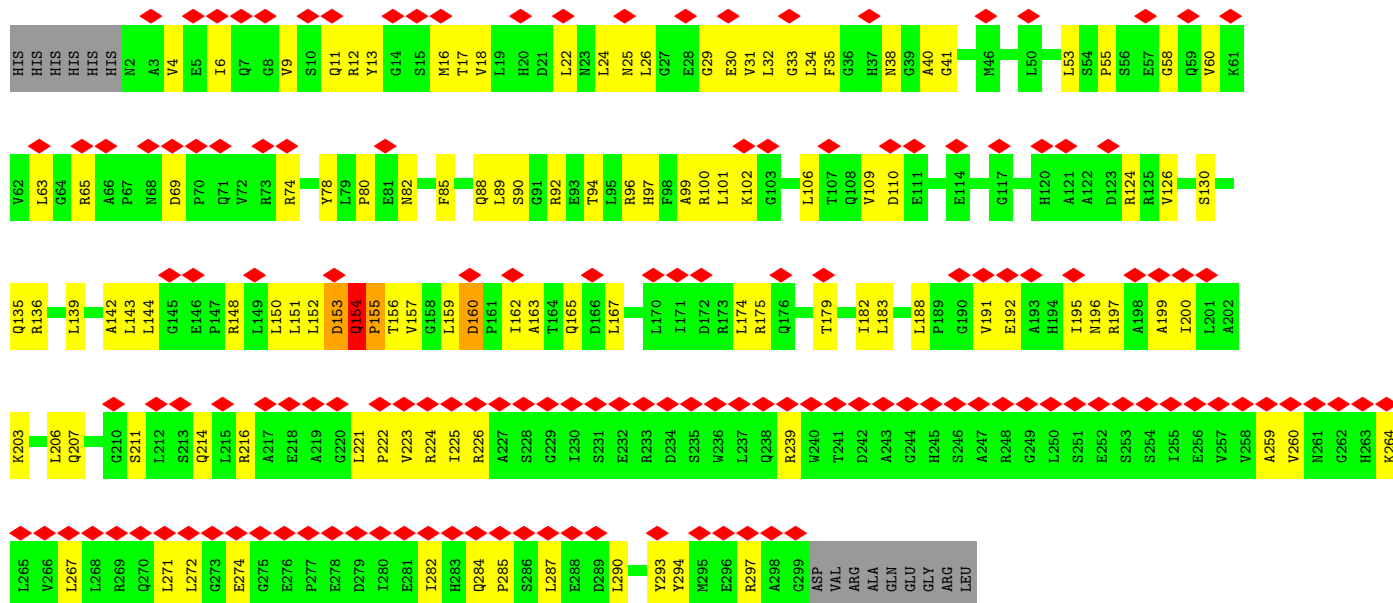
- Molecule 2: Probable ABC transporter ATP-binding protein NosF

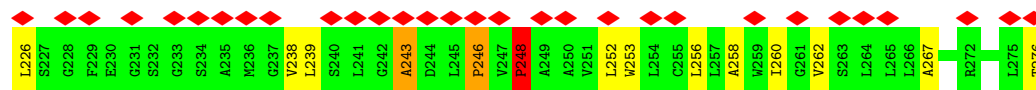




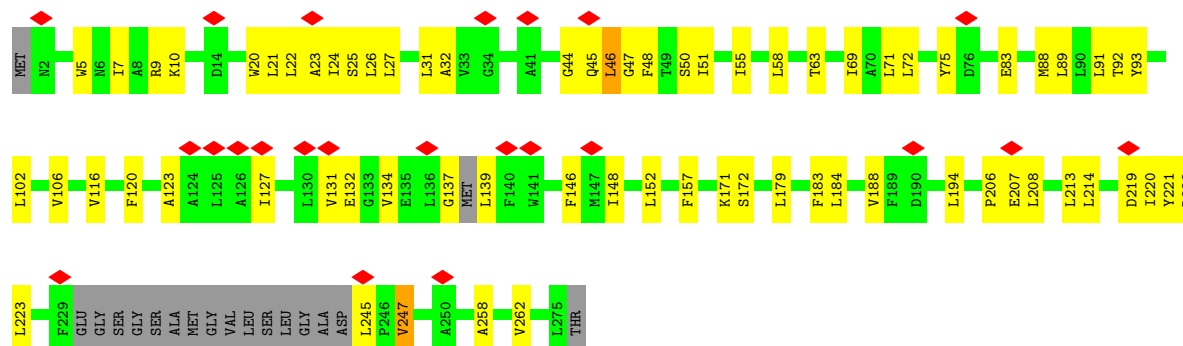
- Molecule 2: Probable ABC transporter ATP-binding protein NosF

Chain C: 46% 59% 35% 5%

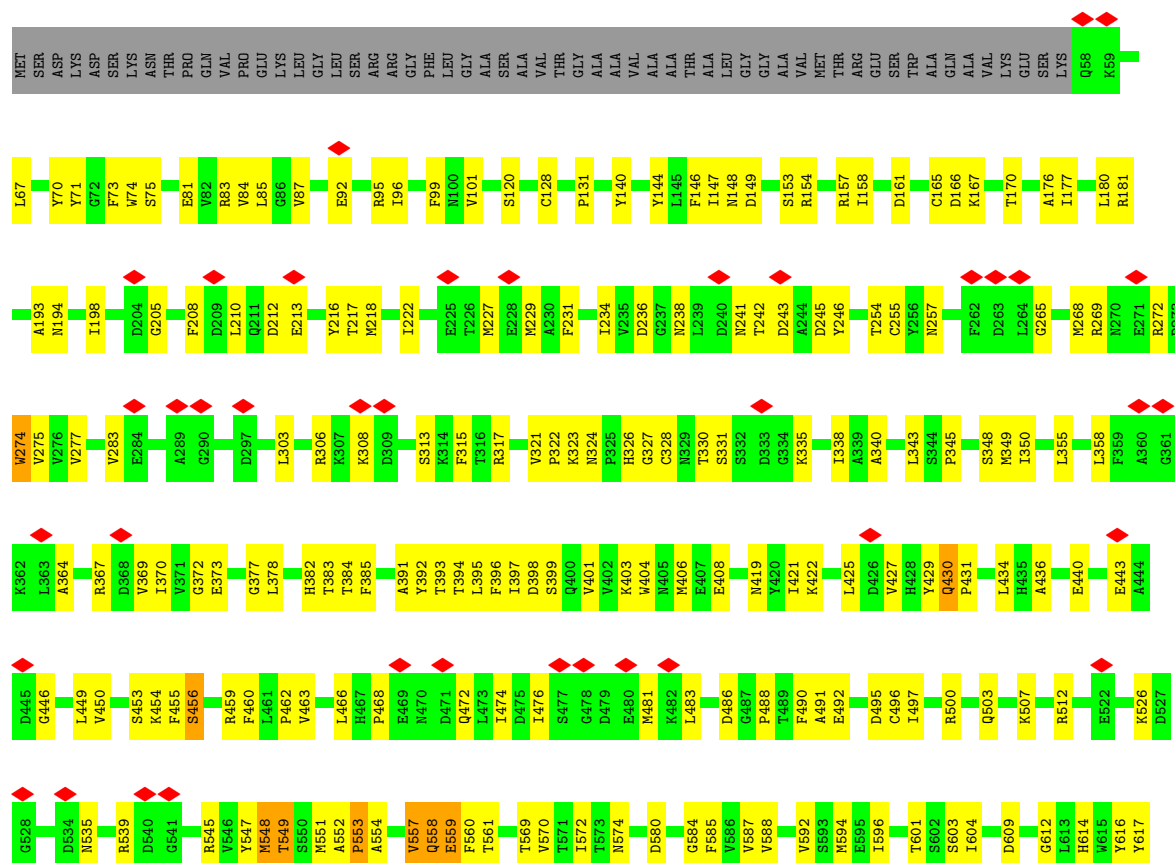


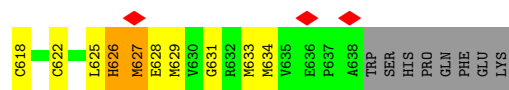


• Molecule 3: Probable ABC transporter permease protein NosY

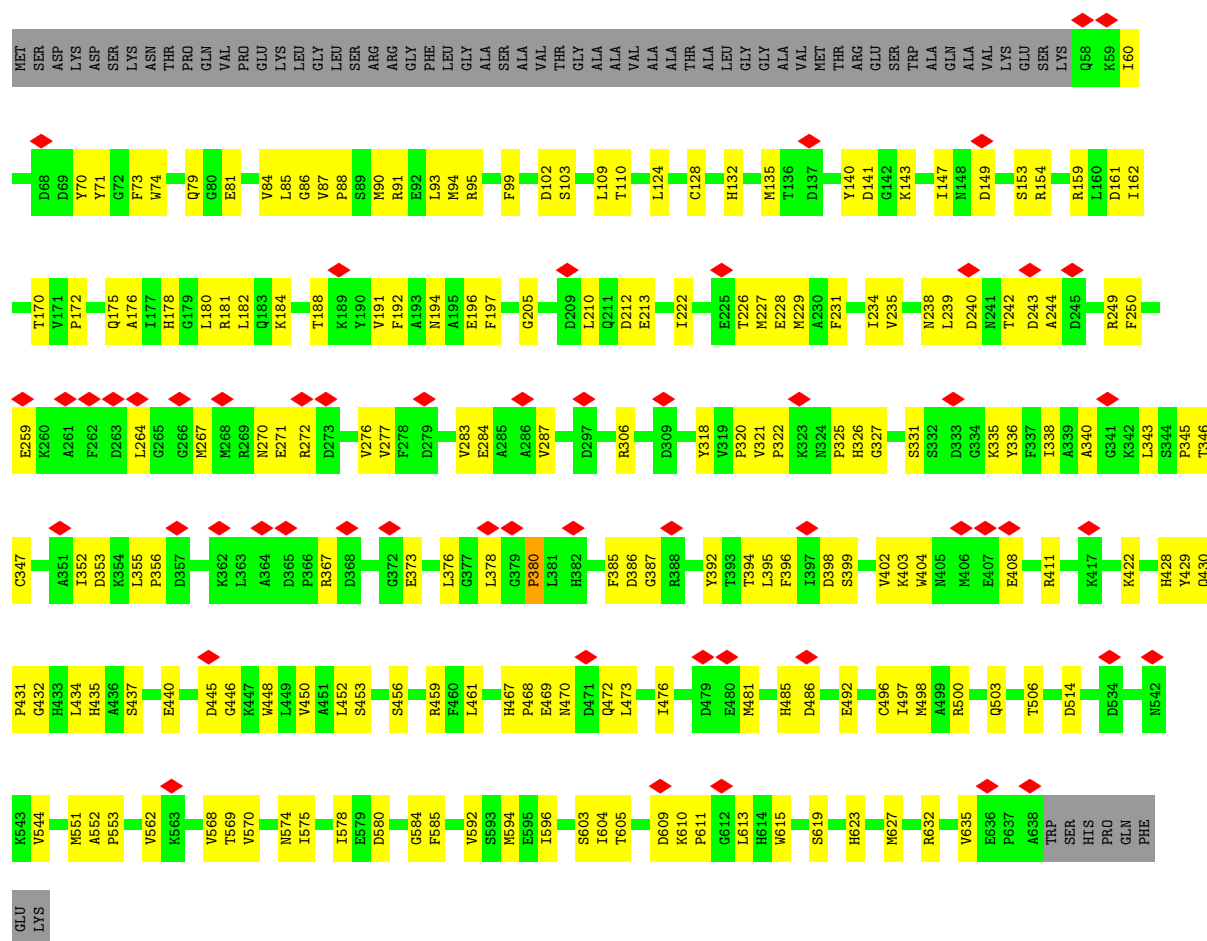


• Molecule 4: Nitrous-oxide reductase





• Molecule 4: Nitrous-oxide reductase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114710	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.954	Depositor
Minimum map value	-1.277	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	208.8, 208.8, 208.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/3213	0.65	4/4361 (0.1%)
2	B	0.36	0/2330	0.70	2/3151 (0.1%)
2	C	0.36	1/2330 (0.0%)	0.68	5/3151 (0.2%)
3	D	0.49	1/2120 (0.0%)	0.85	16/2892 (0.6%)
3	E	0.27	0/2011	0.52	3/2743 (0.1%)
4	H	0.38	1/4693 (0.0%)	0.67	7/6356 (0.1%)
4	I	0.31	1/4679 (0.0%)	0.60	5/6337 (0.1%)
All	All	0.35	4/21376 (0.0%)	0.67	42/28991 (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
3	D	0	2
3	E	0	1
4	H	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	196	LEU	C-O	-7.45	1.15	1.24
4	H	456	SER	CA-CB	-6.54	1.44	1.53
2	C	130	SER	CA-CB	-5.51	1.45	1.53
4	I	380	PRO	CG-CD	-5.47	1.32	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	PRO	N-CA-C	-13.58	90.30	110.80
4	H	274	TRP	N-CA-C	9.36	121.92	110.41
3	D	200	SER	N-CA-C	-9.25	101.42	112.89
4	I	380	PRO	N-CD-CG	-8.69	90.16	103.20
3	D	200	SER	CA-C-N	-8.38	110.33	123.23
3	D	200	SER	C-N-CA	-8.38	110.33	123.23
2	C	160	ASP	CB-CA-C	-7.00	96.78	109.45
3	D	198	VAL	CA-C-N	-6.95	110.40	122.36
3	D	198	VAL	C-N-CA	-6.95	110.40	122.36
3	D	195	ALA	N-CA-C	-6.76	103.93	111.71
4	H	257	ASN	CB-CA-C	-6.59	103.00	111.50
3	D	3	GLN	N-CA-C	-6.48	105.23	113.01
2	B	13	TYR	CB-CA-C	6.48	123.32	110.42
4	I	346	THR	CB-CA-C	-6.34	101.05	110.62
3	D	196	LEU	CA-C-O	-6.22	114.28	120.82
2	C	155	PRO	CB-CA-C	-6.13	100.87	110.49
2	C	153	ASP	CA-C-O	-6.08	114.28	121.16
4	I	380	PRO	CA-N-CD	-6.07	103.50	112.00
3	D	248	PRO	N-CA-C	6.00	124.84	112.47
3	E	47	GLY	N-CA-C	5.98	120.39	111.18
3	D	208	LEU	N-CA-C	5.91	119.67	112.23
3	D	196	LEU	N-CA-C	-5.88	104.77	111.07
4	I	345	PRO	N-CA-C	-5.84	107.97	114.92
4	H	553	PRO	N-CA-CB	-5.59	96.45	102.60
3	D	246	PRO	N-CA-C	-5.53	101.08	112.47
1	A	362	ASN	CB-CA-C	-5.46	101.57	110.85
4	H	549	THR	N-CA-C	-5.46	101.96	110.42
3	D	54	THR	CB-CA-C	5.45	119.54	110.81
4	H	627	MET	N-CA-C	-5.41	106.38	112.87
2	C	156	THR	N-CA-C	-5.41	106.53	113.02
2	C	80	PRO	CB-CA-C	-5.41	102.90	110.63
4	H	558	GLN	N-CA-C	-5.39	105.93	112.88
4	H	455	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	361	ASN	N-CA-C	-5.33	103.50	110.53
4	I	422	LYS	N-CA-C	-5.19	106.03	112.93
1	A	34	THR	CB-CA-C	-5.15	109.66	115.79
3	E	46	LEU	CA-C-N	-5.15	117.15	121.58
3	E	46	LEU	C-N-CA	-5.15	117.15	121.58
3	D	207	GLU	O-C-N	-5.14	115.95	122.27
3	D	210	PRO	CB-CA-C	-5.14	104.14	112.62
2	B	153	ASP	CB-CA-C	-5.11	100.01	109.37
3	D	243	ALA	N-CA-C	-5.05	105.86	111.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	196	LEU	Mainchain
3	D	197	LEU	Mainchain
3	E	50	SER	Mainchain
4	H	548	MET	Mainchain

5.2 Too-close contacts

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	3149	0	3023	138	0
2	B	2295	0	2346	93	0
2	C	2295	0	2346	82	0
3	D	2073	0	2196	82	0
3	E	1966	0	2091	56	0
4	H	4575	0	4448	167	0
4	I	4567	0	4439	156	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	31	0	12	1	0
6	C	31	0	12	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
All	All	20986	0	20913	692	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (692) 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:B:233:ARG:HE	2:B:253:SER:HB2	1.08	1.15
2:B:233:ARG:CG	2:B:253:SER:HA	1.85	1.06
2:B:233:ARG:HG2	2:B:253:SER:CA	1.90	1.00
2:B:233:ARG:HG2	2:B:253:SER:HA	0.96	0.95
1:A:407:VAL:HG12	1:A:408:ILE:HD12	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:394:THR:HG23	4:H:434:LEU:HD22	1.60	0.84
3:E:214:LEU:HA	3:E:220:ILE:HD11	1.61	0.82
1:A:33:THR:HG22	1:A:34:THR:H	1.45	0.81
3:D:14:ASP:OD1	3:D:17:ARG:NH2	2.14	0.81
4:I:271:GLU:HG3	4:I:272:ARG:HG3	1.62	0.81
4:H:396:PHE:CE1	4:H:430:GLN:HG3	2.16	0.80
4:I:243:ASP:OD1	4:I:244:ALA:N	2.14	0.80
2:B:233:ARG:NE	2:B:253:SER:HB2	1.93	0.80
2:B:199:ALA:HB1	2:B:206:LEU:HD11	1.65	0.79
3:D:172:SER:HB2	3:E:20:TRP:HE1	1.48	0.79
2:B:37:HIS:HE1	2:B:203:LYS:HB3	1.48	0.78
1:A:352:TRP:NE1	1:A:415:ASP:OD2	2.17	0.77
3:D:168:VAL:HG11	3:D:174:ALA:HB2	1.66	0.77
1:A:373:ASN:ND2	3:D:43:SER:O	2.18	0.77
3:D:199:LEU:HB2	3:E:45:GLN:HB3	1.67	0.77
4:I:613:LEU:HD11	4:I:632:ARG:HB2	1.67	0.77
1:A:111:ILE:HD12	1:A:134:VAL:HG12	1.66	0.76
4:H:539:ARG:NH2	4:H:561:THR:O	2.19	0.75
4:H:592:VAL:HG13	4:H:604:ILE:HD13	1.69	0.75
2:B:147:PRO:HB3	2:B:150:LEU:HD13	1.69	0.74
4:I:182:LEU:HD22	4:I:191:VAL:HG22	1.69	0.74
2:B:134:ARG:HH12	2:C:82:ASN:ND2	1.86	0.74
1:A:151:ALA:HA	1:A:158:ARG:HH12	1.52	0.74
4:I:592:VAL:HG13	4:I:604:ILE:HD13	1.69	0.74
2:B:90:SER:HA	2:B:125:ARG:HA	1.70	0.73
2:C:259:ALA:HB1	2:C:264:LYS:HD2	1.69	0.73
4:H:627:MET:HE3	4:I:326:HIS:HE1	1.53	0.73
4:I:184:LYS:NZ	4:I:244:ALA:O	2.22	0.72
1:A:274:THR:O	4:H:419:ASN:ND2	2.22	0.72
3:D:34:GLY:O	3:D:39:GLY:N	2.23	0.72
3:D:55:ILE:CD1	3:D:142:ALA:HB1	2.19	0.72
4:H:392:TYR:HE1	4:H:403:LYS:HG3	1.55	0.72
1:A:311:HIS:CE1	1:A:334:LYS:HD3	2.26	0.71
3:E:219:ASP:OD1	3:E:222:ARG:NH2	2.23	0.71
4:I:394:THR:HG23	4:I:434:LEU:HD22	1.70	0.71
4:H:392:TYR:CE1	4:H:403:LYS:HG3	2.26	0.71
4:I:184:LYS:NZ	4:I:243:ASP:OD1	2.22	0.70
1:A:385:GLN:HE22	3:E:245:LEU:HG	1.56	0.70
1:A:243:SER:OG	1:A:246:ASP:OD2	2.09	0.70
3:D:80:GLY:HA2	3:D:171:LYS:HE2	1.73	0.70
4:H:243:ASP:OD2	4:H:330:THR:OG1	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:LEU:HD21	2:C:167:LEU:HD13	1.74	0.70
4:I:367:ARG:NH2	4:I:373:GLU:OE2	2.24	0.70
2:B:134:ARG:HH12	2:C:82:ASN:HD22	1.40	0.69
2:B:37:HIS:CE1	2:B:203:LYS:HB3	2.27	0.69
4:H:241:ASN:ND2	4:H:326:HIS:O	2.26	0.69
4:H:616:TYR:CZ	4:H:631:GLY:HA3	2.27	0.69
4:H:396:PHE:HE1	4:H:430:GLN:HG3	1.56	0.69
4:I:172:PRO:HD2	4:I:229:MET:HE3	1.75	0.68
4:H:268:MET:HE3	4:H:343:LEU:HD13	1.75	0.68
4:I:352:ILE:HA	4:I:355:LEU:HD12	1.74	0.68
2:B:233:ARG:HE	2:B:253:SER:CB	1.96	0.68
2:B:264:LYS:CE	2:B:282:ILE:HD13	2.22	0.68
4:H:212:ASP:OD1	4:H:213:GLU:N	2.27	0.68
2:B:38:ASN:HD22	2:C:136:ARG:HE	1.42	0.67
4:H:408:GLU:OE1	4:H:422:LYS:NZ	2.27	0.67
4:H:272:ARG:HG2	4:H:322:PRO:HB3	1.76	0.67
3:D:223:LEU:HD23	3:D:252:LEU:HD11	1.75	0.67
1:A:57:THR:HG22	1:A:82:LEU:HB2	1.77	0.66
4:H:83:ARG:HH22	4:H:491:ALA:HB3	1.60	0.66
4:H:554:ALA:HB2	4:I:264:LEU:HD11	1.77	0.66
1:A:156:GLN:HG2	4:H:373:GLU:HG2	1.77	0.66
4:H:120:SER:OG	4:H:154:ARG:NH1	2.29	0.66
4:H:161:ASP:HB2	4:H:507:LYS:HG3	1.77	0.66
2:B:134:ARG:HH22	2:C:82:ASN:ND2	1.92	0.66
4:H:574:ASN:HB2	4:H:596:ILE:HG22	1.76	0.66
4:H:627:MET:HE3	4:I:326:HIS:CE1	2.30	0.66
2:B:230:ILE:HG13	2:B:231:SER:H	1.61	0.66
4:I:456:SER:OG	4:I:468:PRO:O	2.13	0.66
2:C:30:GLU:HA	2:C:175:ARG:HH12	1.60	0.65
2:B:47:LYS:NZ	3:E:88:MET:SD	2.69	0.65
4:H:548:MET:HB3	4:H:557:VAL:HG13	1.77	0.65
3:E:48:PHE:HB3	3:E:131:VAL:HG11	1.79	0.65
4:H:377:GLY:HA3	4:H:395:LEU:HD13	1.78	0.65
2:C:6:ILE:HG13	2:C:60:VAL:HG23	1.78	0.64
2:C:239:ARG:HH12	2:C:274:GLU:HG2	1.62	0.64
4:H:198:ILE:O	4:I:615:TRP:NE1	2.28	0.64
4:I:321:VAL:HG22	4:I:322:PRO:HD2	1.78	0.64
4:I:161:ASP:OD1	4:I:162:ILE:N	2.30	0.64
1:A:373:ASN:HB3	1:A:376:VAL:HG12	1.80	0.64
4:I:110:THR:HG22	4:I:594:MET:HE2	1.80	0.64
2:B:35:PHE:HE2	2:B:287:LEU:HD21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:44:GLY:C	3:E:46:LEU:HD13	2.23	0.63
4:H:466:LEU:HD23	4:I:94:MET:HE1	1.81	0.63
2:B:46:MET:HE2	2:B:153:ASP:OD1	1.97	0.63
2:B:264:LYS:HA	2:B:267:LEU:HB2	1.80	0.63
3:D:194:LEU:HD12	3:D:238:VAL:HG22	1.81	0.63
4:I:234:ILE:HG21	4:I:306:ARG:HH11	1.62	0.63
3:E:5:TRP:O	3:E:9:ARG:HG2	1.98	0.63
2:C:101:LEU:HD22	3:D:95:LEU:HD11	1.81	0.63
4:H:331:SER:HA	4:H:385:PHE:CE2	2.34	0.63
3:D:179:LEU:HD12	3:E:72:LEU:HD12	1.81	0.62
1:A:164:LEU:HD23	1:A:167:VAL:HG11	1.81	0.62
4:H:449:LEU:HD22	4:H:474:ILE:HD12	1.81	0.62
1:A:125:MET:HE3	1:A:147:ILE:HG12	1.81	0.62
1:A:169:GLY:H	1:A:191:GLY:HA3	1.64	0.62
2:B:78:TYR:HD2	3:E:92:THR:HG21	1.64	0.62
2:B:268:LEU:HD23	2:B:271:LEU:HD12	1.81	0.62
2:C:78:TYR:HD2	3:D:92:THR:HG21	1.64	0.61
3:E:48:PHE:CZ	3:E:51:ILE:HG12	2.35	0.61
1:A:398:LEU:O	1:A:402:GLN:HG2	1.99	0.61
2:B:141:GLN:NE2	3:E:93:TYR:OH	2.32	0.61
4:H:234:ILE:HG22	4:H:306:ARG:HG3	1.83	0.61
4:H:454:LYS:NZ	4:H:492:GLU:OE2	2.26	0.61
4:H:101:VAL:HG11	4:I:124:LEU:HD23	1.82	0.61
4:I:327:GLY:H	4:I:340:ALA:HB3	1.66	0.61
4:H:472:GLN:HE21	4:H:486:ASP:CG	2.08	0.61
4:H:74:TRP:CZ3	4:H:85:LEU:HB2	2.36	0.61
4:H:548:MET:HE2	4:H:557:VAL:HG13	1.83	0.61
1:A:200:GLU:OE2	1:A:222:ARG:NH1	2.33	0.60
1:A:261:ILE:HB	1:A:298:ILE:HG12	1.83	0.60
3:D:55:ILE:HD13	3:D:142:ALA:HB1	1.83	0.60
4:H:154:ARG:HG2	4:H:170:THR:HG22	1.81	0.60
3:D:55:ILE:HG22	3:D:55:ILE:O	2.01	0.60
4:H:313:SER:O	4:H:317:ARG:NH1	2.34	0.60
4:I:85:LEU:HD23	4:I:91:ARG:C	2.26	0.60
1:A:388:LEU:HD22	3:E:223:LEU:HD21	1.83	0.60
1:A:105:MET:SD	4:H:269:ARG:NH1	2.75	0.60
4:I:431:PRO:HA	4:I:453:SER:HA	1.83	0.60
3:E:48:PHE:HZ	3:E:51:ILE:HG12	1.67	0.59
2:B:118:LEU:HD21	2:B:133:MET:HB3	1.83	0.59
3:E:83:GLU:OE2	3:E:171:LYS:N	2.28	0.59
4:I:459:ARG:HD3	4:I:470:ASN:HD22	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:CE2	4:H:378:LEU:HD21	2.37	0.59
1:A:231:MET:HE1	4:H:378:LEU:HD22	1.85	0.59
2:B:229:GLY:N	2:B:254:SER:OG	2.35	0.59
3:D:223:LEU:HD11	3:D:243:ALA:HA	1.83	0.59
2:B:134:ARG:HH22	2:C:82:ASN:HD21	1.50	0.59
4:H:331:SER:OG	4:H:335:LYS:N	2.35	0.58
2:B:192:GLU:HB3	2:B:287:LEU:HD22	1.86	0.58
4:H:158:ILE:HA	4:H:165:CYS:HA	1.85	0.58
4:I:376:LEU:HD11	4:I:404:TRP:CD1	2.38	0.58
2:C:211:SER:OG	2:C:214:GLN:OE1	2.15	0.58
3:D:138:MET:HA	3:D:141:TRP:NE1	2.18	0.58
4:H:554:ALA:HB2	4:I:264:LEU:CD1	2.32	0.58
2:B:216:ARG:HG3	2:B:290:LEU:HD11	1.85	0.58
2:C:153:ASP:O	2:C:154:GLN:C	2.45	0.58
3:D:71:LEU:HD23	3:D:161:ALA:HB2	1.86	0.58
4:H:144:TYR:CD1	4:H:157:ARG:HD2	2.39	0.58
4:H:434:LEU:HD12	4:H:449:LEU:HD11	1.86	0.58
4:I:159:ARG:NH1	4:I:514:ASP:OD1	2.37	0.58
1:A:294:LEU:HD13	4:I:578:ILE:HG23	1.85	0.58
2:B:30:GLU:OE2	2:B:197:ARG:NH2	2.36	0.58
4:H:338:ILE:HD12	4:H:385:PHE:CZ	2.38	0.58
1:A:312:LEU:HD23	1:A:335:TYR:HD1	1.68	0.58
1:A:238:VAL:HG12	1:A:264:ASN:HD21	1.69	0.57
1:A:169:GLY:N	1:A:191:GLY:O	2.37	0.57
1:A:332:GLN:HE22	1:A:354:ASP:HB2	1.69	0.57
2:B:155:PRO:HD2	2:B:185:SER:HB3	1.86	0.57
2:B:183:LEU:HD23	2:B:195:ILE:HD11	1.86	0.57
4:I:395:LEU:O	4:I:399:SER:N	2.37	0.57
4:I:500:ARG:HH12	4:I:503:GLN:HE21	1.53	0.57
4:I:161:ASP:HA	4:I:506:THR:HA	1.85	0.57
2:C:22:LEU:HD12	2:C:206:LEU:HB2	1.86	0.57
1:A:195:GLU:HA	1:A:217:ILE:O	2.05	0.57
2:B:159:LEU:HA	2:C:38:ASN:HD21	1.69	0.57
4:I:99:PHE:CE2	4:I:149:ASP:HB2	2.40	0.57
1:A:249:TYR:OH	4:H:398:ASP:OD1	2.23	0.57
3:E:88:MET:HA	3:E:91:LEU:HD12	1.86	0.57
2:B:32:LEU:HD23	2:B:33:GLY:N	2.20	0.57
4:H:74:TRP:CD1	4:H:496:CYS:HB3	2.40	0.57
4:H:324:ASN:ND2	4:I:627:MET:HE1	2.20	0.57
2:B:191:VAL:O	2:B:195:ILE:HG12	2.05	0.56
2:C:151:LEU:HD23	2:C:182:ILE:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:55:ILE:CD1	3:D:142:ALA:CB	2.83	0.56
3:E:20:TRP:O	3:E:24:ILE:N	2.36	0.56
4:H:628:GLU:HB3	4:I:267:MET:SD	2.46	0.56
1:A:177:VAL:HG13	1:A:199:ILE:HG23	1.85	0.56
1:A:203:ARG:HH12	4:H:345:PRO:HG2	1.70	0.56
4:I:135:MET:HE2	4:I:140:TYR:HE1	1.69	0.56
1:A:185:TYR:CE1	1:A:187:ASP:HB2	2.40	0.56
4:I:235:VAL:HG11	4:I:239:LEU:HD11	1.88	0.56
1:A:343:TRP:CZ2	1:A:413:VAL:HG11	2.41	0.56
2:B:226:ARG:HB2	2:B:281:GLU:HB2	1.88	0.56
3:E:58:LEU:HG	3:E:146:PHE:CZ	2.41	0.56
3:D:246:PRO:HD2	3:D:248:PRO:HD3	1.88	0.56
4:H:99:PHE:CZ	4:H:149:ASP:HB2	2.41	0.56
4:H:70:TYR:HB2	4:H:87:VAL:HB	1.89	0.55
4:H:213:GLU:O	4:H:306:ARG:NH1	2.39	0.55
4:H:181:ARG:HD2	4:H:243:ASP:HA	1.87	0.55
1:A:148:ASP:OD1	1:A:149:GLY:N	2.40	0.55
3:D:51:ILE:HD11	3:D:139:LEU:HD12	1.88	0.55
4:H:392:TYR:HD2	4:H:449:LEU:HD12	1.71	0.55
4:I:194:ASN:HD22	4:I:239:LEU:HD23	1.71	0.55
1:A:312:LEU:HD23	1:A:335:TYR:CD1	2.41	0.55
4:H:75:SER:HB2	4:H:128:CYS:SG	2.46	0.55
1:A:294:LEU:HD22	4:I:578:ILE:HA	1.87	0.55
4:I:428:HIS:HB3	4:I:429:TYR:CD2	2.42	0.55
1:A:47:LEU:HD13	1:A:64:LEU:HD21	1.87	0.55
4:I:386:ASP:HB2	4:I:446:GLY:HA3	1.88	0.55
4:H:431:PRO:HA	4:H:453:SER:HA	1.88	0.55
4:I:135:MET:SD	4:I:184:LYS:HG2	2.47	0.55
4:I:452:LEU:HB3	4:I:469:GLU:OE2	2.06	0.55
4:I:609:ASP:OD1	4:I:610:LYS:N	2.40	0.55
4:I:102:ASP:OD1	4:I:103:SER:N	2.40	0.54
2:B:221:LEU:O	2:B:261:ASN:ND2	2.41	0.54
2:C:264:LYS:HB2	2:C:267:LEU:HD12	1.88	0.54
3:D:35:ILE:HD11	3:D:61:LEU:HD12	1.89	0.54
2:C:192:GLU:HB3	2:C:287:LEU:HD22	1.89	0.54
3:D:55:ILE:O	3:D:55:ILE:CG2	2.55	0.54
1:A:76:GLY:O	1:A:99:GLY:HA2	2.07	0.54
4:H:463:VAL:HG11	4:I:93:LEU:HB3	1.90	0.54
1:A:234:ARG:HD2	4:I:551:MET:HE1	1.90	0.54
2:B:113:LEU:HD21	2:B:122:ALA:HB2	1.90	0.54
4:I:132:HIS:CD2	4:I:181:ARG:HD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:222:ARG:O	3:D:226:LEU:HG	2.08	0.54
1:A:256:ILE:O	1:A:293:SER:HB2	2.08	0.54
2:B:240:TRP:HZ3	2:B:267:LEU:HD22	1.73	0.54
3:E:116:VAL:HG13	3:E:120:PHE:HD2	1.73	0.54
1:A:213:GLU:HA	1:A:235:LYS:O	2.08	0.53
3:D:201:GLU:HG2	3:D:205:ASN:H	1.73	0.53
4:H:495:ASP:OD1	4:H:496:CYS:N	2.40	0.53
1:A:172:VAL:HG13	1:A:175:ASN:HD22	1.72	0.53
2:B:153:ASP:O	2:B:154:GLN:C	2.51	0.53
2:C:85:PHE:HB2	2:C:126:VAL:HG11	1.91	0.53
3:E:89:LEU:O	3:E:92:THR:OG1	2.18	0.53
4:I:570:VAL:O	4:I:603:SER:HA	2.09	0.53
4:I:74:TRP:CD1	4:I:496:CYS:HB2	2.43	0.53
4:I:86:GLY:O	4:I:90:MET:N	2.37	0.53
1:A:78:GLY:HA3	1:A:106:ASP:HB3	1.90	0.53
4:H:393:THR:HG23	4:H:404:TRP:HE1	1.73	0.53
3:E:137:GLY:O	3:E:139:LEU:N	2.42	0.53
3:D:20:TRP:NE1	3:E:172:SER:O	2.42	0.53
3:D:120:PHE:O	3:D:124:ALA:N	2.30	0.53
3:D:194:LEU:O	3:D:198:VAL:HG22	2.08	0.53
3:D:75:TYR:HH	3:E:75:TYR:HH	1.55	0.53
4:I:403:LYS:HB2	4:I:481:MET:HE3	1.90	0.53
2:B:26:LEU:HB3	2:B:32:LEU:HD12	1.91	0.53
3:D:12:LEU:HA	3:D:111:ILE:HD11	1.91	0.53
2:C:142:ALA:HB1	2:C:150:LEU:HD11	1.91	0.53
3:D:156:VAL:HB	3:D:260:ILE:HG12	1.91	0.53
3:E:51:ILE:O	3:E:55:ILE:HG12	2.09	0.53
1:A:74:SER:HB2	1:A:98:TRP:HA	1.90	0.52
3:D:60:SER:O	3:D:63:THR:HG22	2.09	0.52
1:A:33:THR:HG22	1:A:34:THR:N	2.19	0.52
2:C:12:ARG:HG2	2:C:17:THR:HG22	1.91	0.52
4:I:178:HIS:ND1	4:I:240:ASP:OD1	2.41	0.52
1:A:47:LEU:HB3	1:A:66:CYS:HB3	1.90	0.52
1:A:322:SER:HB3	1:A:345:VAL:HG22	1.91	0.52
4:I:392:TYR:CD2	4:I:481:MET:HE2	2.44	0.52
3:D:24:ILE:O	3:D:28:PHE:HB2	2.10	0.52
3:E:214:LEU:HD11	3:E:247:VAL:HG11	1.92	0.52
4:H:246:TYR:OH	4:H:440:GLU:O	2.22	0.52
4:H:456:SER:HB3	4:H:468:PRO:O	2.09	0.52
4:I:73:PHE:HB2	4:I:497:ILE:HG22	1.91	0.52
3:D:4:VAL:HG13	3:D:103:GLY:HA2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:210:LEU:HD12	4:I:632:ARG:HH11	1.74	0.52
1:A:33:THR:CG2	1:A:34:THR:H	2.21	0.52
1:A:313:THR:HG22	1:A:336:VAL:HG21	1.92	0.52
3:D:77:ALA:O	3:D:104:LYS:NZ	2.41	0.52
3:D:198:VAL:HG23	3:E:45:GLN:HB2	1.92	0.52
4:I:335:LYS:HE2	4:I:336:TYR:CE1	2.45	0.52
1:A:343:TRP:HB2	1:A:415:ASP:OD1	2.10	0.52
2:B:2:ASN:N	2:B:26:LEU:O	2.42	0.52
1:A:82:LEU:HD23	1:A:110:PHE:HB3	1.90	0.52
1:A:270:GLN:HG2	1:A:271:ARG:H	1.75	0.52
3:D:102:LEU:O	3:D:106:VAL:HG23	2.10	0.52
4:H:384:THR:OG1	4:H:436:ALA:N	2.35	0.52
2:C:197:ARG:HA	2:C:211:SER:HA	1.91	0.52
1:A:270:GLN:HG2	1:A:271:ARG:N	2.25	0.51
2:B:78:TYR:HE1	2:B:153:ASP:OD2	1.93	0.51
2:C:13:TYR:HD2	2:C:18:VAL:HG21	1.74	0.51
2:C:33:GLY:HA2	2:C:183:LEU:O	2.10	0.51
2:C:97:HIS:NE2	3:D:10:LYS:HD2	2.25	0.51
4:H:349:MET:HB2	4:H:372:GLY:O	2.10	0.51
4:I:500:ARG:HB3	4:I:503:GLN:HG3	1.92	0.51
4:H:535:ASN:HA	4:H:547:TYR:O	2.10	0.51
2:B:223:VAL:HA	2:B:285:PRO:HD3	1.93	0.51
2:C:143:LEU:HD21	2:C:174:LEU:HD11	1.93	0.51
2:C:175:ARG:NH2	2:C:196:ASN:HD22	2.07	0.51
1:A:244:GLU:O	1:A:246:ASP:N	2.44	0.51
3:D:55:ILE:HD12	3:D:142:ALA:HB1	1.91	0.51
2:B:154:GLN:HA	2:B:185:SER:HA	1.92	0.51
4:I:386:ASP:OD1	4:I:387:GLY:N	2.44	0.51
4:I:128:CYS:HB2	4:I:147:ILE:HD11	1.92	0.51
4:H:95:ARG:CZ	4:I:95:ARG:HH21	2.24	0.50
4:I:380:PRO:HA	4:I:394:THR:O	2.12	0.50
1:A:167:VAL:HG13	1:A:192:ASN:HD21	1.76	0.50
4:H:383:THR:HG22	4:H:385:PHE:CE1	2.46	0.50
4:I:81:GLU:OE2	4:I:95:ARG:NH2	2.43	0.50
1:A:252:LEU:HD13	4:H:378:LEU:HD12	1.94	0.50
3:D:20:TRP:O	3:D:24:ILE:HG22	2.11	0.50
2:B:153:ASP:C	2:B:155:PRO:HD3	2.36	0.50
4:I:408:GLU:HG2	4:I:411:ARG:HH21	1.76	0.50
1:A:170:ALA:HB3	1:A:192:ASN:HD22	1.77	0.50
1:A:238:VAL:HG12	1:A:241:ASN:HD22	1.77	0.50
2:B:124:ARG:O	2:B:125:ARG:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:321:VAL:HG11	4:I:325:PRO:HG3	1.93	0.50
1:A:212:ASN:OD1	1:A:234:ARG:HB2	2.11	0.50
2:B:35:PHE:CE2	2:B:287:LEU:HD21	2.44	0.50
3:D:108:HIS:ND1	3:D:162:TYR:OH	2.40	0.50
3:E:23:ALA:O	3:E:27:LEU:HB2	2.11	0.50
4:H:500:ARG:HB2	4:H:503:GLN:HG3	1.94	0.50
4:H:617:TYR:HB3	4:I:197:PHE:HZ	1.77	0.50
4:I:153:SER:OG	4:I:176:ALA:N	2.37	0.50
3:D:7:ILE:HA	3:D:10:LYS:HG2	1.94	0.50
4:H:425:LEU:HD21	4:H:483:LEU:HD12	1.94	0.50
4:H:627:MET:HE2	4:H:627:MET:H	1.77	0.50
4:I:84:VAL:HG12	4:I:93:LEU:HB2	1.92	0.50
4:I:392:TYR:HD2	4:I:481:MET:HE2	1.76	0.50
1:A:130:PHE:HA	1:A:160:ASN:O	2.12	0.50
1:A:279:MET:HE3	4:H:421:ILE:HG22	1.94	0.50
1:A:383:TYR:CD1	3:E:206:PRO:HB3	2.47	0.50
3:D:179:LEU:HD11	3:E:69:ILE:HG12	1.92	0.50
4:H:338:ILE:HD12	4:H:385:PHE:HZ	1.77	0.50
4:H:572:ILE:O	4:H:601:THR:HA	2.12	0.50
4:I:459:ARG:HD3	4:I:470:ASN:ND2	2.25	0.50
3:D:3:GLN:HB2	3:D:99:GLN:NE2	2.27	0.49
2:C:102:LYS:HD3	2:C:144:LEU:HD23	1.95	0.49
2:C:223:VAL:HG23	2:C:284:GLN:HA	1.94	0.49
4:H:554:ALA:CB	4:I:264:LEU:HD11	2.42	0.49
1:A:247:GLN:HG2	1:A:248:ASN:OD1	2.12	0.49
2:B:292:ARG:CZ	2:C:165:GLN:HE22	2.25	0.49
4:H:74:TRP:HZ3	4:H:85:LEU:HB2	1.75	0.49
1:A:388:LEU:HD23	3:E:213:LEU:HD13	1.95	0.49
4:I:500:ARG:NH1	4:I:503:GLN:HE21	2.11	0.49
2:B:246:SER:HB2	2:B:248:ARG:HH12	1.78	0.49
3:E:20:TRP:O	3:E:24:ILE:HG22	2.12	0.49
4:H:83:ARG:NH1	4:H:490:PHE:O	2.43	0.49
1:A:47:LEU:HD21	1:A:52:TYR:HE2	1.78	0.49
2:B:4:VAL:HB	2:B:26:LEU:HG	1.94	0.49
2:B:38:ASN:HD21	2:C:159:LEU:HA	1.76	0.49
2:B:134:ARG:NH1	2:C:82:ASN:HD22	2.07	0.49
3:D:197:LEU:O	3:D:198:VAL:C	2.56	0.49
4:H:157:ARG:HB3	4:H:167:LYS:HB2	1.95	0.49
4:H:367:ARG:HG2	4:H:370:ILE:HG13	1.94	0.49
4:I:74:TRP:HZ2	4:I:450:VAL:HG11	1.77	0.49
4:I:321:VAL:CG2	4:I:322:PRO:HD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:435:HIS:CE1	4:I:497:ILE:HD12	2.47	0.49
2:C:135:GLN:HG2	2:C:157:VAL:O	2.12	0.49
4:I:552:ALA:HB1	4:I:623:HIS:HB2	1.95	0.49
4:I:562:VAL:HG23	4:I:635:VAL:HG22	1.95	0.49
1:A:261:ILE:O	1:A:298:ILE:HA	2.13	0.49
4:H:570:VAL:O	4:H:603:SER:HA	2.13	0.49
4:I:437:SER:OG	4:I:445:ASP:OD1	2.27	0.49
1:A:161:GLY:O	1:A:184:ILE:HA	2.13	0.48
2:B:248:ARG:HA	2:B:248:ARG:NE	2.28	0.48
3:D:189:PHE:CD1	3:D:216:ASN:HB2	2.48	0.48
3:D:189:PHE:CZ	3:D:215:LEU:HB2	2.48	0.48
2:B:6:ILE:HD11	2:B:49:ILE:HD11	1.93	0.48
2:B:76:LEU:HD23	2:B:77:GLY:N	2.28	0.48
3:D:189:PHE:HZ	3:D:215:LEU:HB2	1.78	0.48
2:B:80:PRO:HG3	3:E:89:LEU:HD12	1.95	0.48
2:C:25:ASN:O	2:C:197:ARG:NH1	2.46	0.48
2:C:99:ALA:HA	2:C:144:LEU:HD21	1.94	0.48
4:I:242:THR:OG1	4:I:243:ASP:N	2.47	0.48
4:I:338:ILE:HD12	4:I:385:PHE:CE1	2.47	0.48
1:A:45:TRP:CD1	1:A:62:MET:HG3	2.49	0.48
1:A:389:LEU:HD21	3:E:194:LEU:HB2	1.95	0.48
3:D:196:LEU:O	3:D:197:LEU:C	2.55	0.48
4:H:71:TYR:HE1	4:I:461:LEU:HB3	1.78	0.48
4:H:255:CYS:HB3	4:H:274:TRP:CD1	2.48	0.48
4:H:338:ILE:HG12	4:H:349:MET:HG2	1.95	0.48
4:I:378:LEU:N	4:I:398:ASP:OD2	2.43	0.48
2:B:156:THR:HA	2:B:159:LEU:HD12	1.94	0.48
2:B:223:VAL:HG23	2:B:284:GLN:HA	1.95	0.48
4:I:180:LEU:HA	4:I:192:PHE:O	2.14	0.48
1:A:258:TYR:N	1:A:295:PHE:O	2.46	0.48
2:C:63:LEU:HD11	2:C:148:ARG:HH21	1.79	0.48
4:H:626:HIS:C	4:H:628:GLU:N	2.70	0.48
1:A:231:MET:HE2	4:H:378:LEU:HD13	1.96	0.48
2:C:100:ARG:NH2	3:D:9:ARG:HD3	2.27	0.48
4:I:181:ARG:HG3	4:I:242:THR:O	2.14	0.48
4:I:276:VAL:HG12	4:I:318:TYR:CE1	2.49	0.48
4:H:358:LEU:HD22	4:H:369:VAL:HG11	1.94	0.48
4:I:376:LEU:HD12	4:I:402:VAL:HG11	1.94	0.48
1:A:359:ASP:HB2	1:A:420:MET:HG3	1.96	0.47
4:H:277:VAL:HG11	4:H:355:LEU:HD13	1.96	0.47
3:D:186:VAL:HG23	3:D:187:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:148:ASN:HB3	4:H:180:LEU:HD22	1.96	0.47
4:H:392:TYR:CD2	4:H:449:LEU:HD12	2.49	0.47
4:I:569:THR:OG1	4:I:605:THR:HG22	2.13	0.47
1:A:137:THR:O	1:A:167:VAL:HG23	2.15	0.47
2:C:63:LEU:HD11	2:C:148:ARG:HE	1.78	0.47
4:H:146:PHE:HE1	4:H:227:MET:HE1	1.80	0.47
4:H:394:THR:HG22	4:H:401:VAL:HG22	1.96	0.47
4:I:320:PRO:O	4:I:367:ARG:NH1	2.44	0.47
4:I:448:TRP:HB3	4:I:473:LEU:HD11	1.96	0.47
1:A:312:LEU:HD11	1:A:316:SER:HB2	1.94	0.47
2:B:152:LEU:HG	2:B:181:ILE:HD11	1.95	0.47
3:D:26:LEU:O	3:D:30:VAL:HG23	2.15	0.47
3:E:45:GLN:N	3:E:46:LEU:CD1	2.77	0.47
4:H:350:ILE:HG12	4:H:370:ILE:HD13	1.96	0.47
1:A:335:TYR:CG	1:A:413:VAL:HG13	2.49	0.47
1:A:399:ARG:O	1:A:403:ARG:HG3	2.14	0.47
4:H:216:TYR:CE2	4:H:218:MET:HE2	2.50	0.47
4:H:429:TYR:O	4:H:453:SER:HB3	2.14	0.47
2:B:78:TYR:CE1	2:B:153:ASP:OD2	2.68	0.47
2:B:134:ARG:NH1	2:C:82:ASN:ND2	2.61	0.47
1:A:363:ASP:O	1:A:364:GLY:C	2.57	0.47
2:B:48:LEU:HD13	2:B:53:LEU:HD22	1.96	0.47
2:B:260:VAL:HG13	2:B:262:GLY:H	1.79	0.47
3:D:153:LEU:HA	3:D:156:VAL:HG12	1.96	0.47
3:E:63:THR:HG22	3:E:221:TYR:HD2	1.80	0.47
3:E:148:ILE:O	3:E:152:LEU:HD23	2.15	0.47
4:H:617:TYR:HB3	4:I:197:PHE:CZ	2.50	0.47
4:I:611:PRO:HA	4:I:635:VAL:HG12	1.96	0.47
2:C:188:LEU:O	2:C:191:VAL:HG22	2.14	0.47
2:C:216:ARG:NH1	2:C:285:PRO:HB2	2.30	0.47
4:H:612:GLY:HA2	4:I:205:GLY:HA2	1.97	0.47
4:I:249:ARG:HD3	4:I:250:PHE:CE1	2.50	0.47
1:A:190:ASN:O	1:A:214:ASN:ND2	2.47	0.47
1:A:332:GLN:HB3	1:A:352:TRP:HZ3	1.80	0.47
1:A:374:ASP:N	1:A:374:ASP:OD1	2.45	0.47
2:C:290:LEU:HD22	2:C:294:TYR:HE2	1.80	0.47
4:H:588:VAL:HG11	4:I:175:GLN:HB3	1.97	0.47
4:I:60:ILE:HD12	4:I:88:PRO:HB2	1.96	0.47
1:A:365:LEU:H	1:A:365:LEU:HD12	1.79	0.47
4:H:378:LEU:HB3	4:H:397:ILE:HB	1.96	0.46
4:I:574:ASN:HD22	4:I:596:ILE:HG22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:TYR:CE2	1:A:372:PRO:HG3	2.51	0.46
2:C:100:ARG:HH21	3:D:9:ARG:HD3	1.81	0.46
2:C:287:LEU:HA	2:C:290:LEU:HB2	1.98	0.46
3:D:160:PHE:O	3:D:163:VAL:HG22	2.15	0.46
1:A:117:ARG:HA	1:A:139:ASP:O	2.16	0.46
1:A:300:ASN:OD1	1:A:424:THR:HG22	2.16	0.46
2:B:224:ARG:HE	2:B:226:ARG:HE	1.64	0.46
3:D:11:GLU:OE1	3:D:108:HIS:NE2	2.49	0.46
4:I:81:GLU:OE1	4:I:95:ARG:NH1	2.48	0.46
1:A:91:GLU:HA	1:A:121:SER:O	2.16	0.46
1:A:137:THR:HG23	1:A:140:VAL:HG21	1.97	0.46
2:B:32:LEU:HD23	2:B:33:GLY:H	1.79	0.46
4:H:460:PHE:CE1	4:H:488:PRO:HD3	2.50	0.46
4:I:74:TRP:CE3	4:I:85:LEU:HB2	2.51	0.46
4:I:551:MET:HB2	4:I:575:ILE:HG13	1.98	0.46
3:E:102:LEU:O	3:E:106:VAL:HG23	2.15	0.46
4:H:216:TYR:CD2	4:H:234:ILE:HG23	2.51	0.46
1:A:260:THR:HG22	1:A:260:THR:O	2.16	0.46
2:C:53:LEU:HD11	3:D:276:THR:HG21	1.97	0.46
4:H:391:ALA:HB2	4:H:406:MET:SD	2.56	0.46
4:H:569:THR:HA	4:H:604:ILE:O	2.16	0.46
3:D:8:ALA:O	3:D:12:LEU:HD23	2.16	0.46
3:D:74:ALA:HB2	3:D:158:LEU:HD22	1.98	0.46
3:E:22:LEU:HA	3:E:26:LEU:HD13	1.97	0.46
4:I:196:GLU:O	4:I:238:ASN:HB2	2.16	0.46
1:A:30:GLN:HG3	1:A:57:THR:OG1	2.16	0.45
1:A:72:ILE:HB	1:A:95:LEU:HD23	1.98	0.45
3:D:69:ILE:HG12	3:E:179:LEU:HD13	1.98	0.45
4:I:210:LEU:H	4:I:210:LEU:HD23	1.80	0.45
4:H:177:ILE:HG23	4:H:193:ALA:HB1	1.99	0.45
4:I:231:PHE:CE1	4:I:283:VAL:HG11	2.51	0.45
1:A:120:ILE:HG22	1:A:145:ASN:HD21	1.81	0.45
3:D:123:ALA:O	3:D:127:ILE:HD12	2.17	0.45
3:E:45:GLN:N	3:E:46:LEU:HD13	2.31	0.45
4:H:222:ILE:HG12	4:H:229:MET:HG2	1.98	0.45
4:I:212:ASP:CG	4:I:213:GLU:H	2.25	0.45
1:A:203:ARG:HH12	4:H:345:PRO:CG	2.29	0.45
1:A:239:THR:HA	1:A:262:THR:O	2.17	0.45
3:D:138:MET:HG3	3:D:141:TRP:CZ2	2.51	0.45
4:H:587:VAL:HB	4:H:592:VAL:HB	1.98	0.45
4:I:87:VAL:HG21	4:I:498:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:446:GLY:O	4:I:476:ILE:HG13	2.16	0.45
4:I:584:GLY:HA3	4:I:619:SER:OG	2.15	0.45
2:C:221:LEU:HD22	2:C:285:PRO:HB3	1.98	0.45
4:H:476:ILE:HG22	4:H:481:MET:HG2	1.98	0.45
1:A:62:MET:O	1:A:88:VAL:HA	2.17	0.45
1:A:351:TYR:HB2	1:A:423:PRO:HD2	1.99	0.45
2:C:78:TYR:CD2	3:D:92:THR:HG21	2.48	0.45
3:D:209:LEU:N	3:D:210:PRO:HD2	2.32	0.45
4:I:212:ASP:OD1	4:I:213:GLU:N	2.50	0.45
2:C:216:ARG:HH12	2:C:285:PRO:HB2	1.82	0.45
3:D:182:TRP:O	3:D:186:VAL:HG22	2.16	0.45
3:E:71:LEU:HD21	3:E:157:PHE:HD1	1.82	0.45
4:I:140:TYR:OH	4:I:497:ILE:HD11	2.16	0.45
2:C:65:ARG:NH2	2:C:69:ASP:OD2	2.50	0.45
2:C:106:LEU:O	2:C:109:VAL:HG22	2.17	0.45
4:H:166:ASP:OD1	4:H:167:LYS:N	2.49	0.45
4:H:622:CYS:SG	4:H:629:MET:SD	2.99	0.45
2:B:6:ILE:HG12	2:B:60:VAL:HG13	1.99	0.45
4:H:322:PRO:HA	4:H:323:LYS:HA	1.73	0.45
1:A:266:VAL:HB	1:A:303:PHE:HD1	1.82	0.44
2:B:126:VAL:O	2:B:129:TYR:HB2	2.18	0.44
4:H:96:ILE:HG21	4:H:158:ILE:HD13	1.99	0.44
2:C:162:ILE:H	2:C:162:ILE:HD12	1.82	0.44
2:C:25:ASN:OD1	2:C:26:LEU:N	2.51	0.44
2:C:223:VAL:HG23	2:C:285:PRO:HD3	1.99	0.44
4:H:70:TYR:HD1	4:H:500:ARG:HA	1.82	0.44
4:H:490:PHE:CD2	4:I:95:ARG:HB2	2.53	0.44
4:H:500:ARG:CZ	4:H:503:GLN:HE21	2.30	0.44
4:H:526:LYS:HD3	4:H:526:LYS:HA	1.79	0.44
4:I:135:MET:HE2	4:I:140:TYR:CE1	2.51	0.44
4:H:303:LEU:HD23	4:H:315:PHE:CE2	2.52	0.44
1:A:236:LEU:H	1:A:236:LEU:HD23	1.82	0.44
2:B:152:LEU:HB3	2:B:155:PRO:HG3	2.00	0.44
4:H:140:TYR:HB2	4:H:503:GLN:OE1	2.17	0.44
4:H:217:THR:HG21	4:H:238:ASN:HA	2.00	0.44
4:H:535:ASN:HD21	4:H:549:THR:HG22	1.82	0.44
4:I:74:TRP:CZ3	4:I:85:LEU:HB2	2.52	0.44
1:A:343:TRP:CH2	1:A:413:VAL:HG11	2.52	0.44
2:B:31:VAL:HG23	2:B:175:ARG:HG3	1.99	0.44
3:D:256:LEU:O	3:D:260:ILE:HG13	2.17	0.44
3:E:21:LEU:O	3:E:25:SER:OG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:HB2	1:A:32:ILE:HG22	2.00	0.44
2:B:97:HIS:O	2:B:101:LEU:HD12	2.17	0.44
3:D:141:TRP:HZ3	3:D:145:ARG:HH12	1.65	0.44
4:H:81:GLU:OE2	4:H:95:ARG:HD3	2.18	0.44
4:I:469:GLU:OE1	4:I:492:GLU:HA	2.18	0.44
4:H:275:VAL:O	4:H:275:VAL:HG13	2.18	0.44
4:I:580:ASP:OD1	4:I:580:ASP:O	2.35	0.44
2:B:161:PRO:HA	2:B:164:THR:HG22	1.99	0.44
4:I:386:ASP:HB3	4:I:392:TYR:CE1	2.53	0.44
1:A:173:LEU:HA	1:A:195:GLU:O	2.18	0.43
2:C:160:ASP:HB2	2:C:163:ALA:H	1.82	0.43
4:H:614:HIS:HB2	4:H:633:MET:HE2	2.00	0.43
1:A:385:GLN:OE1	1:A:385:GLN:HA	2.19	0.43
2:B:188:LEU:HD23	2:B:288:GLU:HA	2.00	0.43
3:D:72:LEU:HD11	3:E:72:LEU:HD21	2.00	0.43
4:H:131:PRO:HB3	4:H:147:ILE:HD12	2.00	0.43
4:I:396:PHE:CE1	4:I:430:GLN:HB3	2.53	0.43
1:A:199:ILE:HD12	1:A:221:THR:HG22	2.00	0.43
2:C:34:LEU:HD23	2:C:199:ALA:HB3	2.00	0.43
4:H:552:ALA:HA	4:H:553:PRO:HA	1.76	0.43
1:A:52:TYR:O	1:A:72:ILE:HA	2.19	0.43
1:A:78:GLY:O	1:A:79:SER:OG	2.32	0.43
1:A:251:ILE:HB	1:A:288:LEU:HD12	2.00	0.43
2:C:9:VAL:HG12	2:C:58:GLY:HA3	2.00	0.43
2:C:24:LEU:HD21	2:C:32:LEU:HD21	2.00	0.43
2:C:293:TYR:O	2:C:297:ARG:HG2	2.18	0.43
3:E:258:ALA:O	3:E:262:VAL:HG22	2.18	0.43
4:I:428:HIS:HA	4:I:429:TYR:HA	1.51	0.43
1:A:186:ILE:HD11	1:A:194:LEU:HD21	2.00	0.43
1:A:308:LEU:HD23	1:A:309:GLY:N	2.33	0.43
1:A:312:LEU:HD11	1:A:316:SER:CB	2.49	0.43
4:I:222:ILE:HG12	4:I:229:MET:SD	2.58	0.43
3:D:258:ALA:O	3:D:262:VAL:HG12	2.18	0.43
4:H:443:GLU:OE2	4:H:443:GLU:HA	2.19	0.43
2:B:116:VAL:HG21	2:B:140:ALA:HB2	2.00	0.43
2:C:92:ARG:HH12	2:C:110:ASP:CG	2.27	0.43
4:H:74:TRP:HZ2	4:H:450:VAL:HG21	1.83	0.43
4:I:73:PHE:HB2	4:I:497:ILE:CG2	2.48	0.43
1:A:181:ARG:HB2	1:A:203:ARG:HE	1.83	0.43
1:A:310:ILE:HD11	1:A:326:PHE:CE1	2.54	0.43
1:A:401:VAL:HG11	3:D:57:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ALA:O	2:B:124:ARG:HB2	2.19	0.43
4:H:512:ARG:HH11	4:H:512:ARG:HA	1.83	0.43
1:A:190:ASN:HA	1:A:212:ASN:O	2.19	0.43
3:E:7:ILE:HD12	3:E:7:ILE:H	1.84	0.43
4:H:67:LEU:HD22	4:I:461:LEU:HD23	2.01	0.43
4:H:205:GLY:HA2	4:H:208:PHE:HE1	1.84	0.43
4:H:625:LEU:HD21	4:I:343:LEU:HD21	2.00	0.43
4:I:259:GLU:CD	4:I:259:GLU:H	2.25	0.43
4:I:331:SER:HA	4:I:385:PHE:CE2	2.54	0.43
4:I:485:HIS:CE1	4:I:486:ASP:O	2.72	0.43
2:B:151:LEU:HG	2:B:182:ILE:HD12	2.01	0.43
4:H:382:HIS:HB3	4:H:434:LEU:HD23	2.00	0.43
4:H:395:LEU:O	4:H:399:SER:N	2.52	0.43
4:I:141:ASP:OD2	4:I:143:LYS:HB2	2.19	0.43
1:A:154:ARG:HD3	1:A:154:ARG:HA	1.82	0.42
2:C:4:VAL:HG22	2:C:26:LEU:HB3	2.01	0.42
3:D:138:MET:HA	3:D:141:TRP:CD1	2.54	0.42
3:D:168:VAL:HG22	3:D:169:ASN:H	1.84	0.42
1:A:185:TYR:HE1	1:A:187:ASP:HB2	1.81	0.42
1:A:203:ARG:HG2	1:A:225:ARG:HE	1.83	0.42
1:A:208:TYR:CZ	1:A:211:ALA:HB3	2.54	0.42
1:A:217:ILE:HA	1:A:239:THR:O	2.19	0.42
1:A:294:LEU:HB3	1:A:295:PHE:CD1	2.54	0.42
3:E:179:LEU:O	3:E:183:PHE:N	2.40	0.42
1:A:136:GLY:N	1:A:165:PHE:O	2.47	0.42
2:C:97:HIS:CE1	2:C:101:LEU:HD11	2.55	0.42
4:I:276:VAL:HG12	4:I:318:TYR:CD1	2.54	0.42
4:I:553:PRO:HG3	4:I:623:HIS:CE1	2.53	0.42
2:B:86:TYR:CE2	3:E:10:LYS:HE3	2.55	0.42
2:C:200:ILE:HG23	2:C:207:GLN:HB2	2.00	0.42
3:E:184:LEU:HA	3:E:188:VAL:HB	2.02	0.42
4:H:177:ILE:HA	4:H:194:ASN:O	2.20	0.42
4:H:245:ASP:HA	4:H:330:THR:HG21	2.01	0.42
1:A:206:VAL:O	1:A:206:VAL:HG23	2.19	0.42
2:C:96:ARG:HH12	2:C:106:LEU:HB2	1.84	0.42
2:C:260:VAL:HG12	2:C:264:LYS:HG2	2.01	0.42
4:H:561:THR:HG22	4:H:634:MET:HB2	2.02	0.42
2:C:11:GLN:OE1	2:C:55:PRO:HA	2.20	0.42
4:H:236:ASP:OD1	4:H:306:ARG:HG2	2.19	0.42
4:H:584:GLY:N	4:H:618:CYS:SG	2.79	0.42
4:H:585:PHE:CD2	4:H:594:MET:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LEU:HA	2:B:197:ARG:O	2.19	0.42
2:C:203:LYS:HD2	2:C:203:LYS:HA	1.87	0.42
2:C:225:ILE:HG23	2:C:282:ILE:HG12	2.00	0.42
3:E:88:MET:O	3:E:92:THR:HG23	2.20	0.42
4:H:73:PHE:HB2	4:H:497:ILE:CG2	2.50	0.42
4:H:153:SER:OG	4:H:176:ALA:N	2.53	0.42
4:H:308:LYS:HD3	4:H:308:LYS:HA	1.92	0.42
4:I:79:GLN:HB3	4:I:81:GLU:HG2	2.02	0.42
4:I:99:PHE:CZ	4:I:149:ASP:HB2	2.54	0.42
4:I:212:ASP:CG	4:I:213:GLU:N	2.78	0.42
4:I:585:PHE:HB3	4:I:594:MET:CG	2.50	0.42
3:E:88:MET:HG3	3:E:89:LEU:N	2.35	0.42
1:A:231:MET:SD	4:H:397:ILE:HD13	2.60	0.42
2:B:134:ARG:NH2	2:C:82:ASN:ND2	2.65	0.42
2:C:88:GLN:O	3:D:17:ARG:NH1	2.53	0.42
4:H:85:LEU:CD2	4:H:92:GLU:HA	2.50	0.42
4:H:626:HIS:C	4:H:628:GLU:H	2.28	0.42
4:I:182:LEU:HB3	4:I:188:THR:HG23	2.01	0.42
1:A:119:GLN:HG2	1:A:141:GLN:HB2	2.02	0.42
3:E:207:GLU:HG2	3:E:208:LEU:HG	2.02	0.42
4:H:545:ARG:HG2	4:H:569:THR:HB	2.01	0.42
4:H:580:ASP:OD1	4:I:467:HIS:HB2	2.19	0.42
2:B:62:VAL:HG12	2:B:63:LEU:HD23	2.02	0.41
2:C:224:ARG:HH21	2:C:226:ARG:NH2	2.17	0.41
3:D:101:LEU:HD11	3:D:267:ALA:HB1	2.02	0.41
4:I:496:CYS:SG	4:I:497:ILE:N	2.92	0.41
2:B:230:ILE:HG13	2:B:231:SER:N	2.30	0.41
2:C:29:GLY:O	2:C:175:ARG:NH1	2.54	0.41
4:H:327:GLY:H	4:H:340:ALA:HB3	1.85	0.41
4:I:73:PHE:CD2	4:I:84:VAL:HG22	2.56	0.41
4:I:181:ARG:NH2	4:I:440:GLU:OE1	2.53	0.41
4:I:249:ARG:HD3	4:I:250:PHE:CZ	2.55	0.41
4:I:544:VAL:O	4:I:568:VAL:HA	2.20	0.41
1:A:235:LYS:HA	1:A:258:TYR:O	2.21	0.41
1:A:250:GLY:N	1:A:286:LYS:O	2.51	0.41
2:C:31:VAL:HG23	2:C:175:ARG:HH11	1.84	0.41
4:H:149:ASP:HB3	4:H:154:ARG:HB2	2.02	0.41
4:I:70:TYR:HB2	4:I:87:VAL:HB	2.02	0.41
4:I:284:GLU:HA	4:I:287:VAL:HG22	2.03	0.41
4:I:432:GLY:N	4:I:452:LEU:O	2.43	0.41
4:I:472:GLN:HG2	4:I:486:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LEU:HD23	2:B:106:LEU:O	2.19	0.41
4:H:558:GLN:O	4:H:559:GLU:HB3	2.20	0.41
2:B:35:PHE:HB2	2:B:200:ILE:HG13	2.02	0.41
3:E:123:ALA:O	3:E:127:ILE:HG12	2.21	0.41
4:H:227:MET:HE2	4:H:227:MET:HB2	1.86	0.41
2:C:90:SER:O	2:C:94:THR:N	2.37	0.41
3:D:61:LEU:HD23	3:D:61:LEU:HA	1.78	0.41
4:I:227:MET:HE2	4:I:227:MET:HB2	1.87	0.41
4:I:353:ASP:O	4:I:356:PRO:HD2	2.21	0.41
1:A:150:ASP:O	1:A:158:ARG:NH1	2.53	0.41
1:A:390:MET:HA	1:A:395:ILE:HG21	2.03	0.41
2:B:264:LYS:HE2	2:B:282:ILE:HD13	1.98	0.41
2:C:31:VAL:HG12	2:C:195:ILE:HD13	2.03	0.41
3:E:31:LEU:HD12	3:E:32:ALA:N	2.36	0.41
4:H:73:PHE:CD1	4:H:84:VAL:HG22	2.55	0.41
4:H:231:PHE:CE1	4:H:283:VAL:HG11	2.55	0.41
4:H:446:GLY:O	4:H:476:ILE:HG13	2.20	0.41
4:H:560:PHE:CZ	4:H:633:MET:HG3	2.55	0.41
1:A:204:TYR:CD1	1:A:226:THR:HB	2.56	0.41
2:B:31:VAL:HB	2:B:196:ASN:H	1.86	0.41
2:B:98:PHE:HB3	2:B:141:GLN:HE21	1.86	0.41
2:C:271:LEU:HG	2:C:272:LEU:HD12	2.03	0.41
4:I:170:THR:O	4:I:172:PRO:HD3	2.21	0.41
1:A:56:PHE:O	1:A:81:LEU:HA	2.21	0.41
1:A:170:ALA:HB3	1:A:192:ASN:ND2	2.34	0.41
1:A:277:ASP:OD1	1:A:277:ASP:N	2.54	0.41
1:A:308:LEU:HA	1:A:331:GLN:O	2.21	0.41
1:A:323:GLY:N	1:A:349:GLY:O	2.49	0.41
2:B:38:ASN:HA	6:B:402:ATP:O1G	2.21	0.41
2:B:141:GLN:HA	2:B:144:LEU:HD12	2.02	0.41
2:C:174:LEU:HB3	2:C:179:THR:OG1	2.21	0.41
3:E:131:VAL:HG12	3:E:132:GLU:N	2.36	0.41
4:H:194:ASN:HD21	4:H:242:THR:HB	1.86	0.41
4:H:321:VAL:HG13	4:H:348:SER:OG	2.21	0.41
4:H:430:GLN:HE21	4:H:430:GLN:HB2	1.73	0.41
4:H:459:ARG:HA	4:H:459:ARG:HD2	1.85	0.41
4:I:109:LEU:HB3	4:I:604:ILE:HD12	2.03	0.41
4:I:277:VAL:HG11	4:I:355:LEU:HD22	2.03	0.41
1:A:229:ALA:HB1	1:A:231:MET:HE3	2.02	0.41
2:B:130:SER:H	2:B:133:MET:HE3	1.85	0.41
3:D:2:ASN:C	3:D:4:VAL:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:54:THR:O	3:D:58:LEU:HB3	2.21	0.41
4:H:609:ASP:OD1	4:H:609:ASP:N	2.47	0.41
2:B:150:LEU:HB3	2:B:181:ILE:CD1	2.51	0.40
3:D:214:LEU:O	3:D:215:LEU:C	2.64	0.40
4:H:254:THR:HG23	4:H:328:CYS:HB2	2.01	0.40
4:I:226:THR:OG1	4:I:228:GLU:OE1	2.32	0.40
2:B:24:LEU:HD11	2:B:32:LEU:HD11	2.04	0.40
2:B:264:LYS:NZ	2:B:282:ILE:HD13	2.36	0.40
2:C:35:PHE:O	2:C:200:ILE:HD12	2.21	0.40
3:D:5:TRP:CD1	3:D:9:ARG:HH12	2.39	0.40
3:D:24:ILE:HG23	3:D:115:ALA:HB1	2.04	0.40
4:H:462:PRO:O	4:I:71:TYR:OH	2.29	0.40
1:A:162:ILE:HB	1:A:184:ILE:HG22	2.04	0.40
1:A:370:TYR:O	1:A:372:PRO:HD3	2.20	0.40
2:C:74:ARG:NH1	3:D:94:PRO:HB2	2.37	0.40
2:C:89:LEU:O	2:C:126:VAL:HG23	2.21	0.40
2:C:221:LEU:HD23	2:C:222:PRO:O	2.20	0.40
3:E:48:PHE:HE2	3:E:134:VAL:HB	1.85	0.40
4:I:140:TYR:HB2	4:I:503:GLN:OE1	2.22	0.40
1:A:144:GLY:HA2	1:A:174:HIS:O	2.21	0.40
1:A:288:LEU:HB3	1:A:310:ILE:HD13	2.03	0.40
2:B:6:ILE:HD12	2:B:24:LEU:HB3	2.04	0.40
2:C:152:LEU:HD23	2:C:155:PRO:CB	2.51	0.40
3:D:152:LEU:HD12	3:D:253:TRP:HZ3	1.86	0.40
4:H:486:ASP:O	4:I:91:ARG:NH1	2.54	0.40
4:I:149:ASP:HB3	4:I:154:ARG:HB2	2.03	0.40
4:I:259:GLU:HG2	4:I:270:ASN:H	1.86	0.40
1:A:188:THR:HG21	4:H:265:GLY:HA3	2.04	0.40
4:H:488:PRO:HD2	4:I:91:ARG:HB3	2.04	0.40
4:I:94:MET:HG3	4:I:95:ARG:N	2.36	0.40
4:I:347:CYS:O	4:I:373:GLU:HA	2.22	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	401/436 (92%)	361 (90%)	37 (9%)	3 (1%)	18	50
2	B	296/313 (95%)	272 (92%)	22 (7%)	2 (1%)	18	50
2	C	296/313 (95%)	280 (95%)	13 (4%)	3 (1%)	12	42
3	D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	30	61
3	E	252/276 (91%)	243 (96%)	9 (4%)	0	100	100
4	H	581/646 (90%)	553 (95%)	27 (5%)	1 (0%)	43	72
4	I	579/646 (90%)	556 (96%)	23 (4%)	0	100	100
All	All	2678/2906 (92%)	2519 (94%)	149 (6%)	10 (0%)	31	61

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	248	PRO
1	A	245	GLN
2	B	13	TYR
2	C	40	ALA
2	B	125	ARG
4	H	364	ALA
1	A	408	ILE
2	C	41	GLY
2	C	154	GLN
1	A	76	GLY

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	340/365 (93%)	340 (100%)	0	100	100
2	B	243/256 (95%)	240 (99%)	3 (1%)	63	71
2	C	243/256 (95%)	240 (99%)	3 (1%)	63	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	211/212 (100%)	208 (99%)	3 (1%)	59	70
3	E	200/212 (94%)	199 (100%)	1 (0%)	81	81
4	H	498/545 (91%)	492 (99%)	6 (1%)	63	71
4	I	496/545 (91%)	496 (100%)	0	100	100
All	All	2231/2391 (93%)	2215 (99%)	16 (1%)	73	77

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	18	VAL
2	B	44	THR
2	B	131	LYS
2	C	16	MET
2	C	124	ARG
2	C	154	GLN
3	D	211	TRP
3	D	218	THR
3	D	239	LEU
3	E	247	VAL
4	H	427	VAL
4	H	430	GLN
4	H	551	MET
4	H	557	VAL
4	H	559	GLU
4	H	626	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	193	HIS
1	A	214	ASN
1	A	311	HIS
1	A	324	ASN
1	A	385	GLN
2	B	37	HIS
2	B	38	ASN
2	B	141	GLN
2	B	154	GLN
2	B	270	GLN

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Mol	Chain	Res	Type
2	C	38	ASN
2	C	82	ASN
2	C	154	GLN
2	C	186	HIS
2	C	196	ASN
3	D	6	ASN
3	E	3	GLN
4	H	232	GLN
4	H	238	ASN
4	H	390	ASN
4	H	430	GLN
4	H	564	GLN
4	H	626	HIS
4	I	152	ASN
4	I	187	HIS
4	I	211	GLN
4	I	326	HIS
4	I	470	ASN
4	I	503	GLN
4	I	574	ASN
4	I	583	HIS
4	I	599	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
6	ATP	B	402	5	32,33,33	0.59	0	48,52,52	0.73	0
6	ATP	C	402	5	32,33,33	0.60	0	48,52,52	0.68	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
6	ATP	B	402	5	-	4/22/38/38	0/3/3/3
6	ATP	C	402	5	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	402	ATP	C5'-O5'-PA-O2A
6	B	402	ATP	C5'-O5'-PA-O3A
6	B	402	ATP	PB-O3B-PG-O1G
6	B	402	ATP	PB-O3B-PG-O3G
6	C	402	ATP	C4'-C5'-O5'-PA
6	C	402	ATP	C3'-C4'-C5'-O5'

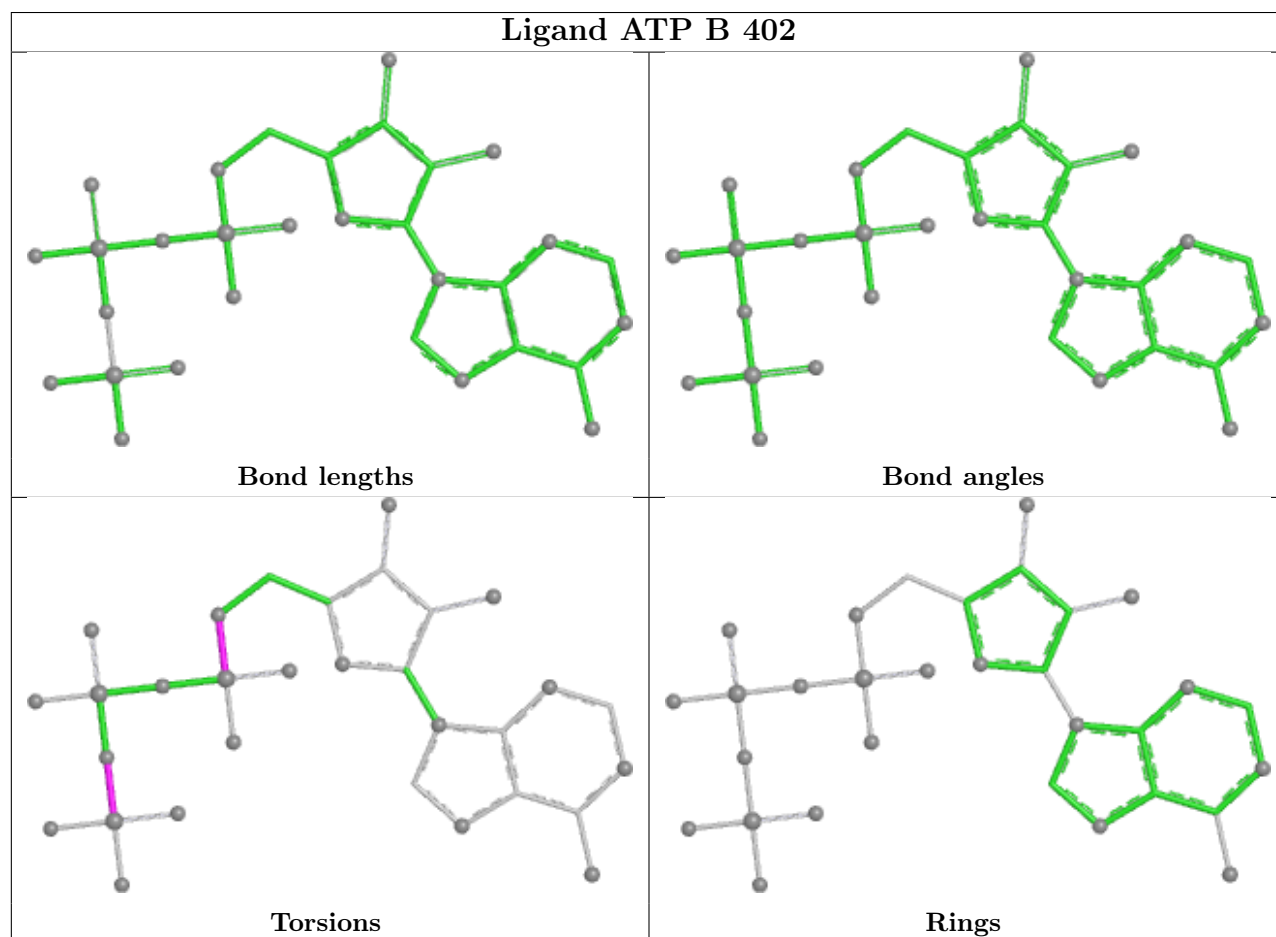
There are no ring outliers.

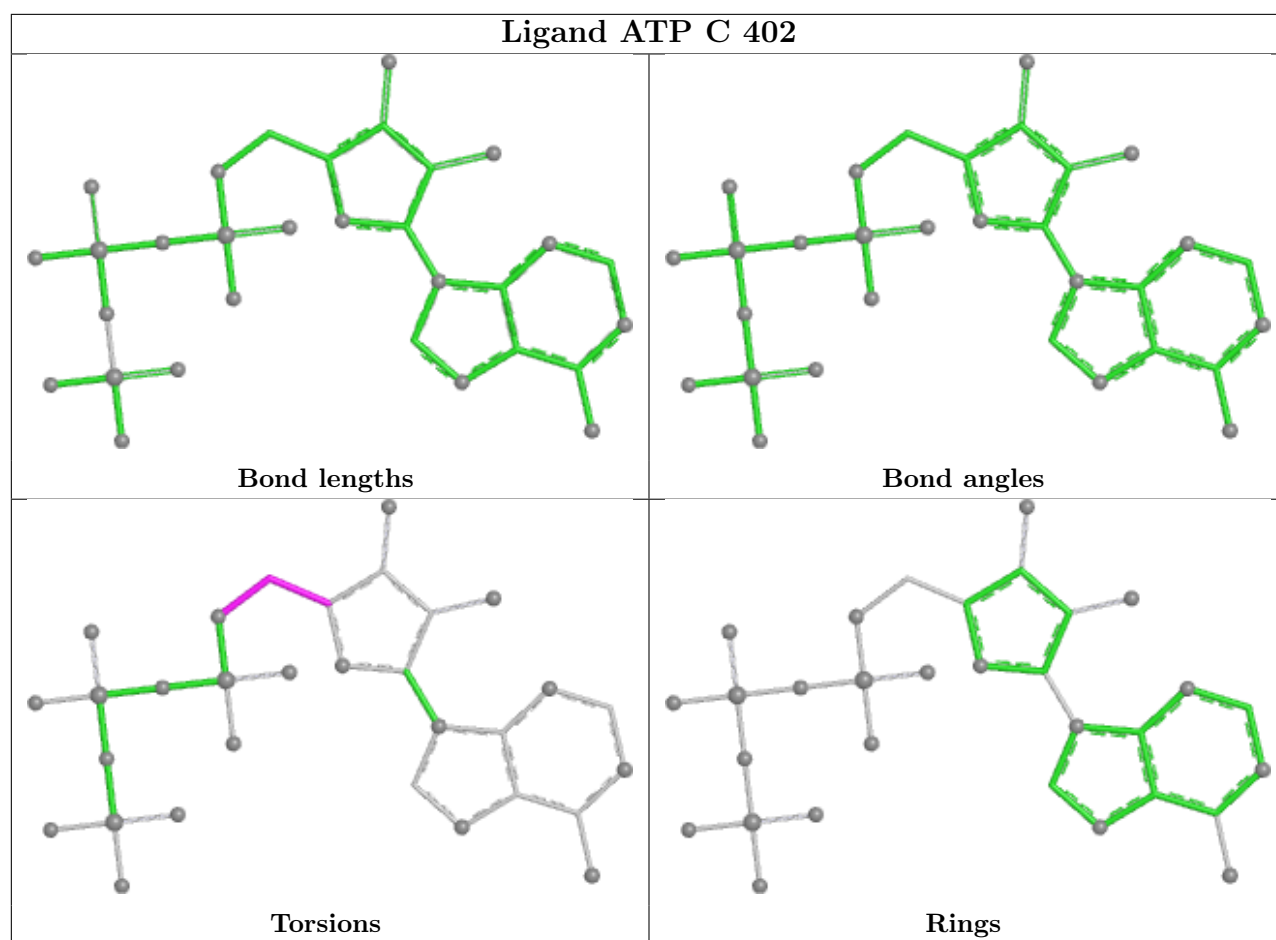
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	402	ATP	1	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.

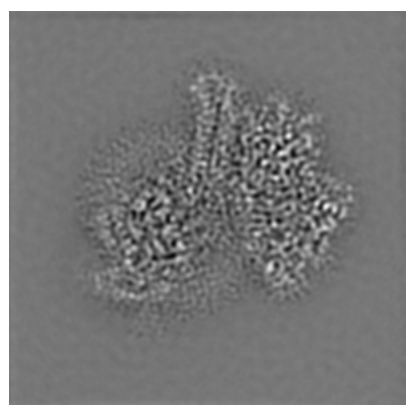
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13885. These allow visual inspection of the internal detail of the map and identification of artifacts.

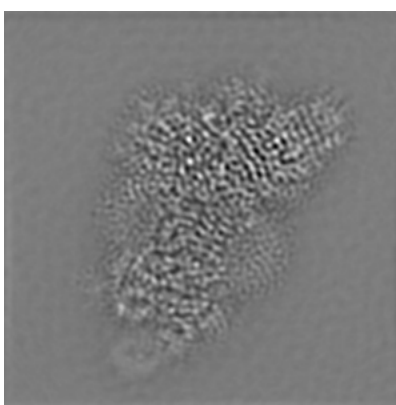
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

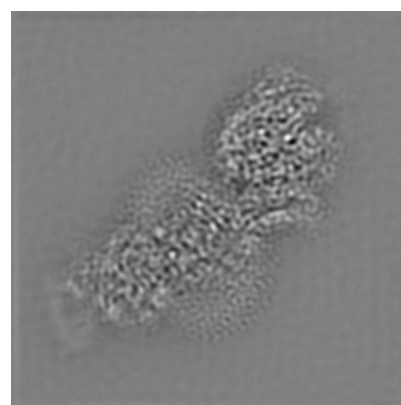
6.1.1 Primary map



X



Y

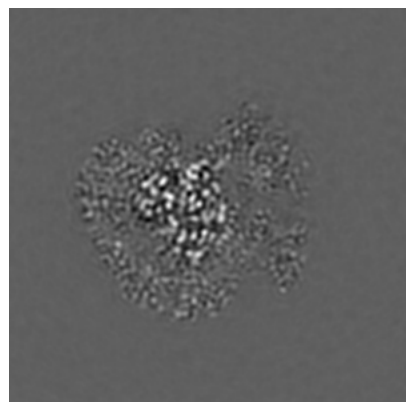


Z

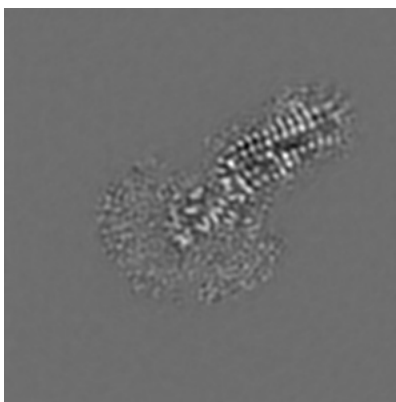
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

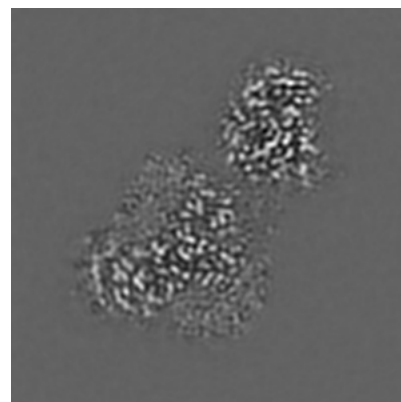
6.2.1 Primary map



X Index: 120



Y Index: 120

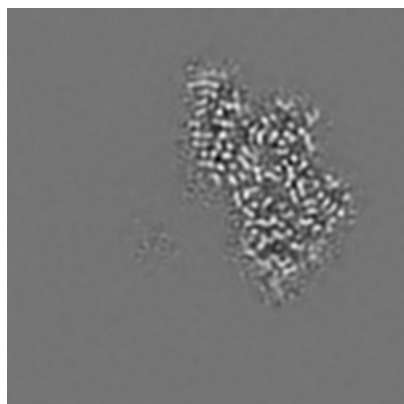


Z Index: 120

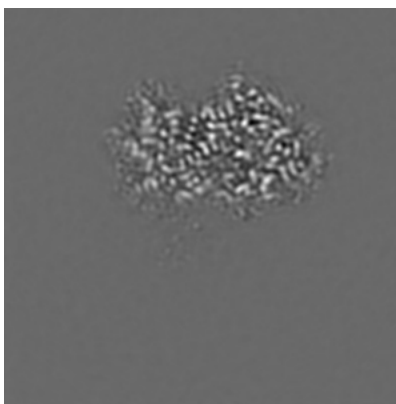
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

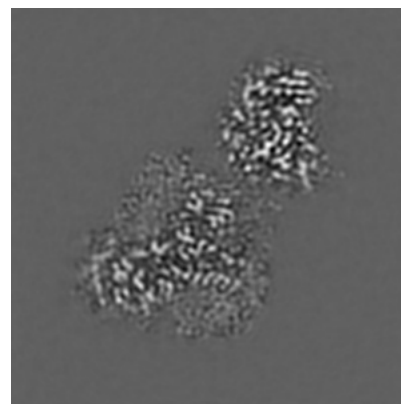
6.3.1 Primary map



X Index: 161



Y Index: 157

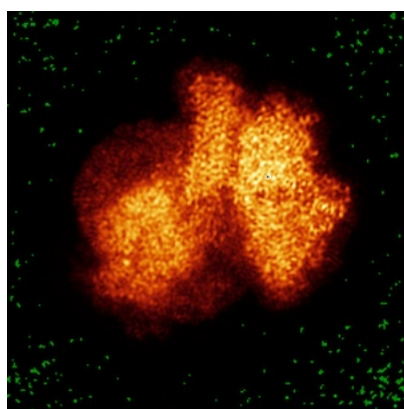


Z Index: 121

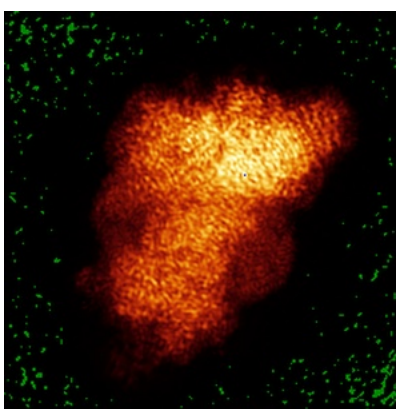
The images above show the largest variance slices of the map in three orthogonal directions.

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

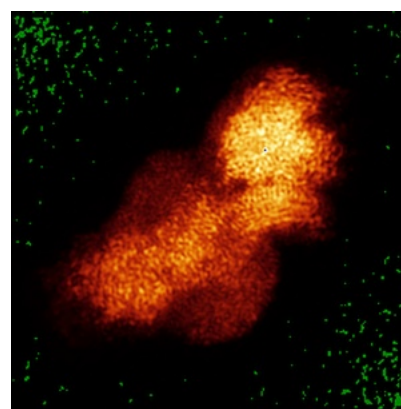
6.4.1 Primary map



X



Y

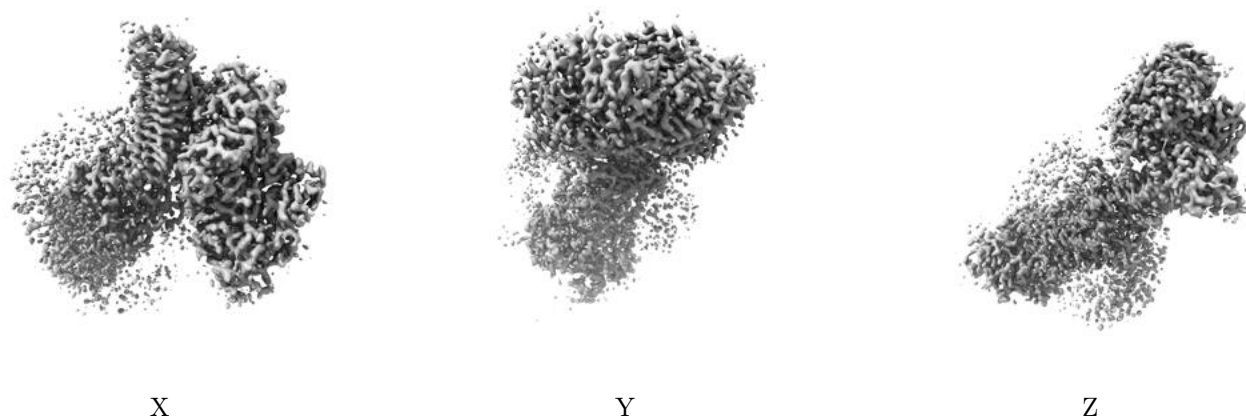


Z

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

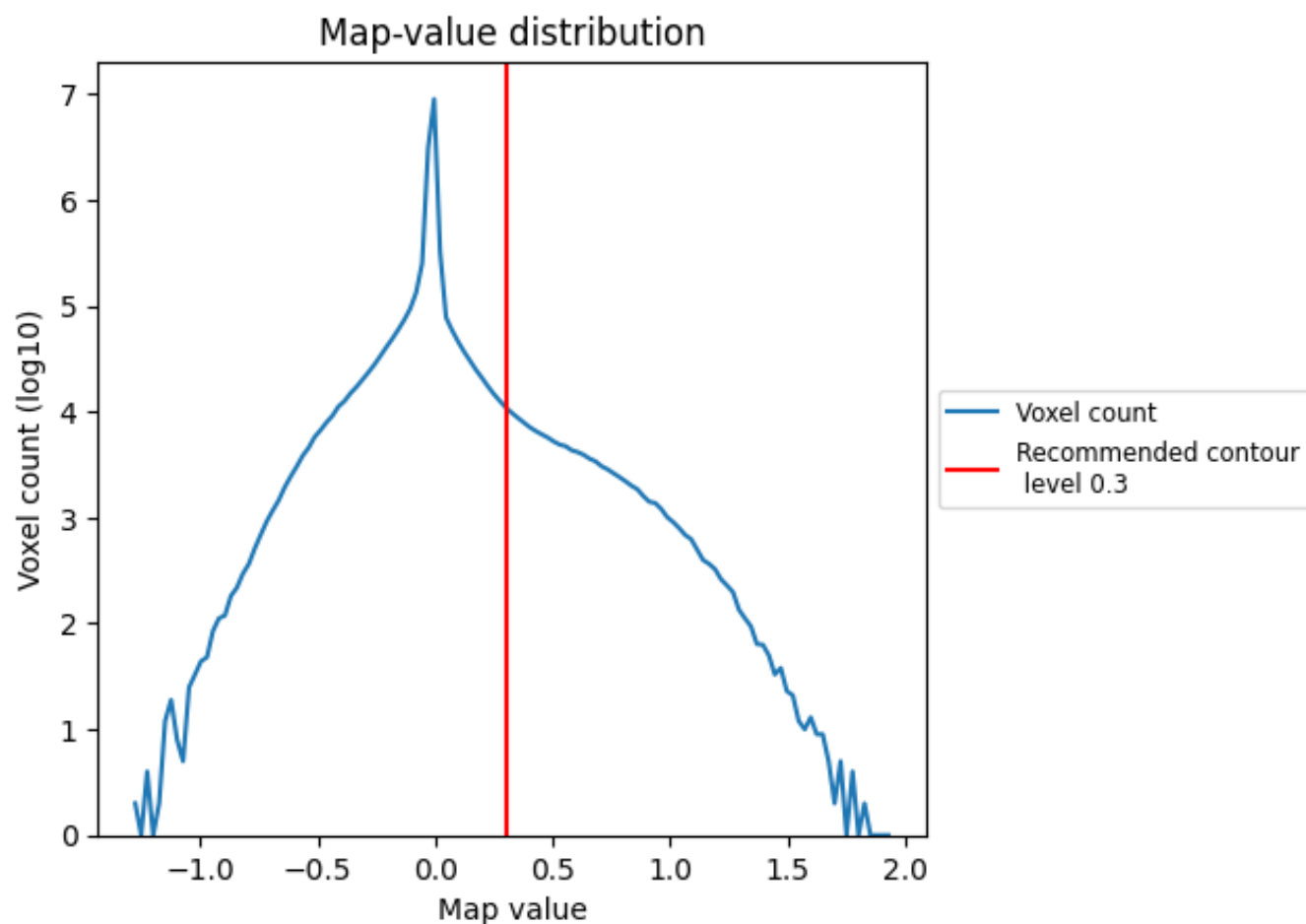
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

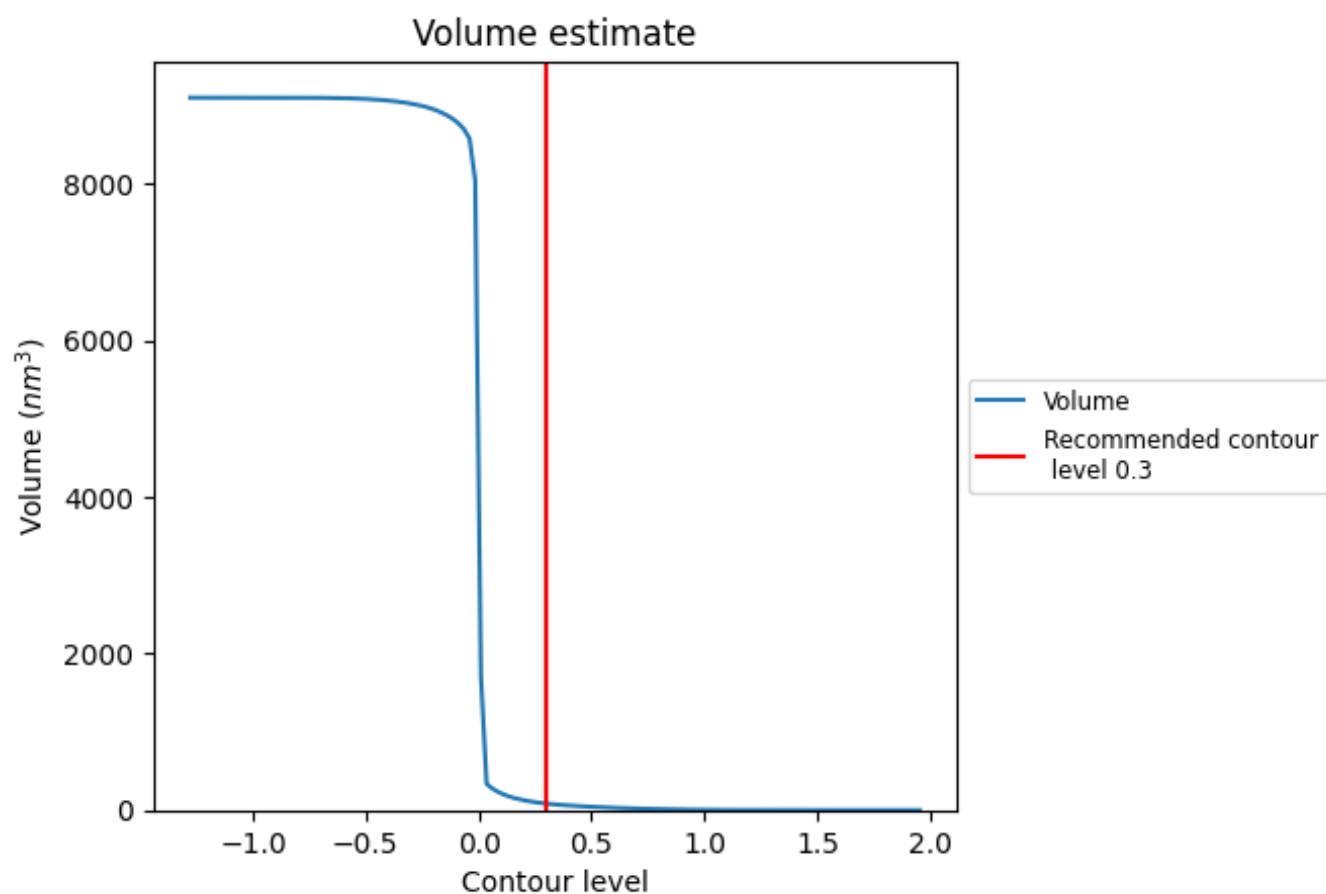
This section contains the results of statistical analysis of the map.

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.

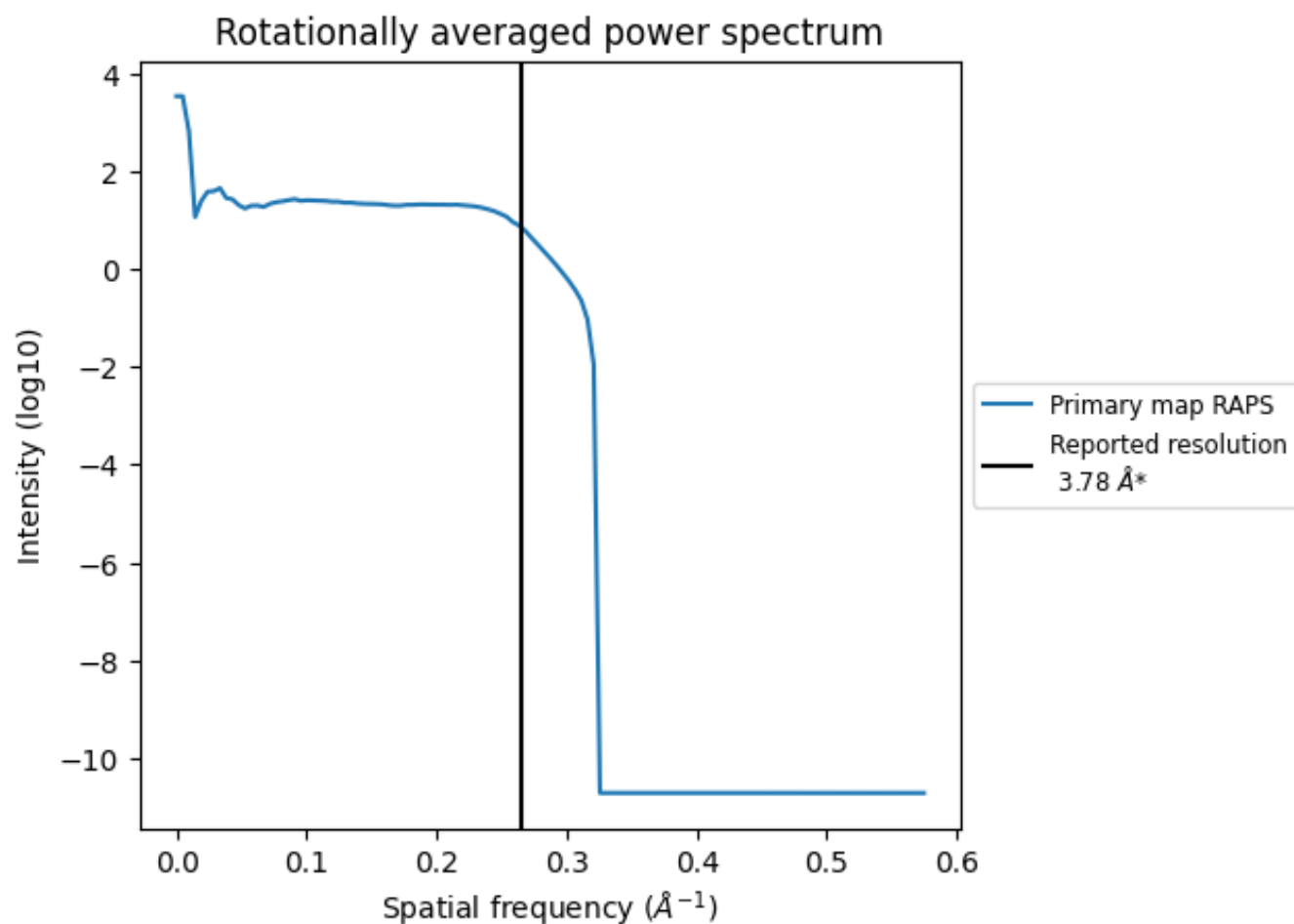
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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 0.265 $\text{\AA}^{-1}$

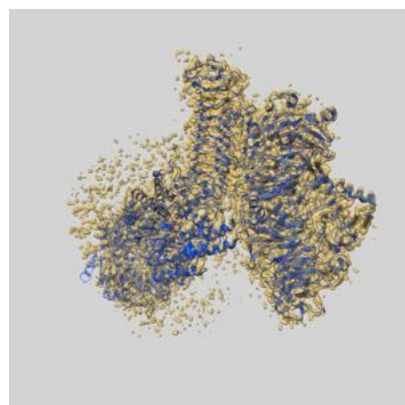
8 Fourier-Shell correlation

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

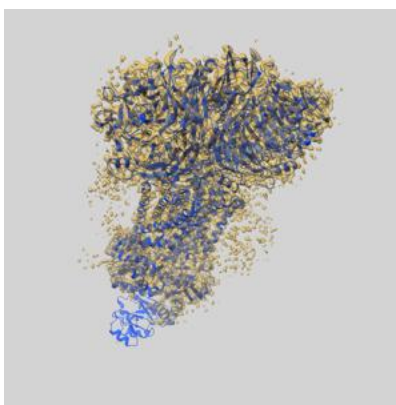
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13885 and PDB model 7QBA. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

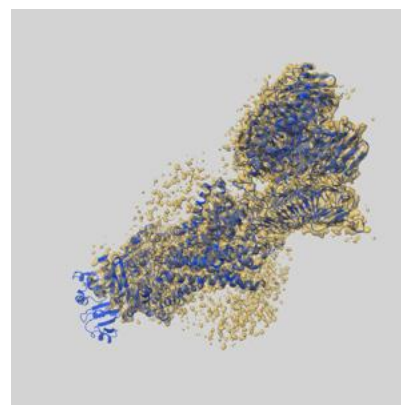
9.1 Map-model overlay [i](#)



X



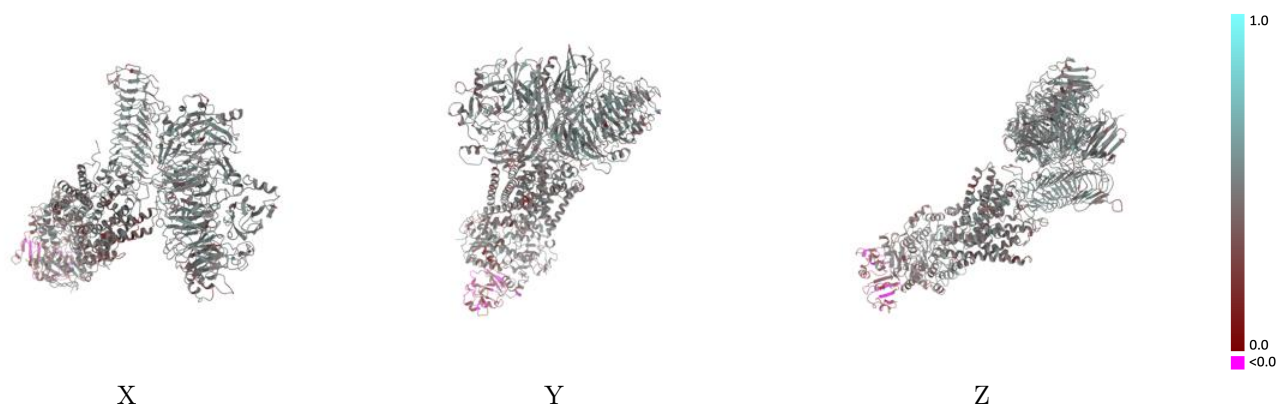
Y



Z

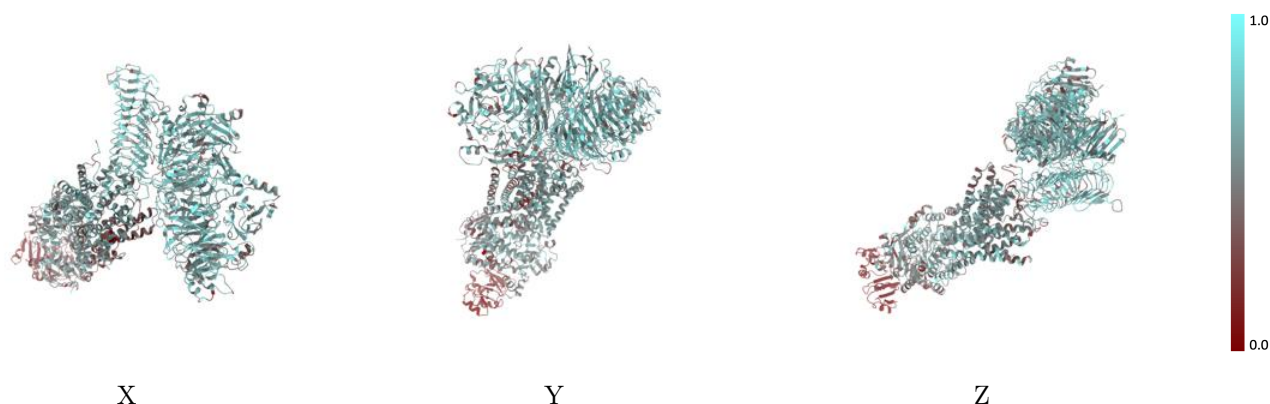
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



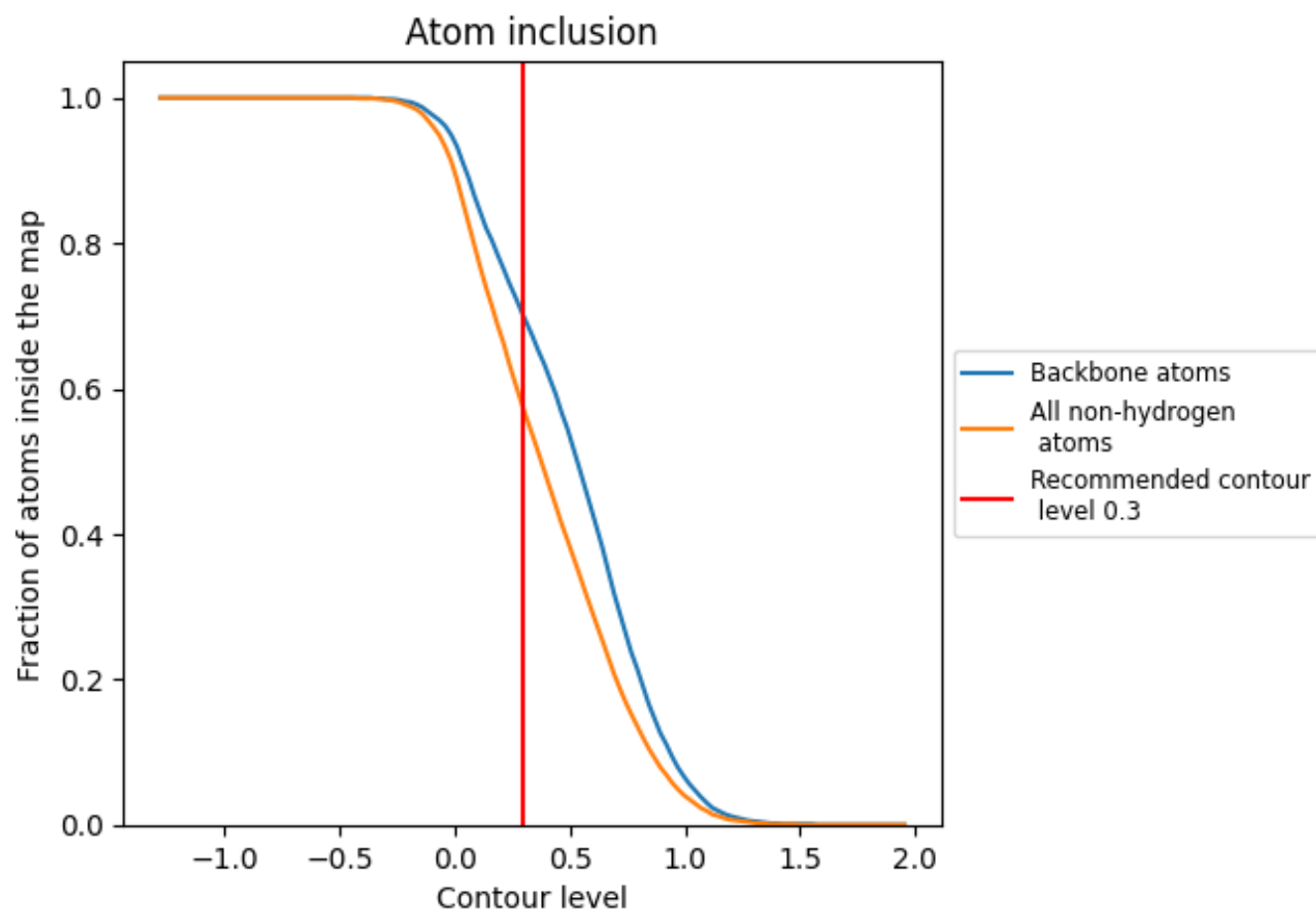
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 57% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5710	0.4500
A	0.6420	0.4870
B	0.4220	0.3660
C	0.3950	0.3580
D	0.5010	0.4260
E	0.5920	0.4540
H	0.6530	0.4920
I	0.6290	0.4810

1.0

0.0

<0.0