



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:19 PM UTC

PDB ID : 7VPN / pdb_00007vpn
Title : Crystal Structure of the dioxygenase CcTet from Coprinopsis cinereain in complex with Mn(II) and N-Oxalylglycine
Authors : Mu, Y.J.; Zhang, L.; Zhang, L.
Deposited on : 2021-10-17
Resolution : 2.60 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

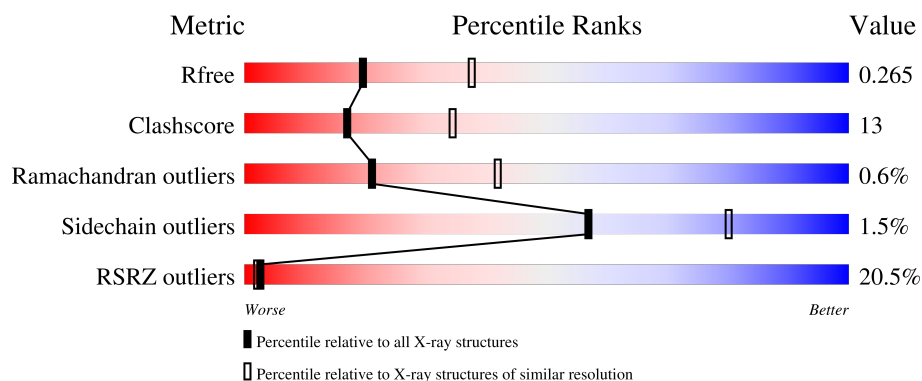
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	430	3% 68% 13% 19%
1	B	430	3% 65% 14% .. 18%
1	C	430	11% 61% 21% . 17%
1	D	430	50% 42% 34% . 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OGA	A	1002	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11103 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.

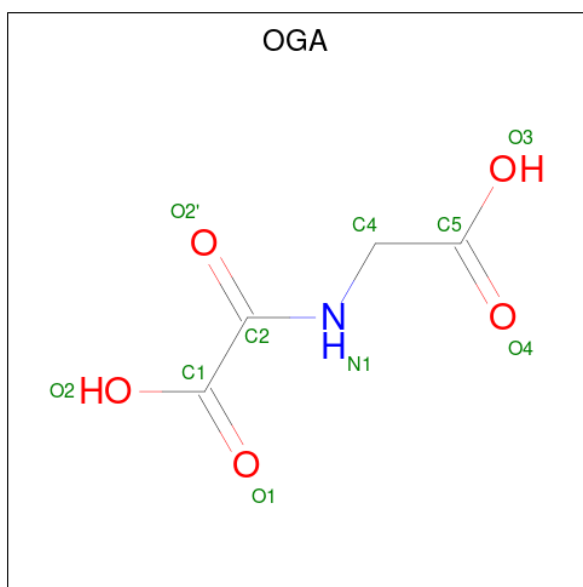
- Molecule 1 is a protein called CcTet molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2715	1743	471	487	14			
1	B	351	Total	C	N	O	S	0	0	0
			2746	1764	474	495	13			
1	C	356	Total	C	N	O	S	0	0	0
			2797	1795	487	502	13			
1	D	334	Total	C	N	O	S	0	0	0
			2626	1689	456	469	12			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	4	1	5		

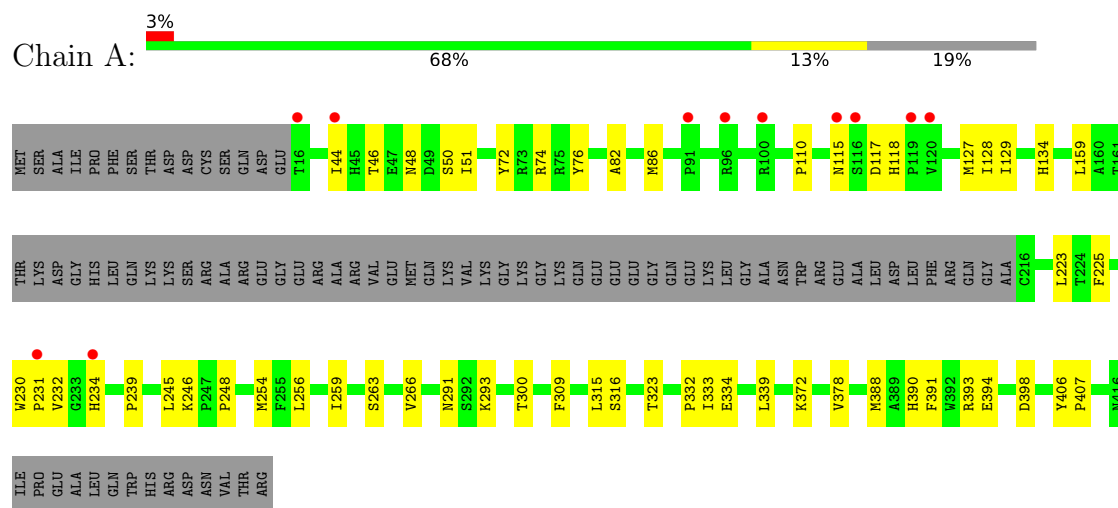
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	97	Total	O	0	0
			97	97		
4	C	31	Total	O	0	0
			31	31		
4	D	4	Total	O	0	0
			4	4		

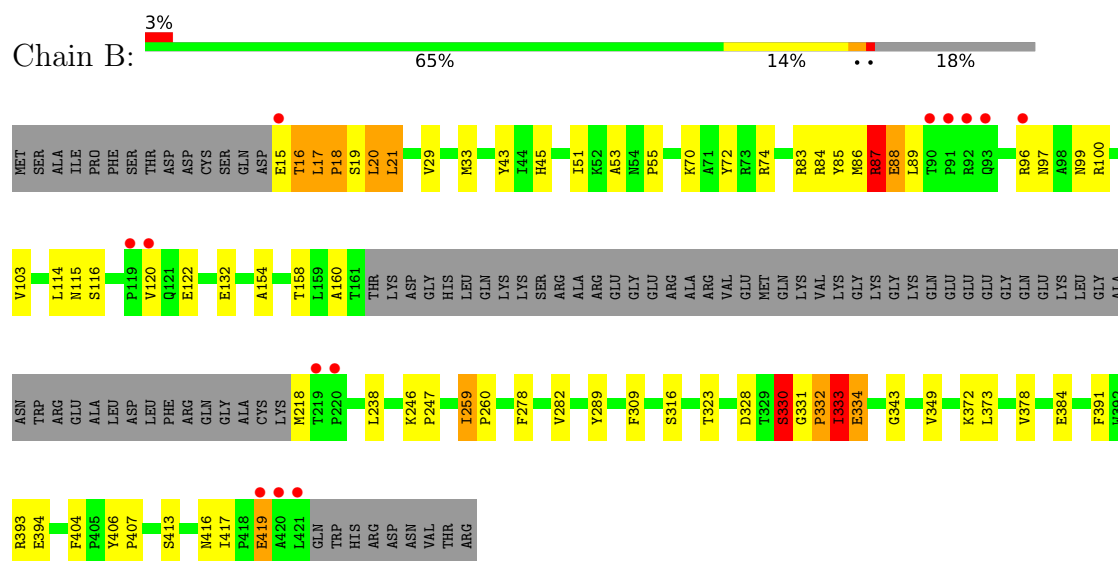
3 Residue-property plots

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CcTet molecule

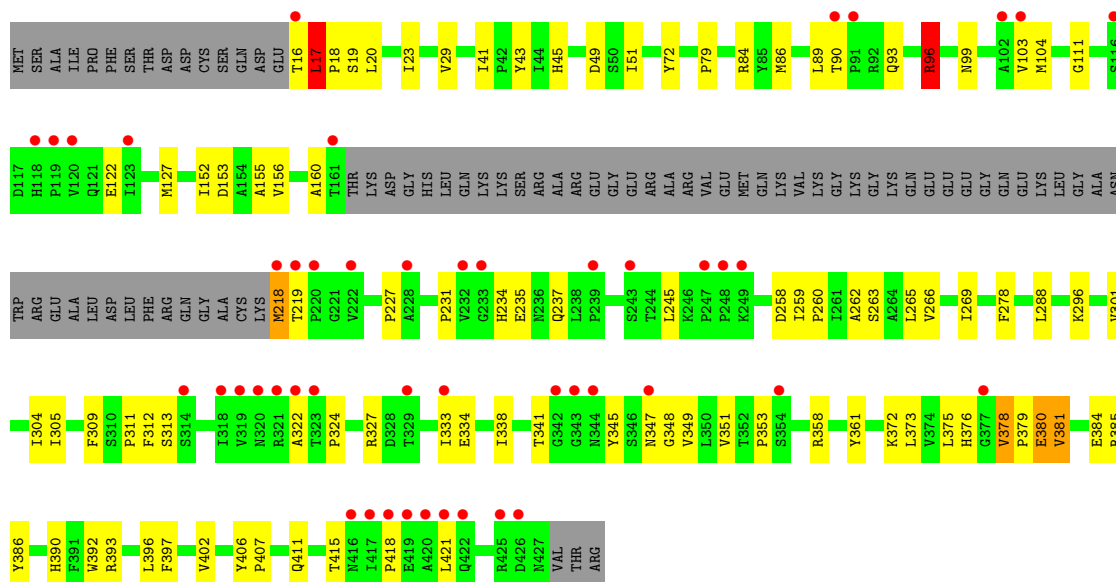


• Molecule 1: CcTet molecule

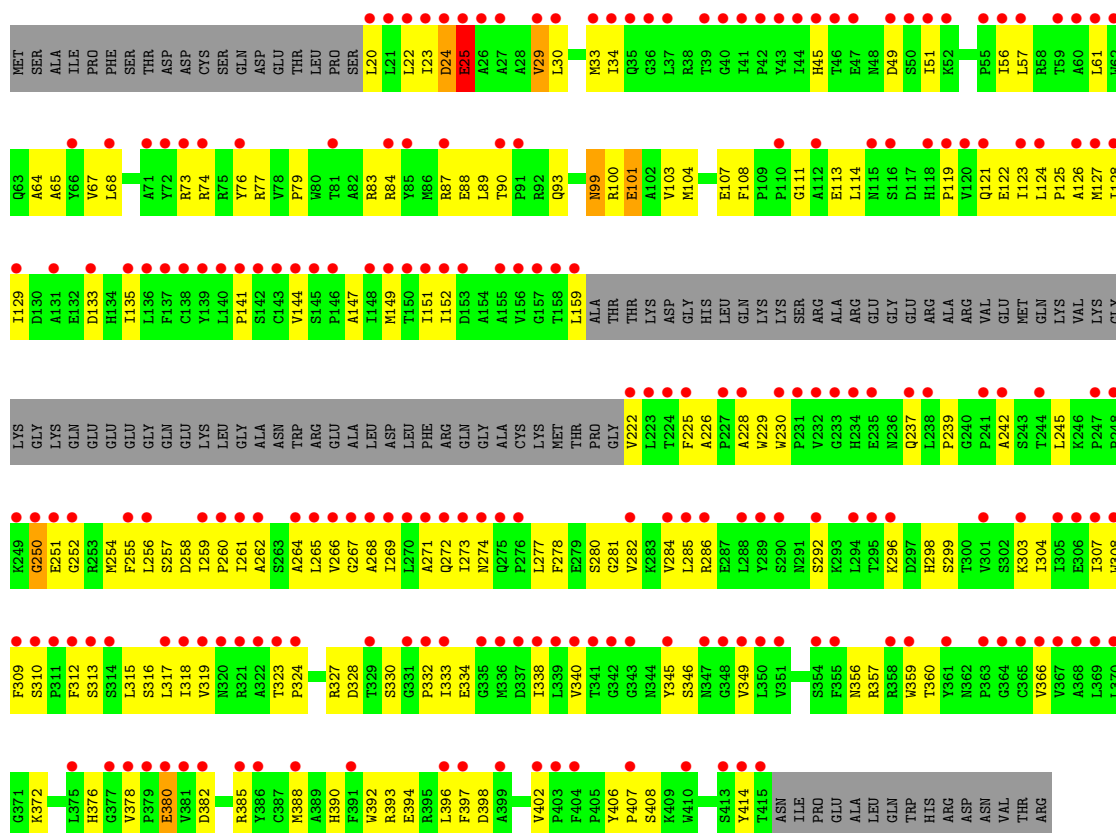
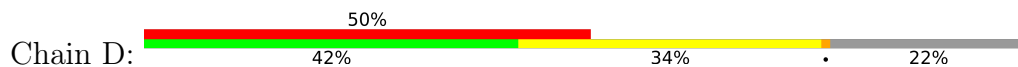


• Molecule 1: CcTet molecule





• Molecule 1: CcTet molecule



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	219.80Å 219.80Å 77.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.16 – 2.60 49.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.3 (49.16-2.60) 91.3 (49.16-2.60)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.217 , 0.266 0.219 , 0.265	Depositor DCC
R_{free} test set	3120 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11103	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OGA, 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	0.49	0/2789	0.73	0/3805
1	B	0.77	15/2821 (0.5%)	0.83	6/3851 (0.2%)
1	C	0.59	4/2875 (0.1%)	0.83	4/3925 (0.1%)
1	D	0.54	2/2698 (0.1%)	0.84	6/3680 (0.2%)
All	All	0.61	21/11183 (0.2%)	0.81	16/15261 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	2
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	PRO	C-O	-11.51	1.10	1.23
1	B	18	PRO	C-O	-8.89	1.12	1.24
1	B	20	LEU	C-O	-8.60	1.13	1.24
1	B	333	ILE	C-O	-7.67	1.14	1.24
1	C	18	PRO	C-O	-7.47	1.14	1.24
1	B	331	GLY	C-O	-7.45	1.14	1.24
1	B	19	SER	C-O	-7.31	1.15	1.24
1	B	17	LEU	C-O	-6.74	1.15	1.24
1	B	85	TYR	C-O	-6.56	1.16	1.24
1	C	379	PRO	C-O	-6.14	1.16	1.23
1	B	21	LEU	C-O	-5.80	1.17	1.24
1	D	376	HIS	CG-ND1	-5.62	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	GLU	C-O	-5.57	1.17	1.24
1	B	18	PRO	N-CA	-5.56	1.40	1.47
1	B	87	ARG	C-O	-5.47	1.17	1.24
1	B	330	SER	CA-CB	-5.45	1.45	1.53
1	C	376	HIS	CG-ND1	-5.44	1.32	1.38
1	D	101	GLU	C-O	-5.40	1.17	1.24
1	C	19	SER	C-O	-5.37	1.17	1.24
1	B	332	PRO	N-CA	-5.20	1.40	1.47
1	B	89	LEU	C-O	-5.12	1.17	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ARG	NE-CZ-NH1	-12.97	108.53	121.50
1	C	96	ARG	CD-NE-CZ	11.69	140.77	124.40
1	D	25	GLU	CA-CB-CG	9.43	132.96	114.10
1	B	16	THR	CA-CB-OG1	-7.83	97.86	109.60
1	B	70	LYS	CD-CE-NZ	-6.86	89.94	111.90
1	D	24	ASP	CA-C-N	-6.45	109.00	121.58
1	D	24	ASP	C-N-CA	-6.45	109.00	121.58
1	D	25	GLU	CG-CD-OE2	-6.13	104.30	118.40
1	B	88	GLU	N-CA-CB	-5.86	100.67	110.22
1	C	18	PRO	N-CA-C	5.68	121.43	113.53
1	B	87	ARG	CB-CG-CD	5.61	124.20	111.30
1	D	25	GLU	N-CA-CB	5.58	119.78	110.41
1	D	49	ASP	CB-CA-C	-5.54	107.48	114.40
1	B	238	LEU	CA-CB-CG	5.38	135.14	116.30
1	B	18	PRO	N-CA-CB	-5.19	97.62	103.33
1	C	17	LEU	N-CA-CB	-5.01	99.05	109.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	96	ARG	Sidechain
1	D	25	GLU	Sidechain
1	D	250	GLY	Peptide

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	2715	0	2725	39	0
1	B	2746	0	2753	50	0
1	C	2797	0	2795	75	0
1	D	2626	0	2633	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	3	4	0
4	A	73	0	0	1	0
4	B	97	0	0	3	0
4	C	31	0	0	1	0
4	D	4	0	0	2	0
All	All	11103	0	10909	277	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 13.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:GLU:HB2	1:C:407:PRO:HD3	1.32	1.05
1:D:274:ASN:HD22	1:D:277:LEU:HB2	1.28	0.95
1:B:86:MET:HE1	1:B:373:LEU:HB2	1.49	0.94
1:A:232:VAL:HB	1:B:97:ASN:HD22	1.32	0.92
1:C:349:VAL:O	1:C:378:VAL:HG23	1.71	0.90
1:B:404:PHE:O	1:D:84:ARG:NH2	2.10	0.84
1:D:129:ILE:HG22	1:D:135:ILE:HA	1.57	0.84
1:C:86:MET:SD	1:C:333:ILE:HD11	2.17	0.83
1:D:312:PHE:HZ	1:D:338:ILE:HD12	1.42	0.83
1:D:99:ASN:OD1	1:D:99:ASN:N	2.13	0.81
1:D:144:VAL:HG11	1:D:149:MET:HE3	1.63	0.80
1:C:96:ARG:HH12	1:C:324:PRO:HG2	1.46	0.79
1:D:77:ARG:HG3	1:D:129:ILE:HG13	1.67	0.77
1:D:274:ASN:ND2	1:D:277:LEU:HB2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LEU:HD22	1:D:319:VAL:HG13	1.66	0.76
1:B:84:ARG:HH22	1:D:394:GLU:HG2	1.52	0.74
1:A:74:ARG:NH2	4:A:1101:HOH:O	2.21	0.73
1:C:333:ILE:HG23	1:C:334:GLU:OE1	1.87	0.73
1:D:312:PHE:CZ	1:D:338:ILE:HD12	2.24	0.73
1:B:332:PRO:HG3	1:B:394:GLU:HB2	1.70	0.72
1:C:122:GLU:OE1	4:C:1101:HOH:O	2.06	0.72
1:D:334:GLU:HB2	1:D:407:PRO:HD3	1.72	0.70
1:D:346:SER:OG	4:D:1101:HOH:O	2.10	0.70
1:C:17:LEU:C	1:C:17:LEU:HD23	2.18	0.69
1:D:225:PHE:HD1	1:D:245:LEU:HD21	1.58	0.68
1:B:120:VAL:O	4:B:1101:HOH:O	2.12	0.68
1:B:15:GLU:O	1:B:15:GLU:HG3	1.92	0.67
1:B:83:ARG:NH1	1:B:132:GLU:OE1	2.29	0.66
1:D:274:ASN:HD22	1:D:277:LEU:CB	2.07	0.66
1:A:316:SER:HB2	1:A:391:PHE:HE2	1.60	0.65
1:D:255:PHE:O	1:D:259:ILE:HG12	1.96	0.65
1:D:265:LEU:O	1:D:269:ILE:HG13	1.97	0.64
1:D:119:PRO:HG3	1:D:356:ASN:O	1.98	0.64
1:D:281:GLY:O	1:D:285:LEU:HD12	1.96	0.64
1:A:332:PRO:HG3	1:A:394:GLU:HB2	1.79	0.64
1:D:242:ALA:HB3	1:D:245:LEU:HD23	1.79	0.64
1:A:334:GLU:HB2	1:A:407:PRO:HD3	1.78	0.63
1:D:230:TRP:CZ2	1:D:239:PRO:HG3	2.33	0.63
1:D:127:MET:HE2	1:D:135:ILE:HG12	1.79	0.63
1:D:30:LEU:O	1:D:34:ILE:HG12	1.99	0.63
1:B:154:ALA:O	1:B:158:THR:HG23	1.99	0.63
1:B:323:THR:HB	1:B:378:VAL:HG12	1.80	0.63
1:D:76:TYR:HB2	1:D:128:ILE:HG12	1.80	0.62
1:D:68:LEU:HD21	1:D:269:ILE:HG23	1.82	0.62
1:D:84:ARG:O	1:D:87:ARG:HG2	1.99	0.62
1:A:246:LYS:O	1:A:248:PRO:HD3	1.99	0.62
1:C:96:ARG:HH12	1:C:324:PRO:CG	2.12	0.61
1:B:74:ARG:NH2	1:B:122:GLU:OE2	2.32	0.61
1:A:398:ASP:OD2	1:C:84:ARG:NH2	2.33	0.61
1:C:45:HIS:HE1	1:C:49:ASP:OD1	1.84	0.61
1:D:313:SER:HB2	1:D:396:LEU:HD12	1.81	0.61
1:D:125:PRO:HB3	1:D:141:PRO:HD2	1.82	0.60
1:C:160:ALA:HB1	1:C:218:MET:HG3	1.82	0.60
1:D:29:VAL:HG21	1:D:51:ILE:HG13	1.82	0.60
1:D:340:VAL:HG22	1:D:366:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:THR:O	1:B:16:THR:HG22	2.02	0.59
1:D:73:ARG:NH1	1:D:414:TYR:OH	2.35	0.59
1:D:378:VAL:HG13	1:D:378:VAL:O	2.02	0.59
1:B:417:ILE:O	1:B:417:ILE:HG13	2.03	0.59
1:D:20:LEU:N	4:D:1102:HOH:O	2.35	0.59
1:D:222:VAL:HG23	1:D:318:ILE:HG13	1.85	0.59
1:D:225:PHE:CD1	1:D:245:LEU:HD21	2.38	0.59
1:C:406:TYR:CG	1:C:407:PRO:HD2	2.38	0.59
1:D:266:VAL:HG21	1:D:390:HIS:CE1	2.37	0.58
1:D:292:SER:HA	1:D:298:HIS:ND1	2.18	0.58
1:A:230:TRP:CE2	1:A:239:PRO:HB3	2.39	0.58
1:D:250:GLY:O	1:D:252:GLY:N	2.36	0.58
1:A:333:ILE:HD12	1:A:372:LYS:HG2	1.85	0.58
1:D:89:LEU:HD23	1:D:104:MET:HE3	1.86	0.58
1:B:43:TYR:OH	1:B:45:HIS:ND1	2.23	0.57
1:D:147:ALA:O	1:D:151:ILE:HG12	2.05	0.57
1:D:333:ILE:H	1:D:333:ILE:HD12	1.69	0.57
1:D:101:GLU:OE1	1:D:101:GLU:HA	2.03	0.57
1:D:330:SER:HB3	1:D:393:ARG:HH12	1.70	0.57
1:C:90:THR:H	1:C:93:GLN:HE21	1.51	0.56
1:D:123:ILE:HG23	1:D:124:LEU:HD12	1.87	0.56
1:C:353:PRO:HD2	1:C:375:LEU:HB3	1.85	0.56
1:D:284:VAL:HG21	1:D:397:PHE:CD1	2.40	0.56
1:C:418:PRO:HA	1:C:421:LEU:HD23	1.87	0.56
1:D:30:LEU:HD13	1:D:61:LEU:HB3	1.87	0.56
1:D:20:LEU:HD12	1:D:22:LEU:H	1.69	0.56
1:A:315:LEU:HD11	1:A:388:MET:HE2	1.87	0.56
1:D:332:PRO:HB3	1:D:394:GLU:HB2	1.88	0.56
1:A:378:VAL:HG11	3:A:1002:OGA:O4	2.06	0.56
1:D:83:ARG:HG3	1:D:406:TYR:OH	2.06	0.55
1:A:291:ASN:OD1	1:A:293:LYS:HG2	2.05	0.55
1:C:90:THR:H	1:C:93:GLN:NE2	2.04	0.55
1:C:288:LEU:HD11	1:C:396:LEU:HD22	1.88	0.55
1:B:316:SER:HB2	1:B:391:PHE:HE1	1.71	0.55
1:A:159:LEU:HD21	1:A:223:LEU:HD23	1.88	0.55
1:B:86:MET:HE2	1:B:373:LEU:HD12	1.89	0.55
1:D:304:ILE:O	1:D:308:TRP:N	2.39	0.55
1:B:84:ARG:NH2	1:D:398:ASP:OD1	2.40	0.55
1:B:17:LEU:HD22	1:B:17:LEU:H	1.73	0.54
1:C:86:MET:HE3	1:C:373:LEU:HD12	1.90	0.54
1:D:255:PHE:CZ	1:D:317:LEU:HD12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:PRO:HB3	1:B:309:PHE:CD1	2.43	0.54
1:C:334:GLU:HB2	1:C:407:PRO:CD	2.23	0.54
1:D:254:MET:O	1:D:258:ASP:N	2.37	0.53
1:D:261:ILE:HD12	1:D:261:ILE:H	1.73	0.53
1:C:90:THR:OG1	1:C:93:GLN:HB2	2.08	0.53
1:C:160:ALA:CB	1:C:218:MET:HG3	2.38	0.53
1:D:397:PHE:HB3	1:D:402:VAL:O	2.09	0.53
1:C:406:TYR:CD2	1:C:407:PRO:HD2	2.43	0.53
1:B:349:VAL:O	1:B:378:VAL:HG23	2.09	0.53
1:C:278:PHE:CD2	1:C:311:PRO:HG3	2.43	0.53
1:A:82:ALA:HB1	1:A:86:MET:HE3	1.91	0.52
1:C:235:GLU:OE2	1:D:324:PRO:HB3	2.09	0.52
1:D:83:ARG:HH12	1:D:84:ARG:NH2	2.07	0.52
1:B:99:ASN:O	1:B:103:VAL:HG23	2.09	0.52
1:C:231:PRO:HD2	1:C:234:HIS:HB2	1.91	0.52
1:D:23:ILE:HG22	1:D:264:ALA:HA	1.92	0.52
1:D:380:GLU:HA	1:D:380:GLU:OE1	2.09	0.51
1:D:345:TYR:CE1	1:D:385:ARG:HG3	2.45	0.51
1:C:29:VAL:HG21	1:C:51:ILE:HG13	1.92	0.51
1:C:99:ASN:O	1:C:103:VAL:HG23	2.09	0.51
1:C:43:TYR:OH	1:C:45:HIS:HD2	1.94	0.51
1:C:334:GLU:OE1	1:C:334:GLU:N	2.40	0.51
1:B:53:ALA:O	1:B:55:PRO:HD3	2.11	0.51
1:C:341:THR:HB	1:C:361:TYR:CZ	2.46	0.51
1:D:64:ALA:O	1:D:67:VAL:HG12	2.11	0.51
1:D:29:VAL:HG12	1:D:33:MET:HE1	1.92	0.50
1:B:160:ALA:HB1	1:B:218:MET:HB3	1.93	0.50
1:D:135:ILE:HD13	1:D:273:ILE:HG23	1.92	0.50
1:D:312:PHE:CG	1:D:390:HIS:HB3	2.46	0.50
1:D:74:ARG:HD3	1:D:126:ALA:HB2	1.93	0.50
1:D:159:LEU:HD12	1:D:255:PHE:HB2	1.94	0.50
1:A:225:PHE:HB3	1:A:245:LEU:HD11	1.94	0.49
1:D:274:ASN:OD1	1:D:408:SER:CB	2.60	0.49
1:B:259:ILE:N	1:B:260:PRO:HD3	2.26	0.49
1:C:266:VAL:HG13	1:C:338:ILE:HG21	1.94	0.49
1:D:122:GLU:HB2	1:D:359:TRP:CE3	2.46	0.49
1:D:245:LEU:HD11	1:D:256:LEU:HD13	1.93	0.49
1:D:271:ALA:HB2	1:D:278:PHE:CD2	2.47	0.49
1:C:411:GLN:HB3	1:C:421:LEU:HB2	1.93	0.49
1:D:260:PRO:HD2	1:D:261:ILE:HD12	1.93	0.49
1:C:89:LEU:HD11	1:C:104:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:VAL:O	1:D:286:ARG:HB2	2.13	0.49
1:A:406:TYR:CD1	1:A:407:PRO:HD2	2.47	0.49
1:C:17:LEU:C	1:C:17:LEU:CD2	2.85	0.49
1:A:129:ILE:HA	1:A:134:HIS:O	2.12	0.48
1:D:274:ASN:OD1	1:D:408:SER:OG	2.22	0.48
1:D:90:THR:OG1	1:D:93:GLN:HB2	2.13	0.48
1:A:231:PRO:HD2	1:A:234:HIS:HB2	1.95	0.48
1:D:79:PRO:HD3	1:D:111:GLY:HA3	1.95	0.48
1:D:267:GLY:O	1:D:278:PHE:HE2	1.95	0.48
1:C:349:VAL:O	1:C:378:VAL:CG2	2.53	0.48
1:C:17:LEU:HD11	1:C:305:ILE:HG22	1.96	0.48
1:B:246:LYS:HB3	1:B:247:PRO:HD3	1.96	0.48
1:D:77:ARG:N	1:D:113:GLU:OE1	2.36	0.48
1:C:327:ARG:HD3	1:C:372:LYS:O	2.13	0.48
1:C:345:TYR:HE2	1:C:348:GLY:HA3	1.78	0.48
1:C:72:TYR:HA	1:C:127:MET:HE3	1.96	0.47
1:C:265:LEU:O	1:C:269:ILE:HG13	2.14	0.47
1:D:45:HIS:HD2	1:D:45:HIS:O	1.97	0.47
1:D:310:SER:HB3	1:D:312:PHE:HD1	1.79	0.47
1:B:83:ARG:NH1	1:D:406:TYR:HB2	2.29	0.47
1:C:313:SER:HB2	1:C:392:TRP:HA	1.97	0.47
1:B:333:ILE:HA	1:B:372:LYS:HG3	1.97	0.47
1:D:77:ARG:NH1	1:D:133:ASP:OD1	2.47	0.47
1:C:322:ALA:N	1:C:380:GLU:OE1	2.48	0.47
1:D:388:MET:SD	1:D:390:HIS:CE1	3.08	0.47
1:C:312:PHE:CG	1:C:390:HIS:HB3	2.50	0.47
1:B:17:LEU:HD21	1:B:289:TYR:CD2	2.50	0.47
1:C:260:PRO:HB3	1:C:309:PHE:CD1	2.49	0.47
1:A:46:THR:HG21	1:A:51:ILE:HB	1.97	0.46
1:B:87:ARG:HH11	1:B:87:ARG:CG	2.28	0.46
1:D:87:ARG:HG3	1:D:88:GLU:N	2.29	0.46
1:B:416:ASN:HB2	4:B:1120:HOH:O	2.14	0.46
1:D:315:LEU:HD21	1:D:388:MET:HG3	1.97	0.46
1:D:56:ILE:HG13	1:D:57:LEU:N	2.30	0.46
1:A:76:TYR:HB2	1:A:128:ILE:HG12	1.98	0.46
1:D:121:GLN:OE1	1:D:349:VAL:HG22	2.16	0.46
1:A:246:LYS:HD2	1:A:300:THR:HG21	1.97	0.46
1:D:123:ILE:HD13	1:D:360:THR:HG21	1.98	0.46
1:B:406:TYR:CD1	1:B:407:PRO:HD2	2.51	0.46
1:C:237:GLN:HE21	1:C:296:LYS:NZ	2.14	0.46
1:A:406:TYR:CG	1:A:407:PRO:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:TYR:CG	1:B:407:PRO:HD2	2.50	0.45
1:C:86:MET:HE3	1:C:373:LEU:CG	2.46	0.45
1:C:393:ARG:HA	1:C:393:ARG:HD3	1.75	0.45
1:D:254:MET:HA	1:D:257:SER:HB2	1.97	0.45
1:C:351:VAL:HG22	1:C:358:ARG:HG3	1.96	0.45
1:B:17:LEU:HG	1:B:20:LEU:HD23	1.98	0.45
1:B:393:ARG:HD3	1:B:393:ARG:HA	1.65	0.45
1:C:41:ILE:O	1:C:41:ILE:HG13	2.17	0.45
1:D:45:HIS:O	1:D:45:HIS:CD2	2.69	0.45
1:C:155:ALA:HB2	1:C:258:ASP:HB3	1.99	0.45
1:C:218:MET:HE3	1:C:218:MET:HB3	1.87	0.45
1:C:245:LEU:HD23	1:C:304:ILE:HG21	1.98	0.45
1:A:245:LEU:HD21	1:A:256:LEU:HD13	1.99	0.44
1:D:152:ILE:HD11	1:D:262:ALA:HB2	1.99	0.44
1:D:328:ASP:O	1:D:372:LYS:HG3	2.17	0.44
1:B:334:GLU:CD	1:B:334:GLU:H	2.25	0.44
1:B:29:VAL:HG11	1:B:51:ILE:HG21	1.98	0.44
1:B:96:ARG:HA	1:B:96:ARG:HD3	1.83	0.44
1:B:86:MET:CE	1:B:373:LEU:HD12	2.47	0.44
1:C:96:ARG:HH12	1:C:324:PRO:CB	2.31	0.44
1:B:419:GLU:CD	1:B:419:GLU:H	2.25	0.44
1:C:347:ASN:OD1	1:C:381:VAL:HG12	2.18	0.44
1:A:72:TYR:HA	1:A:127:MET:HE3	2.00	0.44
1:D:56:ILE:HG13	1:D:57:LEU:H	1.83	0.44
1:D:226:ALA:HB3	1:D:229:TRP:HB2	1.99	0.44
1:D:237:GLN:OE1	1:D:296:LYS:NZ	2.26	0.44
1:D:245:LEU:HB3	1:D:304:ILE:HD11	2.00	0.43
1:C:218:MET:N	1:C:384:GLU:OE1	2.52	0.43
1:A:117:ASP:OD1	1:A:118:HIS:N	2.51	0.43
1:C:86:MET:HE3	1:C:373:LEU:HG	2.01	0.43
1:D:307:ILE:O	1:D:309:PHE:HD1	2.01	0.43
1:C:152:ILE:HD11	1:C:262:ALA:HB1	2.01	0.43
1:D:388:MET:SD	1:D:390:HIS:NE2	2.91	0.43
1:A:339:LEU:HD13	3:A:1002:OGA:C4	2.48	0.43
1:B:29:VAL:O	1:B:33:MET:HG3	2.18	0.43
1:B:114:LEU:C	1:B:116:SER:H	2.26	0.43
1:C:96:ARG:HH12	1:C:324:PRO:HB2	1.84	0.43
1:D:267:GLY:O	1:D:278:PHE:CE2	2.71	0.43
1:B:278:PHE:O	1:B:282:VAL:HG23	2.19	0.42
1:C:153:ASP:OD1	1:C:386:TYR:OH	2.36	0.42
1:C:156:VAL:HG21	1:C:386:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ILE:CD1	1:D:65:ALA:HA	2.48	0.42
1:B:87:ARG:HH11	1:B:87:ARG:HG2	1.84	0.42
1:D:64:ALA:O	1:D:65:ALA:C	2.61	0.42
1:D:304:ILE:HA	1:D:307:ILE:CG2	2.49	0.42
1:C:86:MET:HE2	1:C:86:MET:HA	2.00	0.42
1:D:228:ALA:HB1	1:D:239:PRO:HB2	1.99	0.42
1:A:254:MET:HE2	1:A:254:MET:HA	2.02	0.42
1:D:88:GLU:C	1:D:104:MET:HE1	2.44	0.42
1:D:114:LEU:O	1:D:357:ARG:NH1	2.52	0.42
1:C:79:PRO:HD3	1:C:111:GLY:HA3	2.01	0.42
1:C:235:GLU:OE1	1:C:235:GLU:N	2.33	0.42
1:B:88:GLU:O	1:B:100:ARG:NH2	2.52	0.42
1:D:45:HIS:HE1	1:D:51:ILE:HB	1.85	0.42
1:D:101:GLU:OE2	1:D:327:ARG:NH1	2.46	0.42
1:C:345:TYR:CE1	1:C:385:ARG:HG3	2.54	0.42
1:D:45:HIS:CE1	1:D:51:ILE:HB	2.55	0.42
1:D:280:SER:O	1:D:284:VAL:HG23	2.20	0.42
1:D:292:SER:HA	1:D:298:HIS:CE1	2.55	0.42
1:A:263:SER:HB3	1:A:309:PHE:O	2.20	0.42
1:A:393:ARG:HD3	1:A:393:ARG:HA	1.78	0.42
1:B:328:ASP:OD2	1:B:330:SER:O	2.37	0.42
1:B:96:ARG:HD3	4:B:1109:HOH:O	2.19	0.41
1:D:323:THR:HA	1:D:324:PRO:HD3	1.85	0.41
1:D:299:SER:O	1:D:303:LYS:HG2	2.19	0.41
1:D:313:SER:OG	1:D:392:TRP:HA	2.19	0.41
1:A:86:MET:HG2	1:A:333:ILE:CG1	2.51	0.41
1:A:323:THR:HB	1:A:378:VAL:HG12	2.02	0.41
1:A:398:ASP:CG	1:C:84:ARG:HH21	2.28	0.41
1:C:86:MET:HE3	1:C:373:LEU:CD1	2.50	0.41
1:C:415:THR:HG23	1:C:421:LEU:HB3	2.02	0.41
1:C:263:SER:HB3	1:C:309:PHE:O	2.20	0.41
1:C:345:TYR:HB2	1:C:381:VAL:HB	2.01	0.41
1:C:378:VAL:O	1:C:378:VAL:HG13	2.21	0.41
1:B:17:LEU:CB	1:B:20:LEU:HD23	2.51	0.41
1:D:93:GLN:NE2	1:D:100:ARG:HG3	2.35	0.41
1:A:339:LEU:HD13	3:A:1002:OGA:H4C2	2.03	0.41
1:D:323:THR:OG1	1:D:378:VAL:HG12	2.21	0.41
1:A:110:PRO:HB2	1:A:115:ASN:HB3	2.03	0.41
1:C:397:PHE:HB3	1:C:402:VAL:O	2.20	0.41
1:D:20:LEU:CD1	1:D:22:LEU:H	2.34	0.41
1:D:285:LEU:HD21	1:D:308:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LEU:HD23	1:D:316:SER:N	2.35	0.41
1:A:48:ASN:OD1	1:A:50:SER:HB2	2.20	0.41
1:C:20:LEU:HA	1:C:23:ILE:HG12	2.03	0.41
1:C:96:ARG:NH1	1:C:324:PRO:HB2	2.36	0.41
1:D:107:GLU:HG2	1:D:108:PHE:CE1	2.55	0.41
1:D:268:ALA:O	1:D:272:GLN:HG2	2.21	0.41
1:A:44:ILE:HA	1:A:44:ILE:HD13	1.82	0.40
1:A:266:VAL:HG21	1:A:390:HIS:NE2	2.35	0.40
1:A:333:ILE:CD1	1:A:372:LYS:HE3	2.51	0.40
1:C:227:PRO:O	1:C:301:VAL:HG13	2.21	0.40
1:D:64:ALA:O	1:D:67:VAL:N	2.54	0.40
1:B:218:MET:HG3	1:B:384:GLU:OE1	2.22	0.40
1:C:45:HIS:CE1	1:C:49:ASP:OD1	2.69	0.40
1:A:378:VAL:CG1	3:A:1002:OGA:O4	2.68	0.40
1:B:72:TYR:CE2	1:B:413:SER:HB2	2.56	0.40
1:B:343:GLY:HA3	1:B:384:GLU:O	2.22	0.40
1:D:278:PHE:O	1:D:282:VAL:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/430 (80%)	328 (96%)	14 (4%)	1 (0%)	36	58
1	B	347/430 (81%)	330 (95%)	14 (4%)	3 (1%)	14	30
1	C	352/430 (82%)	329 (94%)	22 (6%)	1 (0%)	36	58
1	D	330/430 (77%)	305 (92%)	22 (7%)	3 (1%)	14	30
All	All	1372/1720 (80%)	1292 (94%)	72 (5%)	8 (1%)	21	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	29	VAL
1	D	24	ASP
1	B	419	GLU
1	B	115	ASN
1	D	251	GLU
1	B	259	ILE
1	C	259	ILE
1	A	259	ILE

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	293/362 (81%)	293 (100%)	0	100	100
1	B	296/362 (82%)	291 (98%)	5 (2%)	53	78
1	C	301/362 (83%)	294 (98%)	7 (2%)	44	71
1	D	282/362 (78%)	277 (98%)	5 (2%)	51	76
All	All	1172/1448 (81%)	1155 (98%)	17 (2%)	57	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	PRO
1	B	21	LEU
1	B	87	ARG
1	B	330	SER
1	B	333	ILE
1	C	16	THR
1	C	17	LEU
1	C	218	MET
1	C	219	THR
1	C	378	VAL
1	C	380	GLU
1	C	381	VAL
1	D	25	GLU
1	D	99	ASN

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Mol	Chain	Res	Type
1	D	103	VAL
1	D	380	GLU
1	D	382	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	347	ASN
1	B	356	ASN
1	C	45	HIS
1	C	93	GLN
1	C	99	ASN
1	C	237	GLN
1	C	291	ASN
1	C	424	HIS
1	D	45	HIS
1	D	54	ASN
1	D	390	HIS

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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
3	OGA	A	1002	2	9,9,9	2.89	5 (55%)	8,11,11	3.50	5 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OGA	A	1002	2	-	3/8/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	OGA	C4-C5	5.13	1.63	1.50
3	A	1002	OGA	C2-N1	4.66	1.41	1.33
3	A	1002	OGA	O3-C5	-3.12	1.20	1.30
3	A	1002	OGA	C4-N1	2.81	1.52	1.45
3	A	1002	OGA	O2-C1	-2.60	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	OGA	O2'-C2-C1	-5.45	114.20	121.36
3	A	1002	OGA	C4-N1-C2	5.17	129.27	121.29
3	A	1002	OGA	C5-C4-N1	4.66	127.55	113.06
3	A	1002	OGA	O2-C1-O1	-2.93	116.91	123.90
3	A	1002	OGA	O3-C5-O4	-2.64	116.55	123.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

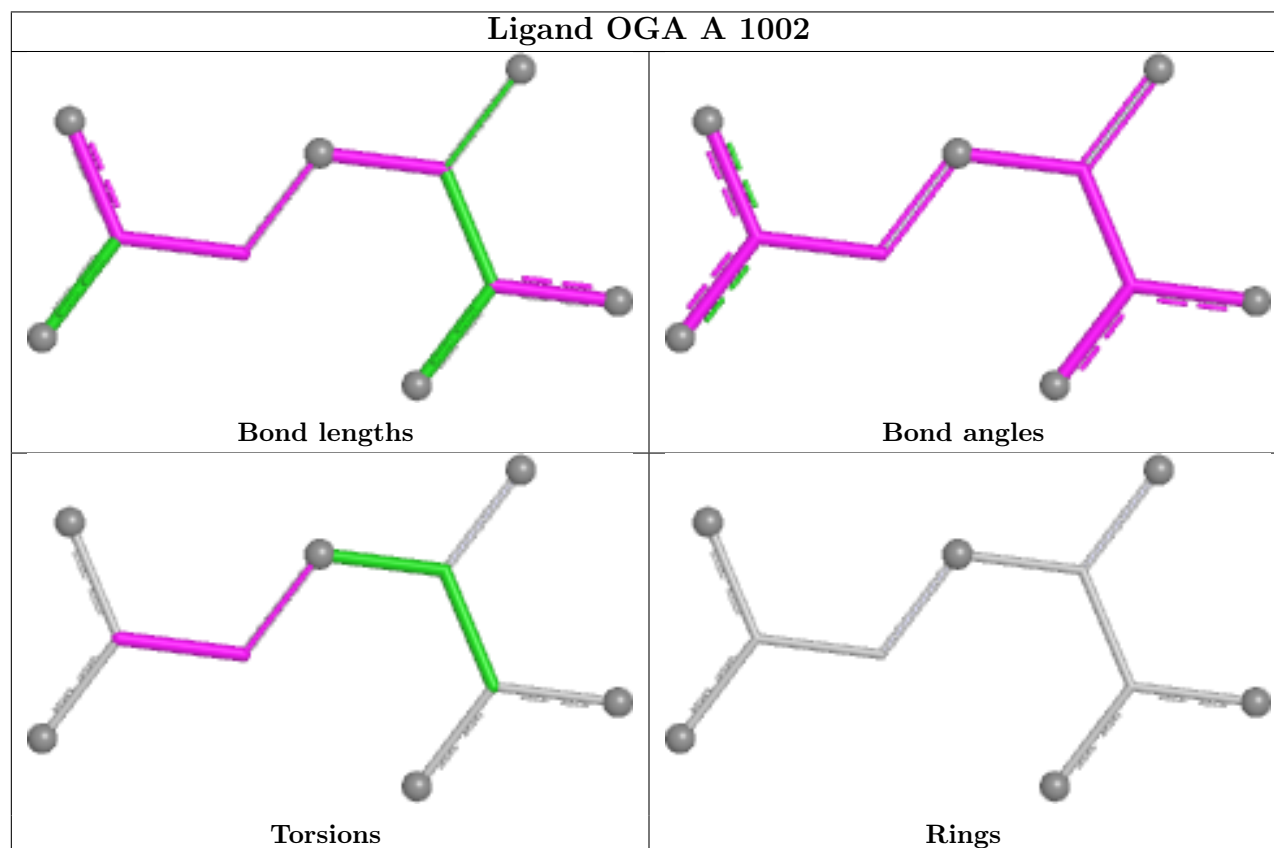
Mol	Chain	Res	Type	Atoms
3	A	1002	OGA	N1-C4-C5-O4
3	A	1002	OGA	N1-C4-C5-O3
3	A	1002	OGA	C5-C4-N1-C2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	OGA	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	347/430 (80%)	-0.07	11 (3%) 50 44	20, 37, 67, 92	0
1	B	351/430 (81%)	-0.09	13 (3%) 45 39	21, 35, 75, 103	0
1	C	356/430 (82%)	0.86	47 (13%) 7 5	29, 58, 92, 156	0
1	D	334/430 (77%)	2.54	214 (64%) 0 0	65, 111, 139, 146	0
All	All	1388/1720 (80%)	0.79	285 (20%) 2 2	20, 50, 131, 156	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	340	VAL	6.7
1	D	343	GLY	6.7
1	D	41	ILE	6.3
1	C	161	THR	5.9
1	D	20	LEU	5.6
1	D	135	ILE	5.5
1	C	418	PRO	5.4
1	D	137	PHE	5.2
1	D	23	ILE	5.2
1	D	255	PHE	5.2
1	D	319	VAL	5.1
1	B	15	GLU	5.0
1	D	124	LEU	4.9
1	D	388	MET	4.9
1	C	417	ILE	4.9
1	D	261	ILE	4.9
1	D	138	CYS	4.8
1	D	123	ILE	4.7
1	D	323	THR	4.7
1	D	359	TRP	4.6
1	D	294	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	247	PRO	4.6
1	D	339	LEU	4.6
1	D	146	PRO	4.6
1	D	336	MET	4.6
1	D	403	PRO	4.6
1	D	324	PRO	4.5
1	D	120	VAL	4.5
1	D	248	PRO	4.5
1	D	320	ASN	4.4
1	D	144	VAL	4.4
1	D	57	LEU	4.3
1	D	350	LEU	4.3
1	D	349	VAL	4.3
1	D	44	ILE	4.2
1	D	156	VAL	4.2
1	D	377	GLY	4.1
1	D	148	ILE	4.1
1	C	419	GLU	4.1
1	D	159	LEU	4.1
1	C	329	THR	4.1
1	D	369	LEU	4.1
1	D	56	ILE	4.0
1	D	43	TYR	4.0
1	D	152	ILE	4.0
1	D	259	ILE	4.0
1	D	396	LEU	4.0
1	D	33	MET	3.9
1	C	420	ALA	3.9
1	C	421	LEU	3.9
1	D	62	TRP	3.9
1	C	416	ASN	3.8
1	D	151	ILE	3.8
1	D	149	MET	3.8
1	D	60	ALA	3.8
1	D	52	LYS	3.8
1	D	313	SER	3.8
1	D	318	ILE	3.8
1	C	91	PRO	3.8
1	D	341	THR	3.8
1	D	256	LEU	3.8
1	D	55	PRO	3.8
1	D	364	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	143	CYS	3.7
1	D	368	ALA	3.7
1	D	66	TYR	3.6
1	D	244	THR	3.6
1	D	270	LEU	3.6
1	D	72	TYR	3.6
1	D	414	TYR	3.6
1	B	92	ARG	3.5
1	B	420	ALA	3.5
1	D	233	GLY	3.5
1	D	21	LEU	3.5
1	D	285	LEU	3.5
1	D	128	ILE	3.5
1	D	370	LEU	3.5
1	D	329	THR	3.5
1	D	241	PRO	3.5
1	D	307	ILE	3.4
1	D	42	PRO	3.4
1	D	227	PRO	3.4
1	D	231	PRO	3.4
1	D	61	LEU	3.4
1	D	232	VAL	3.4
1	B	91	PRO	3.4
1	D	262	ALA	3.4
1	D	347	ASN	3.4
1	D	265	LEU	3.4
1	C	218	MET	3.4
1	D	311	PRO	3.4
1	B	421	LEU	3.3
1	D	385	ARG	3.3
1	D	234	HIS	3.3
1	D	222	VAL	3.3
1	D	365	CYS	3.3
1	D	22	LEU	3.3
1	B	93	GLN	3.3
1	D	264	ALA	3.3
1	B	120	VAL	3.3
1	D	40	GLY	3.3
1	D	223	LEU	3.2
1	D	367	VAL	3.2
1	C	119	PRO	3.2
1	D	332	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	292	SER	3.2
1	D	155	ALA	3.2
1	B	96	ARG	3.2
1	D	310	SER	3.2
1	D	153	ASP	3.2
1	D	415	THR	3.2
1	D	333	ILE	3.2
1	D	289	TYR	3.1
1	B	90	THR	3.1
1	D	59	THR	3.1
1	D	36	GLY	3.1
1	C	248	PRO	3.1
1	C	425	ARG	3.0
1	D	118	HIS	3.0
1	D	386	TYR	3.0
1	D	121	GLN	3.0
1	D	338	ILE	3.0
1	D	145	SER	3.0
1	B	119	PRO	3.0
1	D	139	TYR	3.0
1	C	232	VAL	3.0
1	D	317	LEU	2.9
1	D	71	ALA	2.9
1	C	377	GLY	2.9
1	D	224	THR	2.9
1	D	225	PHE	2.9
1	D	366	VAL	2.9
1	D	272	GLN	2.9
1	D	290	SER	2.9
1	D	90	THR	2.9
1	D	295	THR	2.9
1	D	322	ALA	2.9
1	D	29	VAL	2.9
1	D	306	GLU	2.8
1	D	308	TRP	2.8
1	D	354	SER	2.8
1	D	115	ASN	2.8
1	D	24	ASP	2.8
1	D	126	ALA	2.8
1	D	402	VAL	2.8
1	D	379	PRO	2.8
1	D	136	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	231	PRO	2.8
1	D	74	ARG	2.8
1	D	142	SER	2.8
1	C	343	GLY	2.8
1	D	26	ALA	2.8
1	D	230	TRP	2.8
1	D	37	LEU	2.8
1	C	219	THR	2.8
1	D	228	ALA	2.8
1	D	345	TYR	2.8
1	A	119	PRO	2.7
1	D	110	PRO	2.7
1	C	319	VAL	2.7
1	D	378	VAL	2.7
1	D	237	GLN	2.7
1	A	116	SER	2.7
1	D	157	GLY	2.7
1	D	27	ALA	2.7
1	D	73	ARG	2.7
1	C	233	GLY	2.7
1	C	342	GLY	2.7
1	C	102	ALA	2.7
1	D	351	VAL	2.7
1	D	119	PRO	2.7
1	D	413	SER	2.7
1	D	242	ALA	2.6
1	D	381	VAL	2.6
1	D	269	ILE	2.6
1	D	68	LEU	2.6
1	A	234	HIS	2.6
1	C	220	PRO	2.6
1	D	260	PRO	2.6
1	C	118	HIS	2.6
1	D	249	LYS	2.6
1	D	251	GLU	2.6
1	C	422	GLN	2.6
1	D	305	ILE	2.6
1	D	238	LEU	2.6
1	D	46	THR	2.5
1	D	116	SER	2.5
1	D	87	ARG	2.5
1	D	321	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	91	PRO	2.5
1	D	404	PHE	2.5
1	D	296	LYS	2.5
1	C	123	ILE	2.5
1	D	51	ILE	2.5
1	D	140	LEU	2.5
1	D	337	ASP	2.5
1	D	380	GLU	2.5
1	B	219	THR	2.4
1	A	96	ARG	2.4
1	D	49	ASP	2.4
1	A	120	VAL	2.4
1	C	90	THR	2.4
1	C	344	ASN	2.4
1	D	141	PRO	2.4
1	D	399	ALA	2.4
1	D	39	THR	2.4
1	D	150	THR	2.4
1	C	320	ASN	2.4
1	C	347	ASN	2.4
1	C	247	PRO	2.4
1	D	284	VAL	2.4
1	D	129	ILE	2.4
1	D	274	ASN	2.4
1	C	426	ASP	2.4
1	B	220	PRO	2.4
1	D	363	PRO	2.4
1	D	252	GLY	2.3
1	C	103	VAL	2.3
1	D	309	PHE	2.3
1	D	391	PHE	2.3
1	D	235	GLU	2.3
1	C	239	PRO	2.3
1	D	335	GLY	2.3
1	D	358	ARG	2.3
1	D	266	VAL	2.3
1	A	115	ASN	2.3
1	D	282	VAL	2.3
1	C	322	ALA	2.3
1	D	112	ALA	2.3
1	C	249	LYS	2.3
1	C	116	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	131	ALA	2.2
1	D	76	TYR	2.2
1	D	84	ARG	2.2
1	D	331	GLY	2.2
1	C	228	ALA	2.2
1	D	276	PRO	2.2
1	D	50	SER	2.2
1	D	342	GLY	2.2
1	D	312	PHE	2.2
1	A	16	THR	2.2
1	D	407	PRO	2.2
1	C	354	SER	2.2
1	C	120	VAL	2.2
1	D	301	VAL	2.2
1	D	81	THR	2.2
1	D	275	GLN	2.2
1	D	30	LEU	2.2
1	D	267	GLY	2.2
1	D	348	GLY	2.2
1	D	127	MET	2.2
1	D	133	ASP	2.2
1	C	243	SER	2.2
1	C	321	ARG	2.1
1	D	85	TYR	2.1
1	C	333	ILE	2.1
1	B	419	GLU	2.1
1	D	25	GLU	2.1
1	A	100	ARG	2.1
1	A	91	PRO	2.1
1	D	303	LYS	2.1
1	D	35	GLN	2.1
1	D	288	LEU	2.1
1	D	375	LEU	2.1
1	C	222	VAL	2.1
1	C	318	ILE	2.1
1	D	382	ASP	2.1
1	D	47	GLU	2.1
1	D	158	THR	2.1
1	D	45	HIS	2.1
1	D	34	ILE	2.1
1	D	273	ILE	2.1
1	D	397	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	314	SER	2.0
1	D	271	ALA	2.0
1	C	16	THR	2.0
1	A	44	ILE	2.0
1	D	250	GLY	2.0
1	D	286	ARG	2.0
1	D	355	PHE	2.0
1	D	268	ALA	2.0
1	D	314	SER	2.0
1	C	323	THR	2.0
1	D	410	TRP	2.0
1	D	361	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

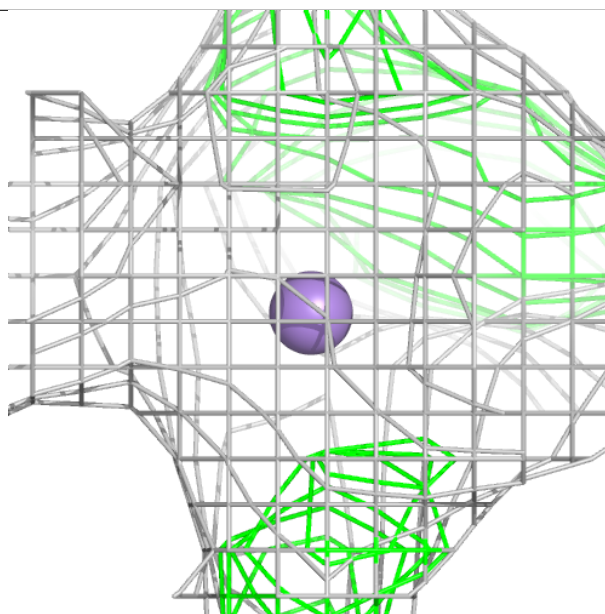
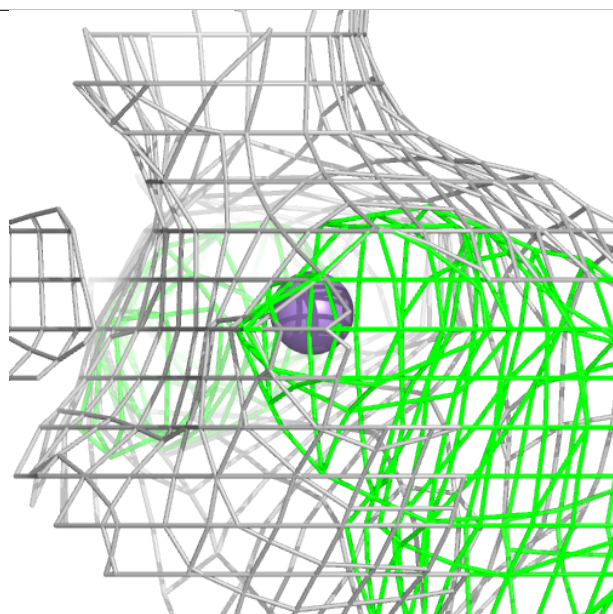
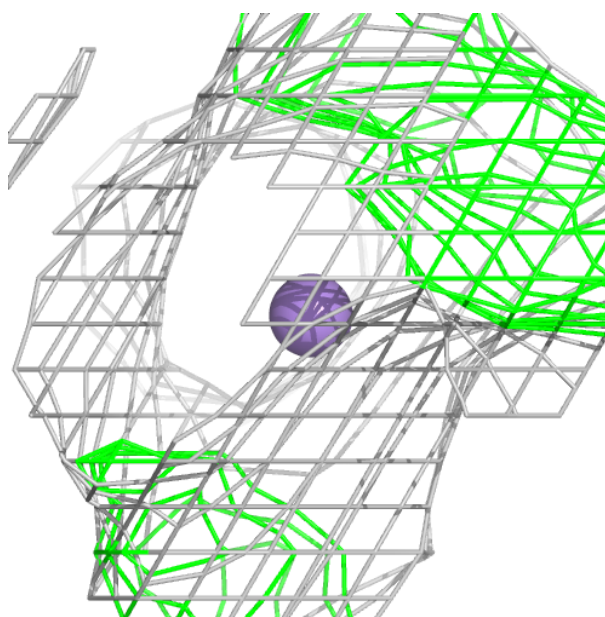
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	1001	1/1	0.71	0.16	89,89,89,89	0
3	OGA	A	1002	10/10	0.75	0.32	13,15,18,20	0
2	MN	C	1001	1/1	0.78	0.16	114,114,114,114	0
2	MN	D	1001	1/1	0.79	0.18	111,111,111,111	0
2	MN	A	1001	1/1	0.82	0.21	59,59,59,59	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.

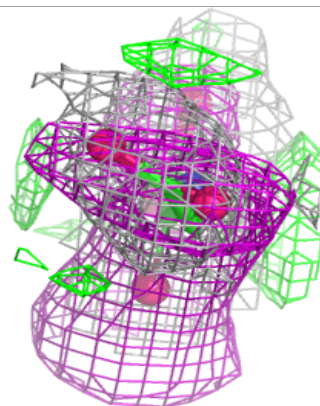
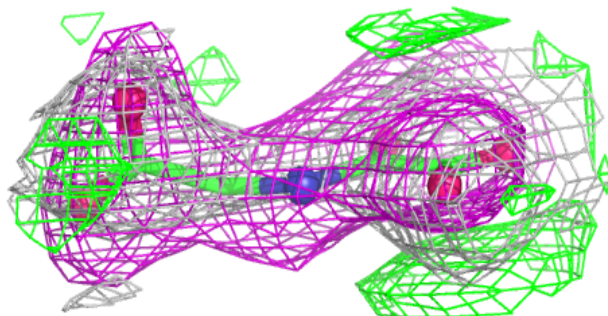
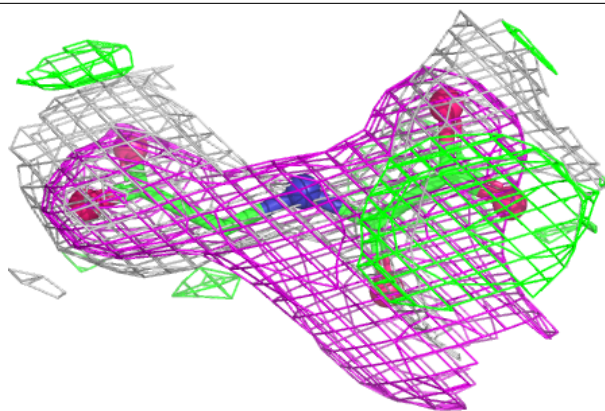
Electron density around MN B 1001:

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



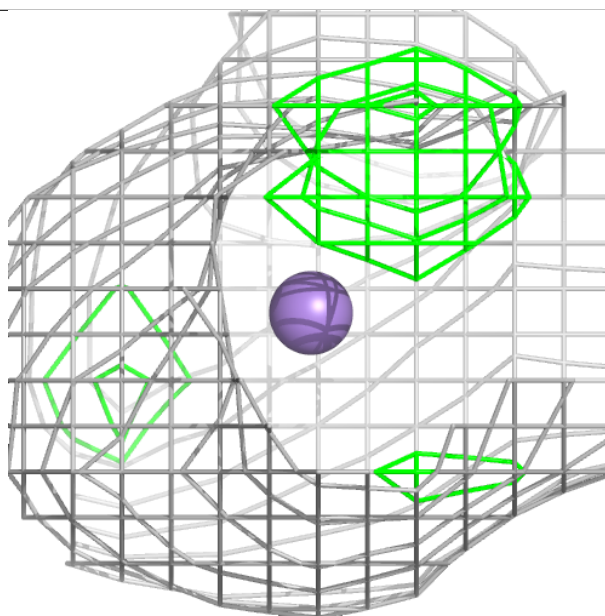
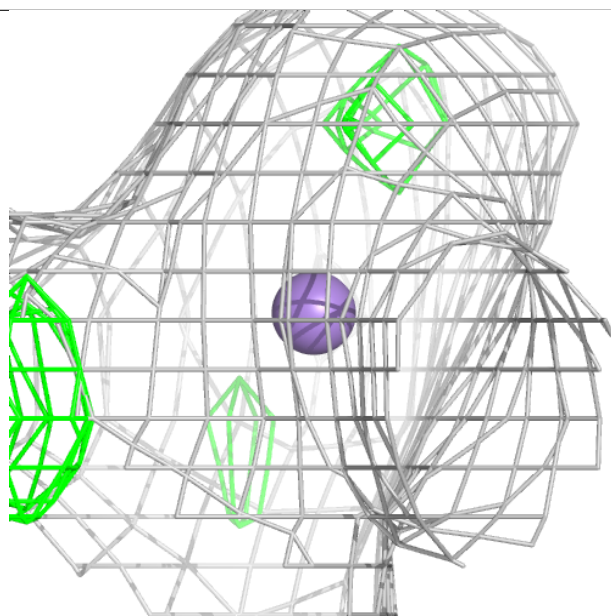
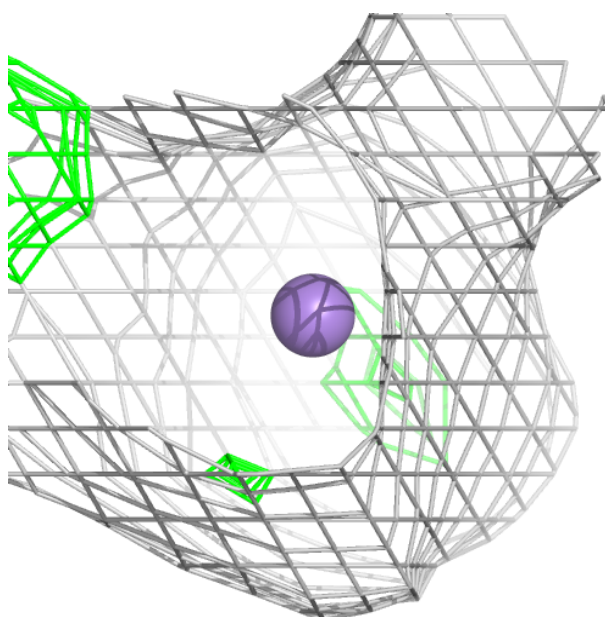
Electron density around OGA A 1002:

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



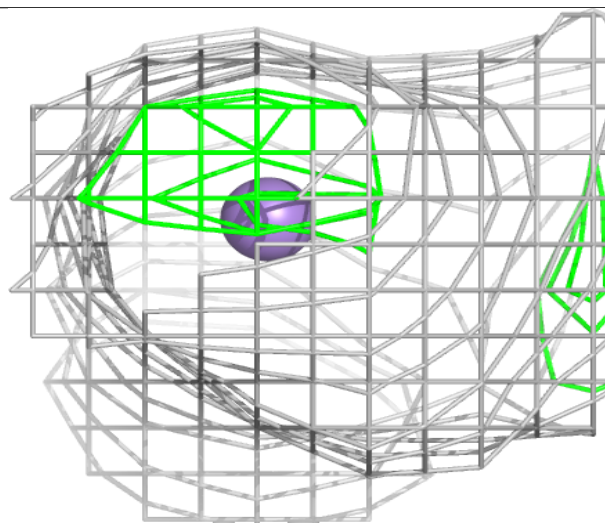
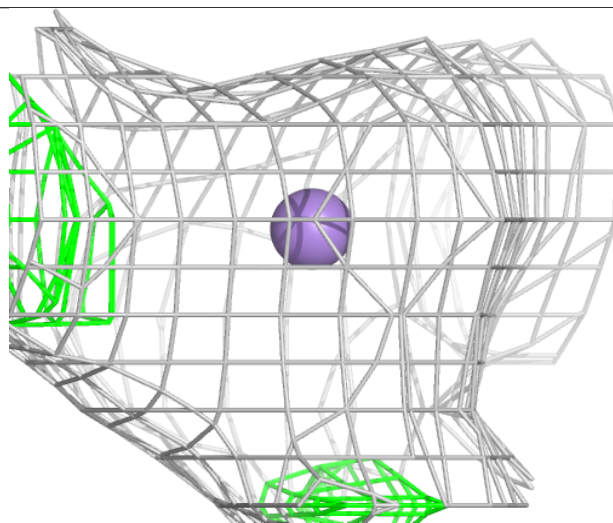
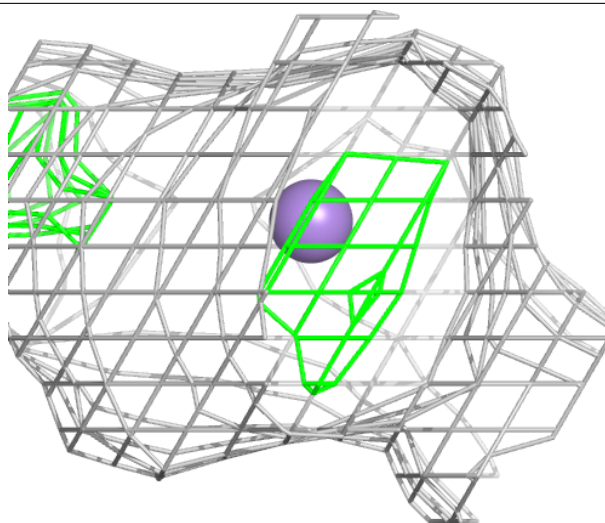
Electron density around MN C 1001:

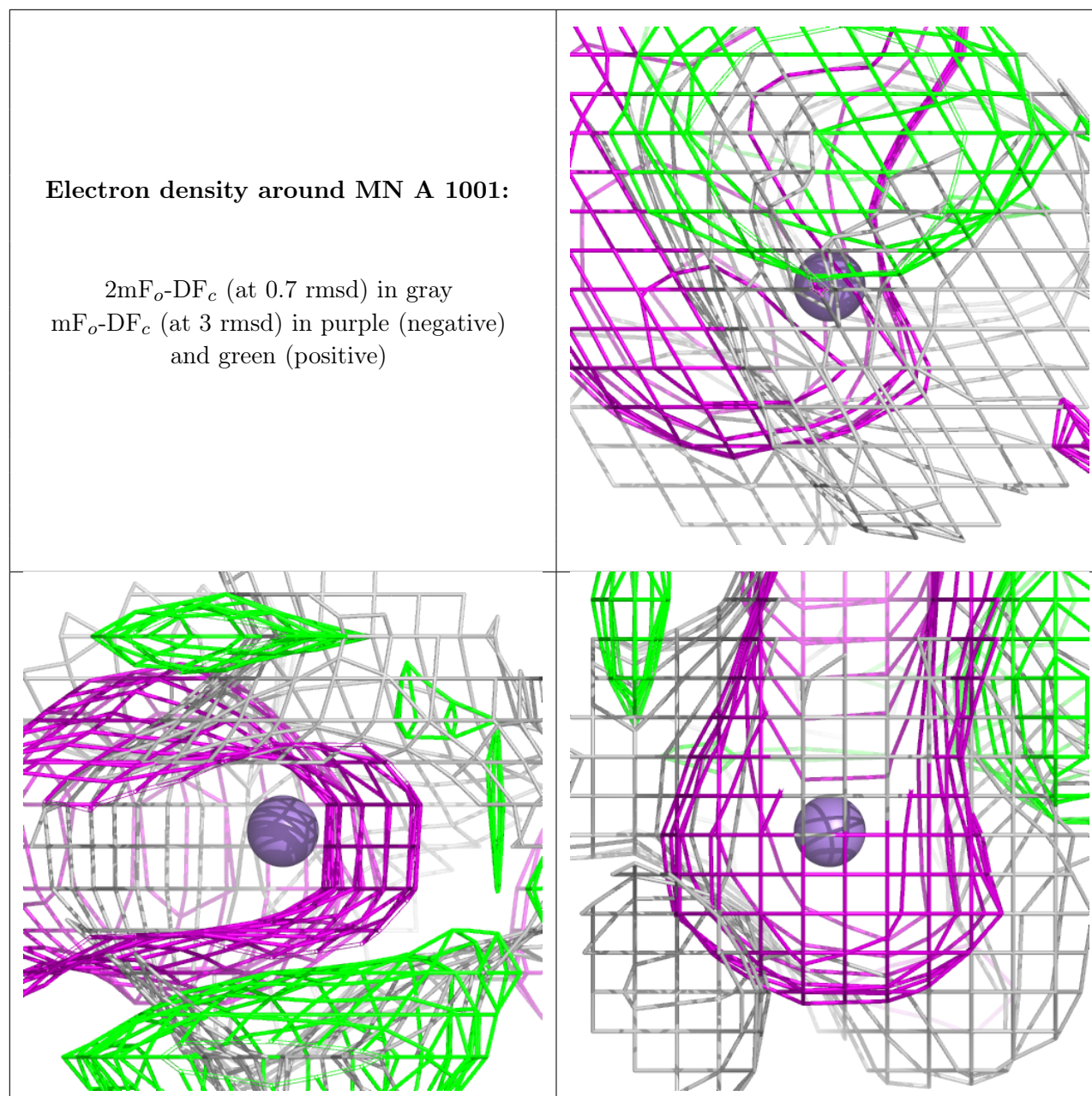
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN D 1001:

$2mF_o-DF_c$ (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.