



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 04:17 PM JST

PDB ID : 7CX7
Title : Crystal structure of Arabinose isomerase from hybrid AI8
Authors : Hoang, N.K.Q.; Dhanasingh, I.; Cao, T.P.; Sung, J.Y.; Shin, S.M.; Lee, D.W.;
Lee, S.H.
Deposited on : 2020-09-01
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

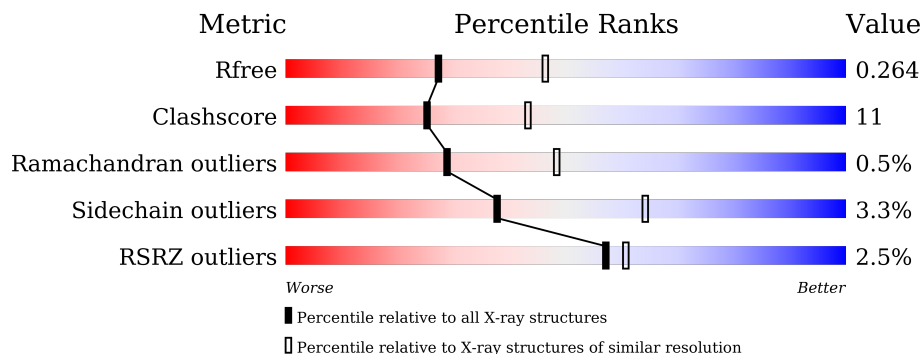
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	 74% 24% .
1	B	497	 74% 25% .
1	C	497	 72% 27% .
1	D	497	 72% 26% ..
1	E	497	 78% 21%
1	F	497	 73% 24% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	E	501	-	-	X	-
4	GOL	C	503	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

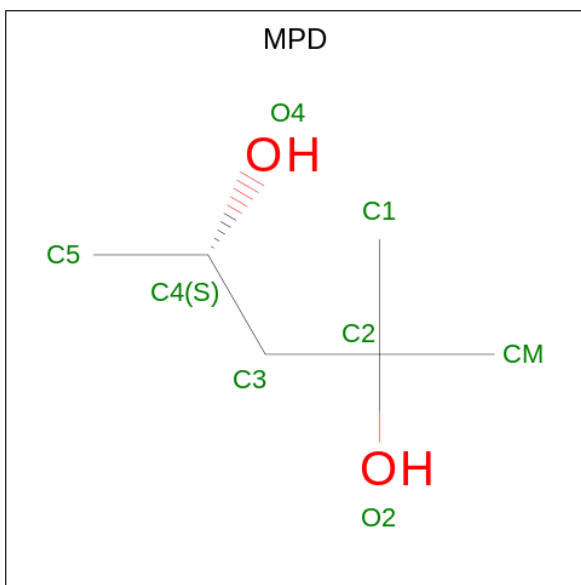
- Molecule 1 is a protein called L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	495	3916	2486	692	714	24	0	0	0
1	B	495	3916	2486	692	714	24	0	0	0
1	C	495	3916	2486	692	714	24	0	0	0
1	D	494	3904	2477	691	712	24	0	0	0
1	E	495	3916	2486	692	714	24	0	0	0
1	F	490	3872	2456	687	705	24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q5KYP7
B	1	MET	-	initiating methionine	UNP Q5KYP7
C	1	MET	-	initiating methionine	UNP Q5KYP7
D	1	MET	-	initiating methionine	UNP Q5KYP7
E	1	MET	-	initiating methionine	UNP Q5KYP7
F	1	MET	-	initiating methionine	UNP Q5KYP7

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

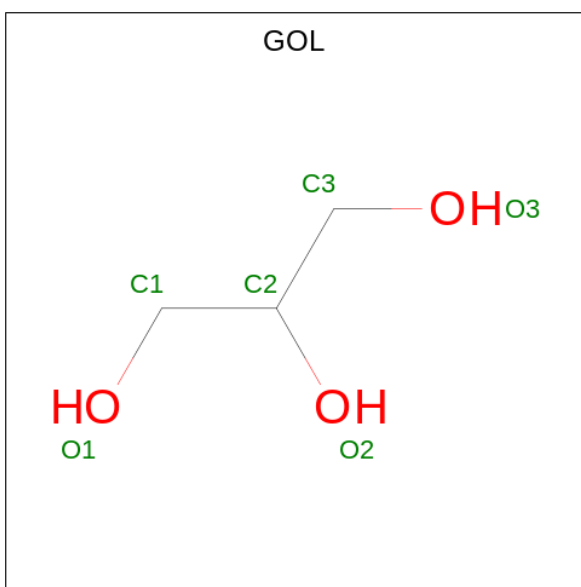
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mn 2 2	0	0
3	B	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mn	0	0
			2	2		
3	D	1	Total	Mn	0	0
			1	1		
3	E	2	Total	Mn	0	0
			2	2		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

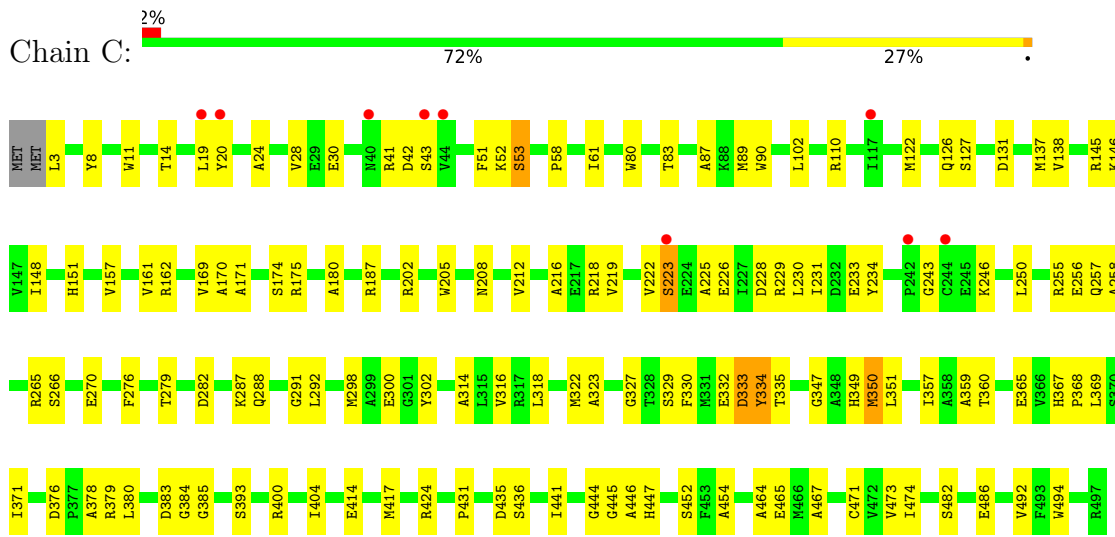
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	72	Total	O	0	0
			72	72		
5	C	66	Total	O	0	0
			66	66		
5	D	59	Total	O	0	0
			59	59		

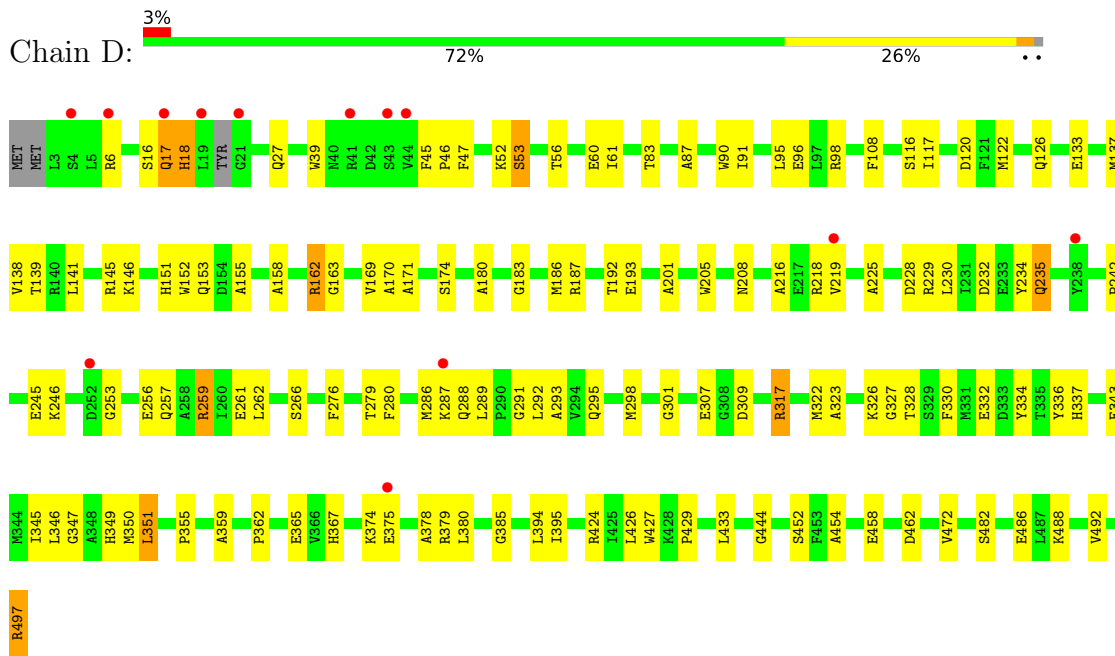
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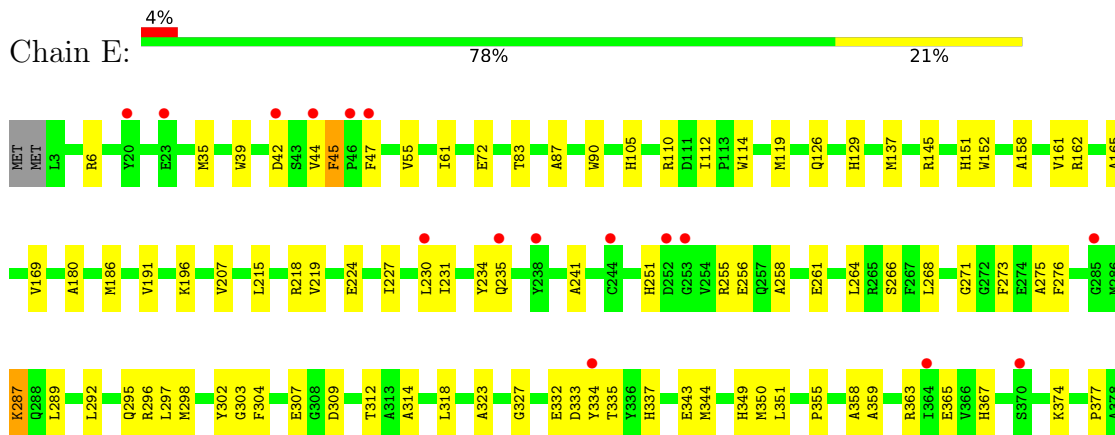
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	47	Total O 47 47	0	0
5	F	52	Total O 52 52	0	0

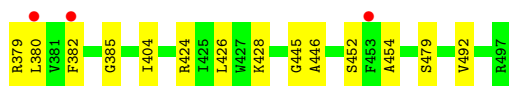


● Molecule 1: L-arabinose isomerase

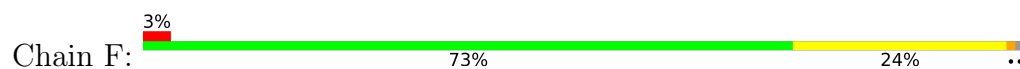


● Molecule 1: L-arabinose isomerase





● Molecule 1: L-arabinose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.59Å 81.91Å 192.00Å 90.00° 117.90° 90.00°	Depositor
Resolution (Å)	48.59 – 2.49 48.54 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.59-2.49) 98.6 (48.54-2.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.268 0.193 , 0.264	Depositor DCC
R_{free} test set	4784 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtrriage
Anisotropy	0.042	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23927	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, GOL, MN

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	0.68	0/4015	0.88	0/5433
1	B	0.68	0/4015	0.85	0/5433
1	C	0.68	0/4015	0.86	0/5433
1	D	0.69	0/4001	0.87	1/5412 (0.0%)
1	E	0.68	0/4015	0.85	0/5433
1	F	0.67	0/3967	0.86	0/5363
All	All	0.68	0/24028	0.86	1/32507 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
1	F	0	4
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	ARG	NE-CZ-NH1	5.51	123.06	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	SER	Peptide
1	C	329	SER	Peptide
1	D	351	LEU	Peptide
1	D	53	SER	Peptide
1	F	245	GLU	Peptide
1	F	329	SER	Peptide
1	F	351	LEU	Peptide
1	F	53	SER	Peptide

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	3916	0	3804	88	0
1	B	3916	0	3804	82	0
1	C	3916	0	3804	103	0
1	D	3904	0	3794	87	0
1	E	3916	0	3804	68	0
1	F	3872	0	3767	88	0
2	A	16	0	28	7	0
2	B	8	0	14	0	0
2	C	16	0	28	6	0
2	E	16	0	28	7	0
2	F	16	0	28	3	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
4	C	6	0	8	4	0
5	A	104	0	0	6	0
5	B	72	0	0	3	0
5	C	66	0	0	2	0
5	D	59	0	0	3	0
5	E	47	0	0	1	0
5	F	52	0	0	1	0
All	All	23927	0	22911	496	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 11.

All (496) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:VAL:HG11	1:B:145:ARG:HD3	1.28	1.15
1:A:138:VAL:HG11	1:A:145:ARG:HD3	1.29	1.05
1:D:98:ARG:NH1	1:F:95:LEU:O	1.91	1.02
1:C:138:VAL:HG11	1:C:145:ARG:HD3	1.43	0.98
1:E:45:PHE:HB2	2:E:501:MPD:H51	1.48	0.92
1:F:138:VAL:HG11	1:F:145:ARG:HD3	1.53	0.90
1:F:200:GLU:HG2	1:F:205:TRP:O	1.72	0.89
1:A:344:MET:CE	1:A:411:VAL:HG21	2.04	0.88
1:D:138:VAL:HG11	1:D:145:ARG:HD3	1.57	0.86
1:F:175:ARG:HG3	2:F:502:MPD:H52	1.56	0.85
1:B:138:VAL:CG1	1:B:145:ARG:HD3	2.08	0.83
1:D:458:GLU:OE2	5:D:601:HOH:O	1.96	0.82
1:A:344:MET:HE2	1:A:411:VAL:HG21	1.61	0.81
1:C:257:GLN:HG2	1:C:288:GLN:HE22	1.47	0.80
1:C:447:HIS:HB2	1:F:129:HIS:HB2	1.64	0.76
1:A:298:MET:CE	1:A:330:PHE:H	1.98	0.75
1:B:344:MET:HE2	1:B:426:LEU:HD13	1.66	0.75
1:D:139:THR:OG1	1:D:145:ARG:NH2	2.20	0.74
1:C:492:VAL:HG21	1:F:493:PHE:HA	1.69	0.74
1:B:231:ILE:HD11	1:B:255:ARG:HA	1.69	0.74
1:D:235:GLN:HE22	1:D:246:LYS:HG3	1.54	0.73
1:D:365:GLU:OE1	1:D:367:HIS:NE2	2.14	0.72
1:B:212:VAL:HG21	1:B:282:ASP:O	1.89	0.72
1:F:35:MET:HA	1:F:152:TRP:CZ3	2.26	0.71
1:B:359:ALA:HB2	1:B:385:GLY:HA2	1.73	0.71
1:C:298:MET:HE1	1:C:330:PHE:H	1.56	0.71
1:A:47:PHE:CE2	1:A:169:VAL:HG21	2.26	0.69
1:A:161:VAL:HG11	2:A:501:MPD:HM3	1.74	0.69
1:B:253:GLY:HA2	1:B:288:GLN:HE22	1.58	0.69
1:C:145:ARG:HG2	1:C:145:ARG:HH11	1.58	0.69
1:B:108:PHE:O	1:B:151:HIS:NE2	2.23	0.68
1:A:200:GLU:HG2	1:A:205:TRP:O	1.93	0.68
1:A:126:GLN:HB3	1:A:129:HIS:NE2	2.08	0.68
1:C:465:GLU:OE2	5:C:601:HOH:O	2.11	0.68
1:A:344:MET:HE1	1:A:411:VAL:HG21	1.75	0.67
1:D:138:VAL:CG1	1:D:145:ARG:HD3	2.24	0.67
1:A:138:VAL:CG1	1:A:145:ARG:HD3	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLU:OE1	5:A:602:HOH:O	2.14	0.66
1:A:486:GLU:OE1	5:A:601:HOH:O	2.13	0.66
1:E:289:LEU:HD23	1:E:351:LEU:HD12	1.78	0.66
1:D:323:ALA:HB1	1:D:454:ALA:HB3	1.76	0.66
1:F:288:GLN:OE1	1:F:377:PRO:HA	1.96	0.66
1:A:87:ALA:HB1	1:A:137:MET:HB2	1.77	0.66
1:C:11:TRP:CD2	1:C:52:LYS:HE3	2.31	0.66
1:F:35:MET:HG2	1:F:152:TRP:CD2	2.30	0.66
1:F:227:ILE:O	1:F:231:ILE:HD12	1.96	0.65
1:A:69:ASN:ND2	1:A:96:GLU:O	2.29	0.65
1:D:218:ARG:HD3	1:D:266:SER:OG	1.96	0.65
1:E:87:ALA:HB1	1:E:137:MET:HB2	1.79	0.65
1:B:231:ILE:CD1	1:B:255:ARG:HG2	2.28	0.64
1:A:298:MET:HE3	1:A:330:PHE:H	1.63	0.64
1:F:186:MET:HB2	1:F:307:GLU:HB3	1.80	0.64
1:F:492:VAL:HG12	1:F:495:ARG:NH2	2.14	0.64
1:F:299:ALA:HB2	1:F:355:PRO:HD2	1.80	0.63
1:F:359:ALA:HB2	1:F:385:GLY:HA2	1.80	0.63
1:F:138:VAL:CG1	1:F:145:ARG:HD3	2.27	0.63
1:A:298:MET:HE1	1:A:330:PHE:H	1.64	0.62
1:F:355:PRO:HG3	1:F:380:LEU:HD12	1.80	0.62
1:A:122:MET:O	1:A:126:GLN:HG2	2.00	0.62
1:A:158:ALA:HA	2:A:501:MPD:H12	1.82	0.62
1:D:359:ALA:HB2	1:D:385:GLY:HA2	1.81	0.62
1:F:289:LEU:HD23	1:F:351:LEU:HD12	1.82	0.62
1:F:298:MET:HE3	1:F:330:PHE:H	1.64	0.62
1:F:332:GLU:OE1	1:F:349:HIS:CD2	2.53	0.61
1:C:180:ALA:O	1:C:276:PHE:HA	2.00	0.61
1:C:257:GLN:HG2	1:C:288:GLN:NE2	2.14	0.61
1:C:83:THR:HA	1:C:126:GLN:HB2	1.82	0.61
1:E:47:PHE:CE2	1:E:169:VAL:HG21	2.35	0.61
1:B:105:HIS:HB3	1:B:149:VAL:HG22	1.82	0.60
1:E:359:ALA:HB2	1:E:385:GLY:HA2	1.84	0.60
1:A:492:VAL:HG11	1:E:492:VAL:HG12	1.82	0.60
1:D:146:LYS:NZ	1:D:458:GLU:OE2	2.35	0.60
1:B:497:ARG:NH1	5:B:601:HOH:O	2.27	0.59
1:E:161:VAL:HG11	2:E:501:MPD:H11	1.85	0.59
1:A:344:MET:HE3	1:A:428:LYS:HE2	1.85	0.59
2:A:502:MPD:O4	2:A:502:MPD:O2	2.15	0.59
1:C:332:GLU:OE1	1:C:349:HIS:CD2	2.56	0.59
1:E:251:HIS:HE1	5:E:625:HOH:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:LEU:HD21	1:D:350:MET:HE3	1.85	0.58
1:E:42:ASP:O	1:E:44:VAL:HG23	2.03	0.58
1:D:98:ARG:CZ	1:F:95:LEU:O	2.51	0.58
1:E:186:MET:HB2	1:E:307:GLU:HB3	1.84	0.58
1:F:244:CYS:SG	1:F:366:VAL:HG23	2.43	0.58
1:E:158:ALA:O	1:E:162:ARG:HB2	2.03	0.58
1:D:180:ALA:O	1:D:276:PHE:HA	2.04	0.58
1:D:497:ARG:HG2	1:D:497:ARG:HH11	1.69	0.58
1:A:138:VAL:HG13	1:A:143:MET:HG3	1.86	0.57
1:B:224:GLU:OE2	1:B:259:ARG:NH2	2.37	0.57
1:C:257:GLN:HE21	1:C:288:GLN:HE21	1.51	0.57
1:B:347:GLY:HA3	1:B:427:TRP:HZ3	1.70	0.57
1:A:375:GLU:OE1	5:A:603:HOH:O	2.17	0.57
1:F:323:ALA:O	1:F:324:ASP:HB2	2.03	0.57
1:D:298:MET:HE1	1:D:330:PHE:H	1.68	0.57
1:D:61:ILE:HG21	1:D:90:TRP:HA	1.87	0.57
1:D:295:GLN:NE2	1:D:380:LEU:HB2	2.20	0.57
1:E:191:VAL:HG21	1:E:446:ALA:HB2	1.87	0.57
1:B:256:GLU:O	1:B:260:ILE:HG12	2.05	0.57
1:F:298:MET:CE	1:F:330:PHE:H	2.17	0.57
1:C:225:ALA:O	1:C:229:ARG:HD2	2.05	0.57
1:C:162:ARG:CG	2:C:501:MPD:HM3	2.35	0.56
1:C:314:ALA:O	1:C:318:LEU:HG	2.05	0.56
1:E:224:GLU:OE1	1:E:255:ARG:NH2	2.36	0.56
1:E:162:ARG:NH2	2:E:501:MPD:O4	2.38	0.56
1:D:151:HIS:HE1	1:D:153:GLN:OE1	1.88	0.56
1:D:350:MET:O	1:D:351:LEU:HD23	2.06	0.56
1:B:139:THR:OG1	1:B:145:ARG:NH2	2.39	0.56
1:C:256:GLU:HG2	1:C:287:LYS:CB	2.36	0.56
1:C:138:VAL:CG1	1:C:145:ARG:HD3	2.27	0.56
1:E:61:ILE:HG21	1:E:90:TRP:HA	1.88	0.56
1:A:39:TRP:HH2	1:A:104:LEU:CD2	2.19	0.56
1:E:227:ILE:HG22	1:E:231:ILE:HD11	1.88	0.56
1:D:257:GLN:HG3	1:D:378:ALA:HB3	1.89	0.55
1:E:45:PHE:CB	2:E:501:MPD:H51	2.30	0.55
1:F:367:HIS:O	1:F:376:ASP:HB3	2.06	0.55
1:A:318:LEU:HD13	1:A:463:PHE:CZ	2.41	0.55
1:A:180:ALA:O	1:A:276:PHE:HA	2.05	0.55
1:F:245:GLU:OE1	1:F:249:PRO:HD2	2.07	0.55
1:C:218:ARG:NH1	1:C:270:GLU:OE1	2.38	0.55
1:C:400:ARG:HD2	1:C:494:TRP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:HD11	1:F:201:ALA:HA	1.89	0.55
1:F:494:TRP:CE3	1:F:497:ARG:HD2	2.41	0.55
1:B:337:HIS:HB3	1:B:344:MET:HG2	1.89	0.54
1:C:219:VAL:HA	1:C:222:VAL:HG23	1.88	0.54
1:D:46:PRO:HD3	1:D:162:ARG:HB3	1.89	0.54
1:D:98:ARG:HH22	1:F:95:LEU:HB3	1.72	0.54
1:C:171:ALA:HB1	2:C:502:MPD:HM2	1.88	0.54
1:C:174:SER:HG	1:C:205:TRP:HE1	1.54	0.54
1:C:87:ALA:HB1	1:C:137:MET:HB2	1.89	0.54
1:E:180:ALA:O	1:E:276:PHE:HA	2.08	0.54
1:B:332:GLU:OE2	1:B:349:HIS:CD2	2.61	0.54
1:B:365:GLU:HB3	1:B:367:HIS:HE2	1.73	0.54
1:C:170:ALA:HB2	1:C:322:MET:HG3	1.89	0.54
1:C:230:LEU:O	1:C:233:GLU:N	2.41	0.54
1:A:359:ALA:HB2	1:A:385:GLY:HA2	1.88	0.54
1:D:56:THR:OG1	1:D:60:GLU:OE1	2.20	0.54
1:F:358:ALA:HB2	1:F:382:PHE:CD1	2.43	0.54
1:B:295:GLN:HG2	1:B:353:VAL:O	2.08	0.54
1:C:8:TYR:CD2	1:C:169:VAL:HG13	2.43	0.54
1:F:158:ALA:HA	2:F:501:MPD:H51	1.89	0.54
1:D:365:GLU:O	1:D:378:ALA:HA	2.08	0.53
1:A:42:ASP:C	1:A:44:VAL:H	2.12	0.53
1:A:265:ARG:NH2	1:A:300:GLU:OE2	2.40	0.53
1:D:47:PHE:CE1	1:D:169:VAL:HG21	2.44	0.53
1:E:112:ILE:HD12	1:E:114:TRP:CH2	2.44	0.53
1:D:186:MET:HA	5:D:615:HOH:O	2.09	0.53
1:E:351:LEU:HD21	1:E:377:PRO:HG2	1.91	0.53
1:A:11:TRP:CD2	1:A:52:LYS:HE3	2.44	0.53
1:C:3:LEU:HD11	1:C:302:TYR:CZ	2.44	0.53
1:D:355:PRO:HG3	1:D:380:LEU:HD12	1.89	0.53
1:F:139:THR:OG1	1:F:145:ARG:NH2	2.42	0.53
1:C:256:GLU:HG2	1:C:287:LYS:HB3	1.91	0.52
1:C:492:VAL:CG2	1:F:493:PHE:HA	2.39	0.52
1:C:51:PHE:CE2	1:C:53:SER:HA	2.44	0.52
1:E:355:PRO:HG3	1:E:380:LEU:CD1	2.39	0.52
1:C:223:SER:O	1:C:226:GLU:N	2.43	0.52
1:B:174:SER:HB2	1:B:318:LEU:HD21	1.92	0.52
1:E:83:THR:HA	1:E:126:GLN:HB2	1.92	0.52
1:C:208:ASN:HB3	1:D:187:ARG:HG2	1.91	0.52
1:C:447:HIS:HB2	1:F:129:HIS:CB	2.38	0.52
1:C:230:LEU:HD23	1:C:258:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ILE:HD11	1:D:122:MET:SD	2.50	0.52
1:D:301:GLY:O	1:D:317:ARG:NH2	2.43	0.52
1:E:241:ALA:HB2	1:E:363:ARG:HD2	1.91	0.52
1:A:146:LYS:NZ	5:A:614:HOH:O	2.43	0.52
1:A:186:MET:HB2	1:A:307:GLU:HB3	1.91	0.52
1:D:186:MET:HB2	1:D:307:GLU:HB3	1.92	0.51
1:E:327:GLY:O	1:E:452:SER:HA	2.11	0.51
1:B:347:GLY:HA3	1:B:427:TRP:CZ3	2.46	0.51
1:A:212:VAL:HG11	1:A:282:ASP:O	2.11	0.51
1:C:61:ILE:HG21	1:C:90:TRP:HA	1.92	0.51
1:E:6:ARG:CZ	1:E:72:GLU:HG2	2.40	0.51
1:C:473:VAL:N	4:C:503:GOL:O2	2.30	0.51
1:D:96:GLU:O	1:D:98:ARG:HG3	2.11	0.51
1:D:155:ALA:O	1:D:158:ALA:HB3	2.11	0.51
1:F:231:ILE:HD11	1:F:255:ARG:HG2	1.91	0.51
1:B:289:LEU:HD12	1:B:290:PRO:HD2	1.92	0.51
1:D:17:GLN:O	1:D:56:THR:HB	2.11	0.51
1:D:39:TRP:CD1	1:D:45:PHE:CZ	2.98	0.51
1:F:61:ILE:HG21	1:F:90:TRP:HA	1.93	0.51
1:B:145:ARG:HG2	1:B:145:ARG:HH11	1.76	0.51
1:C:122:MET:O	1:C:126:GLN:HG2	2.10	0.51
1:C:228:ASP:OD1	1:C:255:ARG:NH1	2.41	0.51
1:E:264:LEU:HB3	1:E:297:LEU:HD11	1.92	0.51
1:E:332:GLU:OE1	1:E:349:HIS:CD2	2.63	0.51
1:F:87:ALA:HB1	1:F:137:MET:HB2	1.92	0.51
1:A:228:ASP:OD1	1:A:255:ARG:NH1	2.34	0.51
1:B:230:LEU:HD22	1:B:262:LEU:HG	1.93	0.51
1:E:271:GLY:HA3	1:E:273:PHE:CE2	2.45	0.51
1:B:405:VAL:HG22	1:B:460:LEU:HD13	1.93	0.50
1:D:162:ARG:HD2	1:D:163:GLY:N	2.25	0.50
1:A:384:GLY:HA3	1:A:425:ILE:HD12	1.92	0.50
1:C:292:LEU:HD13	1:C:380:LEU:HG	1.94	0.50
1:E:47:PHE:CD2	1:E:169:VAL:HG21	2.47	0.50
1:F:215:LEU:O	1:F:219:VAL:HG23	2.11	0.50
1:F:327:GLY:O	1:F:452:SER:HA	2.10	0.50
1:B:227:ILE:HG23	1:B:258:ALA:HB3	1.91	0.50
1:D:216:ALA:O	1:D:219:VAL:HG22	2.10	0.50
1:E:323:ALA:HB1	1:E:454:ALA:HB3	1.94	0.50
1:D:95:LEU:HD21	1:D:141:LEU:HD22	1.94	0.50
1:F:224:GLU:OE1	1:F:255:ARG:NH2	2.38	0.50
1:F:351:LEU:HD21	1:F:377:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:MET:HE1	1:A:330:PHE:N	2.26	0.50
1:B:113:PRO:HB2	1:B:116:SER:HB3	1.94	0.50
1:B:344:MET:CE	1:B:426:LEU:HB3	2.42	0.50
1:E:196:LYS:HD3	1:E:207:VAL:HG12	1.94	0.50
1:B:225:ALA:O	1:B:228:ASP:HB2	2.12	0.50
1:D:280:PHE:HB3	1:D:289:LEU:HD13	1.94	0.50
1:C:464:ALA:CB	1:C:471:CYS:HB2	2.42	0.50
1:B:493:PHE:CZ	1:B:497:ARG:HD2	2.47	0.49
1:E:110:ARG:HA	1:E:151:HIS:CD2	2.47	0.49
1:F:264:LEU:O	1:F:268:LEU:HG	2.12	0.49
1:B:337:HIS:O	1:B:343:GLU:HA	2.12	0.49
1:E:191:VAL:CG2	1:E:446:ALA:HB2	2.42	0.49
1:A:257:GLN:HG2	1:A:288:GLN:OE1	2.11	0.49
1:A:344:MET:HB3	1:A:428:LYS:HD3	1.93	0.49
1:A:447:HIS:HB2	1:E:129:HIS:CB	2.42	0.49
1:C:162:ARG:HG2	2:C:501:MPD:HM3	1.93	0.49
1:C:216:ALA:HA	1:C:219:VAL:HG22	1.94	0.49
1:D:183:GLY:HA3	1:D:279:THR:HG22	1.95	0.49
1:D:374:LYS:NZ	5:D:607:HOH:O	2.45	0.49
1:C:243:GLY:O	1:C:250:LEU:N	2.40	0.49
1:D:192:THR:HG22	1:D:309:ASP:CG	2.33	0.49
1:D:292:LEU:HD13	1:D:380:LEU:HG	1.93	0.49
1:E:39:TRP:CD2	2:E:501:MPD:H12	2.48	0.49
1:E:275:ALA:HA	1:E:303:GLY:O	2.12	0.49
1:B:61:ILE:HG21	1:B:90:TRP:HA	1.93	0.49
1:B:170:ALA:HB2	1:B:322:MET:HG3	1.95	0.49
1:B:327:GLY:O	1:B:452:SER:HA	2.12	0.49
1:B:344:MET:HE2	1:B:426:LEU:HB3	1.95	0.49
1:D:83:THR:HA	1:D:126:GLN:HB2	1.94	0.49
1:F:13:VAL:O	1:F:79:THR:HA	2.13	0.48
1:A:336:TYR:CE2	1:E:105:HIS:NE2	2.81	0.48
1:C:350:MET:HE2	1:C:369:LEU:HD21	1.94	0.48
1:E:344:MET:SD	1:E:426:LEU:HD13	2.53	0.48
1:A:334:TYR:HE2	1:A:349:HIS:HA	1.77	0.48
1:A:110:ARG:HA	1:A:151:HIS:CD2	2.49	0.48
1:C:291:GLY:HA3	1:C:351:LEU:HD13	1.95	0.48
1:D:87:ALA:HB1	1:D:137:MET:HB2	1.95	0.48
1:F:60:GLU:O	1:F:64:VAL:HG23	2.14	0.48
1:B:14:THR:HA	1:B:80:TRP:O	2.14	0.48
1:C:447:HIS:CB	1:F:129:HIS:HB2	2.39	0.48
1:B:28:VAL:HA	1:B:82:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:HA	1:A:26:LYS:HG3	1.96	0.48
1:B:87:ALA:HB2	1:B:133:GLU:HG3	1.96	0.48
1:F:177:LEU:HD21	1:F:314:ALA:HA	1.95	0.48
1:B:472:VAL:HG13	1:B:483:PHE:CE1	2.49	0.47
1:D:347:GLY:HA3	1:D:427:TRP:CZ3	2.49	0.47
1:B:332:GLU:OE1	1:B:447:HIS:HD2	1.97	0.47
1:C:357:ILE:O	1:C:384:GLY:HA2	2.14	0.47
1:D:253:GLY:HA2	1:D:288:GLN:HE22	1.78	0.47
1:C:417:MET:HG2	1:F:117:ILE:CG2	2.44	0.47
1:B:408:VAL:HG12	1:B:429:PRO:HA	1.97	0.47
1:D:225:ALA:O	1:D:228:ASP:HB2	2.14	0.47
1:F:191:VAL:HG21	1:F:446:ALA:HB2	1.96	0.47
1:B:365:GLU:HB3	1:B:367:HIS:NE2	2.29	0.47
1:E:215:LEU:O	1:E:219:VAL:HG23	2.15	0.47
1:E:358:ALA:HB2	1:E:382:PHE:CD2	2.50	0.47
1:A:47:PHE:CD2	1:A:169:VAL:HG21	2.49	0.47
1:B:28:VAL:HG12	1:B:54:VAL:HG21	1.97	0.47
1:D:16:SER:OG	1:D:83:THR:HG21	2.14	0.47
1:F:110:ARG:HG3	1:F:151:HIS:CG	2.49	0.47
1:F:245:GLU:O	1:F:251:HIS:CE1	2.67	0.47
1:F:332:GLU:HB2	1:F:349:HIS:HD2	1.78	0.47
1:A:145:ARG:HG2	1:A:145:ARG:HH11	1.80	0.47
1:A:280:PHE:HA	1:A:283:LEU:HD11	1.97	0.47
1:C:52:LYS:O	1:C:53:SER:O	2.33	0.47
1:F:440:TRP:NE1	1:F:445:GLY:HA3	2.30	0.47
1:C:333:ASP:N	1:C:333:ASP:OD1	2.47	0.47
1:F:36:VAL:O	1:F:40:ASN:ND2	2.48	0.47
1:D:261:GLU:HA	1:D:293:ALA:HB1	1.96	0.46
1:E:45:PHE:CZ	1:E:165:ALA:HB3	2.50	0.46
1:E:268:LEU:HD13	1:E:302:TYR:CE2	2.49	0.46
1:F:39:TRP:CZ2	1:F:152:TRP:HB2	2.50	0.46
1:F:52:LYS:O	1:F:53:SER:O	2.33	0.46
1:A:365:GLU:OE1	1:A:367:HIS:NE2	2.34	0.46
1:B:344:MET:HE3	1:B:411:VAL:CG2	2.45	0.46
1:C:359:ALA:HB2	1:C:385:GLY:HA2	1.98	0.46
1:E:218:ARG:HD3	1:E:266:SER:HB3	1.97	0.46
1:C:323:ALA:HB1	1:C:454:ALA:HB3	1.96	0.46
1:A:56:THR:OG1	1:A:60:GLU:OE1	2.29	0.46
1:B:298:MET:CE	1:B:316:VAL:HG11	2.46	0.46
1:C:157:VAL:O	1:C:161:VAL:HG23	2.15	0.46
1:D:298:MET:CE	1:D:330:PHE:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ALA:CB	1:A:471:CYS:HB2	2.46	0.46
1:C:365:GLU:OE1	1:C:367:HIS:NE2	2.32	0.46
1:D:146:LYS:NZ	1:D:462:ASP:OD2	2.43	0.46
1:E:44:VAL:HB	1:E:162:ARG:NH1	2.30	0.46
1:B:16:SER:O	1:B:56:THR:HA	2.15	0.46
1:D:253:GLY:HA2	1:D:288:GLN:NE2	2.29	0.46
1:D:337:HIS:O	1:D:343:GLU:HA	2.16	0.46
1:F:472:VAL:HG22	1:F:483:PHE:CE1	2.51	0.46
1:A:157:VAL:O	1:A:161:VAL:HG23	2.15	0.46
1:A:447:HIS:HB2	1:E:129:HIS:HB2	1.98	0.46
1:C:265:ARG:NH1	1:C:300:GLU:OE1	2.49	0.46
1:B:363:ARG:NE	1:B:365:GLU:OE2	2.49	0.46
1:A:488:LYS:O	1:A:492:VAL:HG23	2.16	0.46
1:B:38:GLU:OE2	1:B:41:ARG:NH2	2.44	0.46
1:B:485:ASN:HB3	1:B:489:TRP:CH2	2.50	0.46
1:C:41:ARG:O	1:C:43:SER:N	2.49	0.46
1:D:170:ALA:HB2	1:D:322:MET:HG3	1.97	0.46
1:E:230:LEU:HD23	1:E:258:ALA:HB1	1.97	0.45
1:A:62:ARG:CZ	1:A:66:LEU:HD11	2.47	0.45
1:C:170:ALA:CB	1:C:322:MET:HG3	2.46	0.45
1:C:383:ASP:OD1	1:C:424:ARG:HD2	2.17	0.45
1:D:17:GLN:O	1:D:18:HIS:ND1	2.49	0.45
1:D:117:ILE:HG23	1:D:117:ILE:O	2.16	0.45
1:B:234:TYR:CE2	1:B:292:LEU:HD21	2.51	0.45
1:E:404:ILE:HD13	1:E:445:GLY:HA2	1.98	0.45
1:A:139:THR:OG1	1:A:145:ARG:NH2	2.49	0.45
1:B:180:ALA:O	1:B:276:PHE:HA	2.16	0.45
1:E:45:PHE:HB2	2:E:501:MPD:C5	2.32	0.45
1:A:61:ILE:HG21	1:A:90:TRP:HA	1.97	0.45
1:C:360:THR:HG23	1:C:383:ASP:HB2	1.97	0.45
1:D:328:THR:HG23	1:D:452:SER:HB2	1.99	0.45
1:E:241:ALA:HB2	1:E:363:ARG:CD	2.47	0.45
1:B:412:LYS:HG3	1:B:413:PRO:HD2	1.98	0.45
1:C:257:GLN:HE21	1:C:288:GLN:NE2	2.14	0.45
1:C:333:ASP:O	1:F:129:HIS:HB3	2.17	0.45
1:D:201:ALA:HA	1:F:95:LEU:HD11	1.98	0.45
1:D:205:TRP:HH2	1:D:394:LEU:HD22	1.82	0.45
1:A:434:ARG:NH1	1:A:435:ASP:OD1	2.50	0.45
1:B:253:GLY:HA2	1:B:288:GLN:NE2	2.29	0.45
1:C:19:LEU:HD23	1:C:20:TYR:CE1	2.51	0.45
1:A:3:LEU:N	5:A:623:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:93:GLY:HA3	1.99	0.45
1:A:472:VAL:HG13	1:A:483:PHE:CE1	2.52	0.45
1:C:334:TYR:HE2	1:C:349:HIS:HA	1.81	0.45
1:F:355:PRO:HA	1:F:382:PHE:CZ	2.51	0.45
1:F:158:ALA:O	1:F:162:ARG:HG3	2.17	0.45
1:C:393:SER:OG	1:C:446:ALA:HB3	2.17	0.44
1:D:288:GLN:NE2	1:D:375:GLU:OE1	2.49	0.44
1:D:429:PRO:HG2	1:D:433:LEU:HA	1.98	0.44
1:B:441:ILE:HA	5:B:614:HOH:O	2.17	0.44
1:C:24:ALA:O	1:C:28:VAL:HG23	2.17	0.44
1:E:309:ASP:OD2	1:E:312:THR:OG1	2.19	0.44
1:F:202:ARG:HD3	1:F:202:ARG:HA	1.87	0.44
1:B:174:SER:HB2	1:B:318:LEU:CD2	2.47	0.44
1:C:175:ARG:HH21	2:C:502:MPD:HM1	1.82	0.44
1:C:404:ILE:HD12	1:C:445:GLY:HA2	1.99	0.44
1:F:103:HIS:HE1	1:F:131:ASP:O	2.00	0.44
1:F:383:ASP:OD1	1:F:424:ARG:HD3	2.17	0.44
1:F:289:LEU:HD22	1:F:350:MET:CE	2.47	0.44
1:A:255:ARG:O	1:A:258:ALA:HB3	2.16	0.44
1:C:234:TYR:CE2	1:C:292:LEU:HD21	2.53	0.44
1:E:261:GLU:OE1	1:E:296:ARG:HD3	2.18	0.44
1:A:82:HIS:CE1	1:A:124:LEU:O	2.71	0.44
1:A:323:ALA:HB1	1:A:454:ALA:HB3	2.00	0.44
1:D:336:TYR:CE1	1:D:345:ILE:HG12	2.52	0.44
1:E:227:ILE:HG22	1:E:231:ILE:CD1	2.48	0.44
1:A:218:ARG:NH2	1:A:270:GLU:OE2	2.43	0.44
1:A:224:GLU:OE2	1:A:255:ARG:NH2	2.49	0.44
1:C:368:PRO:HA	1:C:376:ASP:OD1	2.18	0.44
1:D:355:PRO:HG3	1:D:380:LEU:CD1	2.47	0.44
1:A:162:ARG:HG3	2:A:501:MPD:H13	2.00	0.44
1:B:31:HIS:O	1:B:35:MET:HG3	2.18	0.44
1:D:46:PRO:HD3	1:D:162:ARG:CB	2.47	0.44
1:E:298:MET:SD	1:E:304:PHE:HB3	2.58	0.44
1:F:327:GLY:O	1:F:453:PHE:N	2.40	0.44
1:A:149:VAL:HG12	1:A:150:GLY:N	2.33	0.44
1:B:400:ARG:HD2	1:B:494:TRP:HB3	2.00	0.44
1:D:16:SER:OG	1:D:83:THR:CG2	2.66	0.44
1:E:35:MET:HG2	1:E:152:TRP:CD2	2.53	0.44
1:E:337:HIS:O	1:E:343:GLU:HA	2.18	0.44
1:B:87:ALA:HB1	1:B:137:MET:HB2	1.99	0.43
1:C:225:ALA:O	1:C:228:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ARG:HD3	1:E:266:SER:CB	2.47	0.43
1:B:10:PHE:CE2	1:B:165:ALA:HB1	2.53	0.43
1:C:265:ARG:NH1	1:C:300:GLU:OE2	2.50	0.43
1:E:234:TYR:CE2	1:E:292:LEU:HD21	2.53	0.43
1:B:219:VAL:HG13	1:B:259:ARG:HG2	1.98	0.43
1:C:14:THR:HA	1:C:80:TRP:O	2.18	0.43
1:C:327:GLY:O	1:C:452:SER:HA	2.18	0.43
1:F:112:ILE:O	1:F:114:TRP:N	2.51	0.43
1:A:82:HIS:ND1	1:A:124:LEU:O	2.52	0.43
1:E:344:MET:HE2	1:E:428:LYS:HE3	1.98	0.43
1:F:58:PRO:HG3	1:F:89:MET:HA	2.00	0.43
1:A:485:ASN:ND2	5:A:604:HOH:O	2.21	0.43
1:D:87:ALA:HB2	1:D:133:GLU:HG3	2.00	0.43
1:D:256:GLU:CD	1:D:287:LYS:HG3	2.38	0.43
1:F:14:THR:HA	1:F:80:TRP:O	2.19	0.43
1:C:174:SER:OG	1:C:205:TRP:NE1	2.45	0.43
1:E:256:GLU:HG2	1:E:287:LYS:HG3	2.01	0.43
1:F:94:LEU:HB3	1:F:143:MET:SD	2.58	0.43
1:A:39:TRP:HH2	1:A:104:LEU:HD21	1.83	0.43
1:A:284:HIS:CG	1:B:213:GLY:HA3	2.54	0.43
1:A:336:TYR:HE2	1:E:105:HIS:NE2	2.16	0.43
1:A:35:MET:HG2	1:A:152:TRP:CD2	2.53	0.43
1:B:157:VAL:O	1:B:161:VAL:HG23	2.18	0.43
1:B:457:THR:HG21	1:B:473:VAL:HG11	2.01	0.43
1:C:58:PRO:HG3	1:C:89:MET:HA	2.00	0.43
1:C:431:PRO:HG2	1:C:435:ASP:HB2	2.00	0.43
1:A:218:ARG:HD2	1:A:267:PHE:HB2	2.01	0.42
1:B:363:ARG:NH1	1:B:365:GLU:OE2	2.52	0.42
1:C:218:ARG:HD2	1:C:266:SER:OG	2.19	0.42
1:F:347:GLY:HA3	1:F:427:TRP:HZ3	1.84	0.42
1:B:193:GLU:O	1:B:311:LYS:NZ	2.46	0.42
1:A:123:ASN:HA	1:A:126:GLN:HE21	1.84	0.42
1:C:350:MET:CE	1:C:369:LEU:HD21	2.49	0.42
1:D:108:PHE:HA	1:D:152:TRP:CD1	2.54	0.42
1:E:45:PHE:CG	2:E:501:MPD:C5	3.02	0.42
1:F:231:ILE:CD1	1:F:255:ARG:HG2	2.50	0.42
1:A:191:VAL:HG21	1:A:446:ALA:HA	2.00	0.42
1:D:17:GLN:O	1:D:18:HIS:CG	2.73	0.42
1:F:173:VAL:HG21	1:F:321:VAL:HG21	2.00	0.42
1:F:195:ASP:OD1	1:F:197:VAL:HB	2.19	0.42
1:F:347:GLY:HA3	1:F:427:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:GLU:CB	4:C:503:GOL:O3	2.68	0.42
1:B:229:ARG:NH2	1:B:229:ARG:HB3	2.35	0.42
1:C:202:ARG:HD2	1:C:467:ALA:O	2.19	0.42
1:C:350:MET:HE3	1:C:371:ILE:HB	2.00	0.42
1:D:332:GLU:OE2	1:D:349:HIS:CD2	2.73	0.42
1:F:432:SER:O	1:F:436:SER:HB3	2.20	0.42
1:A:485:ASN:HB3	1:A:489:TRP:CZ2	2.55	0.42
1:C:223:SER:HB2	1:C:226:GLU:H	1.85	0.42
1:E:365:GLU:OE1	1:E:367:HIS:NE2	2.48	0.42
1:A:14:THR:HA	1:A:80:TRP:O	2.19	0.42
1:A:52:LYS:O	1:A:53:SER:C	2.58	0.42
1:A:161:VAL:CG1	2:A:501:MPD:HM3	2.46	0.42
1:B:138:VAL:HG11	1:B:145:ARG:CD	2.22	0.42
1:B:231:ILE:O	1:B:235:GLN:HG3	2.20	0.42
1:C:145:ARG:HG2	1:C:145:ARG:NH1	2.30	0.42
1:D:91:ILE:HD13	1:F:200:GLU:HB2	2.02	0.42
1:A:28:VAL:HA	1:A:82:HIS:CD2	2.55	0.42
1:C:127:SER:HB3	1:C:131:ASP:OD2	2.19	0.42
1:C:212:VAL:HG11	1:C:282:ASP:O	2.19	0.42
1:A:42:ASP:O	1:A:44:VAL:HG12	2.20	0.41
1:D:171:ALA:O	1:D:174:SER:HB3	2.19	0.41
1:B:107:GLN:O	1:B:151:HIS:HD2	2.02	0.41
1:C:231:ILE:HD11	1:C:255:ARG:HA	2.02	0.41
1:D:488:LYS:O	1:D:492:VAL:HG23	2.20	0.41
1:F:234:TYR:OH	1:F:258:ALA:HA	2.20	0.41
1:B:472:VAL:CG1	1:B:483:PHE:CZ	3.03	0.41
1:C:332:GLU:O	1:C:347:GLY:HA2	2.20	0.41
1:D:482:SER:O	1:D:486:GLU:HG3	2.20	0.41
1:F:346:LEU:HD11	1:F:424:ARG:HB2	2.01	0.41
1:D:234:TYR:CE2	1:D:292:LEU:HD21	2.55	0.41
1:F:337:HIS:O	1:F:343:GLU:HA	2.21	0.41
1:F:355:PRO:CG	1:F:380:LEU:HD12	2.49	0.41
1:B:358:ALA:HB2	1:B:382:PHE:CD1	2.56	0.41
1:C:436:SER:HA	1:C:474:ILE:HG21	2.02	0.41
1:E:295:GLN:OE1	1:E:380:LEU:N	2.53	0.41
1:B:294:VAL:O	1:B:298:MET:HG3	2.21	0.41
1:C:53:SER:O	5:C:602:HOH:O	2.22	0.41
1:C:298:MET:HE1	1:C:316:VAL:HG11	2.02	0.41
1:D:362:PRO:HB2	1:D:380:LEU:HD22	2.01	0.41
1:A:17:GLN:O	1:A:25:LEU:HD21	2.20	0.41
1:B:210:TYR:CD1	1:B:267:PHE:HZ	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLY:HA3	1:B:273:PHE:CE2	2.56	0.41
1:C:486:GLU:HB3	4:C:503:GOL:HO3	1.86	0.41
1:D:286:MET:O	1:D:374:LYS:HE2	2.21	0.41
1:E:55:VAL:HB	1:E:61:ILE:HG13	2.01	0.41
1:E:314:ALA:O	1:E:318:LEU:HD13	2.21	0.41
1:F:245:GLU:HG2	1:F:251:HIS:HB2	2.03	0.41
1:B:107:GLN:O	1:B:151:HIS:CD2	2.74	0.41
1:F:10:PHE:CZ	1:F:168:ALA:HB3	2.55	0.41
1:F:161:VAL:CG1	2:F:501:MPD:H53	2.51	0.41
1:F:181:ARG:HD3	1:F:310:TRP:HB3	2.03	0.41
1:A:355:PRO:HA	1:A:382:PHE:CZ	2.56	0.41
1:B:295:GLN:HB3	1:B:355:PRO:HD3	2.03	0.41
1:B:310:TRP:O	1:B:313:ALA:HB3	2.21	0.41
1:B:328:THR:HG23	1:B:450:CYS:SG	2.61	0.41
1:B:346:LEU:HD11	1:B:424:ARG:HG3	2.02	0.41
1:C:110:ARG:HA	1:C:151:HIS:CD2	2.56	0.41
1:C:441:ILE:HA	5:F:615:HOH:O	2.21	0.41
1:D:395:ILE:HD13	1:D:444:GLY:O	2.20	0.41
1:F:52:LYS:O	1:F:53:SER:C	2.58	0.41
1:F:288:GLN:CD	1:F:377:PRO:HA	2.42	0.41
1:A:231:ILE:HD13	1:A:231:ILE:HA	1.94	0.41
1:A:332:GLU:OE1	1:A:447:HIS:HD2	2.04	0.41
1:C:257:GLN:HG3	1:C:378:ALA:HB3	2.03	0.41
1:C:486:GLU:HB3	4:C:503:GOL:O3	2.21	0.41
1:D:346:LEU:HA	1:D:426:LEU:HD23	2.03	0.41
1:A:400:ARG:HD2	1:A:494:TRP:HB3	2.03	0.40
1:A:492:VAL:CG1	1:E:492:VAL:HG12	2.51	0.40
1:C:102:LEU:CD1	1:C:148:ILE:HD12	2.51	0.40
1:C:265:ARG:HH12	1:C:300:GLU:CD	2.24	0.40
1:C:444:GLY:O	1:F:136:PHE:HB2	2.21	0.40
1:D:193:GLU:OE2	1:D:193:GLU:HA	2.21	0.40
1:A:45:PHE:HB2	2:A:501:MPD:O4	2.21	0.40
1:A:491:GLU:O	1:A:495:ARG:HG3	2.21	0.40
1:D:218:ARG:O	1:D:218:ARG:CG	2.69	0.40
1:D:230:LEU:HD22	1:D:262:LEU:HG	2.04	0.40
1:F:456:THR:OG1	1:F:459:GLN:HG3	2.21	0.40
1:B:186:MET:SD	1:B:307:GLU:HG2	2.61	0.40
1:C:298:MET:CE	1:C:330:PHE:H	2.30	0.40
1:E:191:VAL:HG21	1:E:446:ALA:CB	2.49	0.40
1:F:257:GLN:HG3	1:F:378:ALA:O	2.22	0.40
1:B:88:LYS:HE3	5:B:616:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ARG:HG3	2:C:501:MPD:HM3	2.03	0.40
2:C:501:MPD:H11	2:C:501:MPD:H4	1.92	0.40
1:E:292:LEU:HD12	1:E:380:LEU:HG	2.04	0.40
2:A:502:MPD:H53	2:A:502:MPD:H13	2.02	0.40
1:B:323:ALA:HB1	1:B:454:ALA:HB3	2.03	0.40
1:C:187:ARG:HG2	1:D:208:ASN:HB3	2.03	0.40
1:C:482:SER:O	1:C:486:GLU:HG3	2.22	0.40
1:D:327:GLY:O	1:D:452:SER:HA	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/497 (99%)	470 (95%)	20 (4%)	3 (1%)	25	43
1	B	493/497 (99%)	471 (96%)	21 (4%)	1 (0%)	47	68
1	C	493/497 (99%)	460 (93%)	30 (6%)	3 (1%)	25	43
1	D	490/497 (99%)	465 (95%)	22 (4%)	3 (1%)	25	43
1	E	493/497 (99%)	458 (93%)	34 (7%)	1 (0%)	47	68
1	F	484/497 (97%)	454 (94%)	27 (6%)	3 (1%)	25	43
All	All	2946/2982 (99%)	2778 (94%)	154 (5%)	14 (0%)	29	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	ASP
1	C	246	LYS
1	F	53	SER
1	B	42	ASP

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Mol	Chain	Res	Type
1	C	350	MET
1	D	18	HIS
1	A	43	SER
1	A	17	GLN
1	D	291	GLY
1	F	239	GLU
1	F	249	PRO
1	E	350	MET
1	A	54	VAL
1	D	242	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	406/408 (100%)	392 (97%)	14 (3%)	37 63
1	B	406/408 (100%)	393 (97%)	13 (3%)	39 65
1	C	406/408 (100%)	396 (98%)	10 (2%)	47 73
1	D	405/408 (99%)	385 (95%)	20 (5%)	25 47
1	E	406/408 (100%)	394 (97%)	12 (3%)	41 68
1	F	401/408 (98%)	390 (97%)	11 (3%)	44 71
All	All	2430/2448 (99%)	2350 (97%)	80 (3%)	38 64

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	20	TYR
1	A	27	GLN
1	A	53	SER
1	A	119	MET
1	A	202	ARG
1	A	242	PRO
1	A	307	GLU

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Mol	Chain	Res	Type
1	A	317	ARG
1	A	334	TYR
1	A	379	ARG
1	A	424	ARG
1	A	465	GLU
1	A	472	VAL
1	B	19	LEU
1	B	53	SER
1	B	82	HIS
1	B	115	ASP
1	B	116	SER
1	B	333	ASP
1	B	334	TYR
1	B	349	HIS
1	B	370	SER
1	B	379	ARG
1	B	424	ARG
1	B	479	SER
1	B	482	SER
1	C	30	GLU
1	C	53	SER
1	C	146	LYS
1	C	223	SER
1	C	279	THR
1	C	333	ASP
1	C	334	TYR
1	C	335	THR
1	C	379	ARG
1	C	414	GLU
1	D	6	ARG
1	D	17	GLN
1	D	27	GLN
1	D	52	LYS
1	D	53	SER
1	D	116	SER
1	D	120	ASP
1	D	162	ARG
1	D	229	ARG
1	D	232	ASP
1	D	235	GLN
1	D	245	GLU
1	D	259	ARG

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Mol	Chain	Res	Type
1	D	317	ARG
1	D	326	LYS
1	D	334	TYR
1	D	379	ARG
1	D	424	ARG
1	D	472	VAL
1	D	497	ARG
1	E	45	PHE
1	E	119	MET
1	E	145	ARG
1	E	235	GLN
1	E	287	LYS
1	E	333	ASP
1	E	334	TYR
1	E	335	THR
1	E	374	LYS
1	E	379	ARG
1	E	424	ARG
1	E	479	SER
1	F	72	GLU
1	F	154	ASP
1	F	162	ARG
1	F	334	TYR
1	F	335	THR
1	F	363	ARG
1	F	376	ASP
1	F	379	ARG
1	F	424	ARG
1	F	436	SER
1	F	479	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	B	288	GLN
1	C	185	ASN
1	C	288	GLN
1	D	126	GLN
1	D	151	HIS
1	F	123	ASN
1	F	185	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	$\# Z > 2$
2	MPD	F	501	-	7,7,7	0.24	0	9,10,10	0.59	0
2	MPD	C	502	-	7,7,7	0.21	0	9,10,10	0.41	0
2	MPD	E	501	-	7,7,7	0.19	0	9,10,10	0.40	0
2	MPD	F	502	-	7,7,7	0.29	0	9,10,10	0.70	0
2	MPD	B	501	-	7,7,7	0.09	0	9,10,10	0.73	0
2	MPD	C	501	-	7,7,7	0.19	0	9,10,10	0.73	0
2	MPD	A	502	-	7,7,7	0.19	0	9,10,10	0.68	0
4	GOL	C	503	-	5,5,5	0.12	0	5,5,5	0.31	0
2	MPD	E	502	-	7,7,7	0.18	0	9,10,10	0.49	0
2	MPD	A	501	-	7,7,7	0.24	0	9,10,10	0.67	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
2	MPD	F	501	-	-	2/5/5/5	-
2	MPD	C	502	-	-	0/5/5/5	-
2	MPD	E	501	-	-	2/5/5/5	-
2	MPD	F	502	-	-	2/5/5/5	-
2	MPD	B	501	-	-	2/5/5/5	-
2	MPD	C	501	-	-	3/5/5/5	-
2	MPD	A	502	-	-	1/5/5/5	-
4	GOL	C	503	-	-	4/4/4/4	-
2	MPD	E	502	-	-	0/5/5/5	-
2	MPD	A	501	-	-	4/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	MPD	C2-C3-C4-O4
4	C	503	GOL	O1-C1-C2-O2
4	C	503	GOL	O1-C1-C2-C3
4	C	503	GOL	C1-C2-C3-O3
4	C	503	GOL	O2-C2-C3-O3
2	A	501	MPD	O2-C2-C3-C4
2	E	501	MPD	C2-C3-C4-C5
2	F	501	MPD	C2-C3-C4-C5
2	F	502	MPD	C2-C3-C4-C5
2	A	501	MPD	C1-C2-C3-C4
2	A	501	MPD	CM-C2-C3-C4
2	A	502	MPD	CM-C2-C3-C4
2	B	501	MPD	C1-C2-C3-C4
2	B	501	MPD	O2-C2-C3-C4
2	C	501	MPD	O2-C2-C3-C4
2	A	501	MPD	C2-C3-C4-C5
2	C	501	MPD	C2-C3-C4-C5
2	C	501	MPD	C2-C3-C4-O4
2	F	501	MPD	C2-C3-C4-O4
2	F	502	MPD	C2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	MPD	2	0
2	C	502	MPD	2	0
2	E	501	MPD	7	0
2	F	502	MPD	1	0
2	C	501	MPD	4	0
2	A	502	MPD	2	0
4	C	503	GOL	4	0
2	A	501	MPD	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/497 (99%)	-0.22	4 (0%) 86 87	24, 39, 64, 99	0
1	B	495/497 (99%)	0.07	16 (3%) 47 51	26, 47, 76, 121	0
1	C	495/497 (99%)	-0.09	9 (1%) 68 71	26, 46, 76, 114	0
1	D	494/497 (99%)	0.03	13 (2%) 56 59	28, 47, 81, 101	0
1	E	495/497 (99%)	0.03	19 (3%) 40 43	28, 48, 88, 121	0
1	F	490/497 (98%)	0.05	13 (2%) 54 58	31, 52, 83, 126	0
All	All	2964/2982 (99%)	-0.02	74 (2%) 57 61	24, 46, 80, 126	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	248	GLY	7.6
1	C	44	VAL	6.0
1	E	252	ASP	4.8
1	E	285	GLY	4.6
1	F	423	ALA	4.6
1	E	238	TYR	4.3
1	D	6	ARG	4.2
1	B	42	ASP	4.0
1	E	44	VAL	3.9
1	E	20	TYR	3.7
1	D	21	GLY	3.5
1	C	20	TYR	3.4
1	F	415	HIS	3.3
1	B	418	PRO	3.3
1	F	366	VAL	3.2
1	F	246	LYS	3.2
1	D	4	SER	3.0
1	B	253	GLY	3.0
1	E	364	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	238	TYR	2.9
1	C	40	ASN	2.9
1	C	43	SER	2.9
1	B	20	TYR	2.9
1	F	244	CYS	2.8
1	F	19	LEU	2.8
1	E	380	LEU	2.8
1	E	334	TYR	2.8
1	A	20	TYR	2.8
1	C	242	PRO	2.8
1	F	388	ALA	2.7
1	B	53	SER	2.7
1	B	266	SER	2.7
1	B	238	TYR	2.7
1	D	375	GLU	2.6
1	E	244	CYS	2.6
1	E	382	PHE	2.6
1	B	252	ASP	2.6
1	D	44	VAL	2.6
1	F	39	TRP	2.6
1	D	219	VAL	2.5
1	E	370	SER	2.5
1	A	46	PRO	2.4
1	B	380	LEU	2.4
1	D	17	GLN	2.4
1	A	43	SER	2.4
1	C	223	SER	2.4
1	C	117	ILE	2.4
1	B	234	TYR	2.4
1	D	252	ASP	2.3
1	C	19	LEU	2.3
1	E	253	GLY	2.3
1	E	47	PHE	2.3
1	B	27	GLN	2.2
1	E	453	PHE	2.2
1	B	124	LEU	2.2
1	E	42	ASP	2.2
1	D	43	SER	2.2
1	E	230	LEU	2.2
1	D	41	ARG	2.2
1	F	363	ARG	2.1
1	F	410	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	14	THR	2.1
1	B	114	TRP	2.1
1	D	287	LYS	2.1
1	E	235	GLN	2.1
1	E	46	PRO	2.1
1	A	42	ASP	2.1
1	F	250	LEU	2.1
1	E	23	GLU	2.1
1	D	19	LEU	2.1
1	F	245	GLU	2.1
1	B	242	PRO	2.0
1	B	415	HIS	2.0
1	C	244	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MPD	C	501	8/8	0.70	0.29	73,86,92,95	0
2	MPD	A	501	8/8	0.88	0.25	73,79,85,89	0
2	MPD	E	502	8/8	0.88	0.27	59,68,83,83	0
2	MPD	F	501	8/8	0.88	0.41	73,88,107,110	0
2	MPD	A	502	8/8	0.90	0.23	56,60,63,64	0
2	MPD	C	502	8/8	0.91	0.22	57,60,66,71	0
2	MPD	E	501	8/8	0.91	0.35	80,83,88,89	0
2	MPD	F	502	8/8	0.91	0.26	59,64,72,76	0
3	MN	E	503	1/1	0.91	0.10	70,70,70,70	0
4	GOL	C	503	6/6	0.91	0.27	77,78,82,85	0

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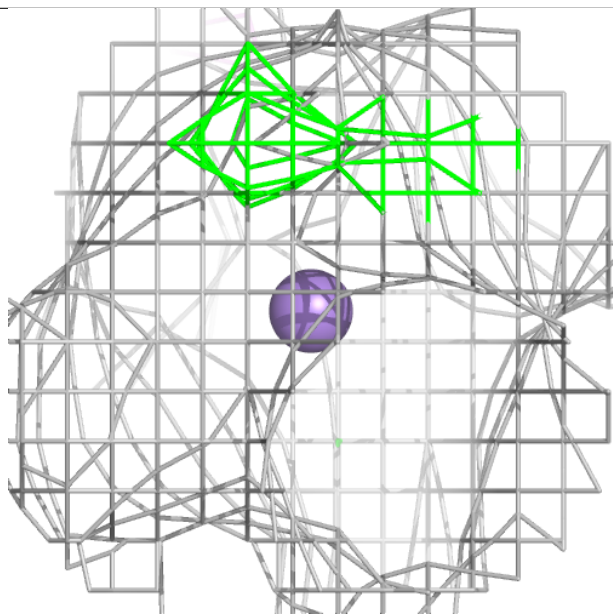
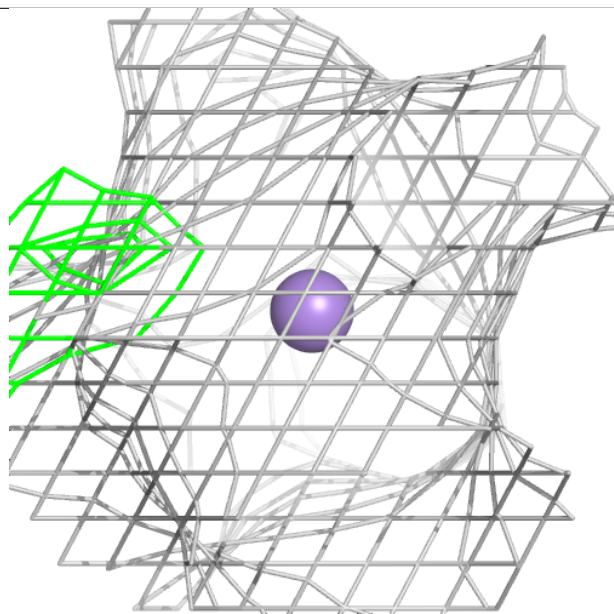
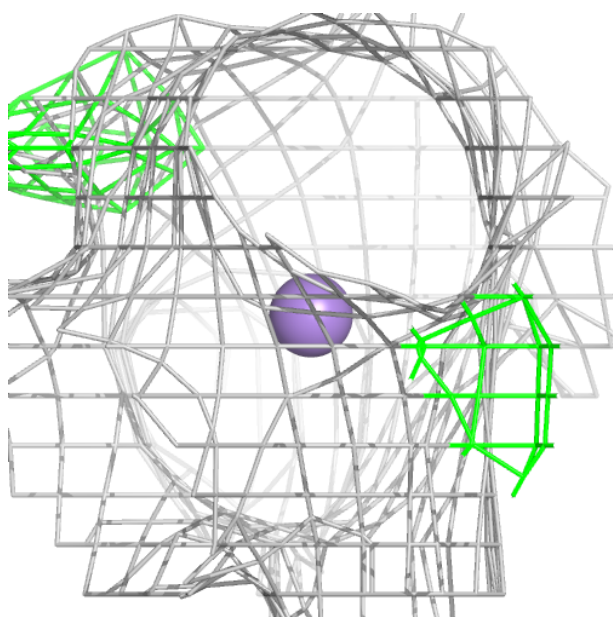
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	MPD	B	501	8/8	0.93	0.24	51,53,67,72	0
3	MN	E	504	1/1	0.97	0.09	58,58,58,58	0
3	MN	C	504	1/1	0.97	0.07	57,57,57,57	0
3	MN	F	503	1/1	0.98	0.09	53,53,53,53	0
3	MN	D	501	1/1	0.99	0.11	43,43,43,43	0
3	MN	A	504	1/1	0.99	0.17	61,61,61,61	0
3	MN	B	502	1/1	0.99	0.14	45,45,45,45	0
3	MN	A	503	1/1	0.99	0.12	40,40,40,40	0
3	MN	C	505	1/1	0.99	0.11	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

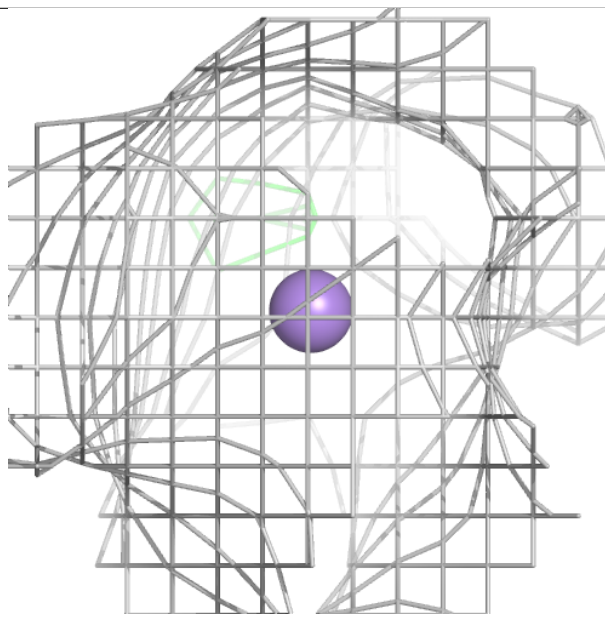
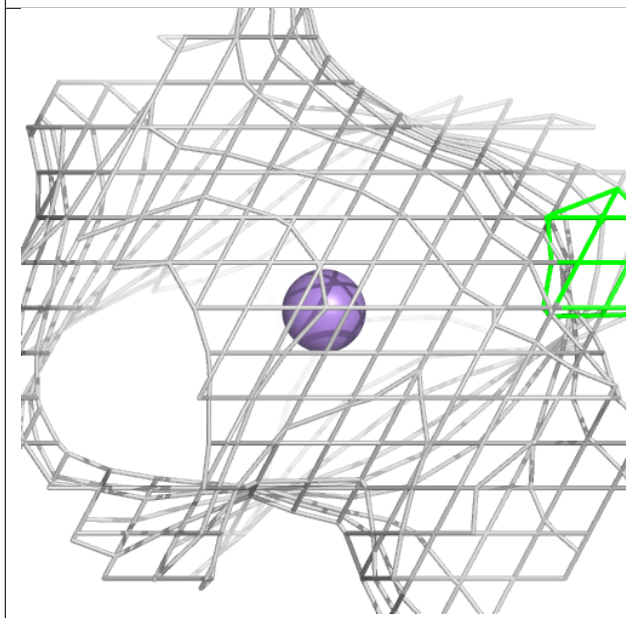
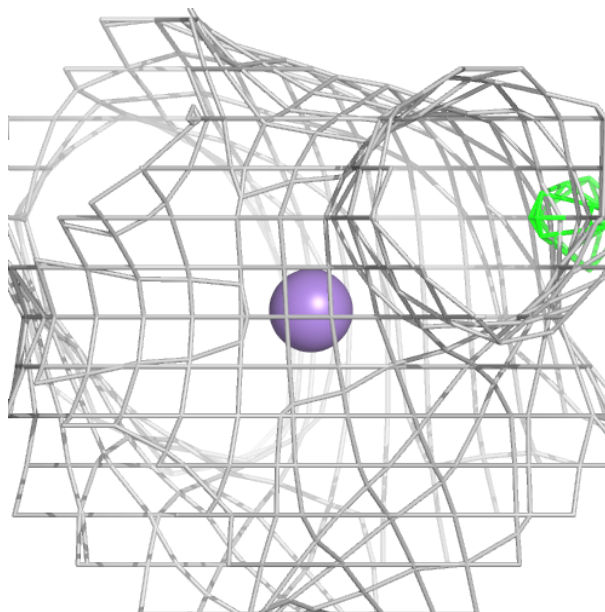
Electron density around MN E 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



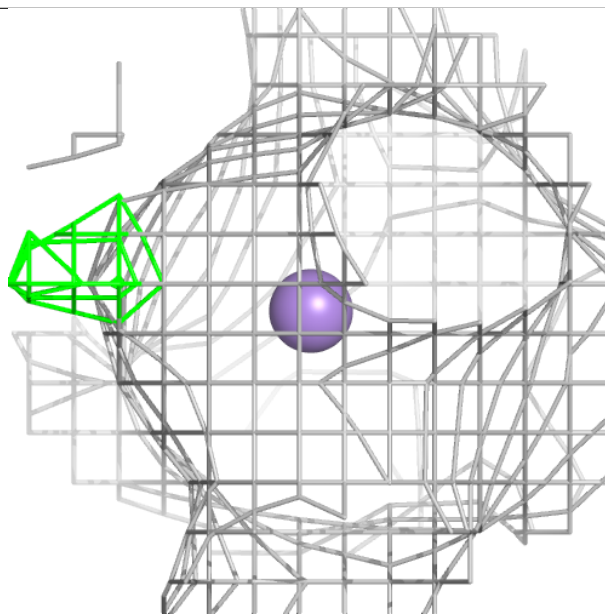
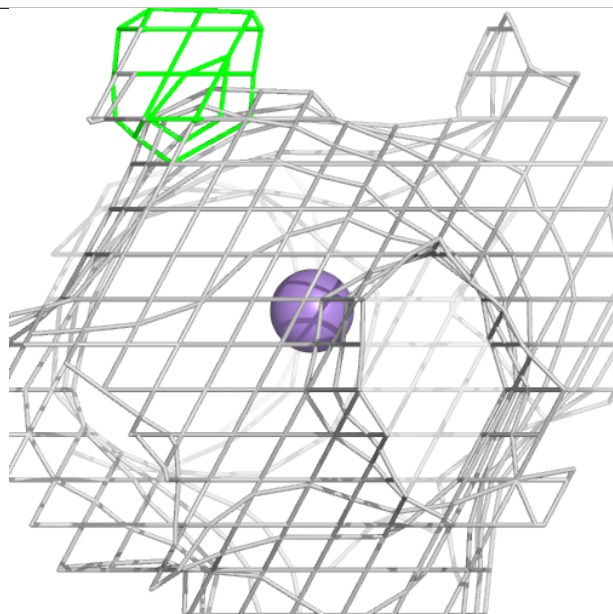
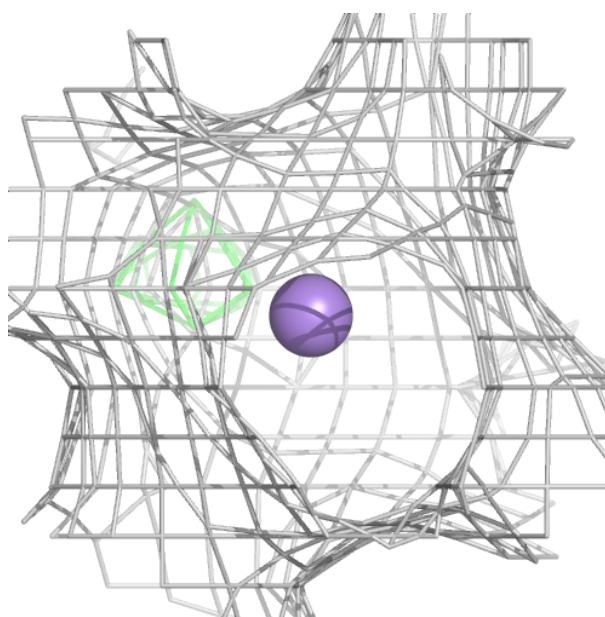
Electron density around MN E 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



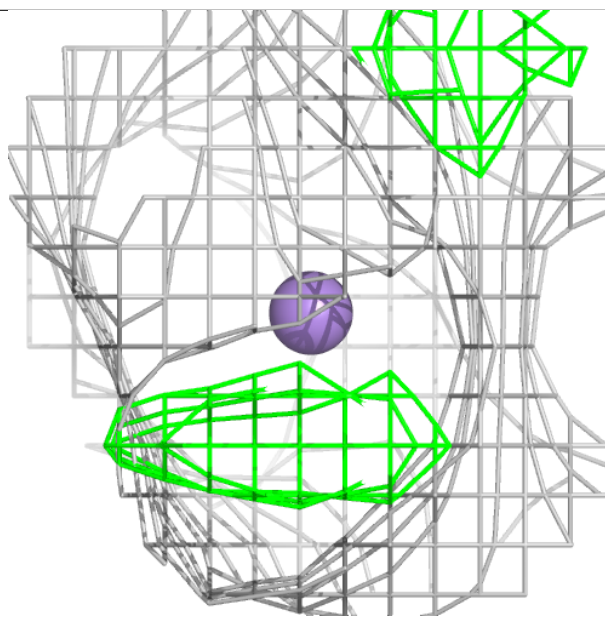
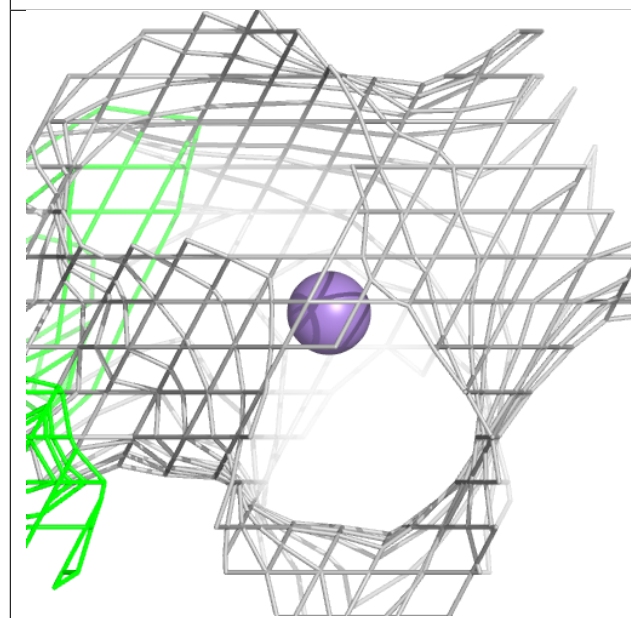
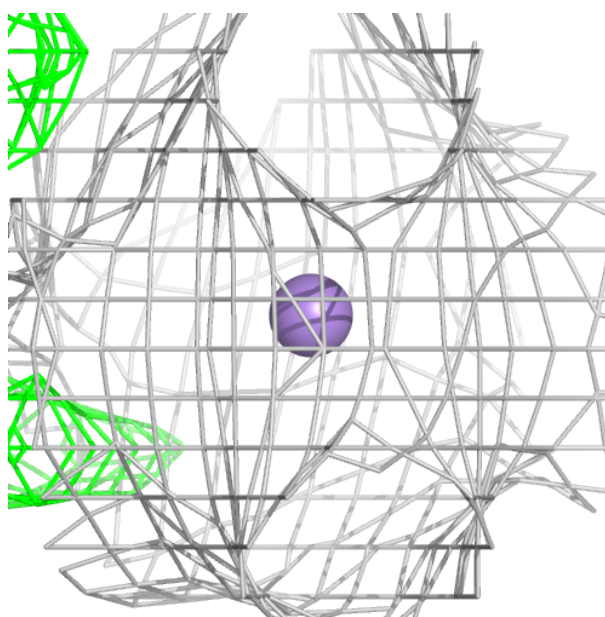
Electron density around MN C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



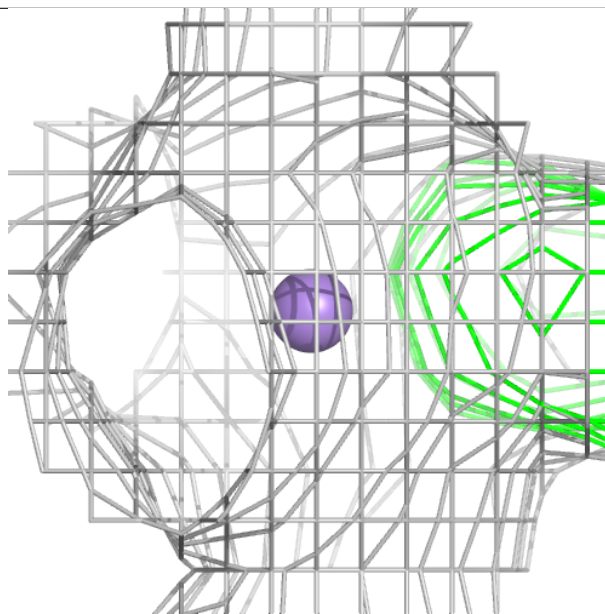
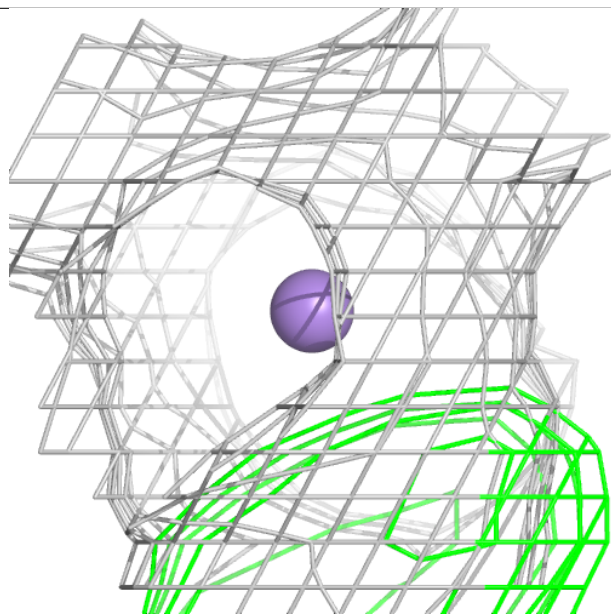
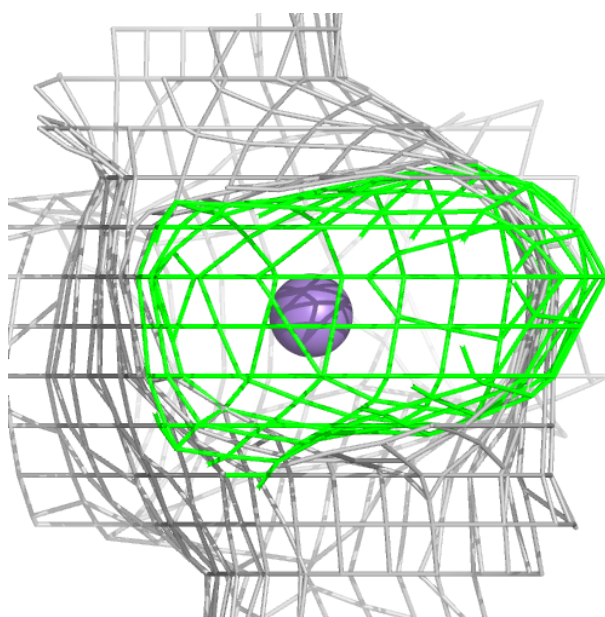
Electron density around MN F 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



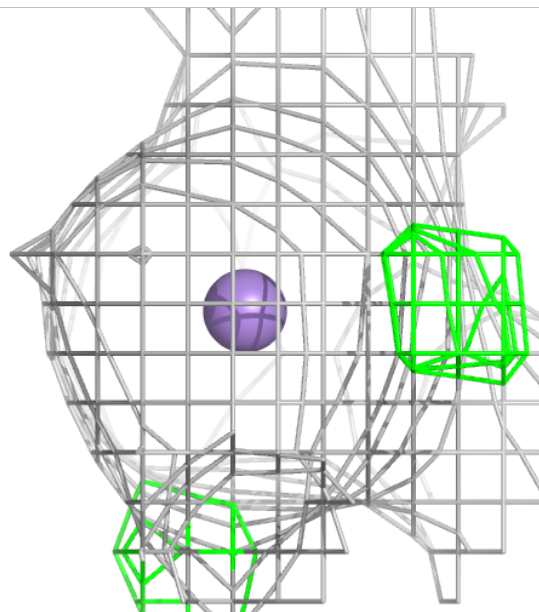
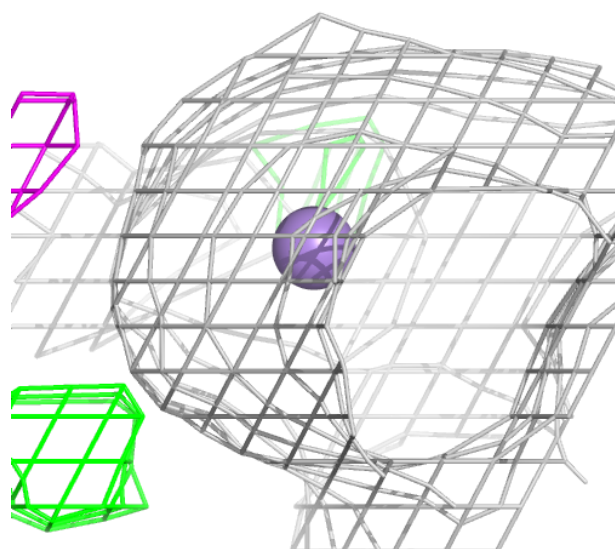
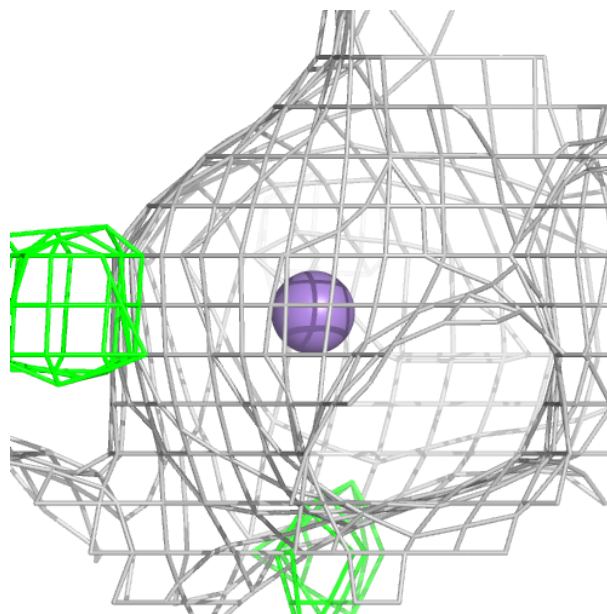
Electron density around MN D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



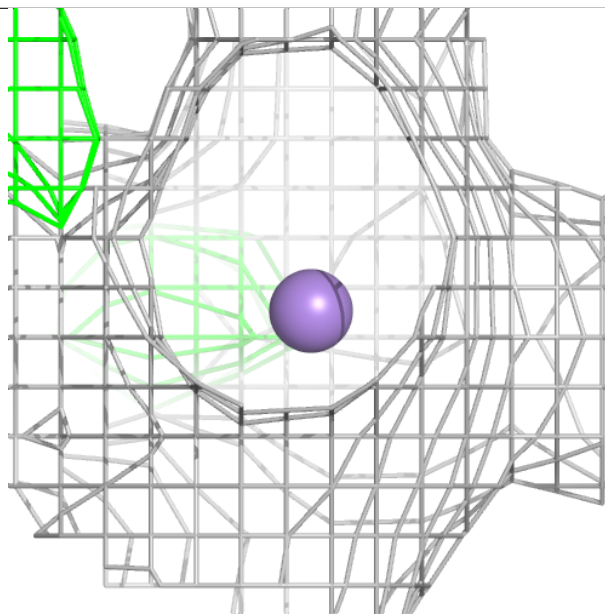
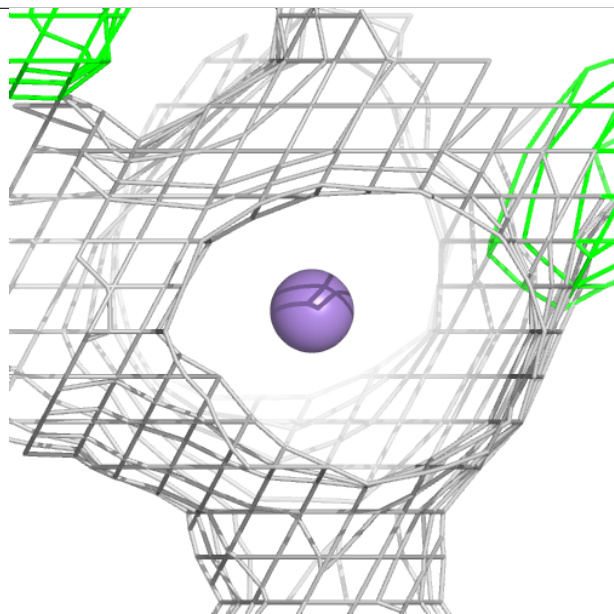
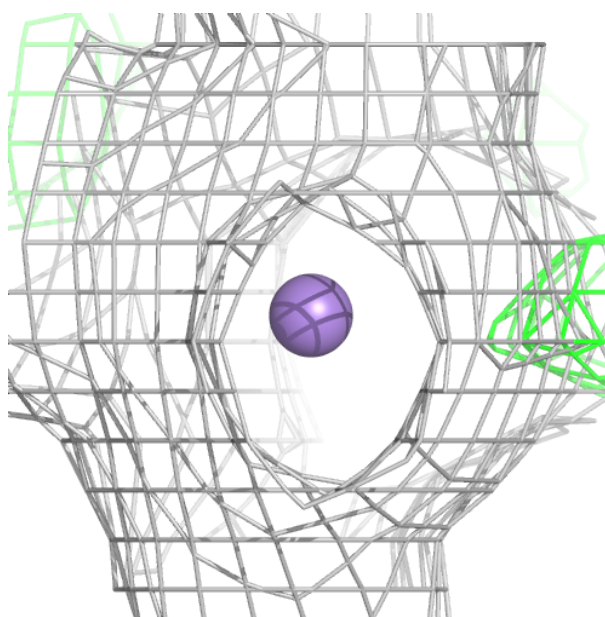
Electron density around MN A 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



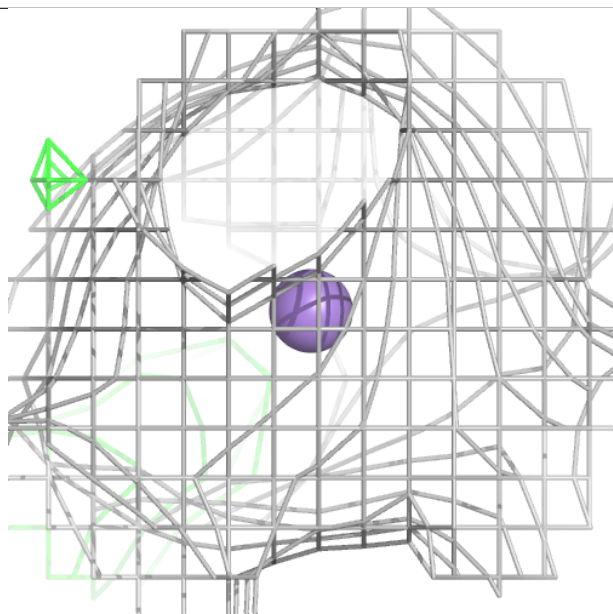
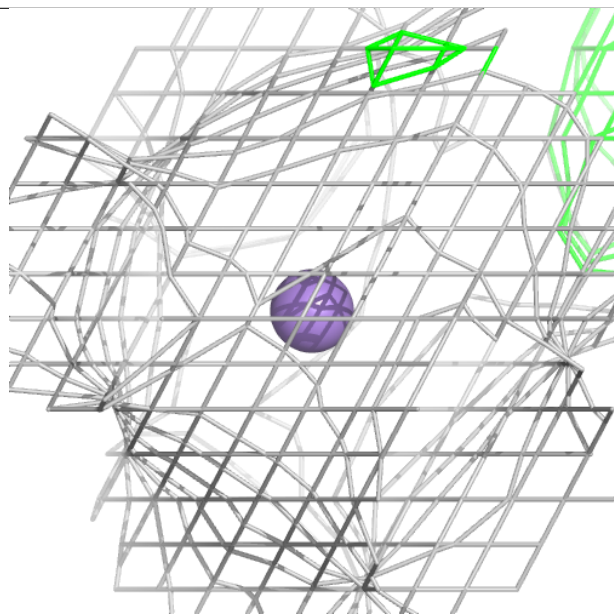
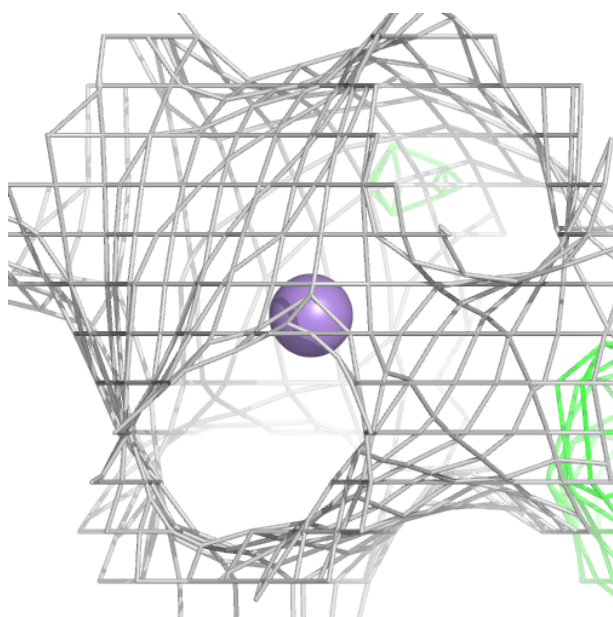
Electron density around MN B 502:

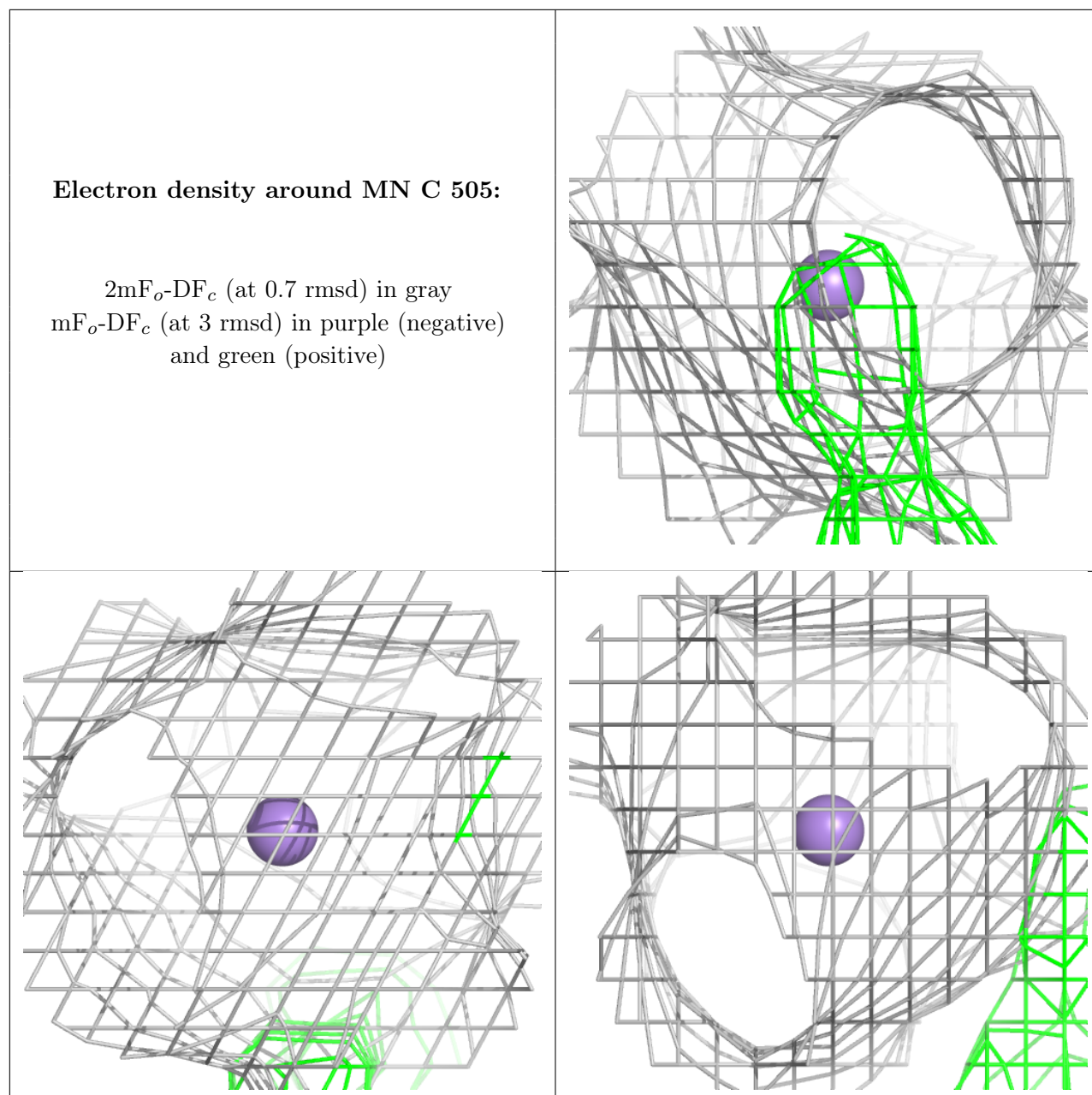
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.