



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:13 PM UTC

PDB ID : 6K73 / pdb_00006k73
Title : Chaperone-tip adhesin complex is vital for synergistic activation of CFA/I fimbriae biogenesis
Authors : Bao, R.; He, L.H.
Deposited on : 2019-06-05
Resolution : 2.77 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:

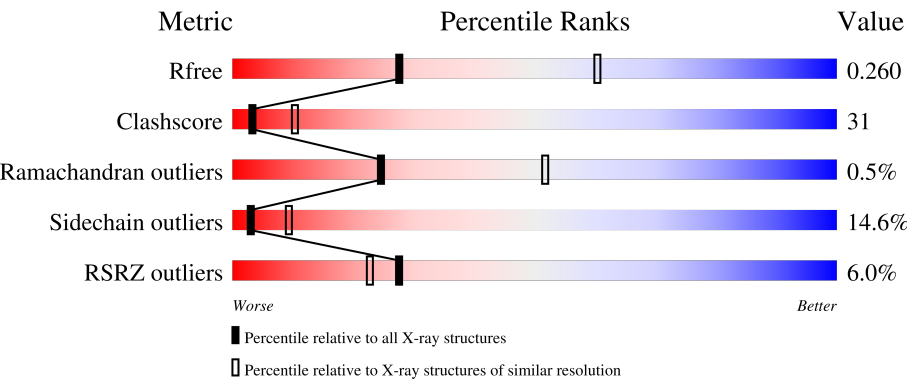
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	221	
1	B	221	
2	C	341	
2	D	341	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8432 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 Colonization factor antigen I chaperone CfaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1642	1062	274	303	3			
1	B	211	Total	C	N	O	S	0	0	0
			1687	1089	281	314	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ILE	THR	engineered mutation	UNP A0A3Y5Z8F9
A	114	ILE	LEU	engineered mutation	UNP A0A3Y5Z8F9
A	116	ILE	VAL	engineered mutation	UNP A0A3Y5Z8F9
A	220	ALA	-	expression tag	UNP A0A3Y5Z8F9
B	112	ILE	THR	engineered mutation	UNP A0A3Y5Z8F9
B	114	ILE	LEU	engineered mutation	UNP A0A3Y5Z8F9
B	116	ILE	VAL	engineered mutation	UNP A0A3Y5Z8F9
B	220	ALA	-	expression tag	UNP A0A3Y5Z8F9

- Molecule 2 is a protein called CFA/I fimbrial subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	320	Total	C	N	O	S	0	0	0
			2491	1561	438	482	10			
2	D	326	Total	C	N	O	S	0	0	0
			2538	1592	446	490	10			

There are 8 discrepancies between the modelled and reference sequences:

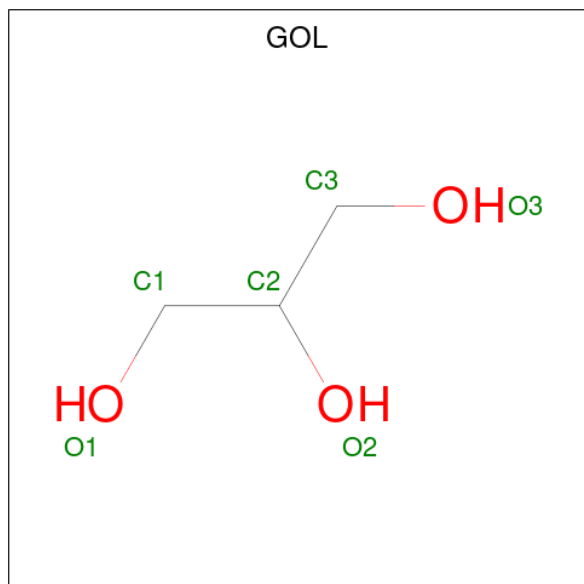
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	HIS	-	expression tag	UNP P25734
C	21	HIS	-	expression tag	UNP P25734
C	22	HIS	-	expression tag	UNP P25734
C	23	HIS	-	expression tag	UNP P25734

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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P25734
D	21	HIS	-	expression tag	UNP P25734
D	22	HIS	-	expression tag	UNP P25734
D	23	HIS	-	expression tag	UNP P25734

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	B	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Ni	0	0
			2	2		

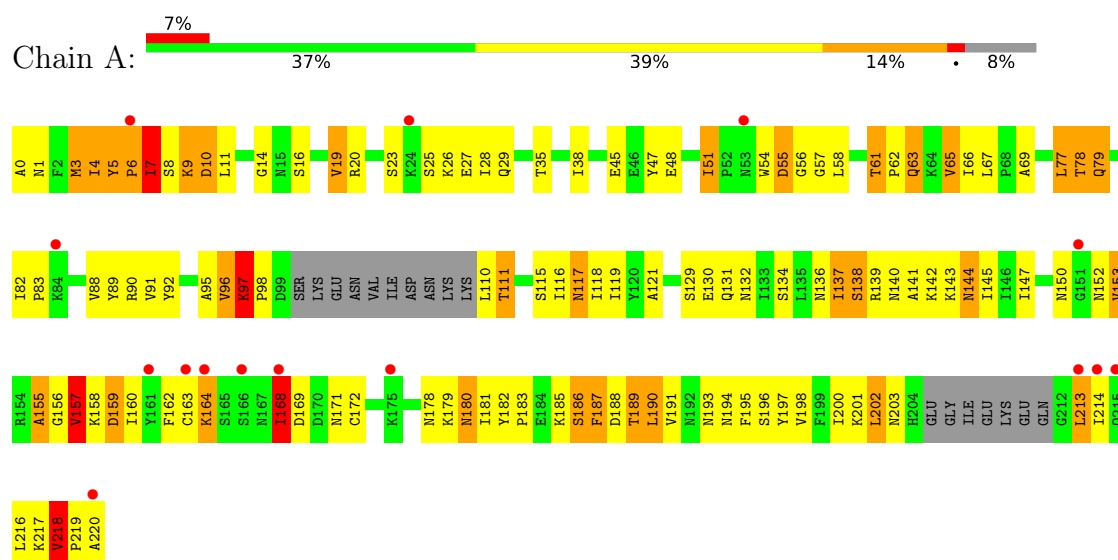
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	14	Total	O	0	0
			14	14		
5	C	14	Total	O	0	0
			14	14		
5	D	11	Total	O	0	0
			11	11		

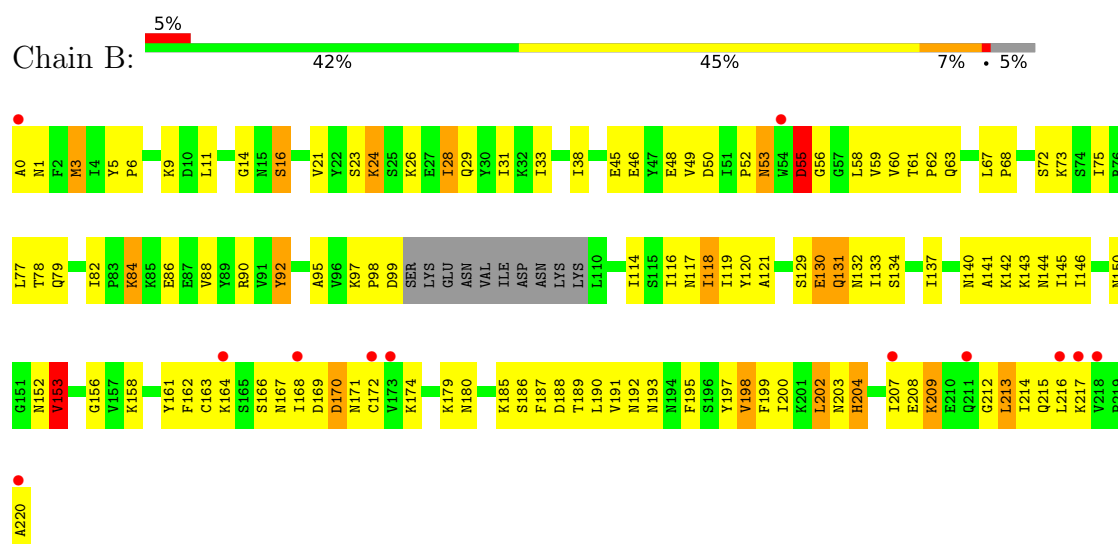
3 Residue-property plots

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: Colonization factor antigen I chaperone CfaA

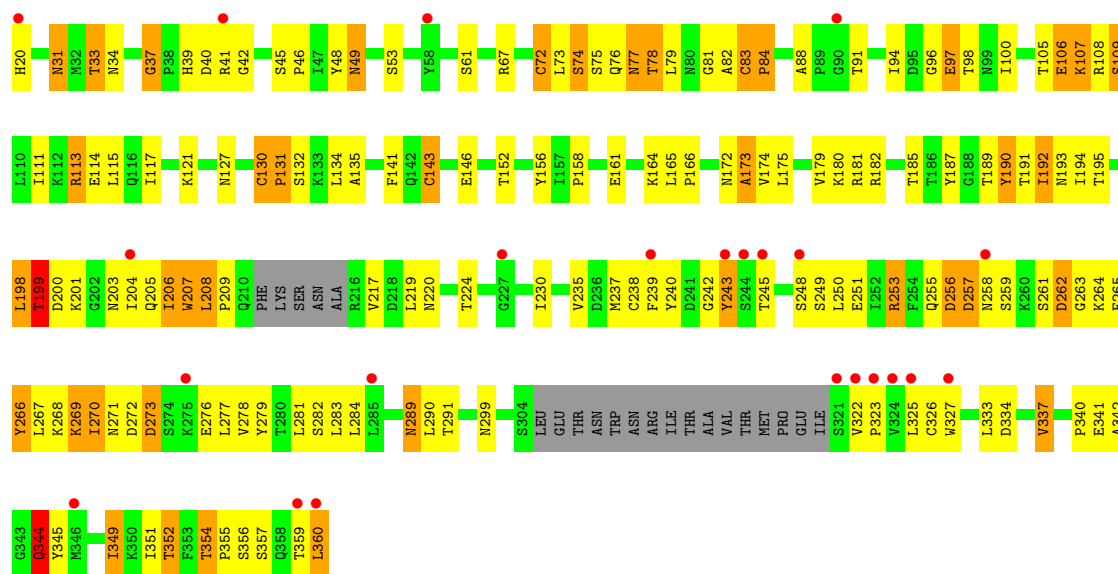


• Molecule 1: Colonization factor antigen I chaperone CfaA

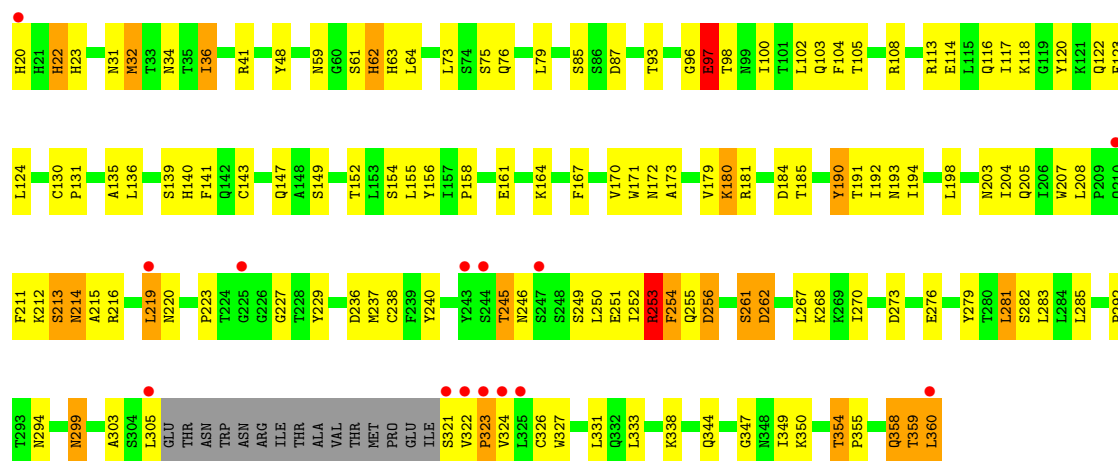


• Molecule 2: CFA/I fimbrial subunit E





• Molecule 2: CFA/I fimbrial subunit E



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	217.16Å 217.16Å 177.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.52 – 2.77 29.52 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.52-2.77) 99.5 (29.52-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.225 , 0.260 0.238 , 0.260	Depositor DCC
R_{free} test set	2000 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8432	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% 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: GOL, NI

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	1.47	15/1672 (0.9%)	1.26	22/2259 (1.0%)
1	B	1.07	7/1718 (0.4%)	0.99	9/2323 (0.4%)
2	C	1.41	33/2542 (1.3%)	1.07	26/3445 (0.8%)
2	D	1.17	31/2591 (1.2%)	0.87	13/3512 (0.4%)
All	All	1.29	86/8523 (1.0%)	1.04	70/11539 (0.6%)

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
2	C	0	1

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	194	ILE	C-O	-9.10	1.14	1.24
2	C	96	GLY	C-O	-9.01	1.17	1.23
2	C	208	LEU	CA-C	-8.41	1.41	1.52
2	D	155	LEU	C-O	-8.19	1.14	1.23
2	D	102	LEU	C-O	-7.86	1.14	1.24
2	C	208	LEU	C-O	-7.80	1.17	1.25
1	A	4	ILE	C-O	-7.69	1.16	1.24
2	C	192	ILE	C-O	-7.65	1.16	1.24
2	D	32	MET	C-O	-7.53	1.14	1.23
2	C	31	ASN	C-O	-7.53	1.15	1.24
2	C	256	ASP	CA-C	-7.04	1.44	1.52
2	D	192	ILE	C-O	-6.92	1.16	1.24
2	C	174	VAL	C-O	-6.90	1.16	1.24
1	B	153	VAL	C-O	-6.89	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	194	ILE	C-O	-6.78	1.16	1.24
2	C	195	THR	C-O	-6.69	1.15	1.24
2	D	254	PHE	C-O	-6.55	1.16	1.24
2	C	84	PRO	C-O	-6.47	1.15	1.23
1	B	92	TYR	C-O	-6.41	1.16	1.24
2	D	36	ILE	C-O	-6.40	1.17	1.24
1	B	114	ILE	C-O	-6.40	1.17	1.24
1	B	46	GLU	C-O	-6.38	1.16	1.24
2	D	154	SER	C-O	-6.36	1.16	1.23
2	C	98	THR	C-O	-6.32	1.16	1.23
2	D	193	ASN	CA-C	-6.29	1.45	1.52
1	A	218	VAL	C-N	6.28	1.39	1.33
2	C	83	CYS	C-O	-6.26	1.16	1.24
2	D	252	ILE	C-O	-6.25	1.17	1.24
2	D	170	VAL	C-O	-6.18	1.17	1.24
2	C	206	ILE	C-O	-6.18	1.17	1.24
2	C	82	ALA	C-O	-6.17	1.16	1.24
2	C	173	ALA	C-O	-6.16	1.16	1.23
1	A	65	VAL	C-O	-6.14	1.16	1.23
2	D	255	GLN	C-O	-6.11	1.16	1.23
2	D	253	ARG	C-O	-6.06	1.16	1.23
1	B	49	VAL	C-O	-6.05	1.18	1.24
2	C	130	CYS	C-O	-6.02	1.18	1.24
2	C	31	ASN	CA-C	-5.97	1.45	1.52
1	A	8	SER	C-O	-5.96	1.16	1.23
2	D	97	GLU	CA-C	-5.93	1.45	1.52
2	C	269	LYS	CA-C	-5.86	1.45	1.52
2	C	189	THR	C-O	-5.85	1.17	1.23
2	C	77	ASN	C-O	-5.84	1.16	1.24
2	D	173	ALA	C-O	-5.84	1.16	1.23
1	A	19	VAL	C-O	-5.81	1.17	1.24
2	D	98	THR	C-O	-5.80	1.16	1.23
2	C	33	THR	C-O	-5.77	1.17	1.24
1	A	95	ALA	C-O	-5.71	1.16	1.23
2	C	191	THR	C-O	-5.68	1.17	1.24
2	C	94	ILE	C-O	-5.66	1.18	1.24
2	D	172	ASN	C-O	-5.66	1.16	1.23
1	B	187	PHE	C-O	-5.61	1.17	1.24
2	D	96	GLY	C-O	-5.60	1.16	1.23
1	A	9	LYS	C-O	-5.56	1.17	1.23
2	D	171	TRP	C-O	-5.55	1.17	1.24
2	D	105	THR	C-O	-5.55	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	208	LEU	C-O	-5.51	1.20	1.25
2	C	74	SER	C-O	-5.48	1.17	1.23
1	A	29	GLN	C-O	-5.47	1.16	1.23
1	A	47	TYR	C-O	-5.45	1.17	1.23
1	B	131	GLN	CA-C	-5.44	1.46	1.52
2	D	135	ALA	C-O	-5.42	1.17	1.23
2	D	103	GLN	C-O	-5.39	1.17	1.24
2	C	81	GLY	C-O	-5.38	1.16	1.23
1	A	180	ASN	C-O	-5.32	1.17	1.23
1	A	182	TYR	C-O	-5.32	1.18	1.23
2	D	114	GLU	C-O	-5.30	1.17	1.24
2	D	104	PHE	C-O	-5.29	1.17	1.24
2	D	256	ASP	C-O	-5.29	1.17	1.23
2	C	34	ASN	C-O	-5.28	1.17	1.24
2	D	191	THR	C-O	-5.25	1.18	1.24
2	D	34	ASN	C-O	-5.25	1.17	1.23
2	C	106	GLU	C-O	-5.22	1.17	1.23
2	D	87	ASP	C-O	-5.20	1.17	1.23
2	D	180	LYS	CA-C	-5.20	1.46	1.52
1	A	82	ILE	C-O	-5.20	1.18	1.25
1	A	179	LYS	C-O	-5.19	1.17	1.23
2	C	198	LEU	C-O	-5.19	1.17	1.23
2	C	173	ALA	CA-C	-5.16	1.46	1.52
1	A	61	THR	C-O	-5.15	1.17	1.24
2	C	190	TYR	C-O	-5.13	1.17	1.24
2	C	198	LEU	CA-C	-5.12	1.46	1.52
2	C	265	PHE	C-O	-5.09	1.17	1.23
1	A	10	ASP	CA-C	-5.03	1.46	1.52
2	D	190	TYR	C-O	-5.02	1.17	1.23
2	C	78	THR	C-O	-5.01	1.17	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ALA	N-CA-C	15.18	127.53	111.14
2	D	214	ASN	N-CA-C	12.56	124.51	111.07
1	B	53	ASN	N-CA-C	11.66	123.99	111.28
1	A	129	SER	N-CA-C	11.50	123.37	111.07
2	C	208	LEU	N-CA-C	-10.71	86.30	109.11
1	A	168	ILE	N-CA-C	10.52	120.42	110.53
2	C	207	TRP	CA-C-O	-9.55	110.61	121.40
2	C	61	SER	N-CA-C	9.39	121.28	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ASN	N-CA-C	-9.22	102.61	113.21
1	A	56	GLY	N-CA-C	-8.64	94.39	110.97
1	A	61	THR	C-N-CD	-8.56	101.77	120.60
2	D	215	ALA	N-CA-C	8.43	122.66	111.28
2	C	107	LYS	N-CA-C	8.39	120.50	111.36
1	A	6	PRO	CA-N-CD	-8.13	100.12	111.50
2	D	136	LEU	N-CA-C	7.96	119.96	111.28
1	B	82	ILE	N-CA-C	-7.76	101.34	108.95
1	B	1	ASN	N-CA-C	7.57	120.97	108.49
2	D	261	SER	N-CA-C	7.36	124.22	113.40
2	C	289	ASN	N-CA-C	7.24	120.32	108.52
2	C	284	LEU	N-CA-C	-7.12	96.91	108.52
1	B	56	GLY	N-CA-C	7.04	123.00	113.99
1	A	5	TYR	CA-C-N	-7.00	110.21	127.00
1	A	5	TYR	C-N-CA	-7.00	110.21	127.00
2	C	263	GLY	N-CA-C	-6.77	105.76	115.64
2	D	192	ILE	N-CA-C	6.60	117.39	107.75
2	C	37	GLY	C-N-CD	-6.58	106.13	120.60
2	D	359	THR	CB-CA-C	-6.57	97.30	110.30
1	A	189	THR	N-CA-C	-6.48	105.19	113.23
2	C	207	TRP	CA-C-N	-6.43	112.65	122.42
2	C	207	TRP	C-N-CA	-6.43	112.65	122.42
1	A	97	LYS	CA-C-N	-6.38	113.21	119.78
1	A	97	LYS	C-N-CA	-6.38	113.21	119.78
2	C	208	LEU	CA-C-N	-6.32	112.12	119.32
2	C	208	LEU	C-N-CA	-6.32	112.12	119.32
1	A	130	GLU	N-CA-C	-6.31	98.61	108.90
2	D	61	SER	N-CA-C	6.22	117.86	111.14
2	C	199	THR	N-CA-C	6.18	121.15	112.93
1	B	129	SER	N-CA-C	6.14	117.64	111.07
1	A	5	TYR	N-CA-C	-6.13	96.27	109.81
2	D	213	SER	N-CA-C	6.11	123.81	110.80
1	A	5	TYR	C-N-CD	6.07	133.96	120.60
2	C	208	LEU	CB-CA-C	6.03	118.57	110.13
2	D	22	HIS	N-CA-C	-5.95	100.01	109.23
2	D	262	ASP	N-CA-C	-5.91	105.83	113.16
1	A	65	VAL	N-CA-C	5.82	116.74	108.42
2	D	23	HIS	N-CA-C	-5.77	101.46	110.17
2	C	96	GLY	N-CA-C	5.76	117.81	110.20
1	B	46	GLU	N-CA-C	5.76	118.92	109.76
1	B	55	ASP	N-CA-C	5.73	120.30	112.68
2	C	270	ILE	N-CA-C	-5.70	102.17	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	337	VAL	N-CA-C	5.61	116.20	108.12
2	C	206	ILE	O-C-N	-5.58	116.85	123.05
2	C	42	GLY	N-CA-C	5.51	119.30	112.64
2	C	73	LEU	N-CA-C	5.45	117.30	111.36
1	A	218	VAL	CA-C-N	-5.42	114.34	120.89
1	A	218	VAL	C-N-CA	-5.42	114.34	120.89
2	C	266	TYR	N-CA-C	5.38	117.57	109.23
2	D	62	HIS	N-CA-C	5.34	117.39	109.69
1	A	51	ILE	CA-C-N	-5.34	114.46	119.85
1	A	51	ILE	C-N-CA	-5.34	114.46	119.85
2	C	344	GLN	N-CA-C	5.32	117.55	110.53
1	A	7	ILE	N-CA-C	5.30	117.71	111.09
2	D	208	LEU	N-CA-C	-5.26	97.90	109.11
2	C	131	PRO	N-CA-CB	-5.23	97.76	103.25
2	C	37	GLY	O-C-N	-5.22	116.55	121.77
2	C	187	TYR	N-CA-C	5.15	119.62	113.23
1	A	157	VAL	CB-CA-C	-5.11	103.49	111.26
1	A	29	GLN	N-CA-C	5.09	117.15	109.41
1	B	209	LYS	N-CA-C	5.08	116.82	111.28
2	C	278	VAL	N-CA-C	5.08	115.89	108.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	37	GLY	Mainchain

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	1642	0	1700	191	0
1	B	1687	0	1733	113	0
2	C	2491	0	2447	195	0
2	D	2538	0	2495	73	0
3	A	6	0	8	0	0
3	C	18	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	7	0	0	2	0
5	B	14	0	0	7	0
5	C	14	0	0	6	0
5	D	11	0	0	3	0
All	All	8432	0	8407	513	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 31.

All (513) 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:C:130:CYS:HB2	2:C:143:CYS:SG	1.52	1.46
1:A:3:MET:CE	2:C:322:VAL:HG21	1.48	1.42
2:C:40:ASP:OD1	2:C:199:THR:CG2	1.66	1.38
1:A:139:ARG:NH1	1:A:194:ASN:HA	1.38	1.36
2:D:238:CYS:HB3	2:D:326:CYS:SG	1.76	1.26
1:B:145:ILE:O	1:B:189:THR:HG22	1.30	1.24
1:A:139:ARG:HD2	1:A:218:VAL:O	1.39	1.21
1:B:197:TYR:O	1:B:217:LYS:HE3	1.42	1.18
2:C:130:CYS:CB	2:C:143:CYS:SG	2.31	1.16
1:A:140:ASN:HB3	1:A:144:ASN:ND2	1.63	1.14
1:A:140:ASN:CB	1:A:144:ASN:ND2	2.13	1.11
1:A:16:SER:HB3	1:A:78:THR:HB	1.19	1.11
1:A:3:MET:HE3	2:C:322:VAL:HG21	1.27	1.11
2:D:256:ASP:OD1	2:D:294:ASN:ND2	1.83	1.10
2:C:258:ASN:HB3	2:C:268:LYS:NZ	1.64	1.10
1:B:145:ILE:HB	1:B:189:THR:HG21	1.27	1.09
2:D:62:HIS:CE1	2:D:64:LEU:HB2	1.88	1.09
1:A:140:ASN:CB	1:A:144:ASN:HD2	1.66	1.07
1:A:197:TYR:CZ	1:A:216:LEU:CD2	2.37	1.07
1:A:3:MET:SD	2:C:322:VAL:HG11	1.95	1.07
1:A:162:PHE:O	1:A:172:CYS:HB3	1.53	1.07
1:A:139:ARG:HH12	1:A:194:ASN:CA	1.69	1.06
2:C:39:HIS:CE1	2:C:46:PRO:HD2	1.91	1.06
2:C:41:ARG:HD3	2:C:200:ASP:CB	1.88	1.04
1:A:3:MET:HE1	2:C:322:VAL:HG21	1.40	1.03
1:A:3:MET:CE	2:C:322:VAL:CG2	2.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ARG:HD3	2:C:200:ASP:HB2	1.07	1.03
1:A:180:ASN:ND2	2:C:359:THR:O	1.93	1.02
1:B:145:ILE:O	1:B:189:THR:CG2	2.07	1.01
2:C:41:ARG:CD	2:C:200:ASP:HB2	1.89	1.01
1:A:197:TYR:CZ	1:A:216:LEU:HD23	1.96	1.00
1:A:97:LYS:HE2	1:A:117:ASN:HD21	1.24	0.99
1:B:197:TYR:C	1:B:217:LYS:HE3	1.87	0.99
1:A:138:SER:HA	1:A:218:VAL:HG11	1.43	0.98
1:A:97:LYS:HE2	1:A:117:ASN:ND2	1.78	0.98
2:C:40:ASP:OD1	2:C:199:THR:HG22	0.79	0.96
2:C:39:HIS:CE1	2:C:46:PRO:CD	2.48	0.96
1:A:139:ARG:HH12	1:A:194:ASN:HA	0.85	0.96
1:A:178:ASN:HA	2:C:360:LEU:HD21	1.45	0.96
1:A:3:MET:HE1	2:C:322:VAL:CG2	1.94	0.95
1:A:16:SER:CB	1:A:78:THR:HB	1.96	0.94
2:C:359:THR:C	2:C:360:LEU:HD12	1.93	0.94
2:D:63:HIS:CD2	2:D:147:GLN:HB2	2.01	0.94
1:A:140:ASN:ND2	1:A:144:ASN:HD21	1.66	0.93
2:C:240:TYR:CE2	2:C:323:PRO:HG3	2.03	0.92
2:C:258:ASN:CB	2:C:268:LYS:NZ	2.33	0.92
1:B:204:HIS:HB2	1:B:207:ILE:HB	1.51	0.92
2:C:258:ASN:HB3	2:C:268:LYS:CE	2.00	0.92
1:A:189:THR:C	1:A:190:LEU:HD13	1.94	0.91
2:C:39:HIS:HE1	2:C:46:PRO:HD3	1.36	0.91
2:D:63:HIS:HD2	2:D:147:GLN:HB2	1.32	0.91
1:A:197:TYR:OH	1:A:216:LEU:HD21	1.69	0.90
2:C:39:HIS:HD1	2:C:48:TYR:HH	0.91	0.90
2:C:256:ASP:OD1	2:C:258:ASN:N	2.04	0.90
1:A:189:THR:O	1:A:190:LEU:HD22	1.71	0.89
1:A:5:TYR:OH	2:C:200:ASP:OD1	1.91	0.89
2:C:258:ASN:HB3	2:C:268:LYS:HZ3	1.33	0.88
1:A:140:ASN:HD22	1:A:144:ASN:ND2	1.71	0.88
1:A:197:TYR:CZ	1:A:216:LEU:HD21	2.06	0.87
2:D:238:CYS:HB3	2:D:326:CYS:HG	1.38	0.87
1:A:139:ARG:HH21	1:A:219:PRO:HA	1.39	0.86
1:A:3:MET:HE1	2:C:322:VAL:CB	2.04	0.85
1:B:189:THR:O	1:B:190:LEU:HB2	1.77	0.85
1:B:158:LYS:NZ	5:B:401:HOH:O	2.06	0.85
1:B:212:GLY:CA	5:B:405:HOH:O	2.24	0.85
2:C:39:HIS:HE1	2:C:46:PRO:CD	1.87	0.85
2:C:203:ASN:HD21	2:C:322:VAL:HA	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:CE1	1:A:216:LEU:HD23	2.12	0.84
1:B:204:HIS:CB	1:B:207:ILE:HB	2.07	0.84
1:B:212:GLY:HA3	5:B:405:HOH:O	1.77	0.84
2:C:268:LYS:HE3	2:C:276:GLU:OE2	1.76	0.83
1:A:0:ALA:HB2	1:A:118:ILE:HB	1.60	0.82
1:A:3:MET:CE	2:C:205:GLN:CD	2.53	0.82
2:C:40:ASP:CG	2:C:199:THR:HG22	1.99	0.81
2:C:78:THR:OG1	2:C:114:GLU:OE1	1.97	0.81
1:B:130:GLU:OE1	1:B:130:GLU:HA	1.81	0.81
1:A:140:ASN:HB2	1:A:144:ASN:HD22	1.44	0.81
1:B:197:TYR:O	1:B:217:LYS:CE	2.26	0.81
2:C:207:TRP:HB2	2:C:238:CYS:HB2	1.64	0.80
2:D:62:HIS:ND1	2:D:64:LEU:HB2	1.95	0.80
1:A:197:TYR:CE1	1:A:216:LEU:CD2	2.64	0.80
1:B:84:LYS:H	1:B:84:LYS:HD2	1.47	0.80
1:B:144:ASN:OD1	1:B:191:VAL:C	2.24	0.80
1:A:213:LEU:HD22	1:A:213:LEU:H	1.46	0.79
2:C:224:THR:HG22	5:C:505:HOH:O	1.82	0.79
2:C:205:GLN:OE1	2:C:323:PRO:HD2	1.82	0.79
1:A:139:ARG:NH1	1:A:194:ASN:CA	2.33	0.79
1:B:24:LYS:NZ	5:B:402:HOH:O	2.15	0.79
2:C:199:THR:HG23	2:C:201:LYS:HG3	1.64	0.79
1:A:140:ASN:ND2	1:A:144:ASN:ND2	2.27	0.78
2:D:251:GLU:OE1	2:D:253:ARG:NH1	2.16	0.78
1:A:3:MET:HE1	2:C:205:GLN:CD	2.09	0.78
2:D:97:GLU:OE1	2:D:156:TYR:OH	2.01	0.78
1:B:140:ASN:ND2	1:B:141:ALA:H	1.81	0.78
2:C:172:ASN:ND2	5:C:501:HOH:O	1.98	0.77
2:C:240:TYR:CE2	2:C:323:PRO:CG	2.68	0.77
2:C:130:CYS:CB	2:C:143:CYS:HG	1.97	0.77
1:A:203:ASN:HD22	2:C:360:LEU:HB3	1.49	0.77
2:C:41:ARG:HH11	2:C:200:ASP:CG	1.93	0.76
1:A:3:MET:CE	2:C:205:GLN:NE2	2.49	0.76
1:A:145:ILE:HD13	1:A:217:LYS:HD3	1.67	0.76
1:B:52:PRO:HG2	1:B:55:ASP:CB	2.16	0.75
2:D:238:CYS:CB	2:D:326:CYS:SG	2.69	0.75
1:A:7:ILE:HG21	2:C:204:ILE:HD12	1.68	0.75
2:C:209:PRO:HG3	2:C:238:CYS:SG	2.26	0.75
2:C:243:TYR:HE2	2:C:327:TRP:HE1	1.34	0.75
2:C:200:ASP:OD2	2:C:203:ASN:ND2	2.13	0.75
1:A:163:CYS:SG	1:A:168:ILE:HG22	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:ASN:CB	2:C:268:LYS:HZ3	1.97	0.74
1:A:144:ASN:HA	1:A:191:VAL:O	1.88	0.74
1:A:138:SER:HA	1:A:218:VAL:CG1	2.17	0.72
1:B:189:THR:HG23	1:B:191:VAL:H	1.53	0.72
2:D:268:LYS:HE2	2:D:276:GLU:HG2	1.70	0.72
2:C:67:ARG:HH22	3:C:403:GOL:H32	1.54	0.71
2:C:262:ASP:N	2:C:262:ASP:OD1	2.21	0.71
1:B:161:TYR:CE2	1:B:174:LYS:HD2	2.26	0.71
2:C:251:GLU:OE1	2:C:253:ARG:NH1	2.23	0.71
1:A:3:MET:SD	2:C:322:VAL:HG21	2.31	0.70
2:C:39:HIS:ND1	2:C:48:TYR:OH	2.14	0.70
1:B:52:PRO:HG2	1:B:55:ASP:HB3	1.74	0.70
1:A:140:ASN:CG	1:A:144:ASN:HD21	1.99	0.69
1:B:208:GLU:HG2	1:B:209:LYS:H	1.56	0.69
1:A:3:MET:HE2	2:C:205:GLN:NE2	2.08	0.69
1:A:196:SER:C	1:A:197:TYR:HD1	2.00	0.69
1:A:178:ASN:CA	2:C:360:LEU:HD21	2.20	0.68
1:B:162:PHE:CE2	1:B:191:VAL:HG21	2.28	0.68
2:D:205:GLN:NE2	2:D:323:PRO:O	2.26	0.68
2:C:239:PHE:H	2:C:326:CYS:HB2	1.58	0.68
2:C:325:LEU:N	2:C:325:LEU:HD12	2.09	0.68
2:C:39:HIS:NE2	2:C:45:SER:HA	2.09	0.68
1:B:212:GLY:C	1:B:213:LEU:HD23	2.19	0.68
1:B:212:GLY:N	5:B:405:HOH:O	2.27	0.67
2:C:172:ASN:OD1	2:C:173:ALA:N	2.28	0.67
2:D:167:PHE:HB3	2:D:323:PRO:HB3	1.76	0.67
1:A:178:ASN:C	2:C:360:LEU:HD11	2.20	0.67
2:C:269:LYS:HB3	2:C:272:ASP:HB3	1.76	0.67
2:C:325:LEU:HD12	2:C:325:LEU:H	1.60	0.67
1:B:213:LEU:HD23	1:B:213:LEU:N	2.10	0.67
2:C:72:CYS:HB2	2:C:83:CYS:SG	2.35	0.66
2:C:270:ILE:O	2:C:271:ASN:HB2	1.96	0.66
2:C:360:LEU:HD12	2:C:360:LEU:N	2.10	0.66
2:C:220:ASN:ND2	5:C:502:HOH:O	2.29	0.66
2:C:273:ASP:OD1	2:C:273:ASP:N	2.23	0.66
1:A:140:ASN:HB3	1:A:144:ASN:HD22	1.29	0.66
1:A:163:CYS:SG	1:A:168:ILE:CG2	2.84	0.66
2:D:41:ARG:HH22	2:D:321:SER:HA	1.61	0.66
1:A:3:MET:HE1	2:C:322:VAL:HB	1.77	0.66
2:C:67:ARG:HH22	3:C:403:GOL:H12	1.61	0.65
1:A:134:SER:HB3	1:A:150:ASN:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:243:TYR:HE2	2:C:327:TRP:NE1	1.94	0.65
1:A:110:LEU:HD12	2:C:341:GLU:O	1.97	0.65
1:A:140:ASN:CG	1:A:144:ASN:ND2	2.53	0.65
2:C:72:CYS:CB	2:C:83:CYS:SG	2.84	0.65
1:A:16:SER:HB3	1:A:78:THR:CB	2.12	0.65
2:C:240:TYR:CD2	2:C:323:PRO:HG2	2.32	0.65
2:C:203:ASN:O	2:C:242:GLY:N	2.27	0.65
1:A:48:GLU:OE1	1:A:92:TYR:OH	2.14	0.64
1:A:96:VAL:HG12	1:A:98:PRO:HD2	1.79	0.64
1:A:97:LYS:HE2	1:A:117:ASN:CG	2.22	0.64
2:C:277:LEU:HD12	2:C:345:TYR:CE2	2.31	0.64
1:A:140:ASN:CB	1:A:144:ASN:HD21	2.07	0.64
1:B:14:GLY:H	1:B:79:GLN:HE21	1.46	0.64
1:B:170:ASP:OD1	1:B:170:ASP:N	2.18	0.64
1:A:178:ASN:O	2:C:360:LEU:HD11	1.98	0.64
2:D:36:ILE:HD12	2:D:48:TYR:HB3	1.80	0.64
1:B:158:LYS:HE3	1:B:203:ASN:HB3	1.79	0.64
1:B:144:ASN:OD1	1:B:191:VAL:O	2.16	0.64
2:C:109:SER:HB2	2:C:111:ILE:HG12	1.80	0.63
2:C:258:ASN:CB	2:C:268:LYS:HZ2	2.08	0.63
2:C:289:ASN:C	2:C:290:LEU:HG	2.22	0.63
1:A:11:LEU:CD1	1:A:58:LEU:HD11	2.28	0.63
1:B:204:HIS:CD2	1:B:207:ILE:HB	2.34	0.63
1:A:3:MET:SD	2:C:322:VAL:CG1	2.81	0.63
2:C:344:GLN:C	2:C:345:TYR:HD1	2.06	0.62
1:B:208:GLU:HG2	1:B:209:LYS:N	2.13	0.62
1:A:9:LYS:NZ	5:A:401:HOH:O	2.33	0.62
1:B:170:ASP:C	1:B:172:CYS:H	2.08	0.62
2:C:325:LEU:H	2:C:325:LEU:CD1	2.13	0.62
2:C:39:HIS:CE1	2:C:45:SER:HA	2.35	0.61
1:B:131:GLN:OE1	5:B:403:HOH:O	2.16	0.61
2:C:41:ARG:HG2	2:C:198:LEU:HG	1.81	0.61
2:C:277:LEU:HD12	2:C:345:TYR:CD2	2.34	0.61
1:B:145:ILE:CB	1:B:189:THR:HG21	2.18	0.61
2:C:205:GLN:OE1	2:C:322:VAL:HB	1.99	0.61
1:B:191:VAL:HG12	1:B:193:ASN:H	1.65	0.61
2:C:277:LEU:HD21	2:C:337:VAL:HG11	1.83	0.61
1:A:3:MET:HE2	2:C:205:GLN:CD	2.26	0.61
1:B:204:HIS:HB2	1:B:207:ILE:CB	2.28	0.61
2:C:49:ASN:ND2	5:C:503:HOH:O	2.29	0.61
2:C:172:ASN:CG	5:C:501:HOH:O	2.38	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:O	1:B:152:ASN:ND2	2.30	0.61
1:B:204:HIS:CG	1:B:207:ILE:HB	2.36	0.60
2:C:205:GLN:NE2	2:C:207:TRP:CZ2	2.69	0.60
2:C:39:HIS:CG	2:C:48:TYR:HH	2.14	0.60
2:C:203:ASN:ND2	2:C:323:PRO:HD3	2.16	0.60
1:A:51:ILE:O	1:A:51:ILE:HG13	2.00	0.60
2:C:219:LEU:HD21	2:C:333:LEU:HB2	1.82	0.60
1:A:155:ALA:HB3	1:A:181:ILE:HB	1.83	0.60
2:D:167:PHE:CB	2:D:323:PRO:HB3	2.32	0.60
1:B:3:MET:HE1	2:D:322:VAL:HG11	1.84	0.60
2:C:208:LEU:HD23	2:C:237:MET:HB3	1.82	0.60
2:D:85:SER:N	5:D:403:HOH:O	2.26	0.60
2:C:113:ARG:HG3	2:C:166:PRO:HD3	1.84	0.59
1:B:52:PRO:HG2	1:B:55:ASP:HB2	1.84	0.59
2:C:41:ARG:CG	2:C:198:LEU:HG	2.32	0.59
1:B:53:ASN:HB2	1:B:63:GLN:OE1	2.03	0.59
2:C:20:HIS:O	2:C:20:HIS:ND1	2.36	0.59
2:C:158:PRO:HD2	2:C:161:GLU:HG3	1.85	0.59
2:C:179:VAL:HG21	2:C:190:TYR:CE1	2.38	0.59
1:A:110:LEU:HD12	2:C:342:ALA:HA	1.85	0.59
1:A:168:ILE:O	1:A:172:CYS:SG	2.54	0.59
1:B:169:ASP:O	1:B:172:CYS:HB2	2.03	0.59
1:A:134:SER:CB	1:A:150:ASN:HB3	2.32	0.58
1:A:139:ARG:HH11	1:A:194:ASN:HA	1.59	0.58
1:A:145:ILE:HD13	1:A:217:LYS:NZ	2.18	0.58
1:A:188:ASP:OD1	1:A:190:LEU:N	2.29	0.58
1:B:145:ILE:HD13	1:B:217:LYS:HD3	1.84	0.58
1:A:189:THR:C	1:A:190:LEU:CD1	2.74	0.58
1:B:48:GLU:OE1	1:B:92:TYR:OH	2.22	0.58
1:B:199:PHE:HA	1:B:213:LEU:O	2.04	0.58
2:D:245:THR:OG1	2:D:246:ASN:N	2.36	0.58
1:A:57:GLY:HA3	1:A:89:TYR:OH	2.04	0.58
1:A:118:ILE:HD13	2:C:351:ILE:HB	1.86	0.58
1:A:189:THR:O	1:A:190:LEU:CD2	2.48	0.58
1:A:144:ASN:ND2	1:A:144:ASN:H	2.02	0.57
1:B:140:ASN:HD22	1:B:141:ALA:H	1.52	0.57
2:C:258:ASN:HB3	2:C:268:LYS:HE2	1.83	0.57
1:A:180:ASN:CG	2:C:359:THR:O	2.47	0.57
2:C:72:CYS:HG	2:C:83:CYS:HG	0.63	0.57
2:D:227:GLY:N	5:D:402:HOH:O	2.26	0.57
1:B:179:LYS:NZ	5:B:407:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:THR:O	1:A:190:LEU:CB	2.52	0.57
1:A:3:MET:HE3	2:C:322:VAL:CG2	2.17	0.57
1:B:158:LYS:HE3	1:B:203:ASN:CB	2.34	0.57
2:D:62:HIS:HE1	2:D:64:LEU:HB2	1.62	0.57
1:A:11:LEU:HD12	1:A:58:LEU:HD11	1.86	0.57
1:A:97:LYS:N	1:A:98:PRO:HD2	2.19	0.57
1:A:218:VAL:HG22	1:A:220:ALA:H	1.70	0.57
1:B:161:TYR:CE2	1:B:174:LYS:CD	2.89	0.56
2:C:205:GLN:NE2	2:C:207:TRP:HE1	2.02	0.56
2:C:205:GLN:NE2	2:C:207:TRP:HZ2	2.03	0.56
1:A:145:ILE:HD13	1:A:217:LYS:CD	2.36	0.56
1:B:98:PRO:HG2	1:B:99:ASP:H	1.70	0.56
2:C:106:GLU:OE2	2:C:108:ARG:N	2.34	0.56
1:B:11:LEU:HD12	1:B:58:LEU:HD11	1.86	0.56
1:A:136:ASN:C	1:A:137:ILE:HD12	2.31	0.56
2:C:258:ASN:ND2	2:C:268:LYS:HD3	2.20	0.56
2:C:41:ARG:NH1	2:C:200:ASP:CG	2.61	0.56
1:A:55:ASP:OD1	1:A:55:ASP:N	2.37	0.56
2:C:41:ARG:HD3	2:C:200:ASP:CG	2.31	0.56
1:A:142:LYS:C	1:A:143:LYS:HG2	2.30	0.56
2:D:62:HIS:C	2:D:63:HIS:ND1	2.64	0.55
2:C:74:SER:OG	3:C:404:GOL:H32	2.05	0.55
1:A:38:ILE:HB	1:A:88:VAL:HG13	1.89	0.55
2:C:269:LYS:HD3	2:C:272:ASP:HB3	1.89	0.55
2:D:211:PHE:N	2:D:211:PHE:CD1	2.75	0.55
1:B:191:VAL:HG13	1:B:193:ASN:OD1	2.06	0.55
1:A:187:PHE:CD1	1:A:187:PHE:C	2.85	0.54
2:C:240:TYR:CD2	2:C:323:PRO:CG	2.90	0.54
1:A:5:TYR:O	1:A:20:ARG:N	2.40	0.54
2:C:269:LYS:HD3	2:C:272:ASP:CB	2.38	0.54
2:C:100:ILE:HB	2:C:117:ILE:HB	1.89	0.54
2:C:266:TYR:HB2	2:C:268:LYS:HZ2	1.73	0.54
1:B:198:VAL:HG23	1:B:217:LYS:CE	2.38	0.54
1:A:137:ILE:HD12	1:A:137:ILE:N	2.23	0.54
1:B:163:CYS:O	1:B:195:PHE:HD2	1.90	0.54
1:A:97:LYS:N	1:A:98:PRO:CD	2.71	0.53
2:C:258:ASN:HB2	2:C:268:LYS:NZ	2.22	0.53
2:C:344:GLN:C	2:C:345:TYR:CD1	2.85	0.53
2:C:208:LEU:O	2:C:209:PRO:C	2.50	0.53
1:A:140:ASN:O	1:A:143:LYS:N	2.40	0.53
1:A:139:ARG:NH2	1:A:219:PRO:HA	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:HG21	2:D:31:ASN:HB3	1.89	0.53
2:D:359:THR:OG1	2:D:360:LEU:N	2.40	0.53
2:D:93:THR:HG21	2:D:141:PHE:HB3	1.91	0.53
2:C:88:ALA:O	2:C:182:ARG:NH2	2.37	0.53
1:A:193:ASN:HB2	1:A:195:PHE:CE1	2.44	0.52
2:C:130:CYS:HB3	2:C:143:CYS:SG	2.43	0.52
2:C:251:GLU:HB2	2:C:356:SER:HB3	1.91	0.52
1:A:137:ILE:N	1:A:137:ILE:CD1	2.73	0.52
1:B:28:ILE:HB	1:B:68:PRO:HA	1.90	0.52
1:B:116:ILE:HD13	2:D:349:ILE:HB	1.89	0.52
2:C:217:VAL:HG11	2:C:235:VAL:HG22	1.91	0.52
1:B:24:LYS:HG3	2:D:207:TRP:CH2	2.45	0.52
1:B:90:ARG:NE	2:D:354:THR:HG21	2.24	0.52
2:C:209:PRO:CG	2:C:238:CYS:SG	2.95	0.52
2:D:41:ARG:HH12	2:D:321:SER:C	2.17	0.52
1:A:26:LYS:HA	1:A:69:ALA:HB1	1.91	0.52
1:A:196:SER:C	1:A:197:TYR:CD1	2.83	0.52
1:B:198:VAL:HG23	1:B:217:LYS:HE2	1.92	0.52
2:C:200:ASP:CG	2:C:203:ASN:HB2	2.35	0.51
1:B:207:ILE:CG2	1:B:208:GLU:N	2.73	0.51
2:C:266:TYR:HB2	2:C:268:LYS:NZ	2.25	0.51
2:C:360:LEU:N	2:C:360:LEU:CD1	2.73	0.51
1:A:0:ALA:HB2	1:A:118:ILE:CB	2.37	0.51
1:A:23:SER:HB2	1:A:67:LEU:HG	1.93	0.51
1:A:158:LYS:HE3	2:C:360:LEU:HD23	1.92	0.51
1:B:48:GLU:OE2	1:B:90:ARG:NH1	2.41	0.51
1:A:141:ALA:C	1:A:143:LYS:H	2.17	0.51
1:B:163:CYS:C	1:B:195:PHE:HD2	2.18	0.51
2:C:258:ASN:HB2	2:C:268:LYS:HZ2	1.74	0.51
1:A:197:TYR:HD1	1:A:197:TYR:N	2.08	0.51
1:B:200:ILE:O	1:B:212:GLY:HA2	2.10	0.51
1:B:118:ILE:HD11	1:B:120:TYR:CE1	2.46	0.50
2:C:257:ASP:C	2:C:259:SER:H	2.16	0.50
2:D:59:ASN:O	2:D:149:SER:HB3	2.11	0.50
1:B:38:ILE:HB	1:B:88:VAL:HG13	1.93	0.50
1:A:110:LEU:CD1	2:C:341:GLU:O	2.60	0.50
2:D:240:TYR:CE2	2:D:323:PRO:HG2	2.46	0.50
2:D:303:ALA:C	2:D:305:LEU:H	2.19	0.50
2:C:172:ASN:OD1	5:C:501:HOH:O	2.19	0.50
1:A:134:SER:OG	1:A:150:ASN:ND2	2.44	0.50
1:A:6:PRO:N	1:A:19:VAL:HG13	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:HD3	1:A:171:ASN:CB	2.42	0.50
1:A:197:TYR:CD1	1:A:197:TYR:N	2.78	0.50
1:B:98:PRO:HG2	1:B:99:ASP:N	2.27	0.50
1:B:16:SER:HB2	1:B:78:THR:HB	1.93	0.49
1:B:170:ASP:C	1:B:172:CYS:N	2.70	0.49
1:A:110:LEU:HB2	2:C:342:ALA:HA	1.94	0.49
1:A:90:ARG:NH2	2:C:356:SER:HA	2.27	0.49
1:A:197:TYR:CE2	1:A:216:LEU:HD23	2.43	0.49
1:B:162:PHE:O	1:B:172:CYS:HB3	2.12	0.49
1:B:213:LEU:HB2	1:B:215:GLN:OE1	2.12	0.49
1:A:152:ASN:OD1	1:A:153:VAL:N	2.45	0.49
1:A:147:ILE:O	1:A:186:SER:HA	2.13	0.49
1:A:168:ILE:N	1:A:168:ILE:HD12	2.28	0.49
2:D:219:LEU:HD22	2:D:333:LEU:HB2	1.94	0.49
1:B:169:ASP:HB3	1:B:172:CYS:SG	2.53	0.49
1:A:3:MET:HE2	2:C:205:GLN:CG	2.43	0.49
1:A:38:ILE:HG12	1:A:48:GLU:HG2	1.94	0.49
1:A:63:GLN:O	1:A:63:GLN:HG2	2.12	0.49
1:A:141:ALA:C	1:A:143:LYS:N	2.70	0.49
2:D:354:THR:HG22	2:D:355:PRO:HD2	1.94	0.49
1:A:16:SER:HB2	1:A:77:LEU:O	2.13	0.48
1:A:38:ILE:HD11	1:A:90:ARG:HD2	1.94	0.48
1:A:140:ASN:C	1:A:143:LYS:H	2.21	0.48
1:A:200:ILE:O	1:A:213:LEU:HD22	2.13	0.48
1:A:213:LEU:N	1:A:213:LEU:HD13	2.28	0.48
1:A:3:MET:CE	2:C:322:VAL:HG11	2.43	0.48
1:A:6:PRO:HD3	1:A:19:VAL:HA	1.95	0.48
2:C:267:LEU:HG	2:C:279:TYR:CD1	2.49	0.48
1:A:1:ASN:HB3	1:A:25:SER:HB2	1.95	0.48
1:A:121:ALA:HB3	2:C:354:THR:HG23	1.96	0.48
1:A:138:SER:CA	1:A:218:VAL:CG1	2.90	0.48
2:D:118:LYS:HG2	2:D:158:PRO:HG3	1.96	0.48
1:B:59:VAL:HB	1:B:78:THR:HG23	1.96	0.47
2:C:198:LEU:HD12	2:C:198:LEU:HA	1.73	0.47
1:A:119:ILE:HB	2:C:352:THR:HG23	1.95	0.47
2:C:262:ASP:HB2	2:C:264:LYS:HG3	1.96	0.47
1:B:189:THR:O	1:B:190:LEU:CB	2.54	0.47
2:C:127:ASN:ND2	2:C:146:GLU:OE2	2.42	0.47
2:C:238:CYS:CB	2:C:326:CYS:HG	2.27	0.47
1:A:35:THR:HG23	1:A:91:VAL:HG22	1.97	0.47
1:B:23:SER:HB2	1:B:67:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:CG2	1:B:217:LYS:HE2	2.45	0.47
2:C:205:GLN:NE2	2:C:207:TRP:NE1	2.62	0.47
2:C:270:ILE:O	2:C:270:ILE:HG23	2.14	0.47
2:D:268:LYS:HE2	2:D:276:GLU:CG	2.41	0.47
1:A:152:ASN:O	1:A:183:PRO:HG3	2.13	0.47
2:D:130:CYS:HB2	2:D:143:CYS:SG	2.54	0.47
1:B:162:PHE:HZ	1:B:189:THR:OG1	1.97	0.46
2:C:239:PHE:N	2:C:326:CYS:HB2	2.29	0.46
2:D:250:LEU:HG	2:D:251:GLU:H	1.80	0.46
2:D:279:TYR:HE2	2:D:349:ILE:HD11	1.81	0.46
1:A:138:SER:CA	1:A:218:VAL:HG11	2.32	0.46
2:C:243:TYR:C	2:C:245:THR:H	2.24	0.46
1:A:110:LEU:N	5:A:403:HOH:O	2.49	0.46
2:D:22:HIS:CD2	2:D:124:LEU:HD13	2.50	0.46
2:D:212:LYS:HA	2:D:212:LYS:HD3	1.68	0.46
2:D:223:PRO:HA	2:D:229:TYR:HA	1.98	0.46
1:A:156:GLY:HA2	1:A:180:ASN:HA	1.98	0.46
1:A:164:LYS:H	1:A:164:LYS:HG2	1.45	0.46
1:B:144:ASN:HA	1:B:191:VAL:O	2.16	0.46
1:B:156:GLY:O	1:B:202:LEU:HA	2.16	0.46
2:C:240:TYR:CZ	2:C:323:PRO:HG3	2.48	0.46
2:D:205:GLN:OE1	2:D:207:TRP:NE1	2.42	0.46
1:B:188:ASP:OD1	1:B:190:LEU:N	2.49	0.46
1:A:163:CYS:O	1:A:195:PHE:HB3	2.16	0.46
1:A:97:LYS:CE	1:A:117:ASN:OD1	2.64	0.45
1:A:145:ILE:HD13	1:A:217:LYS:HZ3	1.80	0.45
1:A:160:ILE:CG2	1:A:198:VAL:HG13	2.46	0.45
1:A:197:TYR:C	1:A:198:VAL:HG23	2.40	0.45
2:C:74:SER:HB3	2:C:77:ASN:HB3	1.98	0.45
2:D:120:TYR:HE1	2:D:156:TYR:HE1	1.64	0.45
2:D:281:LEU:N	5:D:401:HOH:O	2.09	0.45
2:C:206:ILE:HD11	2:C:239:PHE:HD1	1.81	0.45
1:A:140:ASN:O	1:A:143:LYS:HA	2.17	0.45
1:A:197:TYR:O	1:A:198:VAL:HG23	2.17	0.45
1:B:119:ILE:HD12	2:D:350:LYS:HG3	1.97	0.45
2:C:39:HIS:CE1	2:C:46:PRO:HD3	2.21	0.45
1:A:164:LYS:HD3	1:A:171:ASN:HB2	1.97	0.45
2:C:41:ARG:HG2	2:C:198:LEU:CG	2.47	0.45
2:C:203:ASN:HD21	2:C:323:PRO:HD3	1.79	0.45
2:D:254:PHE:CD1	2:D:292:PRO:HB3	2.52	0.45
1:B:145:ILE:HB	1:B:189:THR:CG2	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ARG:NH1	2:C:200:ASP:OD2	2.50	0.45
1:A:190:LEU:HD13	1:A:190:LEU:N	2.30	0.45
1:B:5:TYR:HA	1:B:6:PRO:HA	1.81	0.45
1:A:90:ARG:NH2	2:C:355:PRO:O	2.45	0.44
1:B:53:ASN:HD21	1:B:60:VAL:H	1.64	0.44
2:C:257:ASP:OD1	2:C:257:ASP:N	2.48	0.44
1:B:163:CYS:C	1:B:195:PHE:CD2	2.95	0.44
2:C:106:GLU:OE2	2:C:107:LYS:N	2.50	0.44
2:C:257:ASP:C	2:C:259:SER:N	2.73	0.44
1:A:159:ASP:N	1:A:159:ASP:OD1	2.50	0.44
1:A:197:TYR:HH	1:A:216:LEU:HD21	1.79	0.44
1:B:207:ILE:HD13	1:B:207:ILE:HA	1.79	0.44
2:D:360:LEU:HD22	2:D:360:LEU:HA	1.75	0.44
1:A:14:GLY:HA2	1:A:79:GLN:HG3	2.00	0.44
2:C:249:SER:HB3	2:C:359:THR:HG22	2.00	0.44
2:C:251:GLU:HG2	2:C:253:ARG:HD2	2.00	0.44
1:B:0:ALA:HA	2:D:213:SER:O	2.17	0.44
1:B:28:ILE:HG12	1:B:29:GLN:N	2.32	0.44
1:B:33:ILE:HD13	1:B:75:ILE:HG12	1.99	0.44
1:B:179:LYS:HG3	1:B:180:ASN:N	2.32	0.44
2:D:181:ARG:HB3	2:D:184:ASP:HB3	1.99	0.44
1:A:5:TYR:HA	1:A:6:PRO:HA	1.47	0.44
1:A:188:ASP:O	1:A:190:LEU:HD13	2.17	0.44
2:C:67:ARG:NH2	3:C:403:GOL:H12	2.31	0.44
1:A:26:LYS:O	1:A:26:LYS:HG2	2.18	0.44
1:A:155:ALA:N	1:A:181:ILE:O	2.36	0.44
2:D:223:PRO:HB3	2:D:229:TYR:CZ	2.52	0.44
1:A:4:ILE:HD11	1:A:7:ILE:HD12	2.00	0.44
2:C:20:HIS:O	2:C:20:HIS:CG	2.68	0.43
2:D:20:HIS:O	2:D:22:HIS:ND1	2.51	0.43
2:D:180:LYS:HE2	2:D:181:ARG:O	2.18	0.43
1:A:190:LEU:N	1:A:190:LEU:CD1	2.81	0.43
1:B:97:LYS:HB3	1:B:98:PRO:HD2	2.01	0.43
2:C:257:ASP:O	2:C:259:SER:N	2.39	0.43
2:D:123:PHE:HE2	2:D:140:HIS:HA	1.84	0.43
2:C:121:LYS:HE2	2:C:135:ALA:O	2.18	0.43
1:A:3:MET:HE1	2:C:322:VAL:CG1	2.48	0.43
1:A:189:THR:O	1:A:190:LEU:CG	2.67	0.43
1:B:180:ASN:OD1	2:D:359:THR:O	2.36	0.43
2:D:267:LEU:HD23	2:D:347:GLY:HA3	2.00	0.43
1:A:121:ALA:O	2:C:354:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:283:LEU:HD12	2:D:331:LEU:HB2	2.00	0.43
1:A:144:ASN:ND2	1:A:144:ASN:N	2.66	0.43
1:B:21:VAL:O	1:B:72:SER:HA	2.19	0.43
1:B:145:ILE:CD1	1:B:217:LYS:HD3	2.49	0.43
2:D:116:GLN:HB2	2:D:161:GLU:OE2	2.19	0.43
1:B:189:THR:HG23	1:B:190:LEU:N	2.33	0.42
1:A:116:ILE:HD13	2:C:349:ILE:HB	2.00	0.42
1:A:188:ASP:O	1:A:190:LEU:CD1	2.67	0.42
1:B:134:SER:O	1:B:150:ASN:N	2.44	0.42
2:C:269:LYS:HG2	2:C:270:ILE:N	2.34	0.42
1:A:3:MET:CE	2:C:205:GLN:CG	2.97	0.42
1:A:178:ASN:CB	2:C:360:LEU:HD21	2.50	0.42
1:B:140:ASN:ND2	1:B:141:ALA:N	2.58	0.42
2:C:277:LEU:HD21	2:C:337:VAL:CG1	2.49	0.42
1:A:142:LYS:O	1:A:143:LYS:HB2	2.20	0.42
1:A:157:VAL:HG13	1:A:200:ILE:CG2	2.50	0.42
1:A:201:LYS:C	1:A:202:LEU:HD13	2.44	0.42
2:C:33:THR:HA	2:C:193:ASN:HB2	2.00	0.42
2:C:97:GLU:OE2	2:C:156:TYR:OH	2.20	0.42
1:A:134:SER:O	1:A:150:ASN:HB3	2.20	0.42
1:A:140:ASN:O	1:A:143:LYS:CA	2.68	0.42
1:B:90:ARG:HE	2:D:354:THR:HG21	1.83	0.42
1:B:146:ILE:HD13	1:B:188:ASP:HA	2.02	0.42
2:C:203:ASN:OD1	2:C:322:VAL:HG12	2.20	0.42
2:C:268:LYS:HG3	2:C:276:GLU:CG	2.50	0.42
1:A:111:THR:O	2:C:344:GLN:HA	2.20	0.42
2:D:358:GLN:H	2:D:358:GLN:HG2	1.40	0.42
1:B:131:GLN:HB3	1:B:153:VAL:HG21	2.01	0.42
2:C:165:LEU:HD12	2:C:198:LEU:HD22	2.02	0.42
1:A:28:ILE:HG23	1:A:28:ILE:O	2.19	0.41
1:A:97:LYS:HE3	1:A:117:ASN:OD1	2.20	0.41
1:A:131:GLN:HG2	1:A:153:VAL:HG21	2.02	0.41
1:B:167:ASN:OD1	1:B:167:ASN:N	2.50	0.41
1:B:26:LYS:HB2	2:D:212:LYS:HG3	2.01	0.41
2:C:115:LEU:HD11	2:C:165:LEU:HD21	2.01	0.41
1:A:116:ILE:HD13	1:A:116:ILE:HA	1.95	0.41
1:B:31:ILE:HD13	1:B:95:ALA:HA	2.01	0.41
2:C:238:CYS:HB3	2:C:326:CYS:HG	1.86	0.41
2:D:100:ILE:HB	2:D:117:ILE:HB	2.01	0.41
2:D:108:ARG:HD3	2:D:108:ARG:HA	1.82	0.41
1:A:203:ASN:ND2	2:C:360:LEU:C	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:O	1:A:143:LYS:CB	2.67	0.41
1:A:195:PHE:CD1	1:A:195:PHE:N	2.88	0.41
1:B:26:LYS:HG2	2:D:212:LYS:HD2	2.01	0.41
2:D:249:SER:OG	2:D:299:ASN:OD1	2.37	0.41
2:D:41:ARG:HG3	2:D:198:LEU:HG	2.02	0.41
1:A:140:ASN:HB3	1:A:144:ASN:H	1.86	0.41
1:A:157:VAL:HG13	1:A:200:ILE:HG23	2.02	0.41
1:B:9:LYS:HD2	1:B:9:LYS:HA	1.97	0.41
1:B:207:ILE:HG23	1:B:208:GLU:H	1.85	0.41
2:C:175:LEU:HD23	2:C:192:ILE:HD12	2.02	0.41
1:A:61:THR:HG22	1:A:62:PRO:HD3	2.03	0.41
1:A:110:LEU:CD1	2:C:342:ALA:HA	2.49	0.41
1:B:121:ALA:HB3	2:D:354:THR:HG23	2.03	0.41
2:C:180:LYS:HG2	2:C:181:ARG:O	2.21	0.41
2:C:200:ASP:OD1	2:C:203:ASN:HB2	2.21	0.41
1:A:1:ASN:HB3	1:A:25:SER:CB	2.51	0.41
1:A:168:ILE:HD12	1:A:168:ILE:H	1.86	0.41
1:B:142:LYS:HE2	1:B:142:LYS:HB3	1.71	0.41
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.79	0.41
1:B:216:LEU:HB3	2:C:33:THR:HG21	2.02	0.41
2:D:214:ASN:HB3	2:D:216:ARG:HD2	2.02	0.41
1:A:97:LYS:H	1:A:98:PRO:CD	2.34	0.41
1:B:61:THR:HA	1:B:62:PRO:HA	1.92	0.41
1:B:137:ILE:CD1	1:B:215:GLN:HE21	2.33	0.41
2:D:73:LEU:HD23	2:D:73:LEU:HA	1.90	0.41
1:A:90:ARG:HH22	2:C:356:SER:HA	1.85	0.40
1:B:143:LYS:HD3	1:B:220:ALA:HB1	2.02	0.40
2:C:277:LEU:CD2	2:C:337:VAL:HG11	2.49	0.40
2:D:179:VAL:HG21	2:D:190:TYR:CE1	2.57	0.40
2:C:219:LEU:HD21	2:C:333:LEU:CB	2.48	0.40
1:A:201:LYS:O	1:A:202:LEU:CD1	2.70	0.40
2:C:134:LEU:HD11	2:C:141:PHE:HE1	1.86	0.40
2:C:250:LEU:O	2:C:299:ASN:HA	2.22	0.40
2:C:251:GLU:N	2:C:354:THR:O	2.48	0.40
2:D:180:LYS:HE3	2:D:180:LYS:HB2	1.86	0.40
2:D:184:ASP:OD1	2:D:185:THR:HG22	2.21	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	198/221 (90%)	190 (96%)	7 (4%)	1 (0%)	24	52
1	B	207/221 (94%)	200 (97%)	7 (3%)	0	100	100
2	C	314/341 (92%)	297 (95%)	15 (5%)	2 (1%)	21	47
2	D	322/341 (94%)	308 (96%)	12 (4%)	2 (1%)	21	47
All	All	1041/1124 (93%)	995 (96%)	41 (4%)	5 (0%)	24	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	323	PRO
2	C	340	PRO
1	A	97	LYS
2	C	131	PRO
2	D	131	PRO

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 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	186/202 (92%)	150 (81%)	36 (19%)	1	4
1	B	189/202 (94%)	160 (85%)	29 (15%)	3	8
2	C	278/298 (93%)	239 (86%)	39 (14%)	3	10
2	D	283/298 (95%)	250 (88%)	33 (12%)	5	15
All	All	936/1000 (94%)	799 (85%)	137 (15%)	3	9

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	7	ILE
1	A	10	ASP
1	A	27	GLU
1	A	45	GLU
1	A	54	TRP
1	A	55	ASP
1	A	63	GLN
1	A	65	VAL
1	A	66	ILE
1	A	77	LEU
1	A	78	THR
1	A	79	GLN
1	A	83	PRO
1	A	96	VAL
1	A	111	THR
1	A	115	SER
1	A	117	ASN
1	A	132	ASN
1	A	137	ILE
1	A	138	SER
1	A	144	ASN
1	A	153	VAL
1	A	157	VAL
1	A	159	ASP
1	A	164	LYS
1	A	168	ILE
1	A	169	ASP
1	A	185	LYS
1	A	186	SER
1	A	187	PHE
1	A	190	LEU
1	A	202	LEU
1	A	213	LEU
1	A	214	ILE
1	A	218	VAL
1	B	3	MET
1	B	16	SER
1	B	24	LYS
1	B	28	ILE
1	B	45	GLU
1	B	50	ASP

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Mol	Chain	Res	Type
1	B	55	ASP
1	B	73	LYS
1	B	77	LEU
1	B	84	LYS
1	B	86	GLU
1	B	117	ASN
1	B	118	ILE
1	B	130	GLU
1	B	132	ASN
1	B	133	ILE
1	B	153	VAL
1	B	164	LYS
1	B	166	SER
1	B	168	ILE
1	B	170	ASP
1	B	185	LYS
1	B	186	SER
1	B	192	ASN
1	B	198	VAL
1	B	202	LEU
1	B	204	HIS
1	B	213	LEU
1	B	214	ILE
2	C	31	ASN
2	C	49	ASN
2	C	53	SER
2	C	72	CYS
2	C	75	SER
2	C	76	GLN
2	C	79	LEU
2	C	84	PRO
2	C	91	THR
2	C	97	GLU
2	C	105	THR
2	C	109	SER
2	C	113	ARG
2	C	132	SER
2	C	143	CYS
2	C	152	THR
2	C	164	LYS
2	C	185	THR
2	C	199	THR

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Mol	Chain	Res	Type
2	C	230	ILE
2	C	243	TYR
2	C	248	SER
2	C	253	ARG
2	C	255	GLN
2	C	257	ASP
2	C	261	SER
2	C	262	ASP
2	C	273	ASP
2	C	281	LEU
2	C	282	SER
2	C	283	LEU
2	C	291	THR
2	C	334	ASP
2	C	344	GLN
2	C	349	ILE
2	C	352	THR
2	C	354	THR
2	C	357	SER
2	C	360	LEU
2	D	32	MET
2	D	75	SER
2	D	76	GLN
2	D	79	LEU
2	D	97	GLU
2	D	113	ARG
2	D	122	GLN
2	D	139	SER
2	D	152	THR
2	D	164	LYS
2	D	203	ASN
2	D	204	ILE
2	D	219	LEU
2	D	220	ASN
2	D	236	ASP
2	D	237	MET
2	D	245	THR
2	D	253	ARG
2	D	261	SER
2	D	262	ASP
2	D	270	ILE
2	D	273	ASP

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Mol	Chain	Res	Type
2	D	281	LEU
2	D	282	SER
2	D	285	LEU
2	D	299	ASN
2	D	324	VAL
2	D	327	TRP
2	D	338	LYS
2	D	344	GLN
2	D	354	THR
2	D	358	GLN
2	D	360	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	144	ASN
1	A	150	ASN
1	A	203	ASN
1	A	204	HIS
1	B	140	ASN
2	C	21	HIS
2	C	116	GLN
2	C	339	ASN
2	D	31	ASN
2	D	34	ASN
2	D	147	GLN
2	D	358	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	GOL	C	404	-	5,5,5	0.37	0	5,5,5	0.38	0
3	GOL	C	403	-	5,5,5	0.40	0	5,5,5	0.28	0
3	GOL	A	301	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	C	402	-	5,5,5	0.37	0	5,5,5	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	404	-	-	4/4/4/4	-
3	GOL	C	403	-	-	4/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
3	GOL	C	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	GOL	C1-C2-C3-O3
3	C	403	GOL	O1-C1-C2-C3
3	C	403	GOL	C1-C2-C3-O3
3	C	404	GOL	O1-C1-C2-C3
3	C	404	GOL	C1-C2-C3-O3
3	C	404	GOL	O1-C1-C2-O2
3	A	301	GOL	C1-C2-C3-O3

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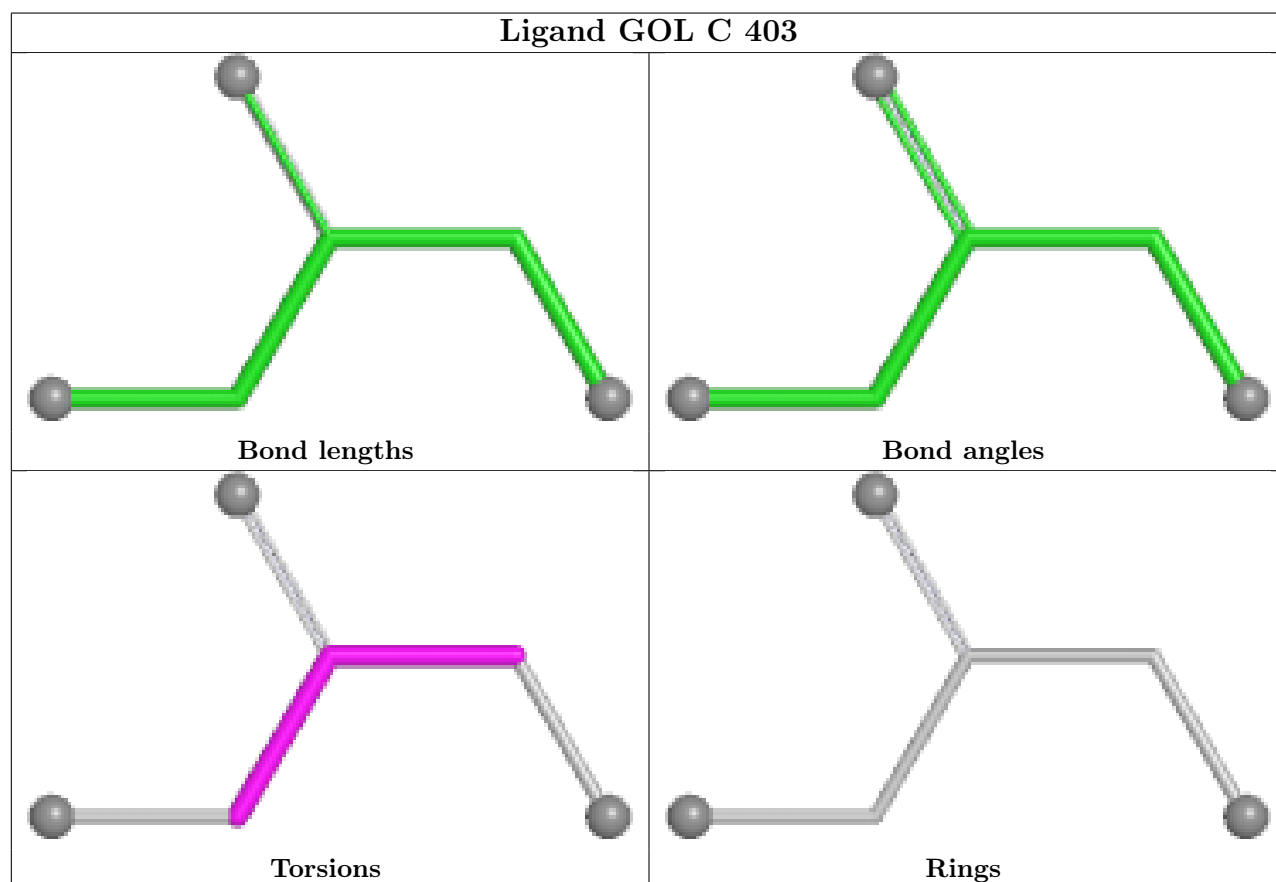
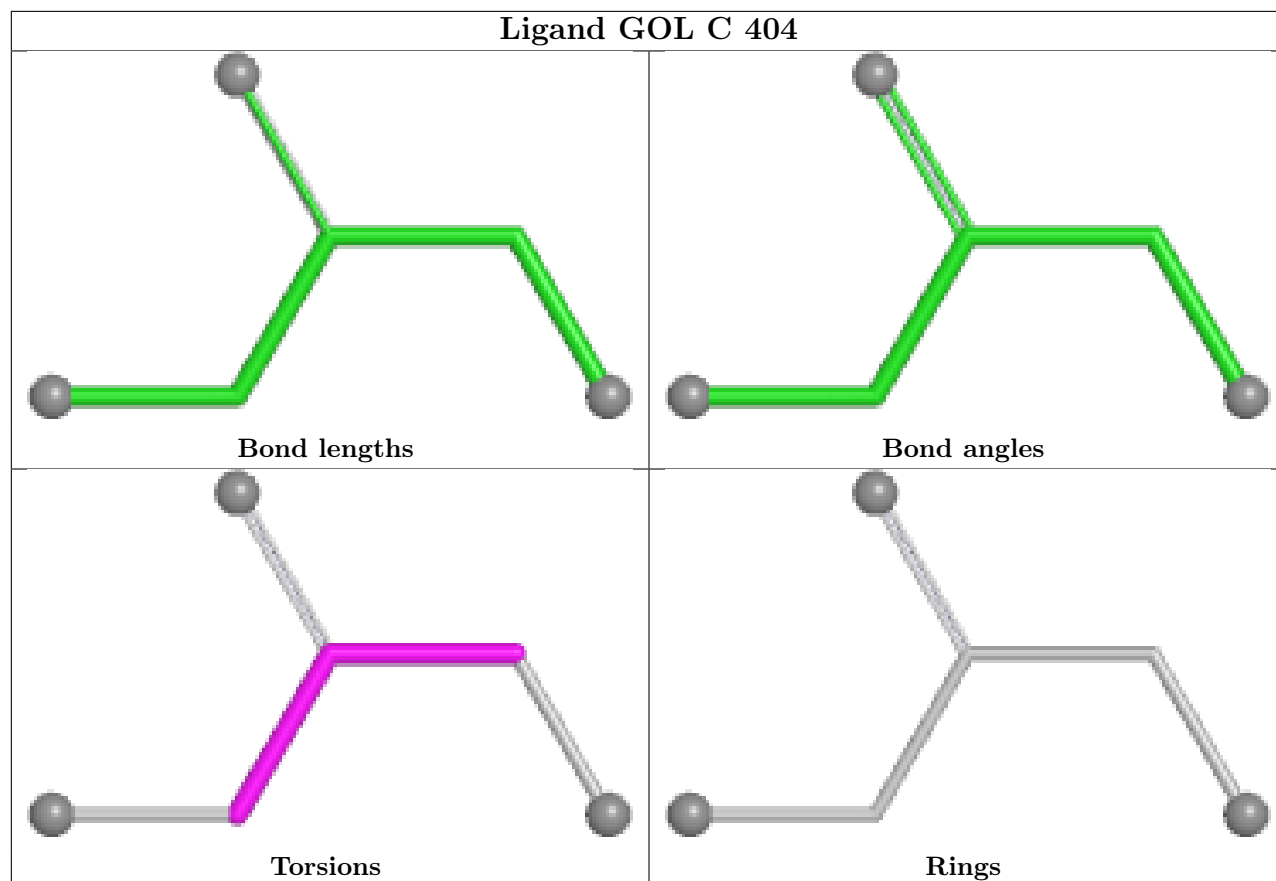
Mol	Chain	Res	Type	Atoms
3	C	402	GOL	O2-C2-C3-O3
3	C	403	GOL	O1-C1-C2-O2
3	C	403	GOL	O2-C2-C3-O3
3	C	404	GOL	O2-C2-C3-O3
3	A	301	GOL	O2-C2-C3-O3

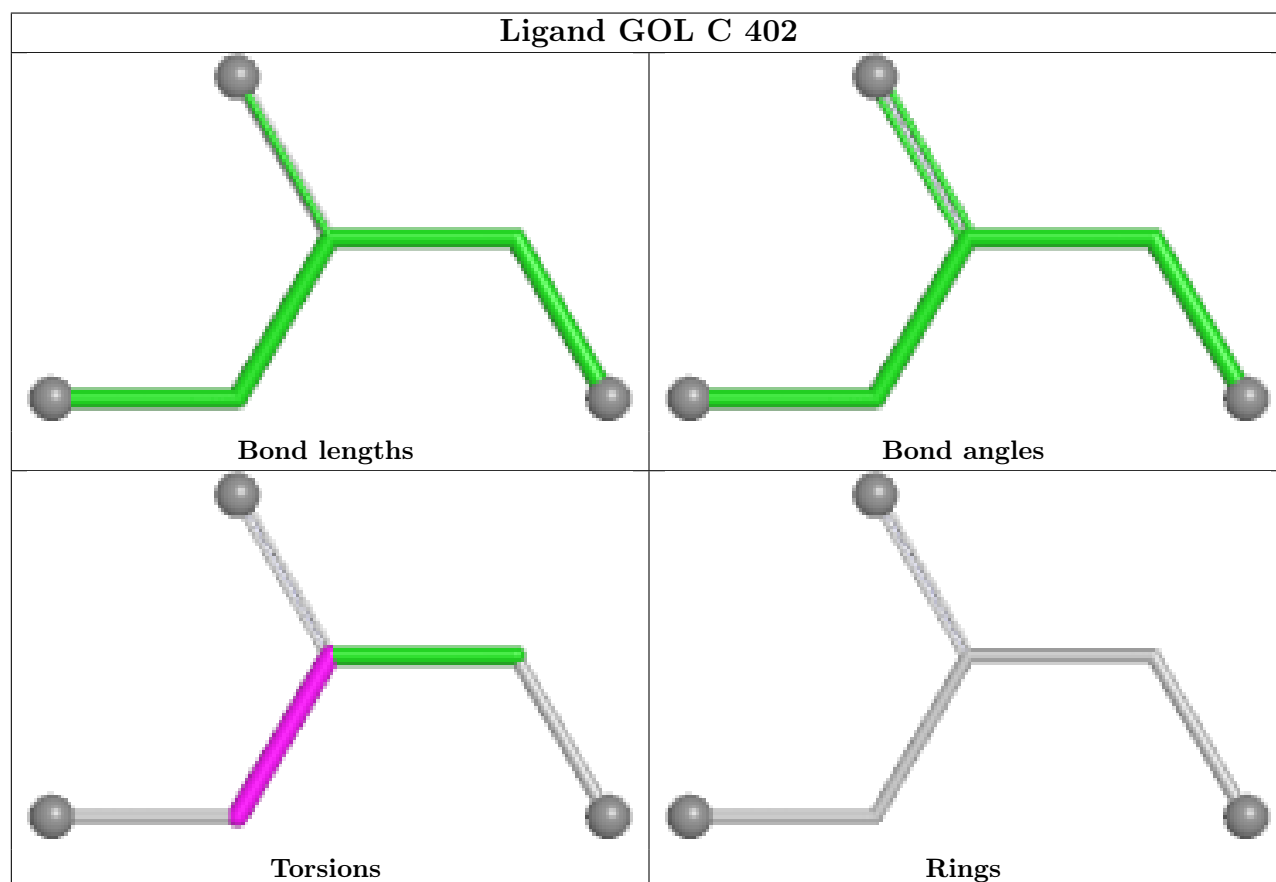
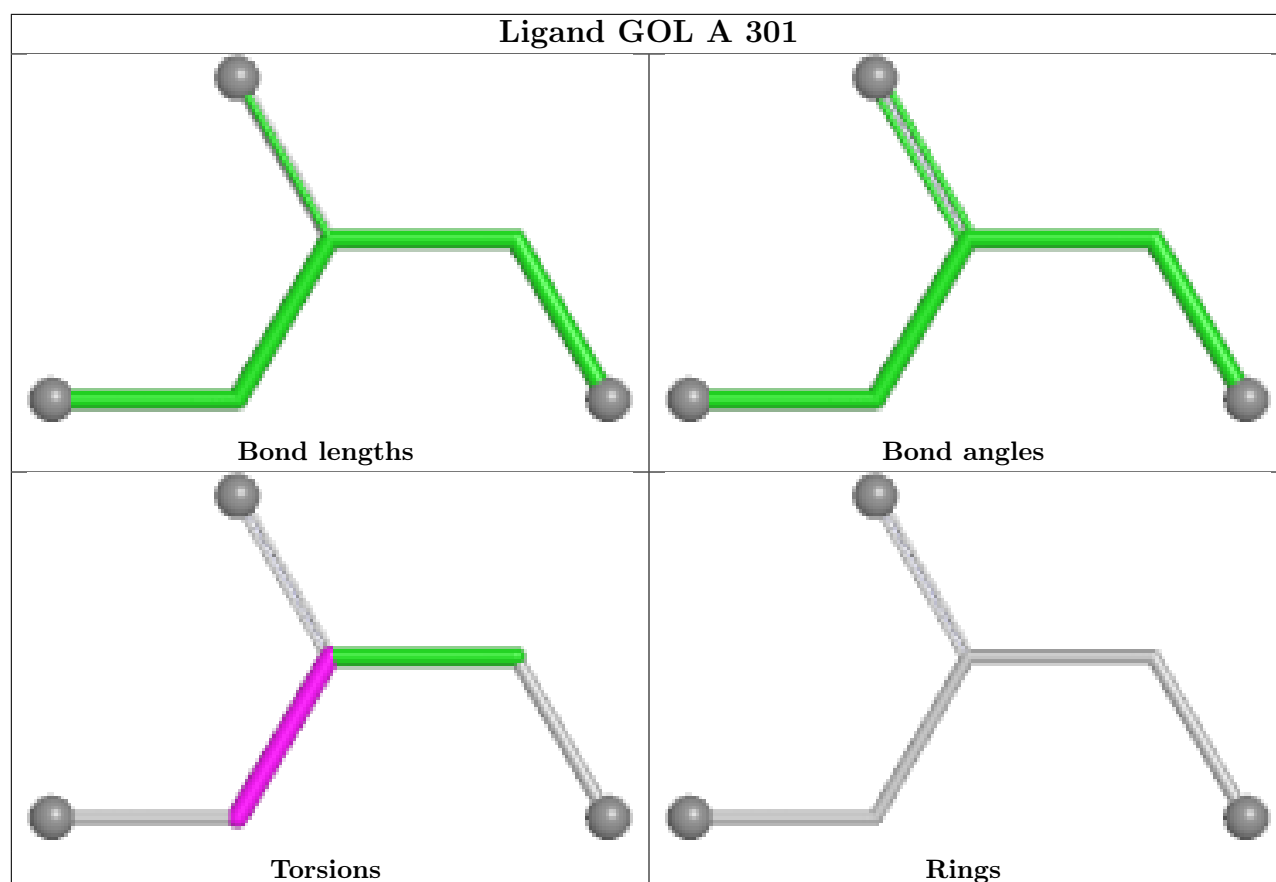
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	404	GOL	1	0
3	C	403	GOL	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	204/221 (92%)	0.46	15 (7%)	20 16	31, 61, 108, 141	0
1	B	211/221 (95%)	0.23	12 (5%)	29 24	28, 52, 120, 155	0
2	C	320/341 (93%)	0.40	23 (7%)	21 17	26, 56, 115, 167	0
2	D	326/341 (95%)	0.24	14 (4%)	40 33	30, 53, 93, 117	0
All	All	1061/1124 (94%)	0.33	64 (6%)	27 23	26, 56, 110, 167	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	324	VAL	7.0
2	C	244	SER	6.8
2	C	325	LEU	5.4
2	C	321	SER	4.9
2	D	360	LEU	4.9
2	D	321	SER	4.2
1	A	53	ASN	3.4
2	D	324	VAL	3.4
2	C	245	THR	3.3
1	B	217	LYS	3.3
2	D	322	VAL	3.3
2	C	360	LEU	3.1
1	B	173	VAL	3.1
2	D	323	PRO	3.0
2	D	225	GLY	2.9
2	C	243	TYR	2.9
2	D	325	LEU	2.8
2	C	20	HIS	2.8
2	C	285	LEU	2.7
1	B	207	ILE	2.7
2	C	346	MET	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	275	LYS	2.7
1	A	6	PRO	2.7
1	A	215	GLN	2.6
1	B	54	TRP	2.6
2	C	322	VAL	2.6
2	C	258	ASN	2.6
1	A	214	ILE	2.6
1	B	0	ALA	2.6
2	D	210	GLN	2.6
2	D	244	SER	2.5
2	C	90	GLY	2.5
1	A	84	LYS	2.5
1	B	172	CYS	2.5
2	C	323	PRO	2.5
2	C	327	TRP	2.4
2	C	204	ILE	2.4
1	A	175	LYS	2.4
1	B	218	VAL	2.4
1	B	220	ALA	2.3
2	D	247	SER	2.3
2	D	219	LEU	2.2
2	D	20	HIS	2.2
2	C	227	GLY	2.2
1	B	164	LYS	2.2
2	C	248	SER	2.2
2	C	239	PHE	2.2
1	B	211	GLN	2.2
1	B	168	ILE	2.2
2	D	243	TYR	2.1
2	D	305	LEU	2.1
1	A	151	GLY	2.1
1	A	161	TYR	2.1
2	C	58	TYR	2.1
1	A	168	ILE	2.1
1	A	166	SER	2.1
1	A	220	ALA	2.1
1	A	164	LYS	2.1
1	A	213	LEU	2.1
1	A	163	CYS	2.1
2	C	359	THR	2.0
1	B	216	LEU	2.0
2	C	41	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	24	LYS	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](#)

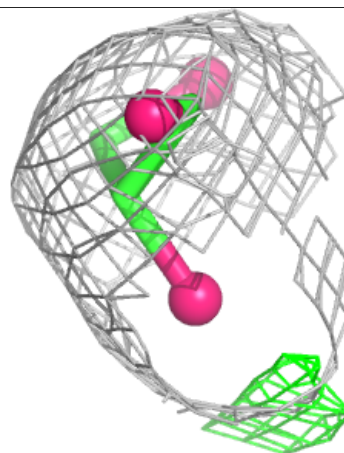
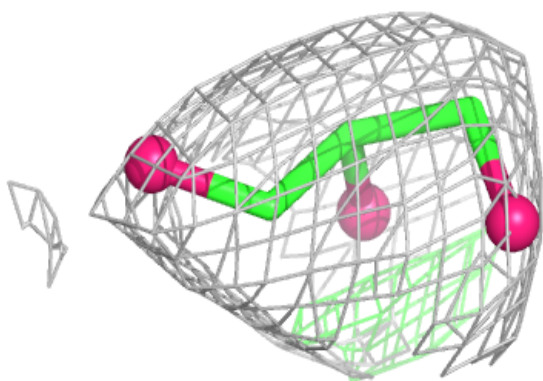
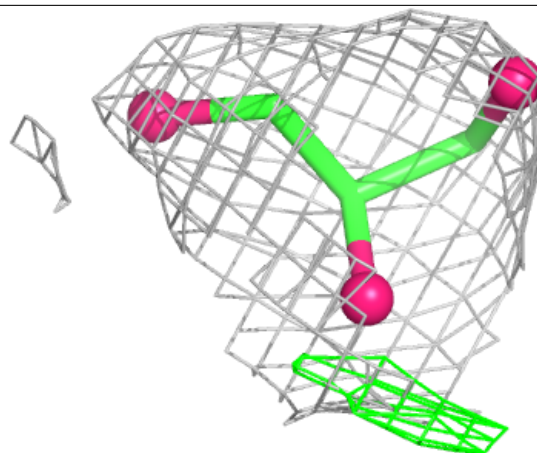
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	402	6/6	0.64	0.16	71,74,84,88	0
3	GOL	A	301	6/6	0.69	0.17	46,57,66,70	0
3	GOL	C	403	6/6	0.85	0.09	55,65,67,69	0
3	GOL	C	404	6/6	0.85	0.09	55,62,63,71	0
4	NI	C	405	1/1	0.87	0.08	131,131,131,131	1
4	NI	A	302	1/1	0.88	0.08	85,85,85,85	0
4	NI	B	301	1/1	0.93	0.06	93,93,93,93	0
4	NI	C	401	1/1	0.94	0.07	88,88,88,88	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.

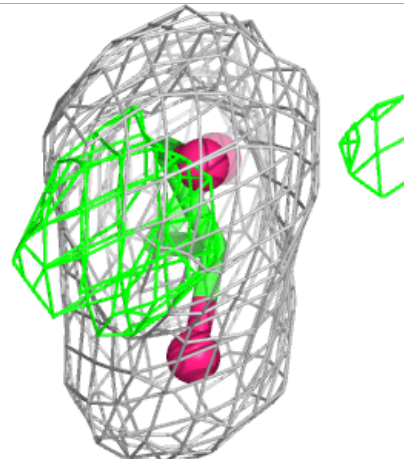
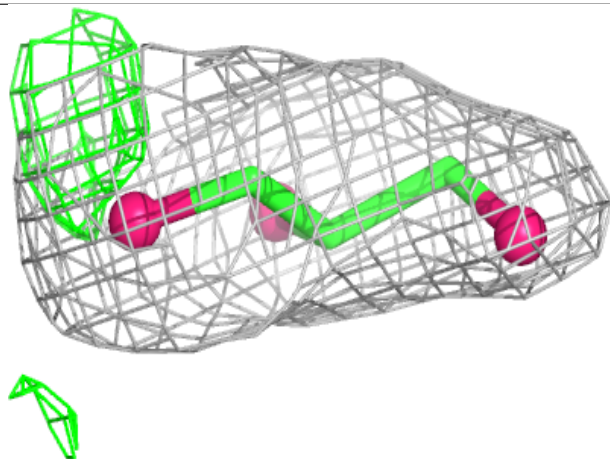
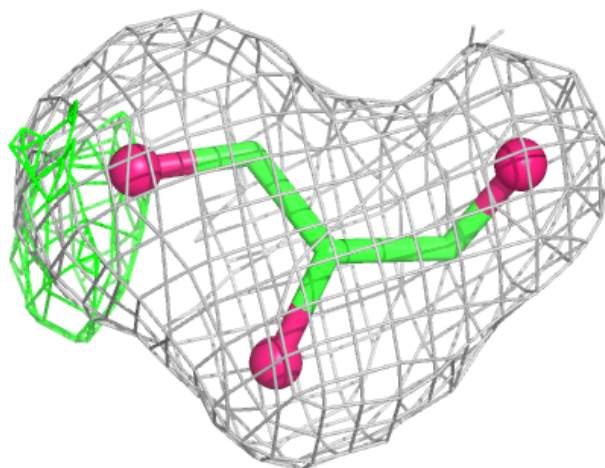
Electron density around GOL C 402:

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



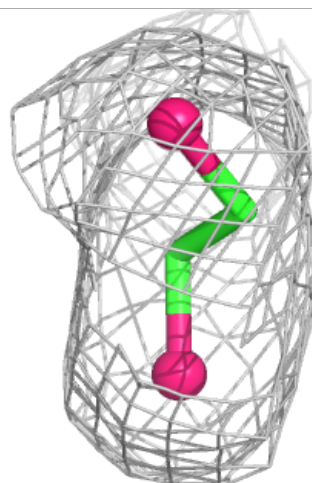
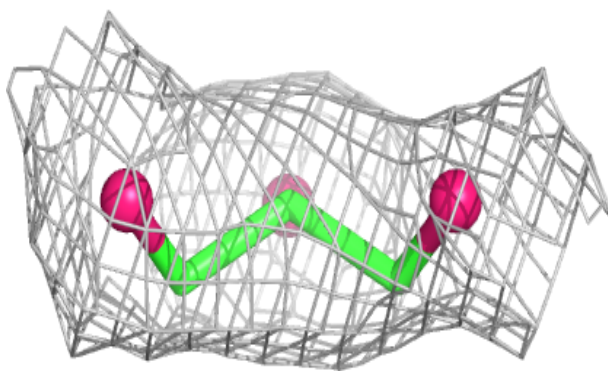
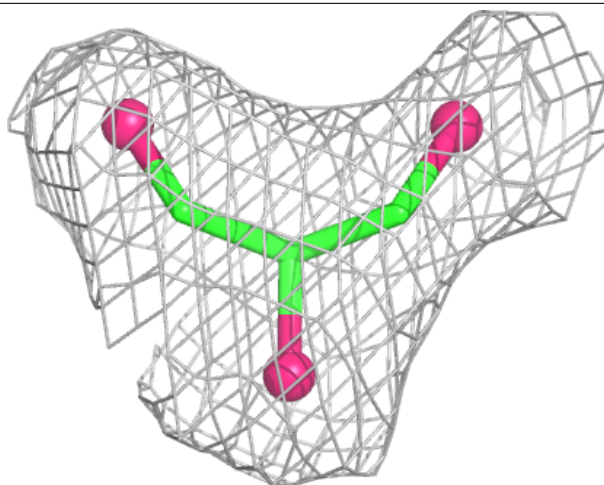
Electron density around GOL A 301:

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



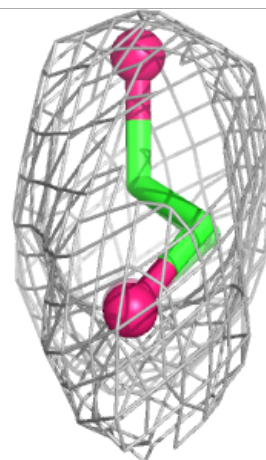
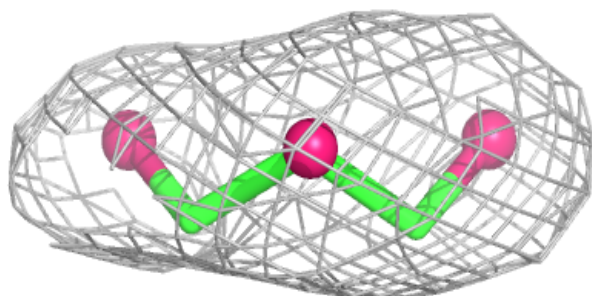
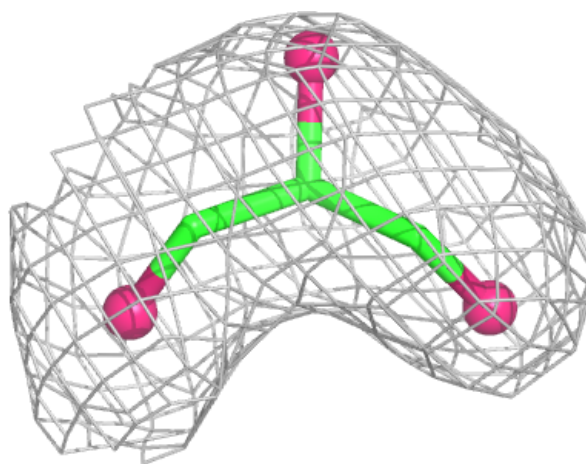
Electron density around GOL C 403:

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



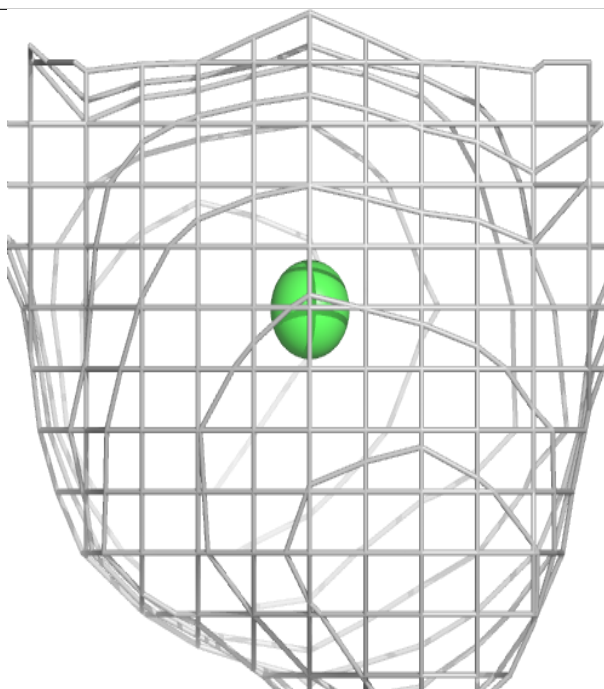
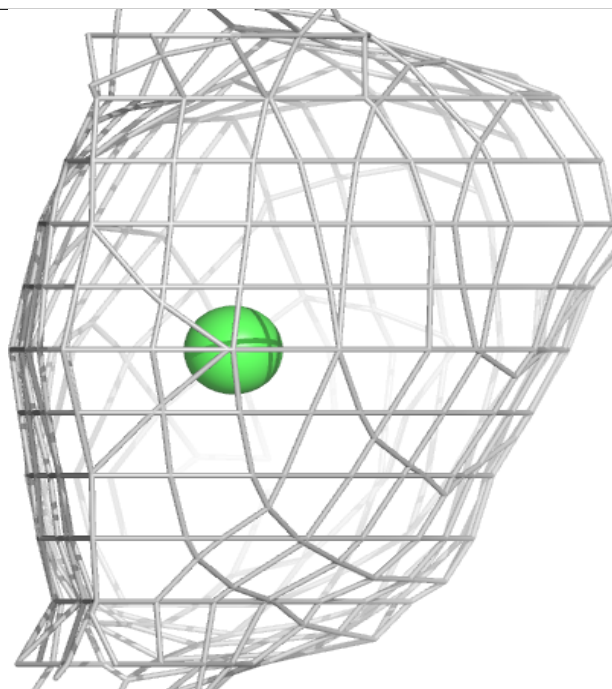
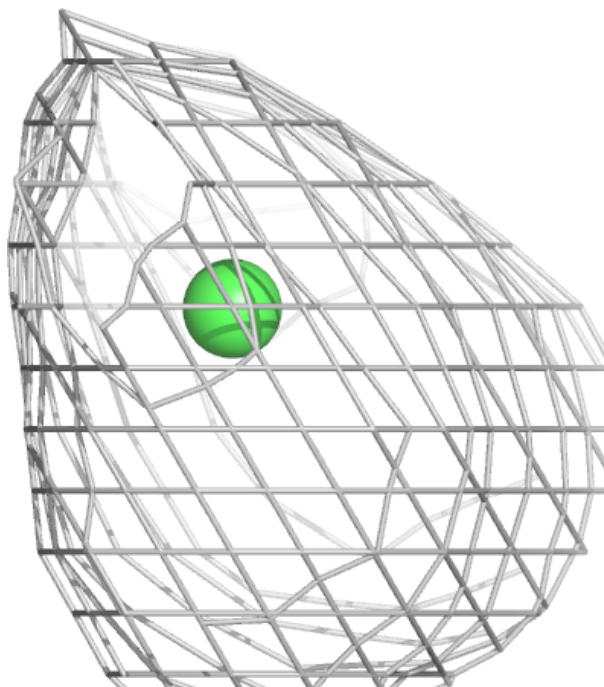
Electron density around GOL C 404:

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



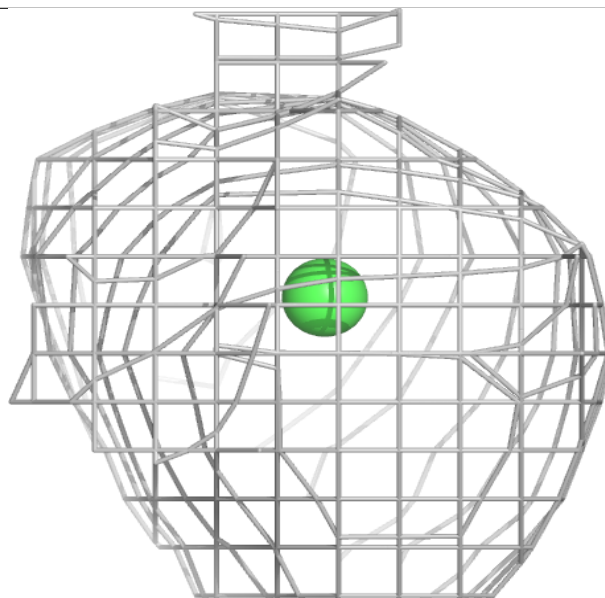
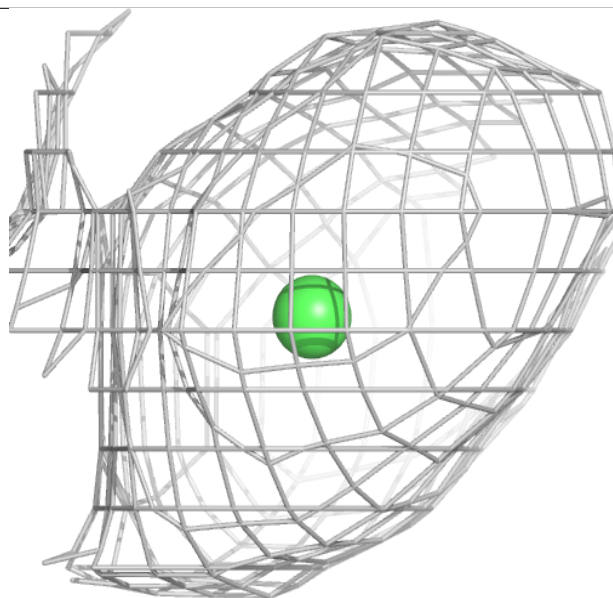
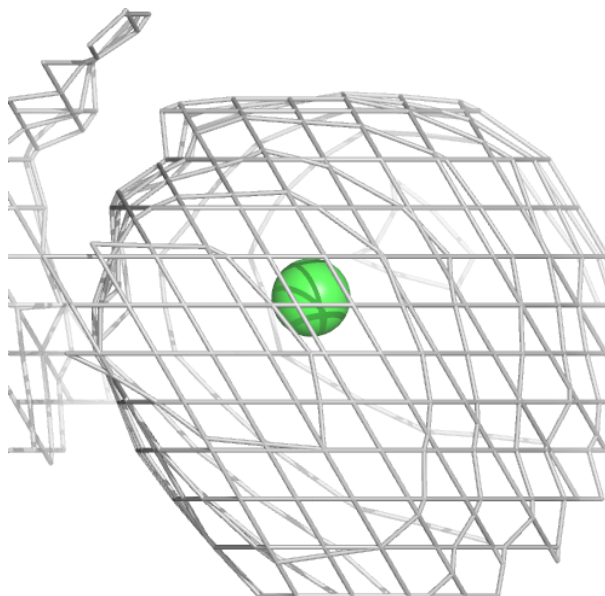
Electron density around NI C 405:

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



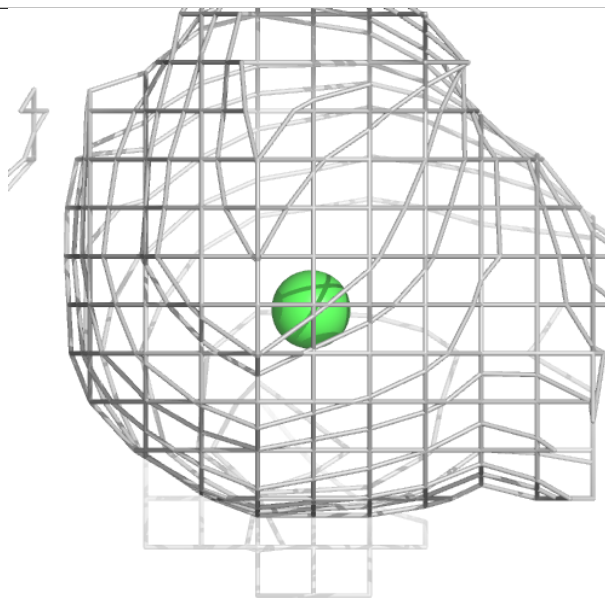
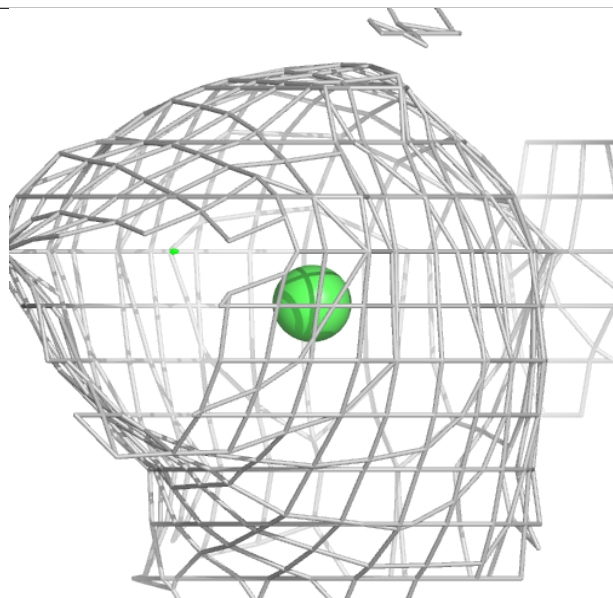
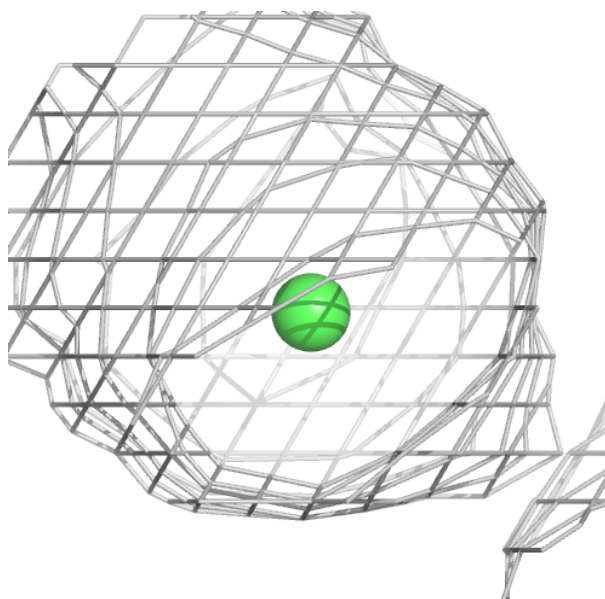
Electron density around NI A 302:

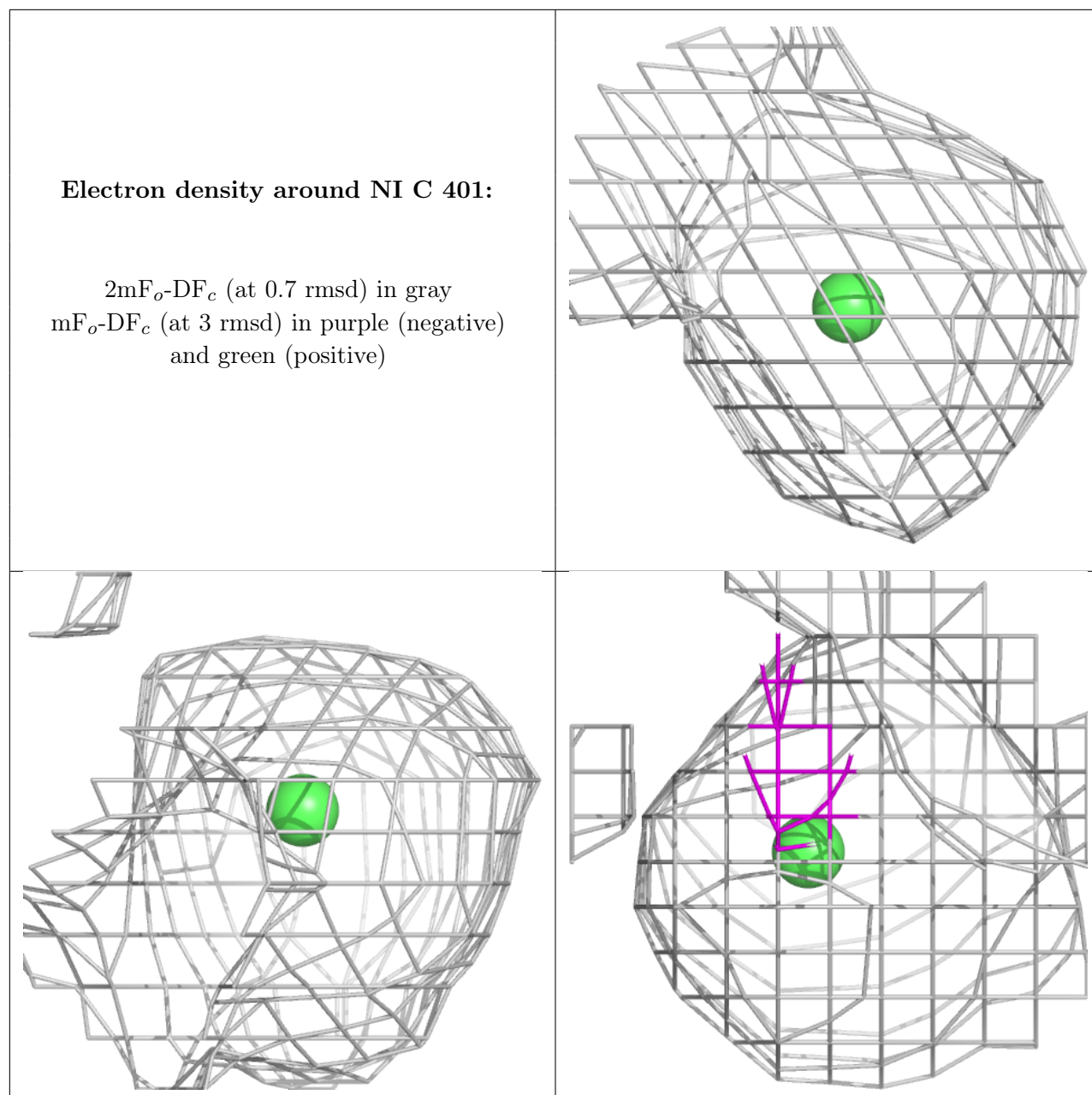
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI B 301:

$2mF_o-DF_c$ (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.