



Full wwPDB X-ray Structure Validation Report

(i)

May 24, 2023 – 04:20 pm BST

PDB ID : 8P3L

Title : The structure of thiocyanate dehydrogenase mutant form with Thr 169 replaced by Ala from Thioalkalivibrio paradoxus

Authors : Varfolomeeva, L.A.; Polyakov, K.M.; Komolov, A.S.; Rakitina, T.V.; Dergousova, N.I.; Dorovatovskii, P.V.; Boyko, K.M.; Tikhonova, T.V.; Popov, V.O.

Deposited on : 2023-05-18

Resolution : 1.80 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 (i) 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 \(1\)](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

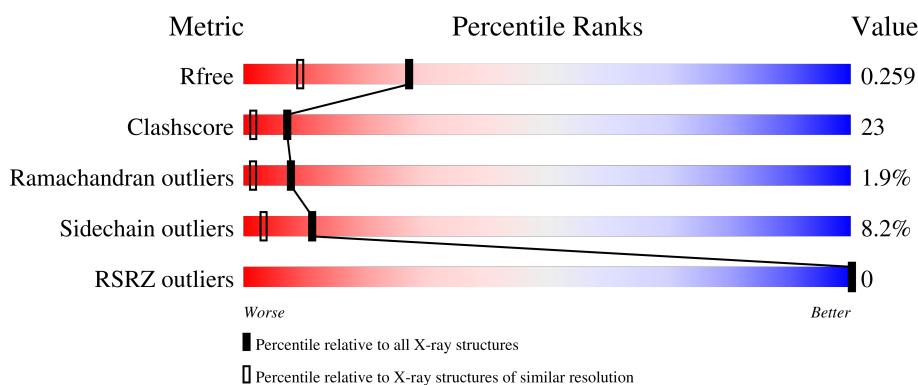
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

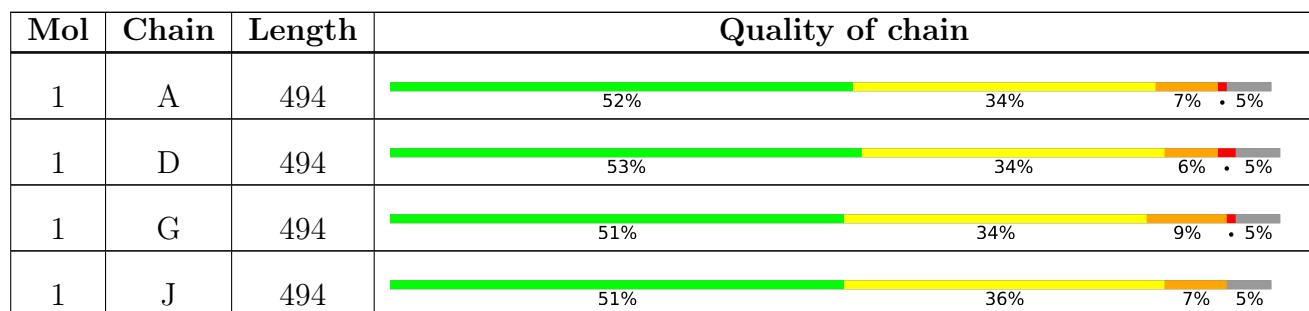
The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15340 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 Twin-arginine translocation signal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S			
			3644	2325	608	693	18	6	1	0
1	D	467	Total	C	N	O	S			
			3644	2325	607	694	18	4	2	0
1	G	467	Total	C	N	O	S			
			3628	2320	599	691	18	4	2	0
1	J	467	Total	C	N	O	S			
			3631	2321	601	691	18	3	2	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	initiating methionine	UNP W0DP94
A	56	SER	-	expression tag	UNP W0DP94
A	57	TYR	-	expression tag	UNP W0DP94
A	58	TYR	-	expression tag	UNP W0DP94
A	59	HIS	-	expression tag	UNP W0DP94
A	60	HIS	-	expression tag	UNP W0DP94
A	61	HIS	-	expression tag	UNP W0DP94
A	62	HIS	-	expression tag	UNP W0DP94
A	63	HIS	-	expression tag	UNP W0DP94
A	64	HIS	-	expression tag	UNP W0DP94
A	65	ASP	-	expression tag	UNP W0DP94
A	66	TYR	-	expression tag	UNP W0DP94
A	67	ASP	-	expression tag	UNP W0DP94
A	68	ILE	-	expression tag	UNP W0DP94
A	69	PRO	-	expression tag	UNP W0DP94
A	70	THR	-	expression tag	UNP W0DP94
A	71	THR	-	expression tag	UNP W0DP94
A	72	GLU	-	expression tag	UNP W0DP94
A	73	ASN	-	expression tag	UNP W0DP94
A	74	LEU	-	expression tag	UNP W0DP94
A	75	TYR	-	expression tag	UNP W0DP94

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Chain	Residue	Modelled	Actual	Comment	Reference
A	76	PHE	-	expression tag	UNP W0DP94
A	77	GLN	-	expression tag	UNP W0DP94
A	78	GLY	-	expression tag	UNP W0DP94
A	79	ALA	-	expression tag	UNP W0DP94
A	80	MET	-	expression tag	UNP W0DP94
A	81	GLY	-	expression tag	UNP W0DP94
A	169	ALA	THR	engineered mutation	UNP W0DP94
D	55	MET	-	initiating methionine	UNP W0DP94
D	56	SER	-	expression tag	UNP W0DP94
D	57	TYR	-	expression tag	UNP W0DP94
D	58	TYR	-	expression tag	UNP W0DP94
D	59	HIS	-	expression tag	UNP W0DP94
D	60	HIS	-	expression tag	UNP W0DP94
D	61	HIS	-	expression tag	UNP W0DP94
D	62	HIS	-	expression tag	UNP W0DP94
D	63	HIS	-	expression tag	UNP W0DP94
D	64	HIS	-	expression tag	UNP W0DP94
D	65	ASP	-	expression tag	UNP W0DP94
D	66	TYR	-	expression tag	UNP W0DP94
D	67	ASP	-	expression tag	UNP W0DP94
D	68	ILE	-	expression tag	UNP W0DP94
D	69	PRO	-	expression tag	UNP W0DP94
D	70	THR	-	expression tag	UNP W0DP94
D	71	THR	-	expression tag	UNP W0DP94
D	72	GLU	-	expression tag	UNP W0DP94
D	73	ASN	-	expression tag	UNP W0DP94
D	74	LEU	-	expression tag	UNP W0DP94
D	75	TYR	-	expression tag	UNP W0DP94
D	76	PHE	-	expression tag	UNP W0DP94
D	77	GLN	-	expression tag	UNP W0DP94
D	78	GLY	-	expression tag	UNP W0DP94
D	79	ALA	-	expression tag	UNP W0DP94
D	80	MET	-	expression tag	UNP W0DP94
D	81	GLY	-	expression tag	UNP W0DP94
D	169	ALA	THR	engineered mutation	UNP W0DP94
G	55	MET	-	initiating methionine	UNP W0DP94
G	56	SER	-	expression tag	UNP W0DP94
G	57	TYR	-	expression tag	UNP W0DP94
G	58	TYR	-	expression tag	UNP W0DP94
G	59	HIS	-	expression tag	UNP W0DP94
G	60	HIS	-	expression tag	UNP W0DP94
G	61	HIS	-	expression tag	UNP W0DP94

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Chain	Residue	Modelled	Actual	Comment	Reference
G	62	HIS	-	expression tag	UNP W0DP94
G	63	HIS	-	expression tag	UNP W0DP94
G	64	HIS	-	expression tag	UNP W0DP94
G	65	ASP	-	expression tag	UNP W0DP94
G	66	TYR	-	expression tag	UNP W0DP94
G	67	ASP	-	expression tag	UNP W0DP94
G	68	ILE	-	expression tag	UNP W0DP94
G	69	PRO	-	expression tag	UNP W0DP94
G	70	THR	-	expression tag	UNP W0DP94
G	71	THR	-	expression tag	UNP W0DP94
G	72	GLU	-	expression tag	UNP W0DP94
G	73	ASN	-	expression tag	UNP W0DP94
G	74	LEU	-	expression tag	UNP W0DP94
G	75	TYR	-	expression tag	UNP W0DP94
G	76	PHE	-	expression tag	UNP W0DP94
G	77	GLN	-	expression tag	UNP W0DP94
G	78	GLY	-	expression tag	UNP W0DP94
G	79	ALA	-	expression tag	UNP W0DP94
G	80	MET	-	expression tag	UNP W0DP94
G	81	GLY	-	expression tag	UNP W0DP94
G	169	ALA	THR	engineered mutation	UNP W0DP94
J	55	MET	-	initiating methionine	UNP W0DP94
J	56	SER	-	expression tag	UNP W0DP94
J	57	TYR	-	expression tag	UNP W0DP94
J	58	TYR	-	expression tag	UNP W0DP94
J	59	HIS	-	expression tag	UNP W0DP94
J	60	HIS	-	expression tag	UNP W0DP94
J	61	HIS	-	expression tag	UNP W0DP94
J	62	HIS	-	expression tag	UNP W0DP94
J	63	HIS	-	expression tag	UNP W0DP94
J	64	HIS	-	expression tag	UNP W0DP94
J	65	ASP	-	expression tag	UNP W0DP94
J	66	TYR	-	expression tag	UNP W0DP94
J	67	ASP	-	expression tag	UNP W0DP94
J	68	ILE	-	expression tag	UNP W0DP94
J	69	PRO	-	expression tag	UNP W0DP94
J	70	THR	-	expression tag	UNP W0DP94
J	71	THR	-	expression tag	UNP W0DP94
J	72	GLU	-	expression tag	UNP W0DP94
J	73	ASN	-	expression tag	UNP W0DP94
J	74	LEU	-	expression tag	UNP W0DP94
J	75	TYR	-	expression tag	UNP W0DP94

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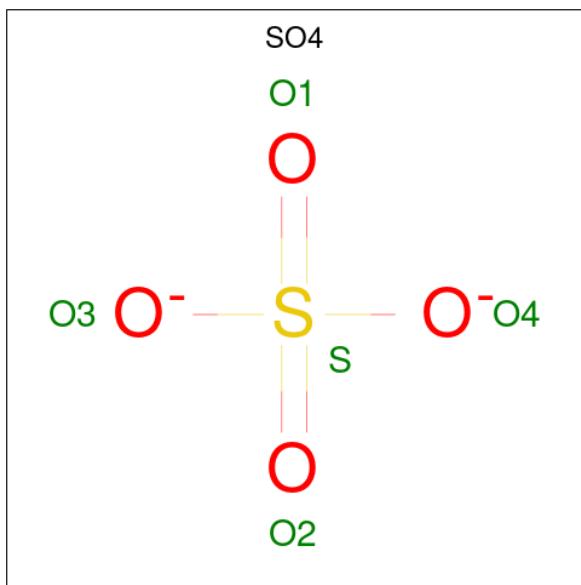
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Chain	Residue	Modelled	Actual	Comment	Reference
J	76	PHE	-	expression tag	UNP W0DP94
J	77	GLN	-	expression tag	UNP W0DP94
J	78	GLY	-	expression tag	UNP W0DP94
J	79	ALA	-	expression tag	UNP W0DP94
J	80	MET	-	expression tag	UNP W0DP94
J	81	GLY	-	expression tag	UNP W0DP94
J	169	ALA	THR	engineered mutation	UNP W0DP94

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	D	2	Total Cu 3 3	0	1
2	G	2	Total Cu 3 3	0	1
2	J	2	Total Cu 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0
4	D	205	Total O 205 205	0	0
4	G	194	Total O 194 194	0	0
4	J	160	Total O 160 160	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Twin-arginine translocation signal domain-containing protein

Chain A: 





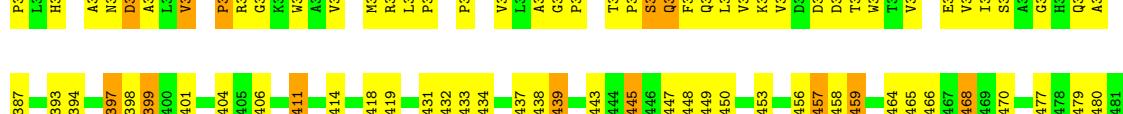
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain G: 51% 34% 9% • 5%



- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain J: 51% 36% 7% 5%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.81 Å 162.24 Å 90.76 Å 90.00° 119.74° 90.00°	Depositor
Resolution (Å)	81.12 – 1.80 81.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (81.12-1.80) 98.9 (81.12-1.80)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.00 (at 1.80 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R , R_{free}	0.186 , 0.254 0.191 , 0.259	Depositor DCC
R_{free} test set	10643 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	1.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.3	EDS
L-test for twinning ²	$< L > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.046 for l,k,-h-l 0.046 for -h-l,k,h 0.048 for -h-l,-k,l 0.045 for h,-k,-h-l 0.447 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15340	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, CU

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	0.81	2/3752 (0.1%)	1.48	37/5119 (0.7%)
1	D	0.93	6/3755 (0.2%)	1.59	43/5124 (0.8%)
1	G	0.94	8/3740 (0.2%)	1.54	39/5104 (0.8%)
1	J	0.80	2/3743 (0.1%)	1.47	33/5110 (0.6%)
All	All	0.87	18/14990 (0.1%)	1.52	152/20457 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	D	0	7
1	G	0	9
1	J	0	5
All	All	0	26

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	288	GLU	CD-OE1	11.34	1.38	1.25
1	G	535	ARG	CD-NE	-10.99	1.27	1.46
1	G	228	GLU	CD-OE1	-10.06	1.14	1.25
1	A	498	SER	CA-CB	-8.71	1.39	1.52
1	D	175	GLU	CD-OE2	-8.57	1.16	1.25
1	G	298	GLU	CD-OE2	8.33	1.34	1.25
1	D	171	GLU	CD-OE2	-7.90	1.17	1.25
1	J	228	GLU	CD-OE1	6.44	1.32	1.25
1	D	212	GLU	CD-OE2	-6.19	1.18	1.25
1	G	294	GLU	CD-OE1	-5.85	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	455	SER	CA-CB	-5.81	1.44	1.52
1	G	395	MET	CG-SD	5.72	1.96	1.81
1	D	395	MET	CG-SD	-5.72	1.66	1.81
1	G	212	GLU	CD-OE1	5.42	1.31	1.25
1	G	511	GLU	CD-OE2	-5.36	1.19	1.25
1	D	148	GLU	CD-OE2	-5.17	1.20	1.25
1	J	397	SER	CB-OG	5.16	1.49	1.42
1	A	516	GLU	CG-CD	-5.11	1.44	1.51

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	249	LYS	CB-CA-C	-10.58	89.25	110.40
1	J	188	ARG	CG-CD-NE	-9.62	91.60	111.80
1	D	535	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	G	456	PRO	N-CA-CB	-9.47	91.94	103.30
1	D	426	PRO	N-CD-CG	-9.36	89.17	103.20
1	G	274	ARG	CG-CD-NE	-9.20	92.47	111.80
1	D	535	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	D	237	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	G	233	THR	CA-CB-OG1	-8.48	91.20	109.00
1	A	262	THR	CA-CB-OG1	-8.44	91.28	109.00
1	J	196	ALA	N-CA-CB	8.19	121.56	110.10
1	D	435	THR	CA-CB-OG1	-8.02	92.16	109.00
1	A	134	MET	CG-SD-CE	7.98	112.97	100.20
1	D	541	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	237	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	G	321	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	J	457	THR	CA-CB-OG1	-7.56	93.13	109.00
1	G	488	TYR	CB-CA-C	7.49	125.39	110.40
1	J	127	TYR	CB-CA-C	7.45	125.31	110.40
1	J	231	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	A	440	PHE	CB-CA-C	-7.42	95.56	110.40
1	A	193	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	399	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	J	468	ASN	CB-CA-C	7.01	124.42	110.40
1	D	250	ASP	CB-CA-C	-7.00	96.41	110.40
1	G	546	THR	CA-CB-OG1	-6.97	94.35	109.00
1	D	237	ARG	CD-NE-CZ	6.92	133.28	123.60
1	G	468	ASN	CB-CA-C	6.87	124.15	110.40
1	G	151	PHE	CB-CA-C	6.83	124.06	110.40
1	A	482	HIS	CB-CA-C	6.81	124.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	231	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	D	232	GLU	CB-CG-CD	-6.78	95.91	114.20
1	J	321	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	D	265	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	D	530	ASN	CB-CA-C	6.57	123.55	110.40
1	A	496	THR	CA-CB-OG1	6.50	122.65	109.00
1	D	154	ASN	CB-CA-C	6.47	123.34	110.40
1	D	141	PRO	CB-CA-C	-6.42	95.95	112.00
1	G	345	PRO	CB-CA-C	-6.38	96.05	112.00
1	G	547	THR	CA-CB-OG1	-6.35	95.67	109.00
1	G	284	LYS	C-N-CA	6.34	137.54	121.70
1	G	105	SER	N-CA-CB	6.30	119.95	110.50
1	D	148	GLU	CB-CA-C	-6.28	97.84	110.40
1	D	262	THR	C-N-CA	6.26	137.35	121.70
1	J	181	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	D	529	ASP	CB-CA-C	6.22	122.84	110.40
1	D	420	LYS	CB-CA-C	6.14	122.68	110.40
1	G	321	ARG	CG-CD-NE	-6.14	98.91	111.80
1	G	502	ASN	CB-CA-C	6.12	122.64	110.40
1	G	454	PRO	N-CD-CG	-6.11	94.03	103.20
1	J	320	PRO	N-CD-CG	-6.09	94.07	103.20
1	D	164	TYR	CB-CA-C	6.01	122.42	110.40
1	D	171	GLU	CB-CG-CD	5.98	130.35	114.20
1	D	388	ASP	CB-CA-C	-5.98	98.44	110.40
1	A	195	ALA	N-CA-CB	-5.96	101.75	110.10
1	J	306	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	541	ARG	CG-CD-NE	-5.94	99.33	111.80
1	J	439	VAL	CA-CB-CG2	5.91	119.76	110.90
1	D	231	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	G	319	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	429	ARG	CG-CD-NE	-5.88	99.46	111.80
1	D	207	VAL	CA-CB-CG1	5.84	119.66	110.90
1	D	170	VAL	CA-CB-CG1	5.84	119.66	110.90
1	G	175	GLU	C-N-CA	-5.83	110.05	122.30
1	A	256	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	A	274	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	G	127	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	A	257	ASP	C-N-CA	-5.80	110.12	122.30
1	G	415	THR	CA-CB-OG1	5.78	121.13	109.00
1	G	388	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	231	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	J	445	LYS	CB-CA-C	5.72	121.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	278	GLN	N-CA-CB	5.71	120.88	110.60
1	A	212	GLU	N-CA-CB	5.67	120.81	110.60
1	D	423	VAL	CA-CB-CG2	5.67	119.40	110.90
1	G	319	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	433	PRO	CB-CA-C	-5.66	97.86	112.00
1	G	535	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	237	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	100	ALA	CB-CA-C	-5.61	101.68	110.10
1	A	238	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	G	394	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	D	367	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	D	429	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	G	138	ALA	CB-CA-C	5.51	118.36	110.10
1	G	153	VAL	CA-CB-CG1	-5.51	102.64	110.90
1	J	212	GLU	CB-CA-C	5.49	121.38	110.40
1	D	134	MET	CG-SD-CE	-5.48	91.43	100.20
1	A	194	ASP	CB-CA-C	5.48	121.35	110.40
1	A	113	LEU	CB-CG-CD1	-5.47	101.70	111.00
1	A	265	ARG	CG-CD-NE	5.45	123.25	111.80
1	G	322	GLY	C-N-CA	5.45	135.32	121.70
1	A	483	THR	CB-CA-C	-5.45	96.90	111.60
1	J	321	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	D	367	ASP	CB-CA-C	-5.42	99.56	110.40
1	D	368	THR	CA-CB-OG1	-5.42	97.61	109.00
1	J	194	ASP	CB-CG-OD2	5.42	123.17	118.30
1	G	231	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	131	CYS	CA-CB-SG	-5.39	104.29	114.00
1	A	321	ARG	CB-CA-C	-5.39	99.61	110.40
1	D	274	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	G	245	ASP	CB-CA-C	5.39	121.18	110.40
1	G	356	PRO	N-CA-C	-5.39	98.09	112.10
1	J	488	TYR	CB-CA-C	5.38	121.16	110.40
1	D	442	PRO	N-CA-CB	-5.38	96.69	102.60
1	J	164	TYR	C-N-CA	-5.37	111.02	122.30
1	D	274	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	G	231	ARG	CG-CD-NE	5.37	123.08	111.80
1	J	286	ASP	CB-CA-C	-5.37	99.66	110.40
1	J	321	ARG	CG-CD-NE	5.37	123.07	111.80
1	A	178	LYS	CB-CA-C	-5.36	99.68	110.40
1	J	151	PHE	CB-CA-C	5.34	121.08	110.40
1	J	314	ASP	CB-CA-C	5.33	121.05	110.40
1	A	544	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	488	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	G	187	THR	CA-CB-OG1	5.29	120.12	109.00
1	D	104	PHE	CB-CG-CD1	-5.28	117.10	120.80
1	D	133	ILE	O-C-N	-5.28	114.25	122.70
1	D	237	ARG	CB-CG-CD	-5.27	97.91	111.60
1	J	536	THR	CA-CB-OG1	-5.27	97.94	109.00
1	G	162	PHE	CB-CG-CD1	5.26	124.48	120.80
1	A	173	PRO	C-N-CA	-5.26	111.25	122.30
1	J	231	ARG	CG-CD-NE	5.25	122.83	111.80
1	A	531	VAL	CA-CB-CG2	5.24	118.76	110.90
1	G	230	ASP	CB-CA-C	-5.24	99.92	110.40
1	A	525	MET	CG-SD-CE	5.23	108.57	100.20
1	J	510	MET	CG-SD-CE	-5.20	91.89	100.20
1	A	301	LYS	CB-CA-C	-5.19	100.02	110.40
1	G	231	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	212	GLU	CB-CA-C	-5.19	100.02	110.40
1	G	135	HIS	CA-CB-CG	-5.18	104.79	113.60
1	A	108	VAL	CA-CB-CG1	5.17	118.65	110.90
1	G	136	HIS	CB-CA-C	5.17	120.73	110.40
1	A	338	PHE	CB-CA-C	-5.16	100.09	110.40
1	D	415	THR	CA-CB-OG1	-5.14	98.20	109.00
1	G	112	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	254	ALA	CB-CA-C	5.12	117.77	110.10
1	G	488	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	J	153	VAL	CA-CB-CG1	5.10	118.55	110.90
1	J	180	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	220	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	J	159	LYS	N-CA-CB	-5.07	101.47	110.60
1	A	228	GLU	CB-CA-C	-5.07	100.27	110.40
1	J	95	LYS	CB-CA-C	5.07	120.54	110.40
1	A	189	MET	CG-SD-CE	-5.06	92.11	100.20
1	D	534	PRO	CB-CA-C	-5.05	99.37	112.00
1	J	477	LEU	C-N-CA	-5.05	111.70	122.30
1	J	149	PHE	CB-CA-C	5.05	120.50	110.40
1	D	103	LYS	CA-CB-CG	-5.04	102.30	113.40
1	G	352	PRO	N-CA-C	5.04	125.19	112.10
1	D	274	ARG	CG-CD-NE	5.02	122.35	111.80
1	J	525	MET	CB-CG-SD	5.02	127.46	112.40

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ALA	Mainchain
1	A	266	LEU	Mainchain
1	A	343	GLN	Peptide
1	A	385	PHE	Peptide
1	A	453	TRP	Peptide
1	D	149	PHE	Sidechain
1	D	316	LEU	Mainchain
1	D	385	PHE	Peptide
1	D	395	MET	Mainchain
1	D	475	VAL	Mainchain
1	D	497	LEU	Peptide
1	D	506	ALA	Peptide
1	G	107	THR	Mainchain
1	G	173	PRO	Peptide
1	G	197	GLU	Mainchain
1	G	198	VAL	Mainchain
1	G	457	THR	Mainchain
1	G	477	LEU	Mainchain
1	G	497	LEU	Mainchain
1	G	514	THR	Peptide
1	G	538	GLU	Mainchain
1	J	117	TRP	Peptide
1	J	272	GLY	Mainchain
1	J	315	ALA	Peptide
1	J	358	GLN	Peptide
1	J	497	LEU	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3644	0	3517	160	0
1	D	3644	0	3509	149	0
1	G	3628	0	3491	169	0
1	J	3631	0	3493	178	0
2	A	2	0	0	0	0
2	D	3	0	0	1	0
2	G	3	0	0	0	0
2	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	D	10	0	0	1	0
3	G	20	0	0	1	0
3	J	5	0	0	0	0
4	A	184	0	0	13	0
4	D	205	0	0	10	0
4	G	194	0	0	4	0
4	J	160	0	0	14	0
All	All	15340	0	14010	647	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 23.

All (647) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:602[B]:CU:CU	4:D:747:HOH:O	0.94	1.12
1:A:265:ARG:HG3	1:A:265:ARG:HH11	1.14	1.09
1:D:236:VAL:HG11	1:D:275:TYR:CE1	1.86	1.08
1:D:465:ASP:HB2	1:D:472:LEU:CD1	1.85	1.06
1:D:103:LYS:HE2	1:D:528:HIS:CE1	1.91	1.04
1:J:265:ARG:HD2	1:J:367:ASP:HB3	1.36	1.03
1:A:290:VAL:HG12	1:A:291:PRO:HD2	1.06	1.02
1:G:160:ASN:HA	1:G:163:ILE:HD11	1.04	1.02
1:G:160:ASN:CA	1:G:163:ILE:HD11	1.88	1.02
1:D:443:ASP:CG	1:D:445:LYS:HE2	1.80	1.01
1:D:465:ASP:HB2	1:D:472:LEU:HD11	1.42	1.01
1:J:352:PRO:HB2	1:J:355:THR:CG2	1.93	0.98
1:J:352:PRO:HB2	1:J:355:THR:HG23	1.47	0.96
1:J:357:SER:HA	1:J:419:LYS:HE2	1.50	0.94
1:G:182:ILE:HG23	1:G:190:ASN:O	1.68	0.93
1:G:160:ASN:HA	1:G:163:ILE:CD1	1.96	0.93
1:J:447[A]:ILE:HG23	1:J:464:ILE:HB	1.49	0.92
1:A:290:VAL:CG1	1:A:291:PRO:HD2	1.98	0.91
1:G:205:VAL:HG12	1:G:206:HIS:H	1.37	0.90
1:A:290:VAL:HG12	1:A:291:PRO:CD	2.00	0.90
1:G:488:TYR:OH	1:G:543:SER:HB2	1.72	0.89
1:J:179:ILE:HG22	1:J:179:ILE:O	1.72	0.89
1:D:407:ASP:OD1	1:D:409:SER:HB2	1.74	0.88
1:J:306:ARG:N	1:J:307:PRO:HD2	1.88	0.88
1:A:112:ASP:OD1	1:A:146:TYR:OH	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:294:GLU:O	1:J:298:GLU:HG3	1.73	0.88
1:A:488:TYR:CD1	1:A:539:ASP:HB3	2.11	0.86
1:D:450:THR:HG21	1:D:482:HIS:O	1.76	0.85
1:G:241:ALA:CB	1:G:266:LEU:HD11	2.05	0.85
3:A:603[A]:SO4:O3	4:A:701:HOH:O	1.92	0.85
1:D:443:ASP:OD2	1:D:445:LYS:HE2	1.76	0.85
1:J:265:ARG:HG2	1:J:265:ARG:HH11	1.39	0.85
1:J:99:VAL:HG11	1:J:137:MET:HE1	1.60	0.84
1:D:236:VAL:HG11	1:D:275:TYR:HE1	1.36	0.83
1:G:377:ILE:HD12	1:G:377:ILE:H	1.44	0.82
1:J:264:LYS:HE3	4:J:747:HOH:O	1.78	0.82
1:J:383:ALA:HA	1:J:393:LEU:O	1.80	0.82
1:A:175:GLU:HG2	1:A:280:SER:HB3	1.62	0.82
1:A:223:LYS:HB3	1:A:225:ILE:HD12	1.62	0.81
1:G:198:VAL:HG11	1:G:234:ASP:HB2	1.63	0.80
1:D:205:VAL:HG23	1:D:220:ASP:HA	1.65	0.78
1:J:299:ASP:OD1	4:J:701:HOH:O	2.00	0.78
1:J:145:PRO:HB3	1:J:533:VAL:HG11	1.65	0.78
1:G:148:GLU:CD	1:G:183:LYS:HE3	2.04	0.78
1:G:477:LEU:HD21	1:G:517:VAL:HG21	1.66	0.78
1:J:265:ARG:HD2	1:J:367:ASP:CB	2.12	0.78
1:D:101:PRO:HG2	4:D:815:HOH:O	1.85	0.77
1:A:179:ILE:HG22	1:A:179:ILE:O	1.84	0.77
1:G:352:PRO:HB2	1:G:355:THR:HG23	1.65	0.77
1:J:185:ASP:OD2	1:J:188:ARG:NH2	2.18	0.77
1:J:348:VAL:HG21	1:J:371:VAL:HG21	1.67	0.77
1:D:153:VAL:O	1:D:153:VAL:HG13	1.85	0.77
1:G:270:LEU:HD21	1:G:276:ASP:HB2	1.65	0.76
1:J:254:ALA:HB3	1:J:255:TRP:CE3	2.21	0.75
1:G:326:VAL:HG11	1:G:392:PHE:CZ	2.22	0.75
1:G:519:GLY:HA3	1:J:86:VAL:HG12	1.68	0.75
1:A:339:ASP:OD1	1:A:342:ASN:HB2	1.85	0.75
1:G:117:TRP:CH2	1:J:479:PRO:HD2	2.21	0.75
1:J:241:ALA:HB2	1:J:266:LEU:HD13	1.69	0.74
1:A:265:ARG:HG3	1:A:265:ARG:NH1	1.95	0.74
1:J:163:ILE:HG22	1:J:164:TYR:CD1	2.22	0.74
1:G:148:GLU:OE2	1:G:183:LYS:HE2	1.88	0.74
1:A:381:HIS:CD2	4:A:702:HOH:O	2.41	0.74
1:A:537:LEU:HD13	4:A:867:HOH:O	1.86	0.74
1:D:236:VAL:HG13	1:D:236:VAL:O	1.86	0.74
1:J:382:GLN:NE2	1:J:382:GLN:HA	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:306:ARG:H	1:J:307:PRO:HD2	1.51	0.73
1:J:350:ALA:O	1:J:419:LYS:NZ	2.21	0.73
1:D:377:ILE:HD12	1:D:377:ILE:H	1.53	0.73
1:G:159:LYS:HD2	1:G:286:ASP:HB3	1.71	0.73
1:J:352:PRO:HB2	1:J:355:THR:HG21	1.70	0.73
1:J:184:TYR:CE2	1:J:186:GLY:HA2	2.24	0.72
1:A:504:ALA:HA	1:D:118:THR:O	1.90	0.71
1:D:465:ASP:HB2	1:D:472:LEU:HD12	1.73	0.71
1:J:99:VAL:CG1	1:J:137:MET:HE1	2.21	0.71
1:J:306:ARG:NH2	1:J:309:HIS:ND1	2.38	0.71
1:G:138:ALA:HB1	1:G:209:ILE:HG12	1.73	0.70
1:J:225:ILE:HA	1:J:240:TRP:O	1.91	0.70
1:G:266:LEU:N	1:G:266:LEU:HD12	2.06	0.70
1:G:241:ALA:HB2	1:G:266:LEU:HD11	1.74	0.70
1:J:450:THR:HG23	1:J:484:LEU:CD1	2.22	0.70
1:A:265:ARG:HH11	1:A:265:ARG:CG	1.94	0.69
1:D:132:PRO:O	1:D:134:MET:HG2	1.92	0.69
1:G:311:VAL:HG21	1:G:329:MET:CE	2.22	0.69
1:G:148:GLU:CD	1:G:183:LYS:CE	2.60	0.69
1:D:90:TYR:HB3	1:D:113:LEU:O	1.93	0.68
1:D:236:VAL:CG1	1:D:275:TYR:HE1	2.05	0.68
1:A:371:VAL:HG22	1:A:373:ILE:CD1	2.23	0.68
1:D:424:GLU:HB3	4:D:785:HOH:O	1.92	0.68
1:G:377:ILE:HD12	1:G:377:ILE:N	2.07	0.68
1:G:403:ILE:HD12	1:G:423:VAL:HG21	1.75	0.68
1:J:163:ILE:HG22	1:J:164:TYR:CE1	2.27	0.68
1:G:403:ILE:HB	1:G:423:VAL:HG23	1.75	0.68
1:J:299:ASP:CB	4:J:701:HOH:O	2.42	0.68
1:D:383:ALA:HB2	1:D:394:PHE:HD1	1.57	0.68
1:D:236:VAL:CG1	1:D:275:TYR:CE1	2.73	0.68
1:J:265:ARG:HG2	1:J:265:ARG:NH1	2.06	0.68
1:G:209:ILE:O	1:G:545:SER:HB2	1.94	0.68
1:A:382:GLN:HB2	1:A:436:PHE:O	1.93	0.67
1:G:498:SER:HA	1:G:505[B]:SER:HB3	1.76	0.67
1:D:154:ASN:HA	1:D:178:LYS:O	1.94	0.67
1:J:411:HIS:O	1:J:411:HIS:ND1	2.27	0.67
1:D:356:PRO:O	1:D:419:LYS:NZ	2.27	0.67
1:J:299:ASP:HB3	4:J:701:HOH:O	1.94	0.67
1:J:306:ARG:N	1:J:307:PRO:CD	2.58	0.67
1:D:345:PRO:HG2	1:D:361:LEU:HD21	1.77	0.66
1:J:399:ARG:HG3	4:J:763:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TRP:HD1	4:A:815:HOH:O	1.77	0.66
1:J:306:ARG:H	1:J:307:PRO:CD	2.08	0.66
1:A:98:LEU:HD12	1:A:531:VAL:O	1.95	0.66
1:A:294:GLU:O	1:A:298:GLU:HG3	1.95	0.66
1:G:182:ILE:HG23	1:G:190:ASN:C	2.16	0.66
1:D:138:ALA:HB1	1:D:209:ILE:HG12	1.77	0.66
1:A:265:ARG:HD3	4:A:788:HOH:O	1.96	0.66
1:G:459:ASN:N	1:G:459:ASN:HD22	1.94	0.65
1:G:387:PRO:HD2	1:G:444:ALA:HB2	1.78	0.65
1:J:382:GLN:HA	1:J:382:GLN:HE21	1.61	0.65
1:G:82:LYS:HD3	1:G:82:LYS:C	2.17	0.65
1:A:153:VAL:HG13	1:A:153:VAL:O	1.97	0.64
1:D:103:LYS:HE2	1:D:528:HIS:ND1	2.12	0.64
1:J:447[A]:ILE:CG2	1:J:464:ILE:HB	2.24	0.64
1:A:326:VAL:HA	1:A:336:VAL:O	1.98	0.64
1:J:502:ASN:O	4:J:702:HOH:O	2.15	0.64
1:J:99:VAL:CG1	1:J:137:MET:CE	2.76	0.64
1:A:214:ASP:OD1	1:A:214:ASP:C	2.36	0.64
1:J:465:ASP:OD2	1:J:468:ASN:HB2	1.98	0.64
1:J:148:GLU:O	1:J:149:PHE:HB3	1.98	0.64
1:J:102:GLY:O	1:J:105:SER:HB3	1.98	0.64
1:A:392:PHE:C	1:A:393:LEU:HD12	2.18	0.63
1:D:225:ILE:HG12	1:D:266:LEU:HD11	1.78	0.63
1:A:238:TYR:CD1	1:A:238:TYR:C	2.72	0.63
1:J:252:LYS:NZ	1:J:299:ASP:OD1	2.31	0.63
1:J:350:ALA:HB2	1:J:359:PHE:CE2	2.33	0.63
1:A:459:ASN:HD22	1:A:459:ASN:H	1.45	0.63
1:D:141:PRO:HA	1:D:534:PRO:O	1.99	0.63
1:A:244:TRP:HA	1:A:244:TRP:CE3	2.34	0.62
1:A:205:VAL:HG12	1:A:206:HIS:H	1.65	0.62
1:J:150:GLU:HG2	1:J:183:LYS:HE2	1.82	0.62
1:J:450:THR:HG21	1:J:482:HIS:O	1.99	0.62
1:J:479:PRO:O	1:J:479:PRO:HG2	1.99	0.62
1:G:161:LEU:HD23	1:G:173:PRO:HG3	1.82	0.62
1:D:481:MET:SD	1:D:497:LEU:HD11	2.40	0.61
1:G:538:GLU:H	1:G:538:GLU:CD	2.03	0.61
1:D:530:ASN:O	1:D:531:VAL:HG12	1.99	0.61
1:A:138:ALA:HB1	1:A:209:ILE:HG12	1.80	0.61
1:G:106:GLY:HA2	1:G:132:PRO:O	1.99	0.61
1:G:241:ALA:HB3	1:G:266:LEU:HD11	1.80	0.61
1:D:434:ASN:HB2	1:D:436:PHE:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:VAL:O	1:D:236:VAL:CG1	2.48	0.61
1:J:448:TYR:CZ	1:J:512:THR:HG22	2.36	0.61
1:J:450:THR:HG23	1:J:484:LEU:HD11	1.83	0.61
1:A:184:TYR:CE2	1:A:186:GLY:HA2	2.36	0.61
1:G:306:ARG:N	1:G:307:PRO:HD3	2.16	0.61
1:D:176:GLY:O	1:D:177:MET:HB2	2.01	0.60
1:A:324:TRP:CZ3	1:A:346:VAL:HG21	2.36	0.60
1:A:326:VAL:HG22	1:A:337:VAL:HG22	1.84	0.60
1:D:357:SER:HA	1:D:419:LYS:CD	2.31	0.60
1:D:459:ASN:HB2	1:D:478:GLY:O	2.01	0.60
1:G:183:LYS:HE2	4:G:742:HOH:O	2.02	0.60
1:G:266:LEU:N	1:G:266:LEU:CD1	2.64	0.60
1:A:321:ARG:HG2	4:A:851:HOH:O	2.01	0.60
1:D:236:VAL:HG11	1:D:275:TYR:CZ	2.36	0.60
1:A:371:VAL:HG22	1:A:373:ILE:HD12	1.85	0.59
1:A:387:PRO:O	1:A:541:ARG:HD3	2.01	0.59
1:A:427:ASP:OD1	1:A:427:ASP:N	2.32	0.59
1:J:290:VAL:HG22	1:J:291:PRO:HD2	1.84	0.59
1:A:289:LEU:HG	4:A:724:HOH:O	2.03	0.59
1:G:148:GLU:OE1	1:G:183:LYS:HE3	2.02	0.59
1:J:179:ILE:O	1:J:179:ILE:CG2	2.47	0.59
1:J:432:TYR:HB3	1:J:433:PRO:HA	1.83	0.59
1:A:240:TRP:CE2	4:A:803:HOH:O	2.52	0.59
1:J:292:GLY:HA2	1:J:294:GLU:HG2	1.84	0.59
1:G:224:ASP:O	1:G:242:PHE:HD1	1.85	0.59
1:G:319:ASP:HB2	1:G:385:PHE:CZ	2.37	0.59
1:J:294:GLU:HG3	1:J:398:LEU:CD2	2.33	0.59
1:D:413:ASP:OD1	1:D:415:THR:HG23	2.02	0.59
1:J:255:TRP:O	1:J:376:VAL:HG23	2.03	0.59
1:A:220:ASP:O	1:A:224:ASP:HA	2.02	0.59
1:D:529:ASP:O	1:D:530:ASN:HB3	2.02	0.59
1:G:251:LEU:HD21	1:G:307:PRO:HB2	1.84	0.59
1:J:352:PRO:O	1:J:355:THR:HG23	2.01	0.58
1:J:251:LEU:O	1:J:298:GLU:HA	2.04	0.58
1:G:433:PRO:HD3	1:G:453:TRP:CZ2	2.39	0.58
1:J:443:ASP:OD1	1:J:445:LYS:HB2	2.04	0.57
1:J:205:VAL:HG23	1:J:220:ASP:HA	1.85	0.57
1:D:465:ASP:OD1	1:D:465:ASP:C	2.42	0.57
1:A:206:HIS:CD2	1:A:315:ALA:HB2	2.39	0.57
1:A:95:LYS:HE2	1:A:114:SER:CB	2.35	0.57
1:A:211:PRO:HD2	1:A:212:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:CYS:SG	1:D:133:ILE:HD12	2.45	0.57
1:G:450:THR:HG21	1:G:482:HIS:O	2.04	0.57
1:J:131:CYS:SG	1:J:157:GLY:HA2	2.45	0.57
1:J:179:ILE:HD12	1:J:196:ALA:HB2	1.88	0.56
1:J:197:GLU:HG2	1:J:278:GLN:OE1	2.05	0.56
1:J:438:MET:SD	1:J:447[A]:ILE:HD11	2.45	0.56
1:D:122:LEU:C	1:D:122:LEU:HD23	2.25	0.56
1:D:380:GLY:HA3	1:D:394:PHE:CZ	2.41	0.56
1:G:205:VAL:HG12	1:G:206:HIS:N	2.14	0.56
1:G:432:TYR:HB3	1:G:433:PRO:HA	1.87	0.56
1:G:103:LYS:HG3	1:G:133:ILE:HG23	1.87	0.55
1:G:453:TRP:CD2	1:G:457:THR:HG21	2.41	0.55
1:G:498:SER:HB3	1:G:526:GLY:HA2	1.87	0.55
1:J:532:ILE:O	1:J:534:PRO:HD3	2.05	0.55
1:A:103:LYS:HB3	1:A:501:GLN:OE1	2.07	0.55
1:A:112:ASP:OD2	1:A:115:THR:HG23	2.06	0.55
1:A:371:VAL:HG22	1:A:373:ILE:HD11	1.88	0.55
1:G:148:GLU:OE2	1:G:183:LYS:CE	2.53	0.55
1:G:160:ASN:O	1:G:163:ILE:HG12	2.07	0.55
1:G:538:GLU:HB3	1:G:541:ARG:NH1	2.21	0.55
1:D:332:PRO:HA	1:D:376:VAL:HG21	1.87	0.55
1:A:443:ASP:O	1:A:444:ALA:HB3	2.07	0.55
1:A:480:ASP:HB2	1:A:500:TYR:CE1	2.42	0.55
1:D:326:VAL:CG1	1:D:335:CYS:HB3	2.36	0.55
1:A:486:ILE:CG2	1:A:542:ILE:HD12	2.37	0.55
1:D:383:ALA:HA	1:D:393:LEU:O	2.07	0.55
1:G:359:PHE:CE2	1:G:373:ILE:HG23	2.42	0.55
1:D:101:PRO:HG3	1:D:135:HIS:O	2.07	0.55
1:J:398:LEU:HD12	1:J:431:ALA:HB1	1.89	0.55
1:D:357:SER:HA	1:D:419:LYS:HD2	1.89	0.54
1:G:153:VAL:HG13	1:G:153:VAL:O	2.07	0.54
1:D:137:MET:HA	1:D:152:VAL:O	2.07	0.54
1:J:99:VAL:HG12	1:J:137:MET:SD	2.47	0.54
1:J:230:ASP:OD1	1:J:237:ARG:NH2	2.40	0.54
1:A:285:ILE:HA	1:A:304:GLY:HA3	1.88	0.54
1:G:228:GLU:HB2	1:G:238:TYR:CZ	2.43	0.54
1:D:401:ASN:ND2	4:D:717:HOH:O	2.40	0.54
1:J:292:GLY:C	1:J:294:GLU:H	2.11	0.54
1:J:433:PRO:HD3	1:J:453:TRP:CZ2	2.43	0.54
1:A:144:ASP:OD2	1:A:147:LYS:HE2	2.08	0.54
1:A:323:LYS:HD3	1:A:324:TRP:CZ2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:331:LEU:O	1:J:376:VAL:HG11	2.08	0.54
1:G:535:ARG:N	1:G:539:ASP:OD2	2.24	0.54
1:A:244:TRP:HA	1:A:244:TRP:HE3	1.71	0.54
1:A:537:LEU:CD1	4:A:867:HOH:O	2.48	0.54
1:D:291:PRO:HB3	1:D:436:PHE:CZ	2.43	0.54
1:G:83:TYR:CD2	1:J:511:GLU:HG2	2.43	0.54
1:A:523:SER:O	1:A:525:MET:N	2.39	0.53
1:D:381:HIS:HB3	4:D:718:HOH:O	2.07	0.53
1:J:456:PRO:O	1:J:457:THR:C	2.42	0.53
1:A:433:PRO:O	1:A:433:PRO:HG2	2.08	0.53
1:A:511:GLU:OE1	1:A:513:GLU:HB3	2.08	0.53
1:G:311:VAL:CG2	1:G:329:MET:CE	2.87	0.53
1:A:511:GLU:HG3	1:A:516:GLU:O	2.09	0.53
1:D:443:ASP:OD2	1:D:445:LYS:CE	2.55	0.53
1:A:433:PRO:HB3	1:A:453:TRP:CE2	2.44	0.53
1:G:417:TRP:CD1	1:G:417:TRP:N	2.73	0.53
1:G:150:GLU:HG2	1:G:183:LYS:HB2	1.91	0.53
1:A:101:PRO:HG3	1:A:137:MET:HG2	1.91	0.53
1:G:311:VAL:HG21	1:G:329:MET:HE1	1.90	0.53
1:J:254:ALA:HB3	1:J:255:TRP:CZ3	2.44	0.53
1:G:122:LEU:HD11	1:G:127:TYR:CE2	2.44	0.53
1:G:159:LYS:HD2	1:G:286:ASP:CB	2.37	0.53
1:G:403:ILE:HD12	1:G:423:VAL:CG2	2.39	0.53
1:J:256:LEU:HD21	1:J:399:ARG:CZ	2.39	0.53
1:G:163:ILE:HG21	1:G:290:VAL:CG1	2.40	0.52
1:D:348:VAL:HG11	1:D:371:VAL:HG21	1.92	0.52
1:G:176:GLY:O	1:G:177:MET:HB2	2.09	0.52
1:D:86:VAL:HG22	1:D:90:TYR:CE2	2.44	0.52
1:A:452:TRP:CZ3	1:A:454:PRO:HD3	2.44	0.52
1:D:163:ILE:HD11	1:D:287:TRP:CE2	2.45	0.52
1:G:109:ALA:HB2	1:G:121:TRP:HB3	1.92	0.52
1:G:407:ASP:N	1:G:420:LYS:HG2	2.24	0.52
1:J:357:SER:OG	1:J:418:GLU:HA	2.10	0.52
1:D:159:LYS:HA	1:D:162:PHE:HD2	1.74	0.52
1:D:203:LEU:HD22	1:D:220:ASP:HB3	1.92	0.52
1:G:377:ILE:H	1:G:377:ILE:CD1	2.21	0.52
1:A:205:VAL:HG12	1:A:314:ASP:O	2.10	0.52
1:D:153:VAL:O	1:D:153:VAL:CG1	2.55	0.52
1:D:172:ASP:HB2	1:J:267:LYS:HB2	1.92	0.52
1:D:265:ARG:NE	1:D:367:ASP:OD1	2.42	0.52
1:G:223:LYS:NZ	1:G:277:LEU:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:445:LYS:O	1:J:466:ALA:HB3	2.10	0.52
1:D:338:PHE:CE1	1:D:345:PRO:HB3	2.45	0.51
1:D:437:HIS:NE2	3:D:604:SO4:O2	2.38	0.51
1:G:101:PRO:HA	1:G:108:VAL:HG23	1.92	0.51
1:G:480:ASP:HB3	1:G:499:GLY:H	1.75	0.51
1:A:163:ILE:HG22	1:A:164:TYR:CD2	2.45	0.51
1:D:220:ASP:O	1:D:224:ASP:HA	2.10	0.51
1:D:320:PRO:HB3	1:D:541:ARG:HG2	1.91	0.51
1:G:433:PRO:HD3	1:G:453:TRP:CE2	2.45	0.51
1:J:317:VAL:HG23	1:J:326:VAL:HB	1.91	0.51
1:A:101:PRO:HD2	1:A:529:ASP:O	2.10	0.51
1:G:98:LEU:HD11	1:G:530:ASN:HB2	1.92	0.51
1:A:112:ASP:HB2	1:A:119:MET:SD	2.50	0.51
1:A:357:SER:HA	1:A:419:LYS:HG3	1.93	0.51
1:A:488:TYR:CE1	1:A:539:ASP:HB3	2.45	0.51
1:D:465:ASP:CB	1:D:472:LEU:HD12	2.37	0.51
1:D:101:PRO:HD3	1:D:137:MET:HG2	1.92	0.51
1:J:148:GLU:HG3	1:J:149:PHE:N	2.25	0.51
1:A:238:TYR:CD1	1:A:238:TYR:O	2.63	0.51
1:D:102:GLY:HA3	1:D:105:SER:OG	2.10	0.51
1:D:530:ASN:O	1:D:531:VAL:CG1	2.59	0.51
1:G:319:ASP:OD1	1:G:321:ARG:HB2	2.10	0.51
1:J:221:GLY:HA3	4:J:722:HOH:O	2.11	0.51
1:J:397:SER:O	1:J:398:LEU:HB3	2.11	0.51
1:J:525:MET:SD	4:J:742:HOH:O	2.59	0.51
1:D:377:ILE:HD12	1:D:377:ILE:N	2.25	0.51
1:D:383:ALA:HB2	1:D:394:PHE:CD1	2.44	0.51
1:A:306:ARG:N	1:A:307:PRO:CD	2.73	0.50
1:J:106:GLY:HA2	1:J:132:PRO:O	2.11	0.50
1:J:387:PRO:HD3	4:J:719:HOH:O	2.11	0.50
1:D:206:HIS:CD2	1:D:315:ALA:HB2	2.46	0.50
1:G:122:LEU:HD12	4:G:712:HOH:O	2.11	0.50
1:A:352:PRO:HG2	4:A:746:HOH:O	2.12	0.50
1:A:488:TYR:CE2	1:A:534:PRO:HA	2.46	0.50
1:D:136:HIS:O	1:D:153:VAL:HA	2.12	0.50
1:G:161:LEU:HD23	1:G:173:PRO:CG	2.42	0.50
1:G:397:SER:O	1:G:398:LEU:HB3	2.12	0.50
1:D:104:PHE:HD2	1:D:166:VAL:HG21	1.77	0.50
1:D:206:HIS:O	1:D:218:VAL:HA	2.11	0.50
1:D:307:PRO:C	1:D:309:HIS:H	2.15	0.50
1:D:481:MET:HG3	1:D:482:HIS:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:O	1:A:153:VAL:CG1	2.59	0.50
1:A:196:ALA:O	1:A:200:GLY:HA2	2.12	0.50
1:D:382:GLN:HG2	1:D:436:PHE:O	2.12	0.50
1:D:488:TYR:CE2	1:D:532:ILE:HG22	2.47	0.50
1:D:304:GLY:N	4:D:713:HOH:O	2.37	0.50
1:G:352:PRO:HB2	1:G:355:THR:CG2	2.41	0.49
1:J:544:ARG:NH1	1:J:548:THR:HA	2.27	0.49
1:A:352:PRO:HA	1:A:396:ASN:ND2	2.27	0.49
1:D:217:ALA:HB1	1:D:316:LEU:HD23	1.94	0.49
1:G:148:GLU:OE1	1:G:183:LYS:CE	2.60	0.49
1:G:459:ASN:HB2	1:G:478:GLY:O	2.12	0.49
1:G:477:LEU:CD2	1:G:517:VAL:HG21	2.38	0.49
1:D:465:ASP:CB	1:D:472:LEU:CD1	2.73	0.49
1:G:477:LEU:HD21	1:G:517:VAL:CG2	2.39	0.49
1:G:488:TYR:OH	1:G:543:SER:CB	2.54	0.49
1:A:447:ILE:HG13	1:A:464:ILE:HB	1.93	0.49
1:D:316:LEU:HD11	1:D:325:ALA:HB1	1.95	0.49
1:G:157:GLY:N	1:G:176:GLY:HA3	2.28	0.49
1:J:253:ARG:O	1:J:254:ALA:C	2.50	0.49
1:J:404:MET:HG3	1:J:406:TRP:CH2	2.47	0.49
1:G:364:VAL:CG2	1:G:370:THR:HG23	2.43	0.49
1:A:329:MET:O	1:A:332:PRO:HD2	2.13	0.49
1:D:355:THR:HB	1:D:356:PRO:HD2	1.95	0.49
1:D:484:LEU:HD23	1:D:495:GLY:HA3	1.95	0.49
1:G:93:LEU:HA	1:G:492:PHE:CE2	2.47	0.49
1:A:513:GLU:HA	1:A:513:GLU:OE1	2.13	0.49
1:D:265:ARG:HG3	1:D:265:ARG:HH11	1.78	0.49
1:A:223:LYS:HB3	1:A:225:ILE:CD1	2.39	0.48
1:A:459:ASN:HD22	1:A:459:ASN:N	2.10	0.48
1:J:352:PRO:CB	1:J:355:THR:HG23	2.33	0.48
1:A:97:VAL:HG21	1:A:145:PRO:HB2	1.95	0.48
1:A:223:LYS:CB	1:A:225:ILE:HD12	2.40	0.48
1:A:465:ASP:C	1:A:465:ASP:OD1	2.52	0.48
1:D:207:VAL:HA	1:D:217:ALA:O	2.13	0.48
1:D:537:LEU:O	1:D:540:LEU:HB2	2.12	0.48
1:J:150:GLU:CG	1:J:183:LYS:HE2	2.43	0.48
1:J:243:ASP:O	1:J:261:MET:HA	2.13	0.48
1:D:136:HIS:HB3	4:D:702:HOH:O	2.13	0.48
1:G:345:PRO:HB2	1:G:361:LEU:HD21	1.94	0.48
1:A:339:ASP:CG	1:A:342:ASN:HB2	2.32	0.48
1:D:382:GLN:C	1:D:382:GLN:NE2	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:GLY:HA3	1:G:229:PHE:O	2.13	0.48
1:J:242:PHE:N	1:J:242:PHE:CD1	2.82	0.48
1:A:291:PRO:HG2	1:A:452:TRP:CH2	2.49	0.48
1:D:306:ARG:NH2	1:D:309:HIS:CG	2.81	0.48
1:J:447[A]:ILE:HG12	1:J:449:VAL:HG13	1.95	0.48
1:G:148:GLU:CD	1:G:183:LYS:HE2	2.31	0.48
1:D:499:GLY:CA	1:D:504:ALA:O	2.62	0.48
1:G:326:VAL:HG11	1:G:392:PHE:HZ	1.74	0.48
1:G:438:MET:HE3	1:G:547:THR:HB	1.95	0.48
1:A:95:LYS:HE2	1:A:114:SER:HB2	1.96	0.48
1:D:289:LEU:CD1	1:D:331:LEU:HD21	2.44	0.48
1:G:244:TRP:HZ3	1:G:373:ILE:HD12	1.78	0.48
1:G:465:ASP:OD2	1:G:468:ASN:HB2	2.13	0.48
1:J:136:HIS:NE2	4:J:708:HOH:O	2.36	0.48
1:G:124:ALA:HB2	1:G:134:MET:CE	2.44	0.48
1:G:147:LYS:O	1:G:148:GLU:HB2	2.14	0.48
1:J:491:LYS:HB3	1:J:492:PHE:CE1	2.49	0.48
1:A:140:PHE:HD2	1:A:150:GLU:HB3	1.79	0.47
1:A:337:VAL:HG11	1:A:414:PRO:HB3	1.96	0.47
1:A:486:ILE:HG21	1:A:542:ILE:HD12	1.95	0.47
1:G:171:GLU:O	1:G:173:PRO:HD3	2.14	0.47
1:G:459:ASN:N	1:G:459:ASN:ND2	2.62	0.47
1:J:317:VAL:O	1:J:326:VAL:N	2.33	0.47
1:D:179:ILE:HD11	1:D:203:LEU:H	1.80	0.47
1:J:193:ARG:HD2	1:J:234:ASP:OD2	2.14	0.47
1:J:202:GLY:O	1:J:223:LYS:NZ	2.28	0.47
1:J:273:GLY:N	4:J:718:HOH:O	2.47	0.47
1:D:222:GLN:HB3	1:D:285:ILE:O	2.14	0.47
1:G:148:GLU:HA	1:G:184:TYR:O	2.15	0.47
1:A:348:VAL:O	1:A:358:GLN:HB3	2.14	0.47
1:D:86:VAL:HG22	1:D:86:VAL:O	2.15	0.47
1:D:427:ASP:OD2	1:D:471:VAL:HG11	2.14	0.47
1:J:306:ARG:O	1:J:309:HIS:HB2	2.15	0.47
1:J:363:LYS:HA	1:J:369:TRP:CD1	2.49	0.47
1:A:267:LYS:HB2	1:G:172:ASP:HB2	1.97	0.47
1:A:453:TRP:CD2	1:A:457:THR:HG21	2.50	0.47
1:A:544:ARG:HA	1:A:544:ARG:HD3	1.69	0.47
1:D:133:ILE:HG21	1:D:156:GLN:HB2	1.96	0.47
1:A:390:GLN:OE1	1:A:409:SER:HB2	2.15	0.47
1:G:200:GLY:HA3	1:G:275:TYR:O	2.15	0.47
1:G:387:PRO:HG3	1:G:542:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:479:PRO:O	1:J:479:PRO:CG	2.63	0.47
1:G:392:PHE:C	1:G:393:LEU:HD12	2.35	0.47
1:D:279:GLY:C	1:D:281:LYS:H	2.18	0.47
1:D:285:ILE:HA	1:D:304:GLY:HA3	1.97	0.47
1:G:495:GLY:HA2	1:G:530:ASN:HD21	1.80	0.47
1:J:105:SER:OG	1:J:107:THR:OG1	2.30	0.47
1:A:96:TYR:HB3	1:A:532:ILE:HG23	1.96	0.46
1:D:326:VAL:HG22	1:D:337:VAL:HG22	1.97	0.46
1:G:226:CYS:HG	1:G:242:PHE:HZ	1.63	0.46
1:G:311:VAL:CG2	1:G:329:MET:HE3	2.46	0.46
1:J:292:GLY:C	1:J:294:GLU:N	2.67	0.46
1:A:150:GLU:HG2	4:A:710:HOH:O	2.15	0.46
1:G:116:GLY:O	1:J:522:PRO:HD3	2.15	0.46
1:G:321:ARG:HB2	1:G:321:ARG:HE	1.39	0.46
1:D:407:ASP:OD1	1:D:409:SER:CB	2.56	0.46
1:J:173:PRO:C	1:J:174:GLY:O	2.54	0.46
1:D:357:SER:HA	1:D:419:LYS:HD3	1.97	0.46
1:J:101:PRO:O	1:J:527:HIS:HB3	2.15	0.46
1:A:172:ASP:O	1:A:173:PRO:C	2.54	0.46
1:A:238:TYR:C	1:A:238:TYR:HD1	2.16	0.46
1:A:286:ASP:OD2	1:A:303:SER:OG	2.23	0.46
1:G:364:VAL:HG23	1:G:370:THR:HG23	1.97	0.46
1:A:181:ARG:NH2	4:A:720:HOH:O	2.46	0.46
1:A:319:ASP:OD2	1:A:324:TRP:HD1	1.99	0.46
1:D:331:LEU:N	1:D:332:PRO:CD	2.78	0.46
1:J:179:ILE:HG22	1:J:195:ALA:HB3	1.98	0.46
1:D:307:PRO:C	1:D:309:HIS:N	2.69	0.46
1:G:206:HIS:O	1:G:218:VAL:HA	2.16	0.46
1:J:178:LYS:HD2	1:J:180:TYR:OH	2.16	0.46
1:J:401:ASN:OD1	1:J:434:ASN:ND2	2.48	0.46
1:A:203:LEU:HB3	1:A:220:ASP:HB2	1.97	0.46
1:J:173:PRO:O	1:J:174:GLY:C	2.53	0.46
1:D:87:GLN:O	1:D:87:GLN:HG3	2.16	0.46
1:J:306:ARG:NH2	1:J:309:HIS:CE1	2.83	0.46
1:A:339:ASP:OD1	1:A:342:ASN:N	2.47	0.46
1:D:481:MET:HA	1:D:497:LEU:HG	1.97	0.46
1:G:473:LYS:NZ	1:G:515:ASP:O	2.39	0.46
1:G:525:MET:HB2	1:G:527:HIS:NE2	2.31	0.46
1:J:179:ILE:CG2	1:J:195:ALA:HB3	2.46	0.46
1:J:393:LEU:HD12	1:J:393:LEU:N	2.31	0.45
1:A:261:MET:HE1	1:A:329:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ILE:CD1	1:A:289:LEU:HD21	2.46	0.45
1:A:540:LEU:HD22	1:A:545:SER:HB2	1.98	0.45
1:D:233:THR:O	1:D:234:ASP:HB2	2.16	0.45
1:D:320:PRO:HD3	1:D:546:THR:HG22	1.98	0.45
1:A:96:TYR:CE2	1:A:487:THR:HB	2.51	0.45
1:A:414:PRO:HA	1:A:417:TRP:CE2	2.52	0.45
1:J:294:GLU:HG3	1:J:398:LEU:HD23	1.98	0.45
1:A:459:ASN:H	1:A:459:ASN:ND2	2.14	0.45
1:A:521:LEU:HA	1:A:522:PRO:HD3	1.70	0.45
1:G:430:GLY:C	1:G:432:TYR:N	2.69	0.45
1:J:101:PRO:HD2	1:J:529:ASP:O	2.16	0.45
1:J:232:GLU:O	1:J:232:GLU:HG3	2.15	0.45
1:J:312:ALA:O	1:J:313:ASN:C	2.55	0.45
1:D:435:THR:CG2	1:D:449:VAL:HB	2.46	0.45
1:D:496:THR:HB	1:D:527:HIS:ND1	2.32	0.45
1:J:161:LEU:HD23	1:J:162:PHE:CE1	2.51	0.45
1:J:439:VAL:CG2	1:J:486:ILE:HG22	2.47	0.45
1:A:297:ILE:HG23	1:A:298:GLU:N	2.32	0.45
1:A:543:SER:O	1:A:545:SER:N	2.44	0.45
1:A:453:TRP:CE3	1:A:457:THR:HG21	2.52	0.45
1:D:306:ARG:N	1:D:307:PRO:CD	2.80	0.45
1:G:241:ALA:HB2	1:G:266:LEU:HD21	1.99	0.45
1:J:102:GLY:HA2	1:J:525:MET:HB3	1.98	0.45
1:J:197:GLU:O	1:J:274:ARG:NH2	2.29	0.45
1:J:205:VAL:HG12	1:J:206:HIS:N	2.32	0.45
1:J:382:GLN:HE21	1:J:382:GLN:CA	2.12	0.45
1:J:511:GLU:OE1	1:J:514:THR:N	2.48	0.45
1:A:197:GLU:HG2	1:A:278:GLN:HE22	1.82	0.44
1:A:425:SER:HA	1:A:426:PRO:HD3	1.83	0.44
1:A:371:VAL:CG2	1:A:373:ILE:HD11	2.47	0.44
1:D:428:TRP:HD1	1:D:433:PRO:HG2	1.82	0.44
1:D:499:GLY:N	1:D:504:ALA:O	2.50	0.44
1:J:290:VAL:HG13	1:J:291:PRO:O	2.16	0.44
1:J:439:VAL:HG22	1:J:486:ILE:CG2	2.47	0.44
1:J:514:THR:O	1:J:515:ASP:HB2	2.17	0.44
1:D:392:PHE:C	1:D:393:LEU:HD12	2.37	0.44
1:J:447[A]:ILE:HG12	1:J:449:VAL:CG1	2.47	0.44
1:J:482:HIS:CD2	1:J:498:SER:HB2	2.52	0.44
1:A:453:TRP:CD1	1:A:453:TRP:N	2.84	0.44
1:J:97:VAL:CG1	1:J:119:MET:CE	2.96	0.44
1:J:150:GLU:OE2	4:J:703:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:VAL:HA	1:D:508:VAL:O	2.18	0.44
1:G:119:MET:O	1:G:120:ALA:HB2	2.17	0.44
1:G:514:THR:O	1:G:515:ASP:HB2	2.17	0.44
1:J:145:PRO:HA	1:J:148:GLU:O	2.18	0.44
1:A:393:LEU:HD23	1:A:403:ILE:HG21	2.00	0.44
1:G:225:ILE:HG12	1:G:266:LEU:HD21	1.99	0.44
1:G:252:LYS:HB3	1:G:252:LYS:HE3	1.69	0.44
1:G:387:PRO:O	1:G:541:ARG:HD3	2.16	0.44
1:A:187:THR:HG23	4:D:765:HOH:O	2.17	0.44
1:G:464:ILE:HD13	1:G:464:ILE:N	2.33	0.44
1:A:135:HIS:HB3	1:A:136:HIS:H	1.54	0.44
1:A:150:GLU:HG3	1:A:183:LYS:HG3	2.00	0.44
1:A:185:ASP:OD1	1:A:185:ASP:C	2.55	0.44
1:D:503:THR:HG23	1:D:504:ALA:H	1.83	0.44
1:G:320:PRO:C	1:G:322:GLY:N	2.71	0.44
1:J:173:PRO:O	1:J:174:GLY:O	2.36	0.44
1:J:322:GLY:C	1:J:324:TRP:H	2.21	0.44
1:A:203:LEU:CD2	1:A:225:ILE:HB	2.48	0.43
1:A:353:LYS:HB2	1:A:400:GLN:OE1	2.18	0.43
1:G:215:GLY:HA2	1:G:231:ARG:HB2	2.00	0.43
1:J:181:ARG:NH2	4:J:703:HOH:O	2.51	0.43
1:J:457:THR:HG22	1:J:458:PRO:O	2.17	0.43
1:D:530:ASN:C	1:D:531:VAL:CG1	2.85	0.43
1:G:241:ALA:N	1:G:266:LEU:HD11	2.33	0.43
1:J:320:PRO:HD3	1:J:546:THR:HG22	2.01	0.43
1:J:358:GLN:NE2	1:J:414:PRO:O	2.51	0.43
1:J:511:GLU:O	1:J:515:ASP:HA	2.18	0.43
1:A:196:ALA:O	1:A:200:GLY:CA	2.66	0.43
1:A:348:VAL:HG23	1:A:361:LEU:HD13	2.00	0.43
1:J:250:ASP:O	1:J:254:ALA:N	2.49	0.43
1:J:294:GLU:HG3	1:J:398:LEU:HD22	2.01	0.43
1:A:428:TRP:CD1	1:A:428:TRP:N	2.87	0.43
1:D:326:VAL:HG13	1:D:335:CYS:HB3	2.00	0.43
1:G:206:HIS:HB2	1:G:315:ALA:HB2	2.01	0.43
1:G:268:PRO:HD2	4:G:728:HOH:O	2.17	0.43
1:A:226:CYS:HG	1:A:242:PHE:HE2	1.66	0.43
1:A:390:GLN:OE1	1:A:409:SER:CB	2.67	0.43
1:D:205:VAL:HB	1:D:206:HIS:H	1.75	0.43
1:G:327:ALA:O	1:G:335:CYS:HA	2.19	0.43
1:J:345:PRO:HB2	1:J:361:LEU:HD21	2.01	0.43
1:D:133:ILE:O	1:D:133:ILE:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:TRP:CZ2	1:D:414:PRO:HD3	2.54	0.43
1:D:486:ILE:HG23	1:D:542:ILE:HD12	1.99	0.43
1:A:137:MET:O	1:A:544:ARG:HG2	2.18	0.43
1:A:251:LEU:HD23	1:A:308:LEU:HD23	2.00	0.43
1:A:434:ASN:HB2	1:A:436:PHE:CZ	2.54	0.43
1:G:226:CYS:HB2	1:G:316:LEU:HD22	2.01	0.43
1:G:460:GLY:C	1:G:461:ILE:HG13	2.38	0.43
1:J:292:GLY:HA2	1:J:398:LEU:HD22	2.01	0.43
1:J:494:VAL:HA	1:J:508:VAL:O	2.19	0.43
1:J:527:HIS:ND1	1:J:527:HIS:N	2.67	0.43
1:A:480:ASP:HB2	1:A:500:TYR:CD1	2.54	0.43
1:A:480:ASP:OD1	1:A:482:HIS:NE2	2.46	0.43
1:G:438:MET:CB	1:G:449:VAL:HG12	2.49	0.43
1:J:166:VAL:O	1:J:168:VAL:HG13	2.18	0.43
1:J:362:VAL:O	1:J:369:TRP:HA	2.18	0.43
1:A:346:VAL:CG2	1:A:414:PRO:HG2	2.49	0.42
1:G:182:ILE:CG2	1:G:190:ASN:O	2.54	0.42
1:G:331:LEU:HD23	1:G:331:LEU:HA	1.85	0.42
1:J:329:MET:O	1:J:332:PRO:HD2	2.20	0.42
1:J:404:MET:HG3	1:J:406:TRP:CZ3	2.54	0.42
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.79	0.42
1:A:404:MET:CG	1:A:406:TRP:CH2	3.02	0.42
1:D:240:TRP:CZ3	1:D:265:ARG:HB2	2.55	0.42
1:D:271:PRO:O	4:D:701:HOH:O	2.22	0.42
1:G:117:TRP:CZ3	1:J:479:PRO:HD2	2.54	0.42
1:G:129:ASP:C	1:G:129:ASP:OD1	2.57	0.42
1:G:276:ASP:O	1:G:281:LYS:HD3	2.19	0.42
1:J:348:VAL:O	1:J:358:GLN:HB3	2.20	0.42
1:D:473:LYS:HD3	1:D:515:ASP:HB2	2.02	0.42
1:D:496:THR:HB	1:D:527:HIS:CG	2.54	0.42
1:J:99:VAL:HG11	1:J:137:MET:CE	2.34	0.42
1:D:176:GLY:HA2	4:D:758:HOH:O	2.18	0.42
1:D:279:GLY:C	1:D:281:LYS:N	2.73	0.42
1:G:320:PRO:C	1:G:322:GLY:H	2.22	0.42
1:G:436:PHE:C	1:G:437:HIS:CG	2.93	0.42
1:A:274:ARG:HH11	1:A:274:ARG:HD3	1.67	0.42
1:A:449:VAL:HG23	1:A:462:ALA:HB3	2.02	0.42
1:G:98:LEU:HG	1:G:99:VAL:N	2.34	0.42
1:J:453:TRP:HB2	1:J:459:ASN:ND2	2.34	0.42
1:J:465:ASP:HB3	1:J:470:GLU:HG2	2.02	0.42
1:D:202:GLY:O	1:D:203:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ALA:HB1	1:D:392:PHE:HZ	1.85	0.42
1:G:350:ALA:HB3	1:G:356:PRO:O	2.18	0.42
1:A:192:GLN:O	1:A:193:ARG:HB3	2.20	0.42
1:J:252:LYS:O	1:J:256:LEU:HD12	2.19	0.42
1:J:516:GLU:HG3	4:J:822:HOH:O	2.19	0.42
1:A:163:ILE:CG2	1:A:164:TYR:CD2	3.03	0.42
1:A:337:VAL:HB	1:A:347:ALA:HB3	2.02	0.42
1:A:339:ASP:OD1	1:A:342:ASN:CB	2.62	0.42
1:D:225:ILE:HA	1:D:240:TRP:O	2.20	0.42
1:D:387:PRO:HG2	1:D:444:ALA:HB2	2.02	0.42
1:G:211:PRO:HD3	1:G:318:PHE:HB3	2.02	0.42
1:J:330:ARG:HA	1:J:380:GLY:O	2.20	0.42
1:G:243:ASP:OD1	1:G:284:LYS:NZ	2.46	0.41
1:A:106:GLY:HA2	1:A:132:PRO:O	2.20	0.41
1:A:252:LYS:NZ	1:A:299:ASP:OD1	2.49	0.41
1:D:138:ALA:CB	1:D:209:ILE:HG12	2.49	0.41
1:D:232:GLU:H	1:D:232:GLU:HG2	1.41	0.41
1:G:266:LEU:CD1	1:G:266:LEU:H	2.33	0.41
1:G:306:ARG:HG2	1:G:309:HIS:CD2	2.55	0.41
1:G:436:PHE:CD2	3:G:606:SO4:O2	2.73	0.41
1:A:499:GLY:C	1:A:501:GLN:N	2.73	0.41
1:A:523:SER:HB3	1:A:527:HIS:NE2	2.35	0.41
1:D:96:TYR:HB2	1:D:113:LEU:HD12	2.01	0.41
1:G:270:LEU:HD12	1:G:274:ARG:HH12	1.84	0.41
1:G:285:ILE:HA	1:G:304:GLY:HA3	2.00	0.41
1:J:159:LYS:HB2	1:J:286:ASP:O	2.21	0.41
1:J:486:ILE:HD13	1:J:486:ILE:HG21	1.77	0.41
1:A:382:GLN:HB2	1:A:436:PHE:C	2.41	0.41
1:D:387:PRO:O	1:D:541:ARG:HD3	2.20	0.41
1:D:533:VAL:HA	1:D:534:PRO:HD3	1.83	0.41
1:G:118:THR:HB	1:J:505:SER:O	2.21	0.41
1:G:306:ARG:N	1:G:307:PRO:CD	2.83	0.41
1:A:405:VAL:HG12	1:A:420:LYS:HE2	2.03	0.41
1:D:126:ASN:N	1:D:126:ASN:OD1	2.53	0.41
1:G:395:MET:SD	1:G:395:MET:N	2.93	0.41
1:J:224:ASP:HB2	1:J:284:LYS:HE3	2.03	0.41
1:A:242:PHE:HA	1:A:262:THR:O	2.20	0.41
1:A:288:GLU:O	1:A:289:LEU:C	2.59	0.41
1:D:210:THR:HA	1:D:211:PRO:HD3	1.99	0.41
1:G:414:PRO:O	1:G:416:THR:N	2.53	0.41
1:G:505[B]:SER:HG	1:J:121:TRP:HE1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:164:TYR:CD2	1:J:501:GLN:HG2	2.56	0.41
1:D:544:ARG:HD2	1:D:548:THR:HG22	2.01	0.41
1:G:214:ASP:C	1:G:214:ASP:OD1	2.59	0.41
1:G:438:MET:HB3	1:G:449:VAL:HG12	2.02	0.41
1:G:538:GLU:CD	1:G:538:GLU:N	2.70	0.41
1:J:292:GLY:CA	1:J:294:GLU:HG2	2.49	0.41
1:J:307:PRO:C	1:J:309:HIS:H	2.23	0.41
1:J:332:PRO:O	1:J:376:VAL:HG13	2.21	0.41
1:A:201:LEU:HD11	1:A:203:LEU:HD21	2.03	0.41
1:D:241:ALA:HB2	1:D:266:LEU:HD21	2.03	0.41
1:D:543:SER:O	1:D:545:SER:N	2.53	0.41
1:G:126:ASN:N	1:G:126:ASN:ND2	2.69	0.41
1:G:159:LYS:C	1:G:161:LEU:N	2.73	0.41
1:G:175:GLU:HB3	1:G:280:SER:OG	2.20	0.41
1:G:216:TYR:OH	1:G:234:ASP:OD1	2.21	0.41
1:G:381:HIS:CD2	1:G:381:HIS:C	2.94	0.41
1:G:414:PRO:O	1:G:415:THR:C	2.59	0.41
1:J:364:VAL:N	1:J:368:THR:O	2.32	0.41
1:J:378:SER:OG	1:J:399:ARG:HB2	2.21	0.41
1:A:242:PHE:O	1:A:284:LYS:NZ	2.50	0.41
1:A:450:THR:HG21	1:A:482:HIS:O	2.20	0.41
1:D:350:ALA:HB3	1:D:356:PRO:O	2.20	0.41
1:G:242:PHE:CD1	1:G:242:PHE:N	2.89	0.41
1:J:350:ALA:HB3	1:J:356:PRO:O	2.21	0.41
1:A:361:LEU:HD12	1:A:361:LEU:HA	1.83	0.40
1:A:443:ASP:O	1:A:444:ALA:CB	2.67	0.40
1:A:483:THR:O	1:A:484:LEU:HD12	2.20	0.40
1:G:98:LEU:HD12	1:G:531:VAL:O	2.21	0.40
1:G:538:GLU:CB	1:G:541:ARG:NH1	2.85	0.40
1:J:351:GLY:O	1:J:404:MET:HG2	2.21	0.40
1:A:136:HIS:HB3	4:A:733:HOH:O	2.20	0.40
1:D:127:TYR:CD2	1:D:191:LEU:HD22	2.57	0.40
1:D:182:ILE:HD13	1:D:182:ILE:HG21	1.76	0.40
1:J:255:TRP:O	1:J:376:VAL:CG2	2.68	0.40
1:J:437:HIS:ND1	1:J:483:THR:HG22	2.37	0.40
1:D:540:LEU:C	1:D:542:ILE:N	2.71	0.40
1:G:535:ARG:HB2	4:G:721:HOH:O	2.22	0.40
1:J:383:ALA:HB2	1:J:394:PHE:HD1	1.87	0.40
1:A:96:TYR:HB3	1:A:532:ILE:CG2	2.52	0.40
1:A:121:TRP:CD1	1:D:524:PRO:HA	2.56	0.40
1:A:404:MET:HG3	1:A:406:TRP:CZ3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ALA:O	1:D:313:ASN:C	2.60	0.40
1:G:197:GLU:HG2	1:G:278:GLN:HE22	1.85	0.40
1:G:270:LEU:CD2	1:G:276:ASP:HB2	2.44	0.40
1:G:332:PRO:HA	1:G:376:VAL:HG21	2.04	0.40
1:G:498:SER:HB3	1:G:526:GLY:CA	2.51	0.40
1:J:433:PRO:HB3	1:J:453:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	466/494 (94%)	420 (90%)	37 (8%)	9 (2%)	8 1
1	D	467/494 (94%)	405 (87%)	51 (11%)	11 (2%)	6 1
1	G	467/494 (94%)	416 (89%)	40 (9%)	11 (2%)	6 1
1	J	467/494 (94%)	411 (88%)	52 (11%)	4 (1%)	17 6
All	All	1867/1976 (94%)	1652 (88%)	180 (10%)	35 (2%)	8 1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	280	SER
1	D	444	ALA
1	G	398	LEU
1	A	323	LYS
1	A	389	GLY
1	A	527	HIS
1	A	544	ARG
1	D	126	ASN
1	D	205	VAL

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Mol	Chain	Res	Type
1	G	160	ASN
1	G	174	GLY
1	G	415	THR
1	J	91	ASP
1	A	398	LEU
1	A	444	ALA
1	D	176	GLY
1	D	366	ASP
1	D	409	SER
1	G	527	HIS
1	J	205	VAL
1	D	333	GLY
1	G	515	ASP
1	G	545	SER
1	J	306	ARG
1	A	280	SER
1	D	133	ILE
1	G	271	PRO
1	G	323	LYS
1	G	473	LYS
1	J	480	ASP
1	D	343	GLN
1	G	205	VAL
1	A	306	ARG
1	A	356	PRO
1	D	167	PRO

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	392/415 (94%)	359 (92%)	33 (8%)	11 3
1	D	392/415 (94%)	358 (91%)	34 (9%)	10 3
1	G	388/415 (94%)	361 (93%)	27 (7%)	15 5
1	J	389/415 (94%)	354 (91%)	35 (9%)	9 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1561/1660 (94%)	1432 (92%)	129 (8%)	11 3

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	MET
1	A	161	LEU
1	A	171	GLU
1	A	192	GLN
1	A	193	ARG
1	A	212	GLU
1	A	223	LYS
1	A	243	ASP
1	A	244	TRP
1	A	249	LYS
1	A	252	LYS
1	A	265	ARG
1	A	301	LYS
1	A	341	GLU
1	A	343	GLN
1	A	361	LEU
1	A	368	THR
1	A	371	VAL
1	A	374	PRO
1	A	382	GLN
1	A	390	GLN
1	A	395	MET
1	A	425	SER
1	A	427	ASP
1	A	434	ASN
1	A	447	ILE
1	A	459	ASN
1	A	483	THR
1	A	502	ASN
1	A	511	GLU
1	A	523	SER
1	A	527	HIS
1	A	529	ASP
1	D	85	LYS
1	D	92	GLN
1	D	103	LYS
1	D	122	LEU

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Mol	Chain	Res	Type
1	D	137	MET
1	D	163	ILE
1	D	191	LEU
1	D	193	ARG
1	D	205	VAL
1	D	207	VAL
1	D	222	GLN
1	D	232	GLU
1	D	249	LYS
1	D	268	PRO
1	D	294	GLU
1	D	336	VAL
1	D	382	GLN
1	D	395	MET
1	D	406	TRP
1	D	409	SER
1	D	412	ASP
1	D	420	LYS
1	D	424	GLU
1	D	434	ASN
1	D	442	PRO
1	D	447	ILE
1	D	472	LEU
1	D	502	ASN
1	D	514	THR
1	D	516	GLU
1	D	523	SER
1	D	527	HIS
1	D	529	ASP
1	D	530	ASN
1	G	82	LYS
1	G	87	GLN
1	G	92	GLN
1	G	98	LEU
1	G	114[A]	SER
1	G	114[B]	SER
1	G	126	ASN
1	G	163	ILE
1	G	177	MET
1	G	178	LYS
1	G	183	LYS
1	G	249	LYS

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Mol	Chain	Res	Type
1	G	250	ASP
1	G	266	LEU
1	G	311	VAL
1	G	357	SER
1	G	377	ILE
1	G	395	MET
1	G	423	VAL
1	G	447	ILE
1	G	456	PRO
1	G	483	THR
1	G	484	LEU
1	G	524	PRO
1	G	527	HIS
1	G	544	ARG
1	G	545	SER
1	J	85	LYS
1	J	88	ASP
1	J	105	SER
1	J	111	THR
1	J	122	LEU
1	J	137	MET
1	J	142	SER
1	J	143	PRO
1	J	147	LYS
1	J	161	LEU
1	J	163	ILE
1	J	172	ASP
1	J	173	PRO
1	J	188	ARG
1	J	249	LYS
1	J	252	LYS
1	J	264	LYS
1	J	265	ARG
1	J	294	GLU
1	J	305	ASP
1	J	314	ASP
1	J	317	VAL
1	J	357	SER
1	J	360	GLN
1	J	366[A]	ASP
1	J	366[B]	ASP
1	J	375	GLU

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Mol	Chain	Res	Type
1	J	377	ILE
1	J	399	ARG
1	J	411	HIS
1	J	459	ASN
1	J	497	LEU
1	J	521	LEU
1	J	522	PRO
1	J	527	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	434	ASN
1	A	468	ASN
1	D	382	GLN
1	D	401	ASN
1	D	434	ASN
1	G	278	GLN
1	J	342	ASN
1	J	360	GLN
1	J	482	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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	SO4	G	606	-	4,4,4	0.28	0	6,6,6	0.69	0
3	SO4	G	604	-	4,4,4	0.62	0	6,6,6	0.24	0
3	SO4	G	605	-	4,4,4	0.86	0	6,6,6	0.62	0
3	SO4	D	604	-	4,4,4	0.55	0	6,6,6	0.66	0
3	SO4	J	603[A]	-	4,4,4	0.44	0	6,6,6	0.44	0
3	SO4	G	603	-	4,4,4	0.68	0	6,6,6	0.21	0
3	SO4	A	603[A]	-	4,4,4	0.47	0	6,6,6	1.14	0
3	SO4	D	603	-	4,4,4	0.72	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	606	SO4	1	0
3	D	604	SO4	1	0
3	A	603[A]	SO4	1	0

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	467/494 (94%)	-0.62	0 [100] 100	9, 19, 28, 42	3 (0%)
1	D	467/494 (94%)	-0.65	0 [100] 100	8, 17, 26, 37	1 (0%)
1	G	467/494 (94%)	-0.69	0 [100] 100	9, 17, 25, 38	1 (0%)
1	J	467/494 (94%)	-0.62	0 [100] 100	10, 19, 30, 37	2 (0%)
All	All	1868/1976 (94%)	-0.65	0 [100] 100	8, 18, 27, 42	7 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates i

There are no monosaccharides in this entry.

6.4 Ligands i

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

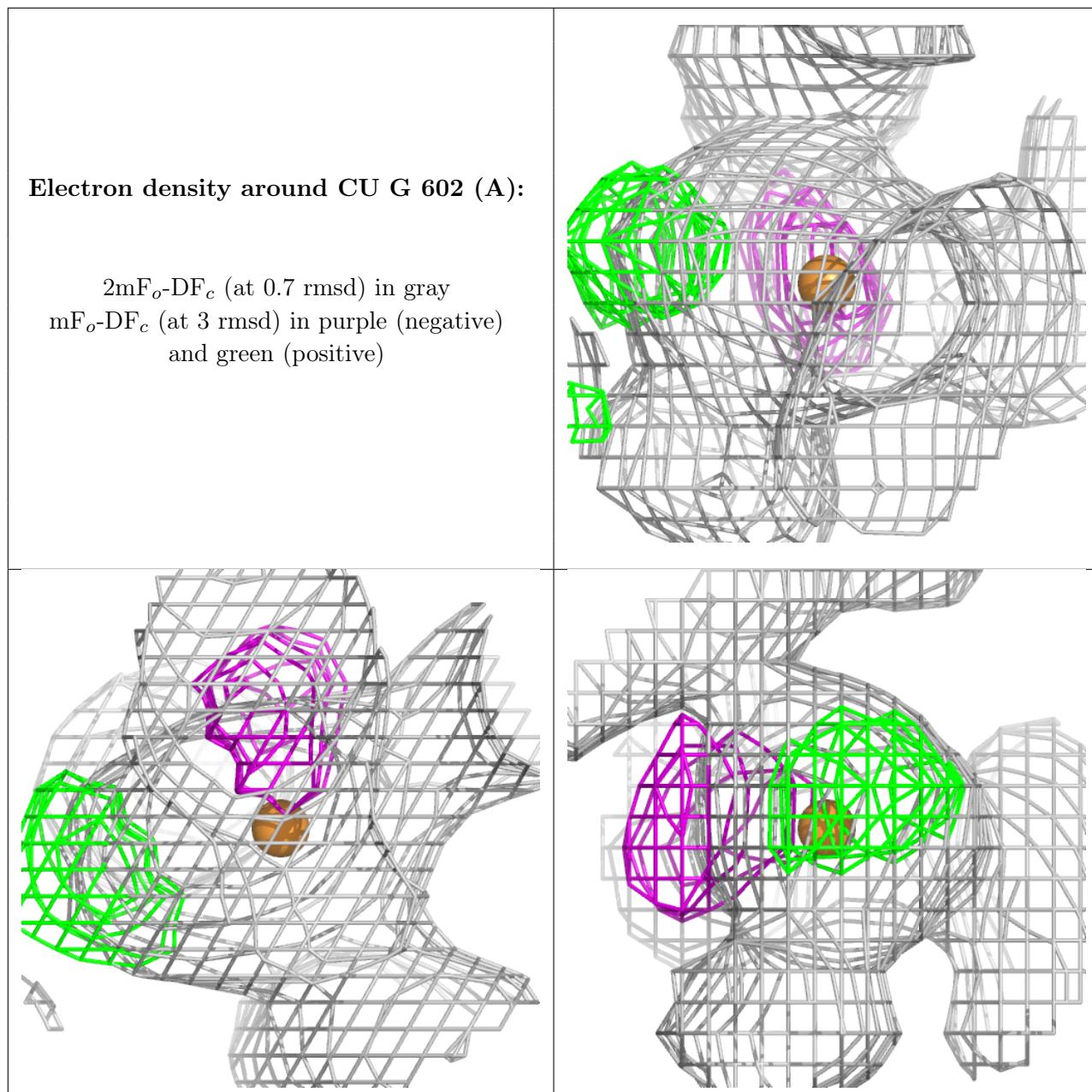
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	G	603	5/5	0.97	0.08	15,19,22,23	0
3	SO4	D	604	5/5	0.98	0.07	9,12,13,14	5
3	SO4	D	603	5/5	0.98	0.09	19,20,24,26	5
3	SO4	G	604	5/5	0.98	0.07	17,17,20,25	5

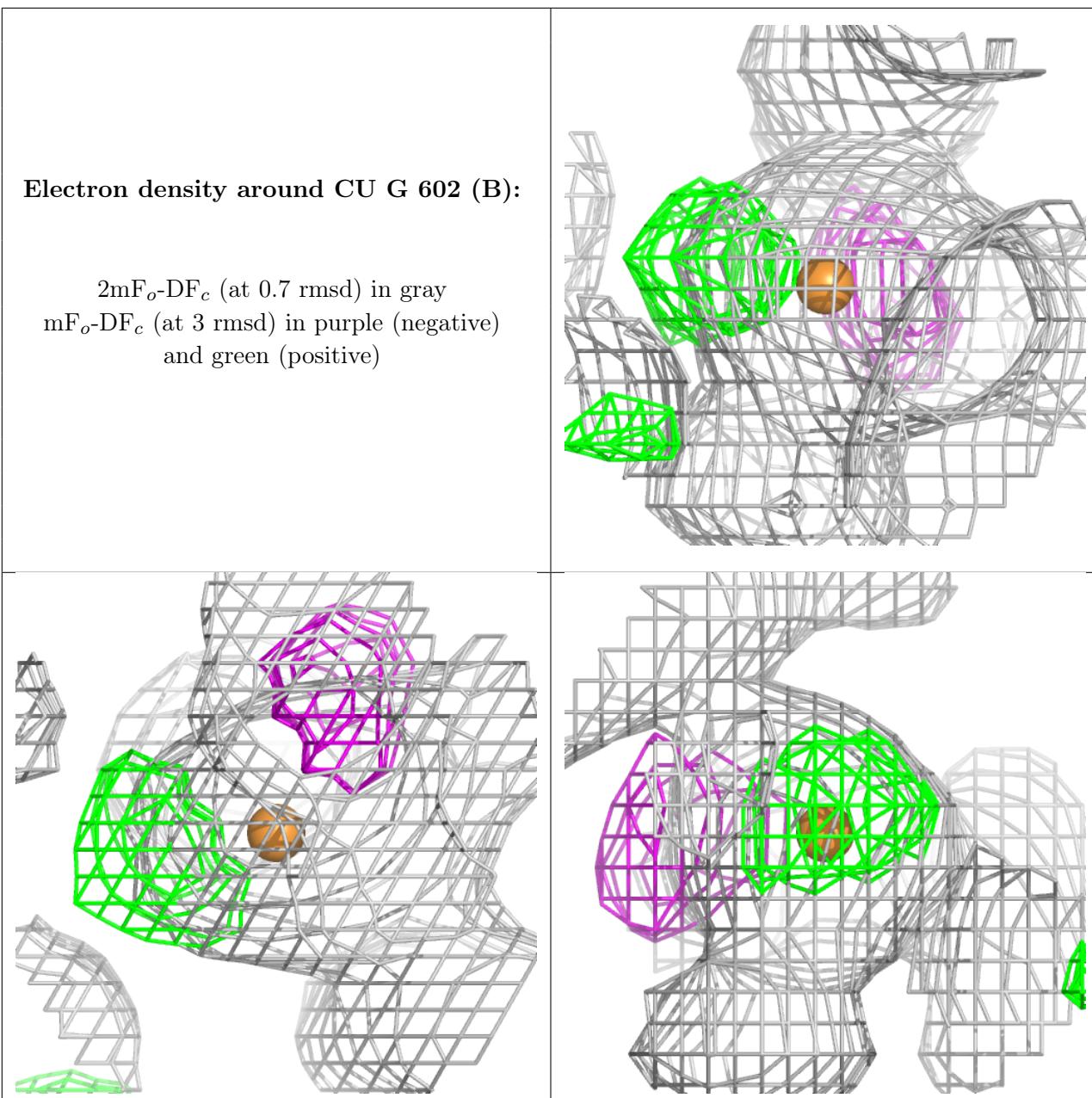
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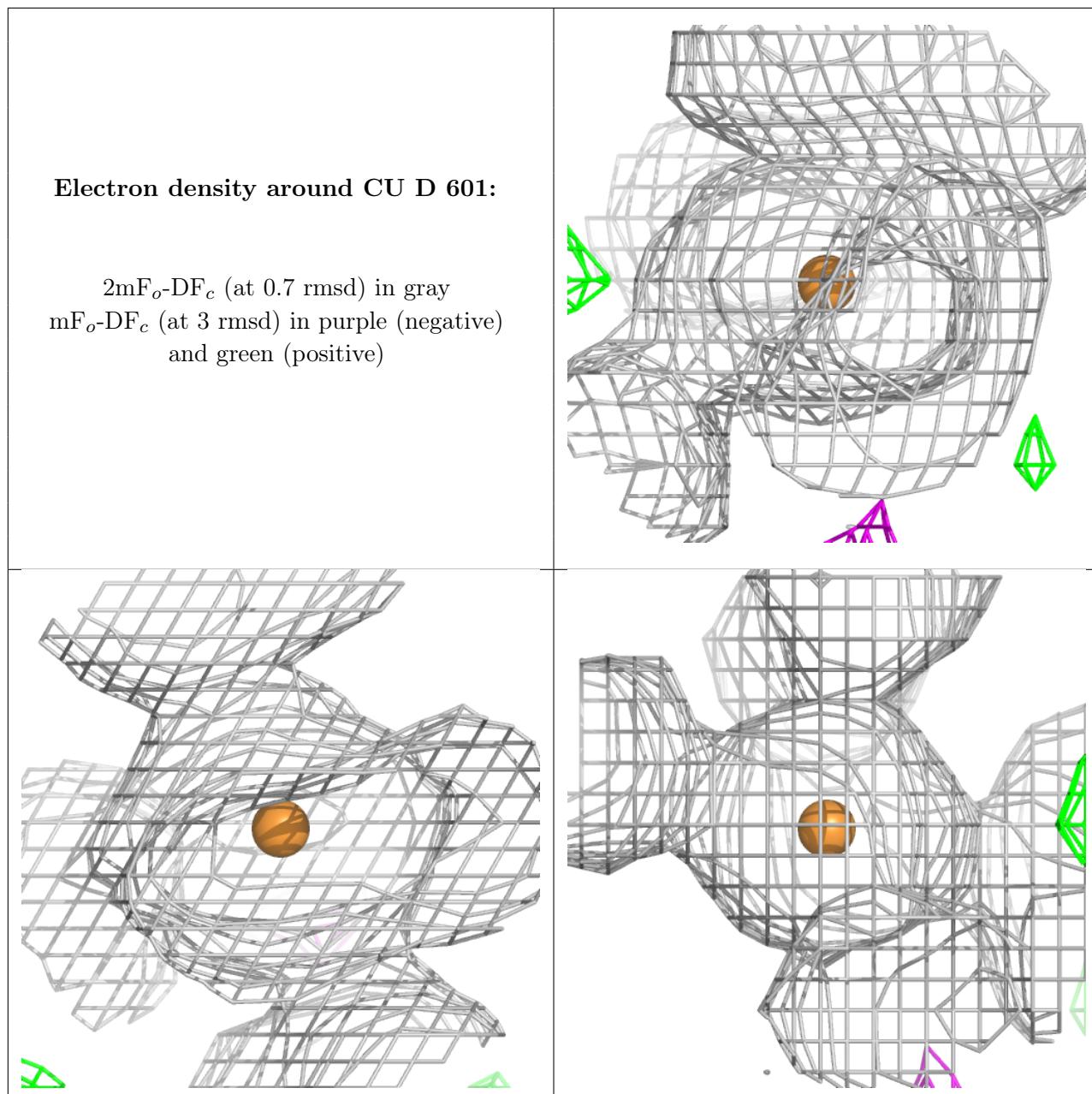
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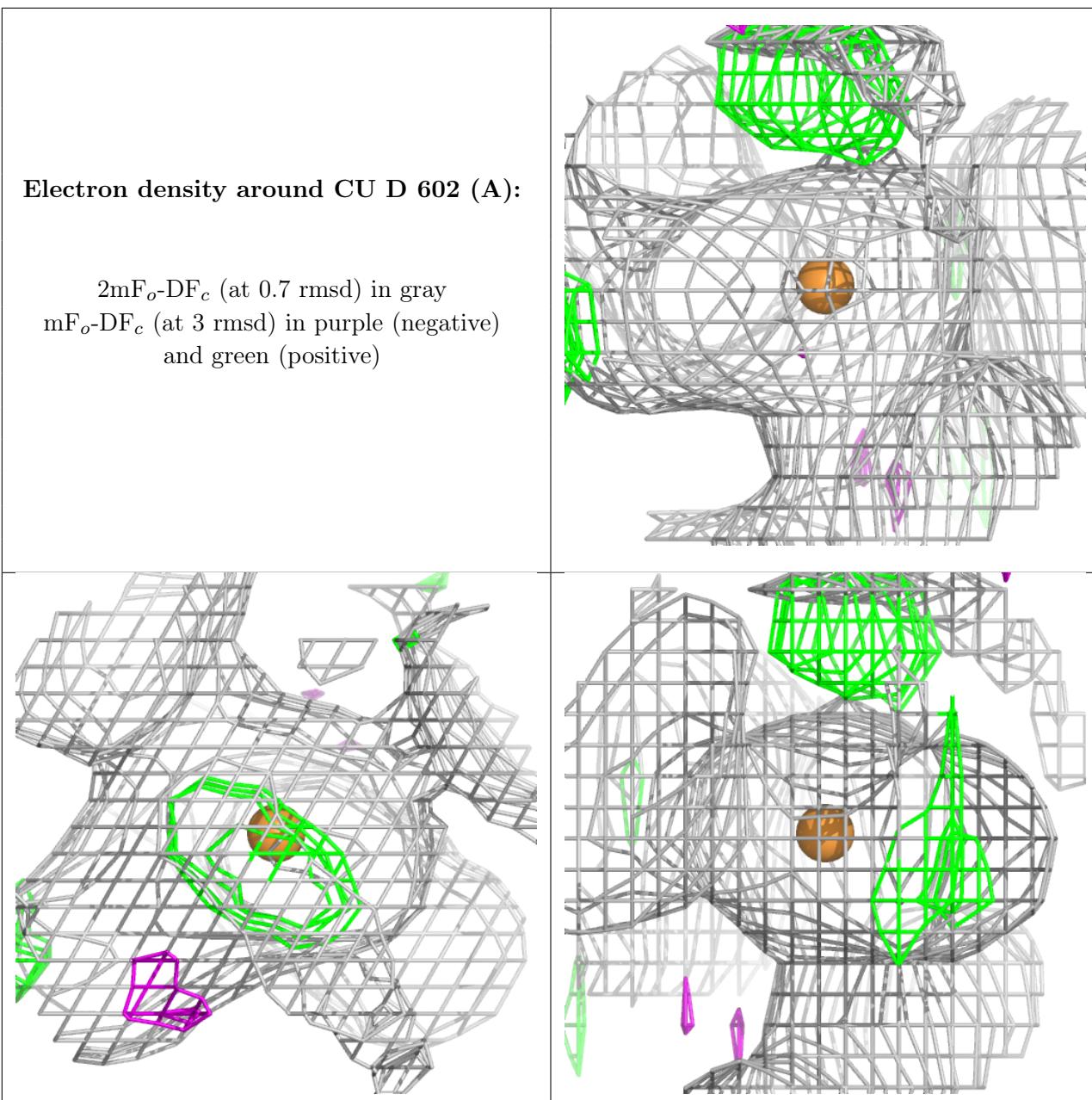
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	G	605	5/5	0.98	0.10	17,18,19,22	5
3	SO4	A	603[A]	5/5	0.99	0.09	8,8,8,11	5
2	CU	G	602[A]	1/1	0.99	0.06	17,17,17,17	1
2	CU	G	602[B]	1/1	0.99	0.06	15,15,15,15	1
3	SO4	G	606	5/5	0.99	0.05	18,19,22,23	0
3	SO4	J	603[A]	5/5	0.99	0.05	18,18,19,23	0
2	CU	D	601	1/1	1.00	0.05	18,18,18,18	0
2	CU	D	602[A]	1/1	1.00	0.05	14,14,14,14	1
2	CU	D	602[B]	1/1	1.00	0.05	6,6,6,6	1
2	CU	G	601	1/1	1.00	0.05	12,12,12,12	0
2	CU	A	601	1/1	1.00	0.05	15,15,15,15	0
2	CU	A	602	1/1	1.00	0.06	22,22,22,22	0
2	CU	J	601	1/1	1.00	0.07	23,23,23,23	0
2	CU	J	602	1/1	1.00	0.04	19,19,19,19	0

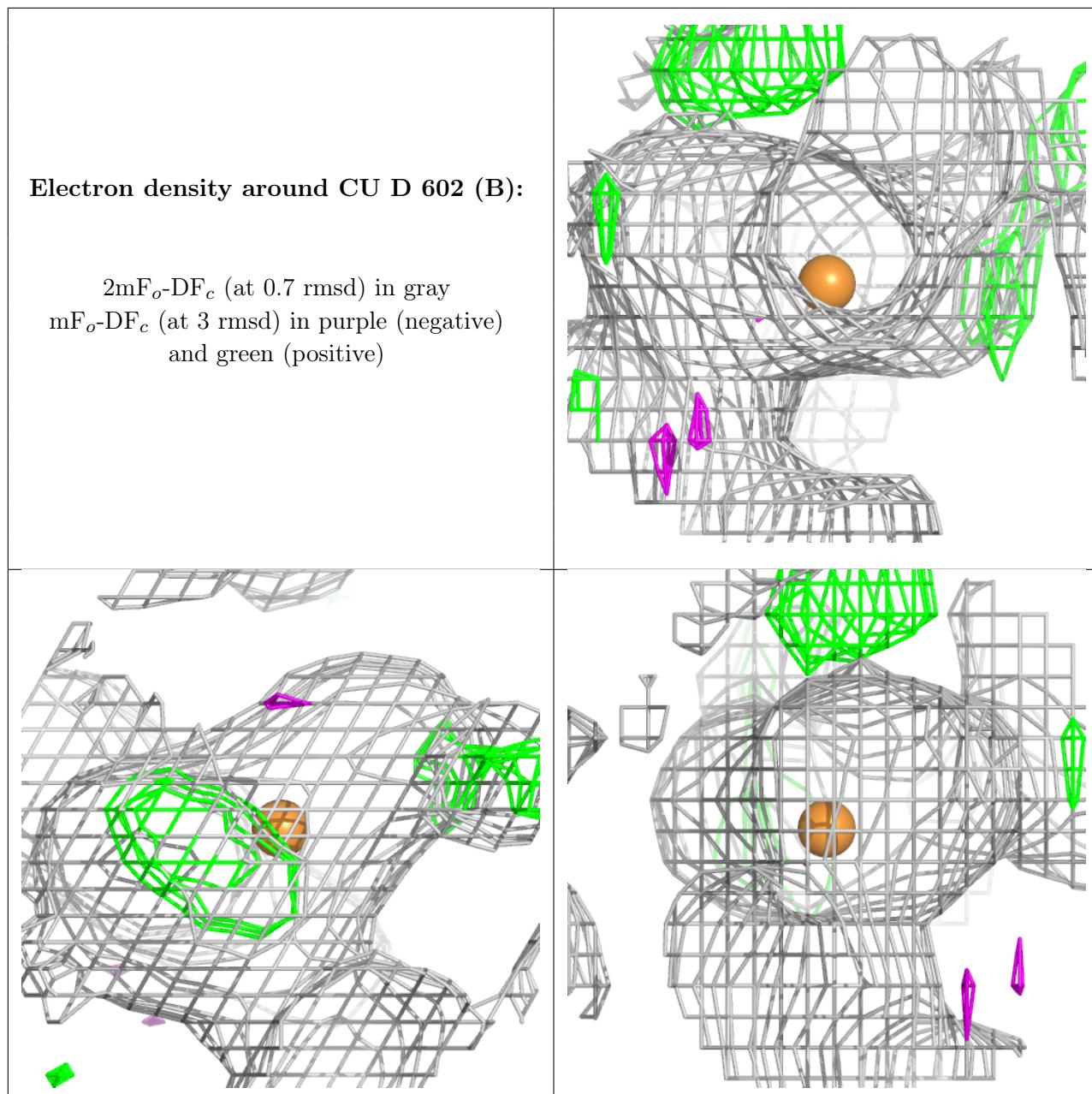
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

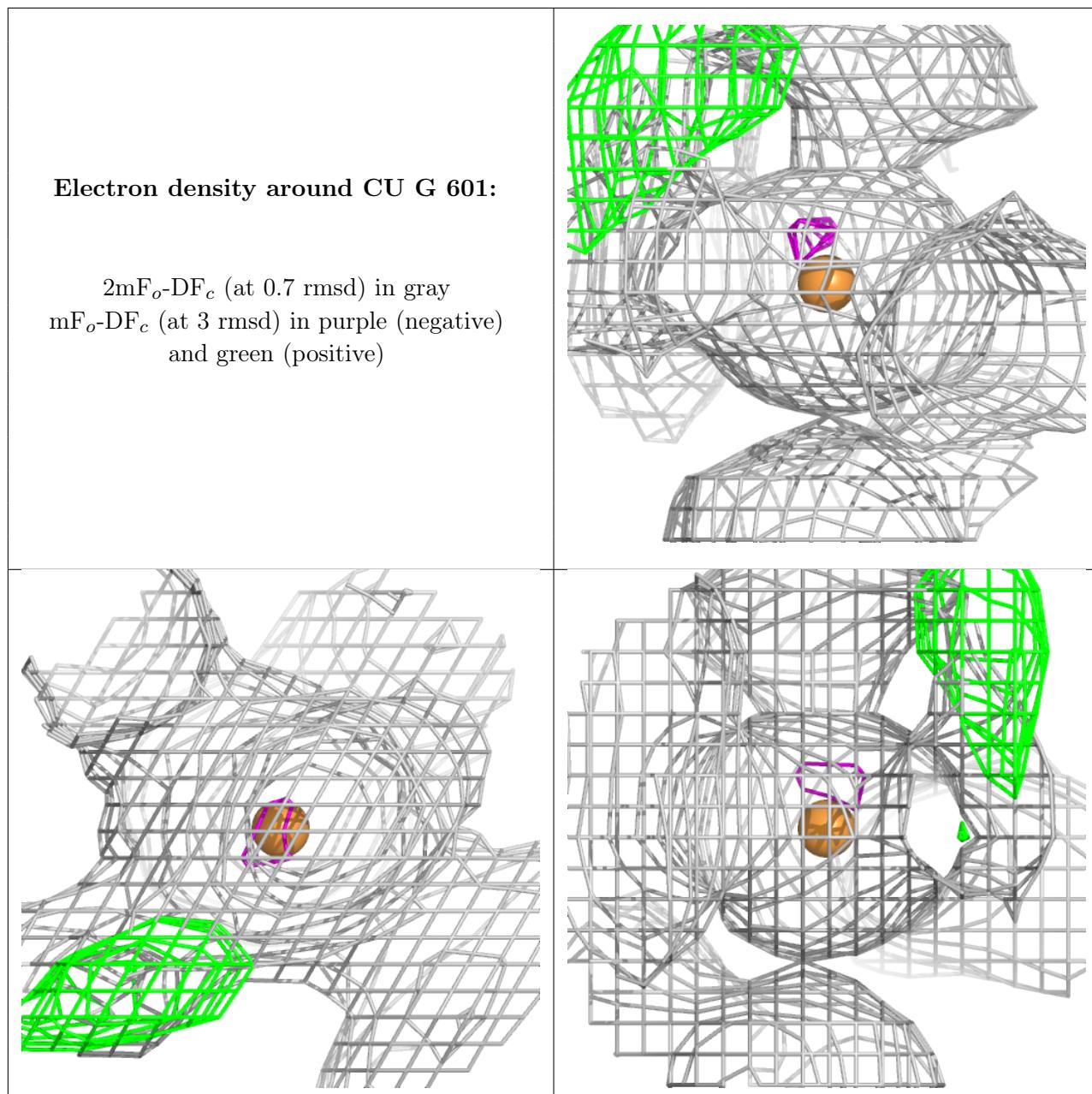


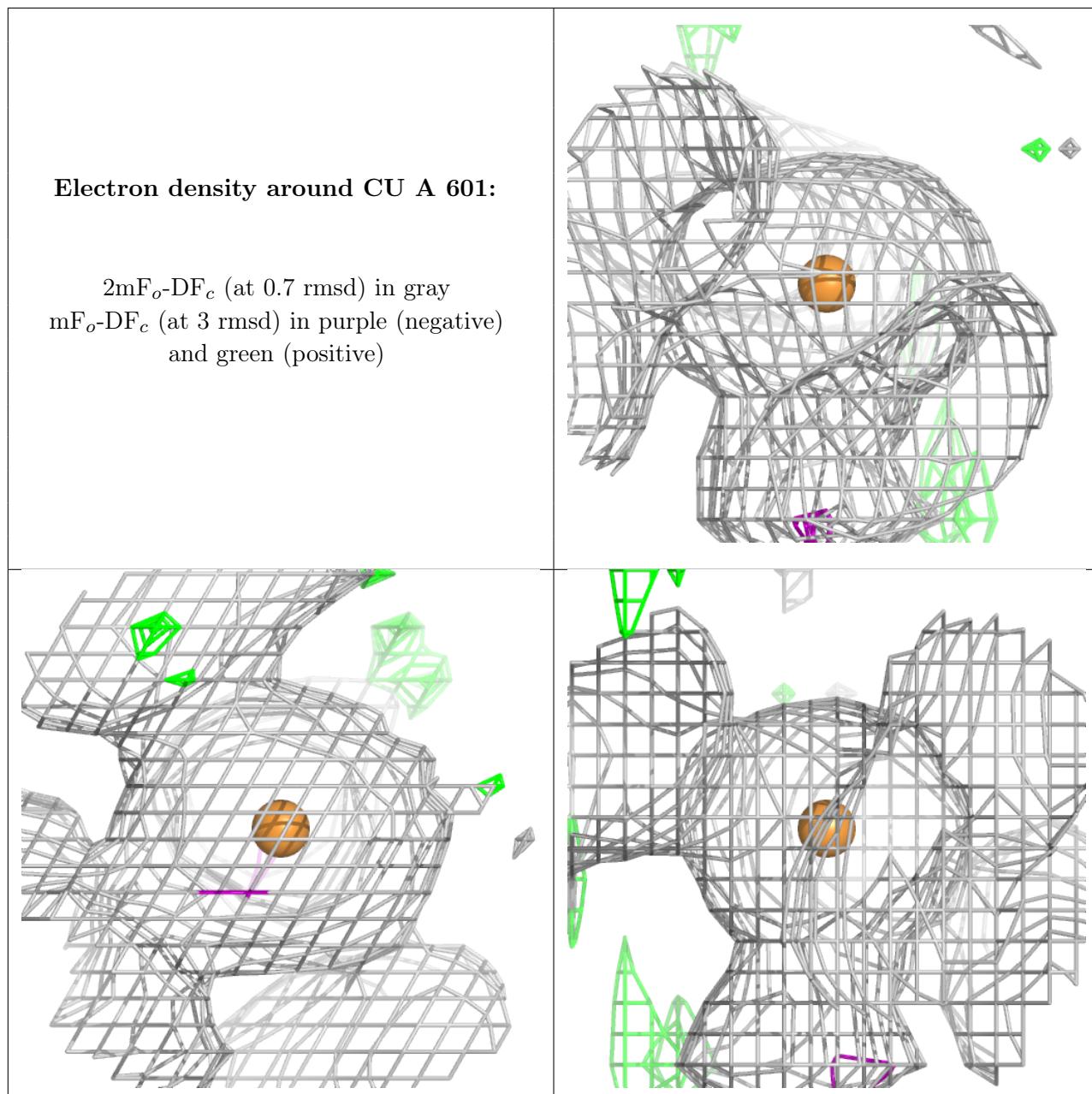


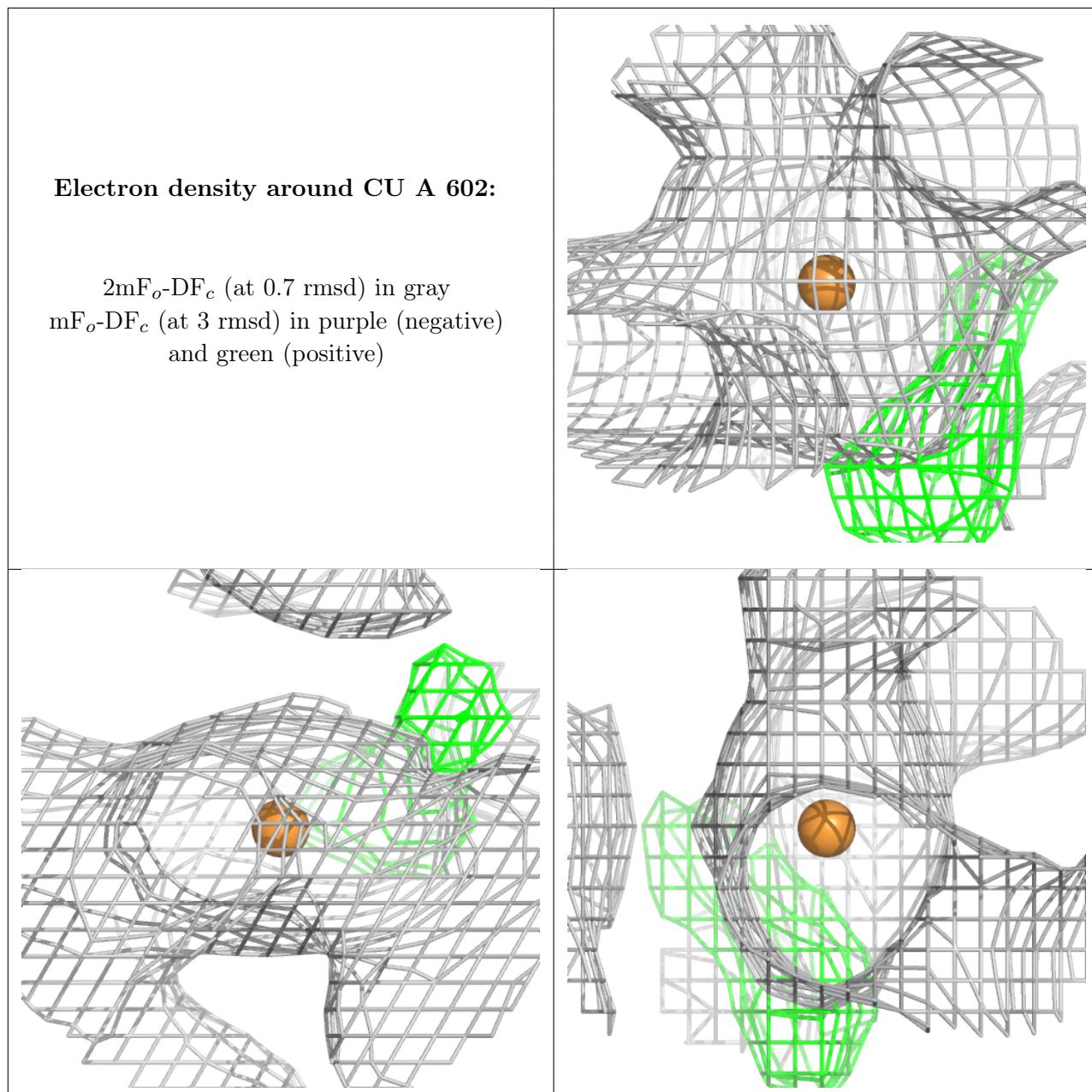


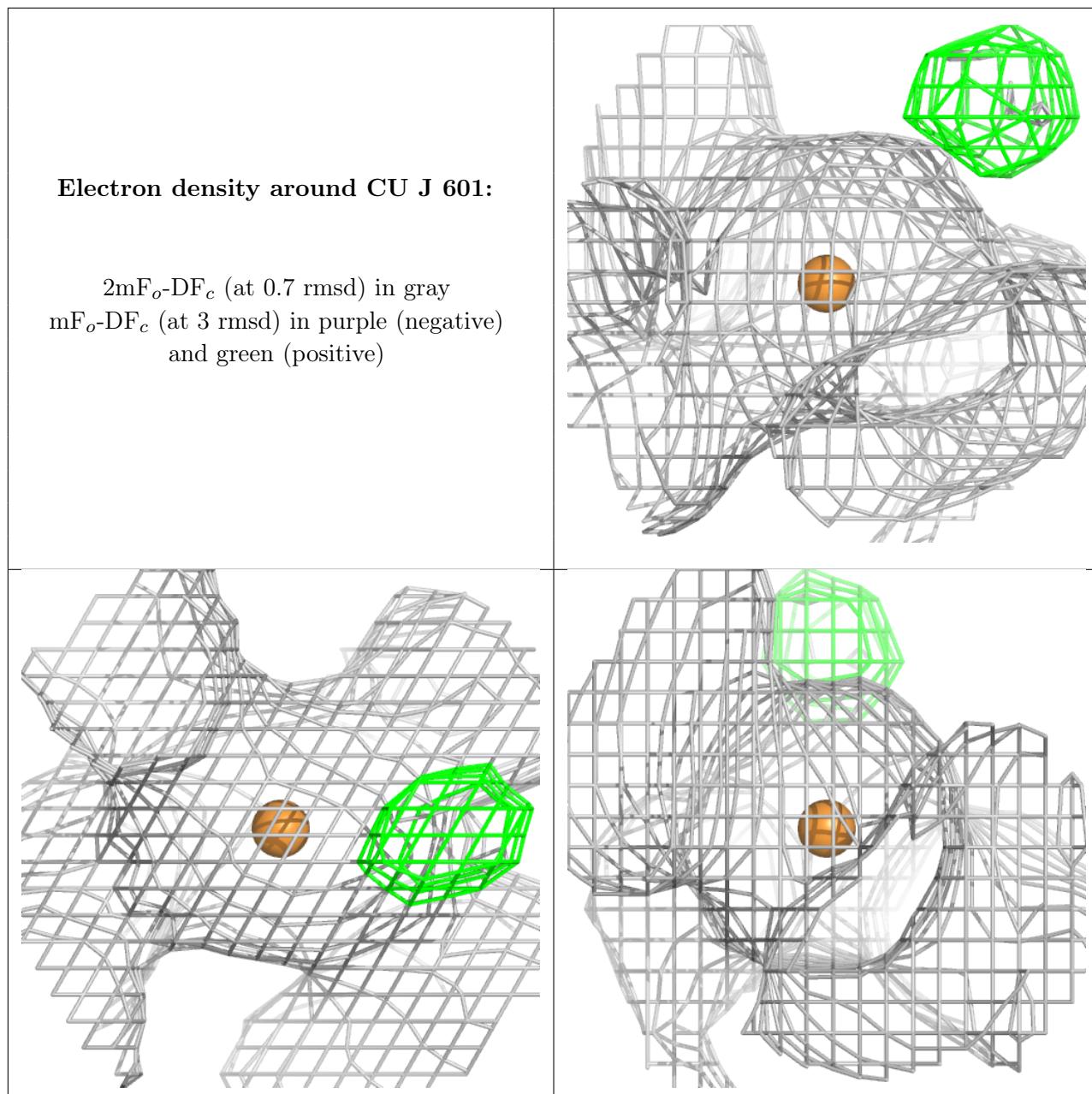


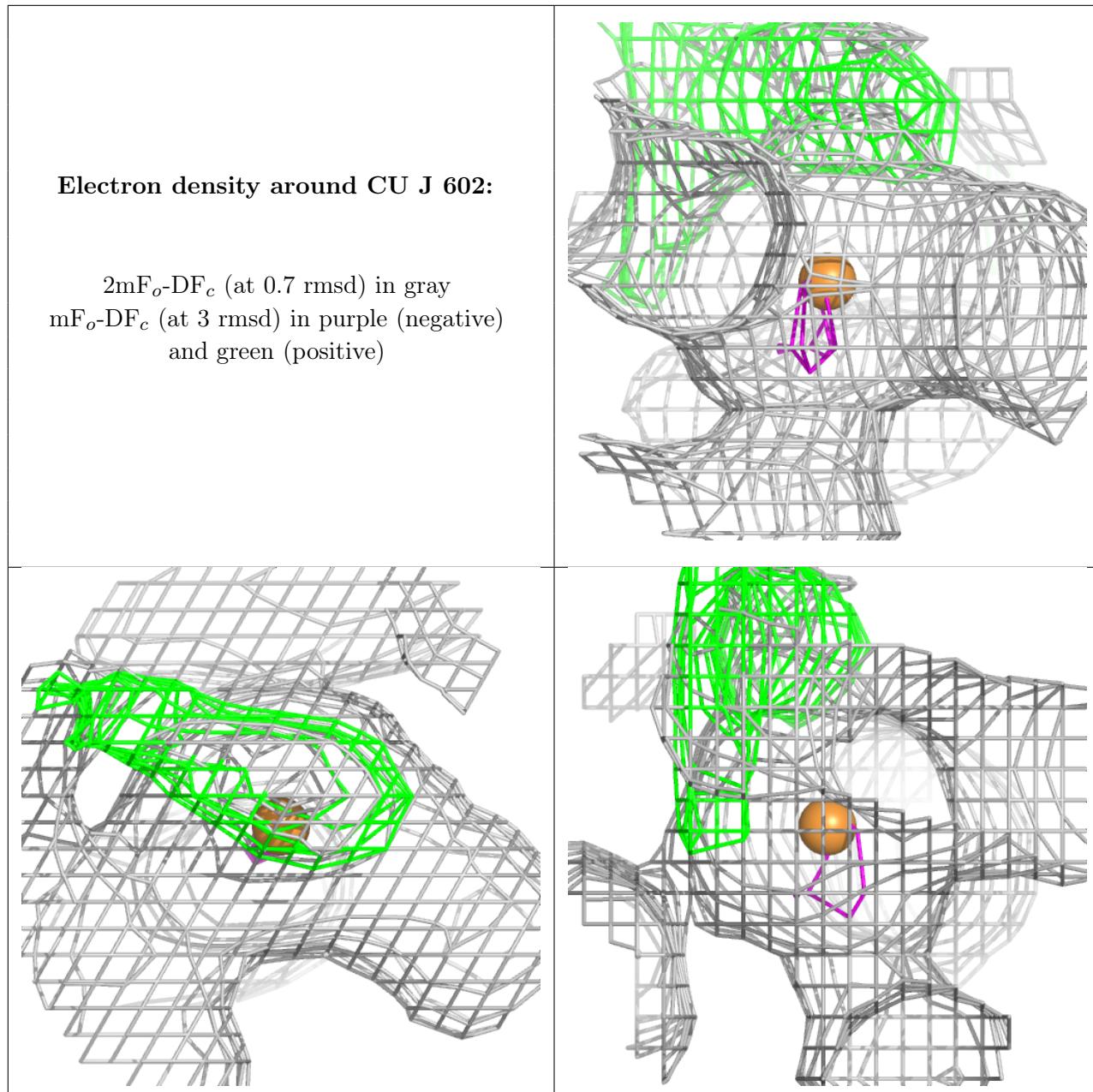












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.