



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:09 PM UTC

PDB ID : 8P3L / pdb_00008p3l
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.; Der-gousova, 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 ⓘ 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

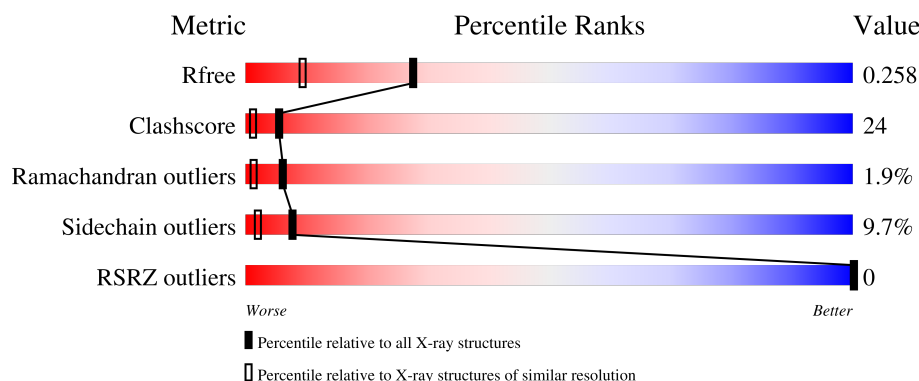
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	494	 44% 36% 13% • 5%
1	D	494	 44% 35% 12% • 5%
1	G	494	 44% 35% 13% • 5%
1	J	494	 45% 35% 13% • 5%

2 Entry composition

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	6	1	0
			3644	2325	608	693	18			
1	D	467	Total	C	N	O	S	4	2	0
			3644	2325	607	694	18			
1	G	467	Total	C	N	O	S	4	2	0
			3628	2320	599	691	18			
1	J	467	Total	C	N	O	S	3	2	0
			3631	2321	601	691	18			

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

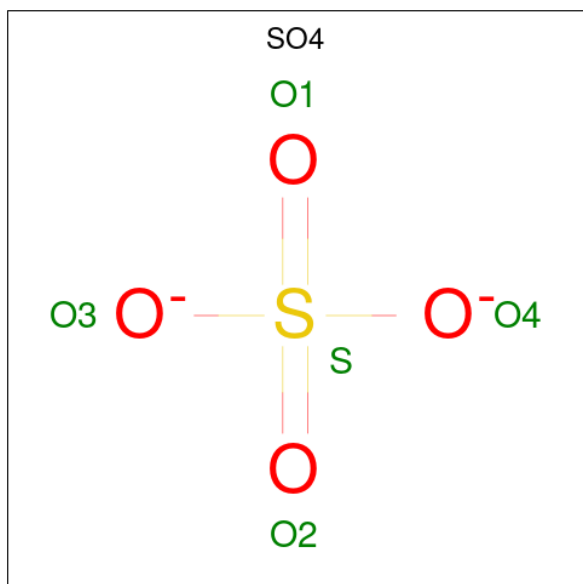
Continued from previous page...

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 (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

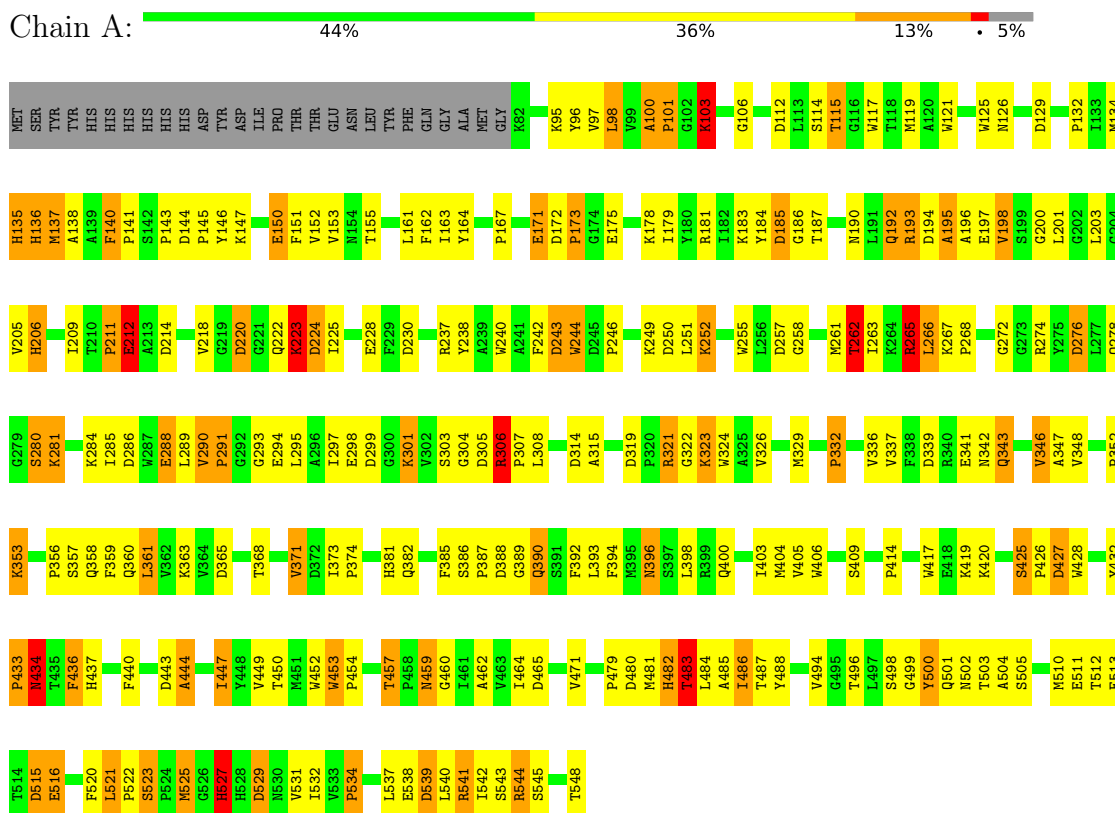
- Molecule 4 is water.

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

3 Residue-property plots

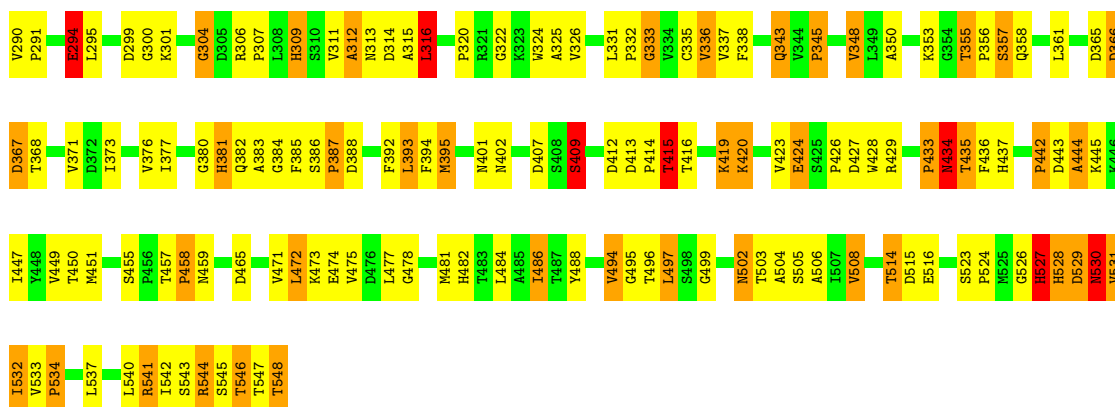
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



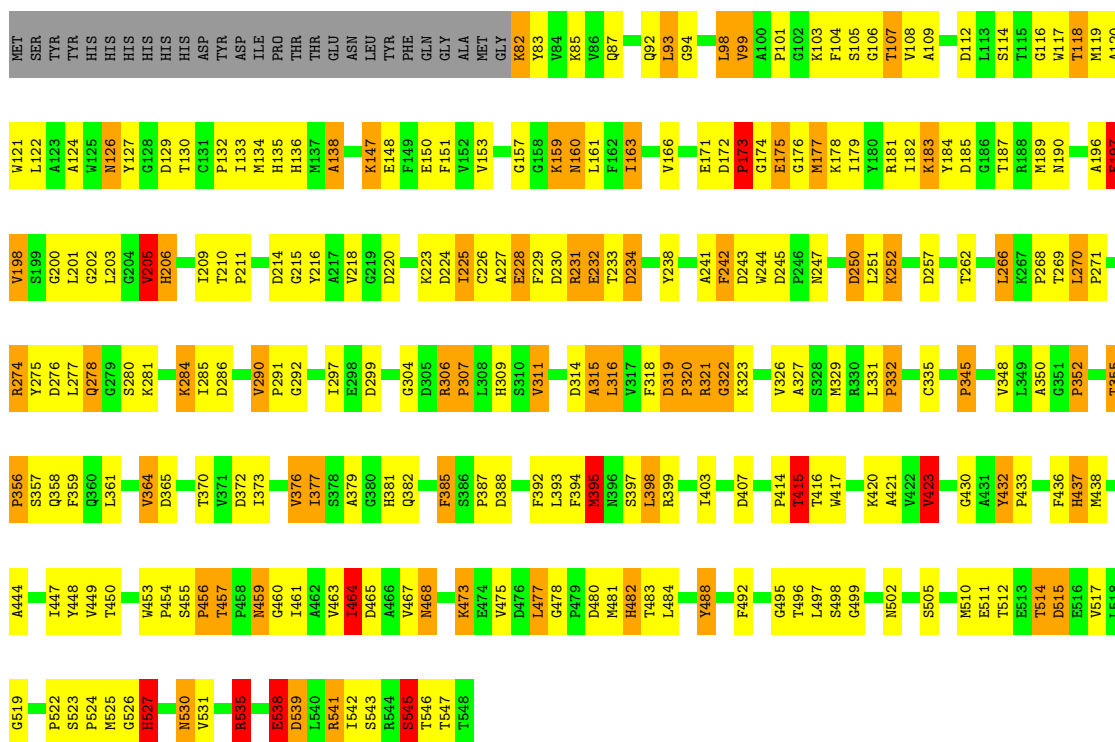
- Molecule 1: Twin-arginine translocation signal domain-containing protein





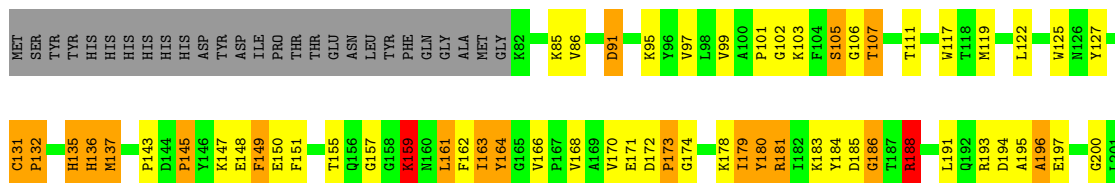
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain G: 44% 35% 13% 5%



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

Chain J: 45% 35% 13% 5%



G202	V290	L361	H437	E511
V206	P291	V362	M438	T512
H206	G292	K363	V439	E513
E212	G293	V364	D443	T514
V218	E294	D365	A444	D515
G219	E298	D366	K445	E516
D220	D299	D367	K446	
G221	D299	T368	I447	L521
G222	V302	W369	Y448	P522
K223	V302	V370	V449	
D224	D306	V371	T450	M525
I225	R306	E376	W453	G526
D230	P307	V376		H527
R231	L308	I377	W453	H528
E232	H309	S378	P456	D529
T233	S310	A379	T457	
D234	V311	G380	P458	I532
M235	A312	H381	K459	V533
V236	N313	Q382	G460	P534
R237	D314	A383	I464	R535
	A315	G384	D465	T536
	L316	F385	A466	L540
	V317	S386	V467	
		P387	M468	R544
V240	P320	Q390	W469	S545
A241	R321	L393	E470	T546
F242	G322	F394	E474	T547
D243	K323	M395		T548
P246	W324	K396		
	A325	S397	L477	
K249	V326	L398	G478	
D250	M329	R399	P479	
L251	R330	Q400	D480	
K252	L331	N401	M481	
R253	P332	W404	H482	
A254	V337	V405	T483	
W255	F338	W406	L484	
L256	D339	D407	A485	
M261	R340		I486	
	E341	H411	T487	
K264			Y488	
L266	P345	P414	K491	
K267	V346	E418	P492	
P268	A347	K419	V493	
T269	V348	V422	V494	
	L349	W426	G495	
G272	A350	P426	T496	
G273	G351		L497	
R274	P352		S498	
	T355	A431	Q501	
Q278	P356	Y432	N502	
N283	S357	P433	T503	
K284	Q358	M434	A504	
I285	F359	T435	S505	
D286	Q360	F436	V508	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.81Å 162.24Å 90.76Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.254 0.190 , 0.258	Depositor DCC
R_{free} test set	10643 reflections (5.06%)	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)	0.38 , 18.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	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	0.95	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	1.05	3/3752 (0.1%)	1.98	134/5119 (2.6%)
1	D	1.19	10/3755 (0.3%)	2.10	142/5124 (2.8%)
1	G	1.24	11/3740 (0.3%)	2.07	134/5104 (2.6%)
1	J	1.06	6/3743 (0.2%)	1.96	131/5110 (2.6%)
All	All	1.14	30/14990 (0.2%)	2.03	541/20457 (2.6%)

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
1	A	0	5
1	D	0	7
1	G	0	9
1	J	0	5
All	All	0	26

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	535	ARG	CD-NE	-13.20	1.27	1.46
1	D	528	HIS	CE1-NE2	10.96	1.43	1.32
1	G	206	HIS	CE1-NE2	10.82	1.43	1.32
1	J	135	HIS	CE1-NE2	9.69	1.42	1.32
1	G	136	HIS	CE1-NE2	9.27	1.41	1.32
1	G	135	HIS	CE1-NE2	8.03	1.40	1.32
1	D	527	HIS	CE1-NE2	7.46	1.40	1.32
1	D	381	HIS	CE1-NE2	-7.08	1.25	1.32
1	D	288	GLU	CD-OE1	6.72	1.38	1.25
1	D	486	ILE	C-O	6.67	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	309	HIS	CE1-NE2	6.65	1.39	1.32
1	J	381	HIS	CE1-NE2	-6.59	1.25	1.32
1	G	206	HIS	CG-ND1	6.58	1.45	1.38
1	A	498	SER	CA-CB	-6.46	1.39	1.53
1	D	135	HIS	CE1-NE2	6.45	1.39	1.32
1	G	437	HIS	CE1-NE2	6.18	1.38	1.32
1	G	395	MET	CG-SD	6.11	1.96	1.80
1	G	455	SER	CA-CB	-5.82	1.44	1.53
1	D	395	MET	CG-SD	-5.79	1.66	1.80
1	J	494	VAL	C-O	5.68	1.30	1.24
1	G	228	GLU	CD-OE1	-5.67	1.14	1.25
1	A	527	HIS	ND1-CE1	5.45	1.38	1.32
1	J	206	HIS	CD2-NE2	5.29	1.43	1.37
1	G	181	ARG	NE-CZ	5.26	1.38	1.33
1	A	140	PHE	C-N	5.23	1.40	1.33
1	D	527	HIS	CG-ND1	5.23	1.44	1.38
1	J	236	VAL	C-O	-5.21	1.18	1.24
1	J	155	THR	C-O	5.16	1.30	1.23
1	D	286	ASP	CG-OD2	-5.14	1.15	1.25
1	G	395	MET	C-O	-5.05	1.18	1.24

All (541) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	VAL	N-CA-C	-12.59	101.75	113.71
1	D	141	PRO	CB-CA-C	-12.36	95.95	111.64
1	G	233	THR	CA-CB-OG1	-12.27	91.20	109.60
1	A	262	THR	CA-CB-OG1	-12.21	91.28	109.60
1	D	435	THR	CA-CB-OG1	-11.63	92.16	109.60
1	G	345	PRO	CB-CA-C	-11.39	96.05	110.98
1	D	262	THR	CA-C-N	11.08	137.35	123.17
1	D	262	THR	C-N-CA	11.08	137.35	123.17
1	J	457	THR	CA-CB-OG1	-10.98	93.13	109.60
1	D	249	LYS	CB-CA-C	-10.64	89.25	110.42
1	J	459	ASN	CA-CB-CG	10.45	123.05	112.60
1	D	171	GLU	CB-CG-CD	10.44	130.35	112.60
1	G	284	LYS	CA-C-N	10.30	137.54	122.71
1	G	284	LYS	C-N-CA	10.30	137.54	122.71
1	G	546	THR	CA-CB-OG1	-10.16	94.35	109.60
1	D	232	GLU	CB-CG-CD	-9.82	95.91	112.60
1	G	456	PRO	N-CA-CB	-9.69	91.94	102.60
1	G	530	ASN	CA-CB-CG	9.44	122.03	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	356	PRO	N-CA-C	-9.38	98.09	111.22
1	D	426	PRO	N-CD-CG	-9.36	89.17	103.20
1	G	547	THR	CA-CB-OG1	-9.29	95.67	109.60
1	J	188	ARG	CG-CD-NE	-9.27	91.60	112.00
1	D	314	ASP	CA-CB-CG	9.20	121.80	112.60
1	J	127	TYR	N-CA-C	-9.09	101.50	112.59
1	G	234	ASP	CA-CB-CG	-9.06	103.54	112.60
1	J	363	LYS	CA-C-N	-9.04	113.28	122.77
1	J	363	LYS	C-N-CA	-9.04	113.28	122.77
1	J	426	PRO	CA-C-N	9.03	133.28	120.28
1	J	426	PRO	C-N-CA	9.03	133.28	120.28
1	G	135	HIS	CA-CB-CG	-9.01	104.79	113.80
1	A	284	LYS	N-CA-C	-8.96	102.50	113.97
1	A	185	ASP	CA-CB-CG	-8.92	103.68	112.60
1	G	352	PRO	N-CA-C	8.89	125.19	111.15
1	G	274	ARG	CG-CD-NE	-8.88	92.47	112.00
1	J	127	TYR	CB-CA-C	8.87	125.31	111.02
1	J	468	ASN	CB-CA-C	8.85	124.42	109.55
1	G	467	VAL	N-CA-C	-8.83	104.64	111.62
1	A	223	LYS	N-CA-C	-8.76	102.73	113.50
1	A	496	THR	CA-CB-OG1	8.70	122.65	109.60
1	D	163	ILE	N-CA-CB	-8.68	102.00	112.33
1	J	305	ASP	CA-CB-CG	-8.68	103.92	112.60
1	G	502	ASN	CB-CA-C	8.66	122.64	109.13
1	G	297	ILE	N-CA-C	-8.52	102.12	110.72
1	J	206	HIS	CA-C-N	8.49	133.72	123.19
1	J	206	HIS	C-N-CA	8.49	133.72	123.19
1	A	135	HIS	CA-CB-CG	-8.45	105.35	113.80
1	A	255	TRP	N-CA-C	-8.43	102.92	113.55
1	D	373	ILE	O-C-N	-8.25	116.17	121.37
1	A	258	GLY	CA-C-O	-8.21	116.04	122.52
1	G	468	ASN	CA-CB-CG	-8.18	104.42	112.60
1	J	200	GLY	CA-C-N	-8.01	111.71	123.00
1	J	200	GLY	C-N-CA	-8.01	111.71	123.00
1	D	368	THR	CA-CB-OG1	-7.99	97.61	109.60
1	D	534	PRO	CB-CA-C	-7.87	99.37	110.63
1	A	173	PRO	CB-CA-C	-7.87	101.32	111.39
1	D	285	ILE	CA-C-O	-7.86	113.94	121.64
1	G	385	PHE	CA-C-O	-7.84	112.02	121.28
1	J	536	THR	CA-CB-OG1	-7.77	97.94	109.60
1	A	246	PRO	CB-CA-C	-7.73	100.85	110.98
1	D	151	PHE	CA-CB-CG	7.71	121.51	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	PRO	CB-CA-C	7.69	120.19	110.27
1	G	415	THR	CA-CB-OG1	7.69	121.13	109.60
1	A	440	PHE	CB-CA-C	-7.68	95.56	109.38
1	G	488	TYR	CB-CA-C	7.67	125.39	110.67
1	G	201	LEU	CA-C-N	-7.65	115.38	122.80
1	G	201	LEU	C-N-CA	-7.65	115.38	122.80
1	A	432	TYR	CB-CA-C	7.62	120.31	108.88
1	G	538	GLU	CA-C-O	-7.61	112.83	120.82
1	D	420	LYS	CB-CA-C	7.60	122.68	109.15
1	D	415	THR	CA-CB-OG1	-7.60	98.20	109.60
1	A	500	TYR	N-CA-C	-7.56	103.63	112.86
1	D	148	GLU	CB-CA-C	-7.55	97.84	109.99
1	J	294	GLU	CB-CG-CD	7.47	125.31	112.60
1	J	482	HIS	CA-CB-CG	-7.46	106.34	113.80
1	D	163	ILE	CB-CA-C	7.43	118.65	110.62
1	J	384	GLY	CA-C-N	-7.42	110.92	122.87
1	J	384	GLY	C-N-CA	-7.42	110.92	122.87
1	A	257	ASP	CA-C-N	-7.42	110.12	122.43
1	A	257	ASP	C-N-CA	-7.42	110.12	122.43
1	D	149	PHE	CA-CB-CG	7.40	121.20	113.80
1	D	541	ARG	N-CA-C	-7.40	103.36	112.38
1	G	151	PHE	CB-CA-C	7.35	124.06	110.24
1	D	458	PRO	CB-CA-C	7.34	123.68	111.56
1	J	302	VAL	N-CA-CB	7.33	121.48	112.10
1	G	423	VAL	N-CA-CB	7.32	119.32	110.31
1	D	366	ASP	CA-CB-CG	-7.30	105.30	112.60
1	D	180	TYR	CA-C-N	7.26	133.23	122.99
1	D	180	TYR	C-N-CA	7.26	133.23	122.99
1	D	502	ASN	CA-CB-CG	7.26	119.86	112.60
1	A	155	THR	CA-CB-OG1	-7.24	98.74	109.60
1	A	276	ASP	CB-CA-C	-7.24	101.82	111.74
1	G	322	GLY	CA-C-N	7.22	135.32	121.54
1	G	322	GLY	C-N-CA	7.22	135.32	121.54
1	D	365	ASP	CA-CB-CG	-7.20	105.40	112.60
1	G	468	ASN	CB-CA-C	7.19	124.15	109.55
1	A	162	PHE	CA-CB-CG	-7.17	106.62	113.80
1	A	218	VAL	CA-C-N	-7.17	116.08	122.47
1	A	218	VAL	C-N-CA	-7.17	116.08	122.47
1	D	388	ASP	CB-CA-C	-7.17	98.44	110.56
1	J	171	GLU	CB-CG-CD	7.17	124.78	112.60
1	D	262	THR	CA-CB-OG1	-7.15	98.88	109.60
1	D	434	ASN	CA-CB-CG	7.13	119.73	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	GLU	CA-C-N	-7.13	115.19	122.74
1	D	171	GLU	C-N-CA	-7.13	115.19	122.74
1	G	464	ILE	CA-C-N	7.09	134.12	122.07
1	G	464	ILE	C-N-CA	7.09	134.12	122.07
1	A	230	ASP	CA-CB-CG	7.06	119.66	112.60
1	J	286	ASP	CB-CA-C	-7.06	99.66	111.02
1	G	189	MET	CA-C-N	-7.05	113.05	122.99
1	G	189	MET	C-N-CA	-7.05	113.05	122.99
1	J	194	ASP	CA-CB-CG	7.05	119.65	112.60
1	G	187	THR	CA-CB-OG1	7.01	120.12	109.60
1	D	387	PRO	CB-CA-C	-7.01	101.90	111.85
1	D	198	VAL	N-CA-CB	7.00	118.56	110.65
1	A	173	PRO	CA-C-N	-6.98	111.25	121.30
1	A	173	PRO	C-N-CA	-6.98	111.25	121.30
1	A	126	ASN	CA-CB-CG	6.96	119.56	112.60
1	J	232	GLU	CB-CG-CD	6.94	124.41	112.60
1	D	508	VAL	O-C-N	-6.94	115.90	123.18
1	G	538	GLU	CB-CG-CD	6.93	124.39	112.60
1	J	246	PRO	CB-CA-C	-6.92	102.01	111.21
1	J	494	VAL	CA-C-N	6.89	129.41	122.66
1	J	494	VAL	C-N-CA	6.89	129.41	122.66
1	J	367	ASP	CA-CB-CG	6.89	119.49	112.60
1	G	197	GLU	CB-CG-CD	-6.87	100.92	112.60
1	D	355	THR	CA-C-O	6.87	129.57	120.16
1	J	196	ALA	N-CA-CB	6.85	121.56	110.40
1	G	220	ASP	CA-CB-CG	-6.84	105.76	112.60
1	G	245	ASP	CB-CA-C	6.84	121.18	110.71
1	J	132	PRO	N-CA-C	-6.83	103.27	112.48
1	D	345	PRO	N-CA-C	-6.77	100.37	111.68
1	A	483	THR	CB-CA-C	-6.76	96.90	111.78
1	A	457	THR	CB-CA-C	-6.74	99.35	109.26
1	A	539	ASP	CA-CB-CG	6.74	119.34	112.60
1	G	94	GLY	CA-C-O	-6.73	117.60	122.45
1	G	319	ASP	O-C-N	-6.73	115.31	121.30
1	G	454	PRO	N-CA-CB	-6.73	97.32	103.31
1	G	512	THR	CA-CB-OG1	-6.71	99.53	109.60
1	G	250	ASP	CA-C-N	6.71	129.57	120.38
1	G	250	ASP	C-N-CA	6.71	129.57	120.38
1	J	332	PRO	N-CA-C	-6.71	105.22	114.27
1	J	435	THR	CA-CB-OG1	-6.69	99.56	109.60
1	D	167	PRO	CB-CA-C	6.69	122.59	111.56
1	G	388	ASP	N-CA-C	-6.68	105.01	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	ILE	O-C-N	-6.65	114.25	122.57
1	D	299	ASP	CA-CB-CG	-6.64	105.96	112.60
1	G	319	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	206	HIS	N-CA-C	6.63	119.59	110.24
1	D	144	ASP	CB-CA-C	-6.62	103.17	110.98
1	G	356	PRO	CA-C-N	6.62	129.15	120.28
1	G	356	PRO	C-N-CA	6.62	129.15	120.28
1	D	148	GLU	CA-C-N	-6.61	110.50	121.80
1	D	148	GLU	C-N-CA	-6.61	110.50	121.80
1	D	530	ASN	CB-CA-C	6.60	123.55	110.42
1	D	203	LEU	CA-C-O	-6.57	113.42	121.11
1	A	98	LEU	CA-C-N	-6.55	111.66	122.67
1	A	98	LEU	C-N-CA	-6.55	111.66	122.67
1	D	268	PRO	CB-CA-C	-6.54	102.85	111.23
1	J	220	ASP	CA-CB-CG	-6.54	106.06	112.60
1	J	459	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	D	288	GLU	CB-CG-CD	-6.51	101.53	112.60
1	J	278	GLN	N-CA-CB	6.51	120.88	110.46
1	D	547	THR	CA-C-O	-6.51	114.48	121.45
1	J	359	PHE	CA-C-N	6.49	132.68	122.17
1	J	359	PHE	C-N-CA	6.49	132.68	122.17
1	D	316	LEU	CA-C-N	-6.48	115.16	122.48
1	D	316	LEU	C-N-CA	-6.48	115.16	122.48
1	J	477	LEU	CA-C-N	-6.48	111.70	121.87
1	J	477	LEU	C-N-CA	-6.48	111.70	121.87
1	J	460	GLY	CA-C-N	-6.44	113.99	122.94
1	J	460	GLY	C-N-CA	-6.44	113.99	122.94
1	G	130	THR	CA-CB-OG1	-6.42	99.98	109.60
1	A	266	LEU	CA-C-O	-6.40	113.93	120.71
1	A	115	THR	CA-CB-OG1	-6.39	100.01	109.60
1	D	250	ASP	CB-CA-C	-6.39	96.41	109.38
1	A	194	ASP	CB-CA-C	6.39	121.35	110.81
1	D	345	PRO	CB-CA-C	6.37	119.74	110.63
1	G	364	VAL	N-CA-C	-6.36	106.60	112.96
1	J	347	ALA	CA-C-N	6.35	130.94	122.93
1	J	347	ALA	C-N-CA	6.35	130.94	122.93
1	D	214	ASP	N-CA-C	-6.35	104.79	113.30
1	G	247	ASN	CA-CB-CG	-6.35	106.25	112.60
1	J	351	GLY	CA-C-N	6.35	127.78	119.84
1	J	351	GLY	C-N-CA	6.35	127.78	119.84
1	D	237	ARG	CD-NE-CZ	6.34	133.28	124.40
1	A	485	ALA	CA-C-N	-6.33	112.62	122.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ALA	C-N-CA	-6.33	112.62	122.69
1	J	266	LEU	N-CA-C	-6.33	98.58	108.90
1	D	358	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	D	184	TYR	N-CA-C	-6.30	98.97	109.24
1	J	265	ARG	CA-C-N	-6.29	114.11	122.99
1	J	265	ARG	C-N-CA	-6.29	114.11	122.99
1	G	320	PRO	N-CA-CB	-6.29	97.61	103.46
1	D	222	GLN	CA-C-N	-6.28	112.27	122.26
1	D	222	GLN	C-N-CA	-6.28	112.27	122.26
1	G	482	HIS	CA-CB-CG	-6.27	107.53	113.80
1	D	474	GLU	CB-CG-CD	6.25	123.23	112.60
1	D	529	ASP	CB-CA-C	6.24	122.84	110.42
1	D	402	ASN	CA-C-N	-6.24	115.01	123.12
1	D	402	ASN	C-N-CA	-6.24	115.01	123.12
1	G	511	GLU	CB-CG-CD	6.23	123.19	112.60
1	A	346	VAL	CB-CA-C	6.22	116.47	110.63
1	D	154	ASN	CB-CA-C	6.21	123.34	111.48
1	A	396	ASN	CB-CA-C	6.21	119.95	109.84
1	A	198	VAL	CA-C-N	6.20	129.20	120.28
1	A	198	VAL	C-N-CA	6.20	129.20	120.28
1	D	373	ILE	CB-CA-C	6.20	118.35	111.04
1	A	212	GLU	N-CA-CB	6.19	120.81	110.41
1	A	194	ASP	CA-C-N	6.18	129.71	120.31
1	A	194	ASP	C-N-CA	6.18	129.71	120.31
1	G	358	GLN	CB-CG-CD	6.18	123.10	112.60
1	G	179	ILE	CA-C-N	-6.15	114.23	122.72
1	G	179	ILE	C-N-CA	-6.15	114.23	122.72
1	G	314	ASP	CA-CB-CG	6.14	118.74	112.60
1	J	382	GLN	CA-C-N	6.12	130.70	121.40
1	J	382	GLN	C-N-CA	6.12	130.70	121.40
1	G	454	PRO	N-CD-CG	-6.11	94.03	103.20
1	J	445	LYS	CB-CA-C	6.09	121.84	110.70
1	J	320	PRO	N-CD-CG	-6.09	94.07	103.20
1	A	527	HIS	CA-CB-CG	6.08	119.88	113.80
1	G	307	PRO	CA-C-N	6.08	129.03	120.28
1	G	307	PRO	C-N-CA	6.08	129.03	120.28
1	D	477	LEU	CA-C-N	-6.07	112.34	121.87
1	D	477	LEU	C-N-CA	-6.07	112.34	121.87
1	G	455	SER	O-C-N	-6.07	114.34	121.32
1	A	512	THR	CA-C-N	6.06	128.68	120.44
1	A	512	THR	C-N-CA	6.06	128.68	120.44
1	A	321	ARG	CB-CA-C	-6.04	99.61	110.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	GLU	CA-C-N	-6.03	113.36	120.72
1	D	197	GLU	C-N-CA	-6.03	113.36	120.72
1	D	548	THR	CB-CA-C	6.03	122.36	109.10
1	D	386	SER	CA-C-N	6.03	125.71	119.56
1	D	386	SER	C-N-CA	6.03	125.71	119.56
1	G	185	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	294	GLU	N-CA-CB	6.01	119.60	110.28
1	G	252	LYS	N-CA-C	-6.01	104.64	111.07
1	A	262	THR	CB-CA-C	-5.98	99.44	109.48
1	A	136	HIS	CA-CB-CG	-5.97	107.83	113.80
1	D	234	ASP	N-CA-C	-5.97	105.94	113.23
1	A	288	GLU	CB-CA-C	5.97	119.21	109.90
1	G	227	ALA	CA-C-O	-5.95	114.32	120.99
1	G	321	ARG	CG-CD-NE	-5.95	98.91	112.00
1	A	479	PRO	CB-CA-C	-5.95	102.46	110.85
1	J	503	THR	CB-CA-C	5.94	122.25	110.42
1	A	516	GLU	CB-CG-CD	5.94	122.70	112.60
1	J	283	ASN	N-CA-C	5.94	119.21	110.30
1	G	147	LYS	N-CA-C	-5.94	105.12	112.90
1	G	197	GLU	CA-C-O	-5.93	114.20	120.55
1	D	433	PRO	CA-C-N	-5.92	113.33	122.87
1	D	433	PRO	C-N-CA	-5.92	113.33	122.87
1	J	132	PRO	N-CA-CB	5.92	106.39	102.25
1	D	217	ALA	CA-C-N	-5.92	113.28	122.69
1	D	217	ALA	C-N-CA	-5.92	113.28	122.69
1	D	442	PRO	N-CA-CB	-5.91	96.69	103.30
1	D	103	LYS	CA-CB-CG	-5.90	102.30	114.10
1	G	104	PHE	CA-C-O	-5.90	114.26	120.63
1	J	173	PRO	N-CA-C	5.89	120.75	111.38
1	D	133	ILE	CA-C-N	-5.89	113.89	122.19
1	D	133	ILE	C-N-CA	-5.89	113.89	122.19
1	G	175	GLU	CA-C-N	-5.89	110.05	121.01
1	G	175	GLU	C-N-CA	-5.89	110.05	121.01
1	J	268	PRO	N-CA-C	5.89	119.46	111.22
1	J	317	VAL	CA-C-N	5.88	131.12	123.00
1	J	317	VAL	C-N-CA	5.88	131.12	123.00
1	A	263	ILE	N-CA-CB	-5.88	105.35	112.35
1	D	117	TRP	O-C-N	5.87	129.64	123.06
1	J	479	PRO	N-CA-CB	-5.87	97.46	103.15
1	J	341	GLU	CB-CA-C	5.87	120.17	110.90
1	D	290	VAL	O-C-N	-5.86	114.42	121.10
1	A	143	PRO	CB-CA-C	5.86	122.28	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	336	VAL	CB-CA-C	5.85	119.50	110.96
1	G	448	TYR	CB-CA-C	5.84	120.13	110.78
1	D	312	ALA	N-CA-C	5.83	119.16	111.28
1	A	178	LYS	CB-CA-C	-5.83	99.68	109.53
1	J	375	GLU	CA-C-N	5.83	129.98	122.93
1	J	375	GLU	C-N-CA	5.83	129.98	122.93
1	J	522	PRO	N-CA-CB	-5.82	98.12	103.25
1	D	237	ARG	CB-CG-CD	-5.82	97.91	111.30
1	A	140	PHE	N-CA-C	5.82	116.29	109.60
1	G	262	THR	CB-CA-C	5.81	119.35	109.53
1	A	262	THR	CA-C-N	5.81	130.61	123.17
1	A	262	THR	C-N-CA	5.81	130.61	123.17
1	J	132	PRO	CA-C-N	-5.81	112.98	122.33
1	J	132	PRO	C-N-CA	-5.81	112.98	122.33
1	A	190	ASN	CB-CA-C	-5.81	101.76	110.24
1	G	269	THR	CA-CB-OG1	-5.81	100.89	109.60
1	J	320	PRO	CB-CA-C	-5.79	102.01	111.56
1	J	265	ARG	N-CA-C	-5.77	101.94	110.48
1	A	129	ASP	CA-C-N	-5.77	113.61	122.60
1	A	129	ASP	C-N-CA	-5.77	113.61	122.60
1	D	182	ILE	N-CA-C	-5.76	100.75	108.35
1	G	372	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	541	ARG	CG-CD-NE	-5.76	99.33	112.00
1	J	407	ASP	CB-CA-C	-5.76	101.92	110.67
1	A	486	ILE	CA-C-N	-5.75	112.07	120.75
1	A	486	ILE	C-N-CA	-5.75	112.07	120.75
1	J	212	GLU	CB-CA-C	5.74	121.38	109.95
1	A	548	THR	OG1-CB-CG2	5.74	120.78	109.30
1	J	496	THR	CA-C-N	5.74	131.82	122.81
1	J	496	THR	C-N-CA	5.74	131.82	122.81
1	A	222	GLN	CB-CA-C	5.73	119.81	110.24
1	D	223	LYS	N-CA-C	-5.73	106.27	113.72
1	D	213	ALA	CA-C-N	5.73	131.37	122.49
1	D	213	ALA	C-N-CA	5.73	131.37	122.49
1	J	456	PRO	CA-C-N	-5.73	112.43	120.39
1	J	456	PRO	C-N-CA	-5.73	112.43	120.39
1	J	488	TYR	CB-CA-C	5.72	121.16	109.55
1	A	436	PHE	CA-C-O	5.72	125.09	118.97
1	J	459	ASN	CB-CG-ND2	5.72	124.98	116.40
1	A	521	LEU	O-C-N	5.71	127.31	121.72
1	A	211	PRO	N-CA-C	-5.71	106.09	113.57
1	D	429	ARG	CG-CD-NE	-5.70	99.46	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	210	THR	CA-CB-OG1	5.70	118.15	109.60
1	G	230	ASP	CB-CA-C	-5.69	99.92	109.65
1	J	522	PRO	O-C-N	5.68	130.10	122.89
1	G	379	ALA	O-C-N	5.67	129.31	122.85
1	G	196	ALA	N-CA-C	-5.66	105.25	111.82
1	A	433	PRO	CB-CA-C	-5.66	97.86	112.00
1	G	322	GLY	O-C-N	5.65	129.18	122.68
1	J	522	PRO	CA-C-O	-5.64	114.98	121.36
1	D	353	LYS	CB-CA-C	-5.64	102.22	110.06
1	A	115	THR	O-C-N	-5.63	116.15	122.34
1	A	293	GLY	N-CA-C	-5.63	107.68	114.66
1	J	151	PHE	CB-CA-C	5.62	121.08	110.62
1	D	243	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	224	ASP	CB-CA-C	-5.61	103.92	111.89
1	G	291	PRO	CB-CA-C	5.61	118.77	111.64
1	G	105	SER	N-CA-CB	5.60	119.95	110.49
1	A	237	ARG	N-CA-CB	-5.59	101.96	110.07
1	A	243	ASP	CA-CB-CG	-5.59	107.01	112.60
1	D	357	SER	CA-C-O	-5.58	114.67	120.92
1	D	271	PRO	CB-CA-C	5.58	118.26	110.95
1	J	360	GLN	N-CA-CB	-5.58	102.16	110.24
1	D	416	THR	CA-CB-OG1	5.57	117.96	109.60
1	D	532	ILE	N-CA-C	-5.57	100.45	108.53
1	G	233	THR	CB-CA-C	-5.57	100.20	109.55
1	A	482	HIS	CA-CB-CG	-5.56	108.24	113.80
1	J	390	GLN	CB-CG-CD	-5.56	103.15	112.60
1	A	141	PRO	N-CA-CB	5.55	108.25	103.31
1	A	394	PHE	CB-CA-C	5.55	119.86	109.86
1	D	193	ARG	CB-CA-C	-5.55	100.95	110.95
1	D	502	ASN	CB-CG-ND2	5.55	124.73	116.40
1	J	181	ARG	O-C-N	-5.54	116.90	123.22
1	G	355	THR	CB-CA-C	5.54	117.40	109.26
1	J	145	PRO	CA-C-N	5.54	128.25	120.28
1	J	145	PRO	C-N-CA	5.54	128.25	120.28
1	D	526	GLY	CA-C-N	5.53	131.54	121.97
1	D	526	GLY	C-N-CA	5.53	131.54	121.97
1	J	400	GLN	N-CA-C	-5.53	100.89	109.24
1	J	498	SER	CA-CB-OG	-5.51	100.07	111.10
1	D	304	GLY	N-CA-C	-5.50	102.71	110.75
1	G	232	GLU	CA-C-N	-5.50	113.51	122.26
1	G	232	GLU	C-N-CA	-5.50	113.51	122.26
1	J	439	VAL	CA-CB-CG2	5.50	119.76	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ALA	N-CA-CB	-5.50	101.75	110.28
1	G	322	GLY	CA-C-O	-5.50	117.51	122.57
1	A	134	MET	CG-SD-CE	5.49	112.97	100.90
1	A	228	GLU	CB-CA-C	-5.48	100.27	109.48
1	G	316	LEU	N-CA-CB	-5.48	101.38	110.47
1	G	541	ARG	N-CA-C	-5.47	105.87	112.54
1	A	534	PRO	CB-CA-C	5.47	118.84	110.75
1	A	534	PRO	N-CA-C	-5.47	102.98	111.13
1	G	173	PRO	CB-CA-C	5.46	118.55	110.85
1	G	538	GLU	CA-C-N	5.46	127.91	120.54
1	G	538	GLU	C-N-CA	5.46	127.91	120.54
1	J	180	TYR	CA-C-N	5.46	130.03	122.77
1	J	180	TYR	C-N-CA	5.46	130.03	122.77
1	D	207	VAL	CA-CB-CG1	5.45	119.66	110.40
1	D	170	VAL	CA-CB-CG1	5.44	119.66	110.40
1	J	291	PRO	CA-C-O	-5.44	115.41	121.23
1	G	394	PHE	CA-CB-CG	5.43	119.23	113.80
1	D	546	THR	CA-CB-OG1	-5.43	101.45	109.60
1	G	243	ASP	CA-CB-CG	-5.43	107.17	112.60
1	G	136	HIS	CB-CA-C	5.41	120.73	110.51
1	A	100	ALA	CB-CA-C	-5.41	101.68	109.63
1	J	265	ARG	CB-CG-CD	-5.41	98.87	111.30
1	J	496	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	460	GLY	CA-C-N	5.40	130.58	122.75
1	A	460	GLY	C-N-CA	5.40	130.58	122.75
1	D	132	PRO	CB-CA-C	-5.40	102.66	111.56
1	G	379	ALA	N-CA-C	-5.40	103.26	110.55
1	D	245	ASP	CA-C-N	5.39	125.65	119.83
1	D	245	ASP	C-N-CA	5.39	125.65	119.83
1	J	385	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	220	ASP	CA-CB-CG	-5.39	107.21	112.60
1	J	223	LYS	CA-C-N	-5.39	114.44	122.36
1	J	223	LYS	C-N-CA	-5.39	114.44	122.36
1	D	419	LYS	CB-CA-C	5.38	118.65	109.72
1	A	436	PHE	N-CA-CB	-5.38	103.20	110.67
1	G	522	PRO	CA-C-N	-5.38	116.35	122.26
1	G	522	PRO	C-N-CA	-5.38	116.35	122.26
1	J	317	VAL	O-C-N	5.37	129.51	122.47
1	D	348	VAL	CA-C-O	-5.37	114.94	120.25
1	G	118	THR	CB-CA-C	5.36	117.88	110.16
1	A	268	PRO	N-CA-C	-5.35	103.16	111.13
1	G	348	VAL	O-C-N	-5.35	117.52	122.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	314	ASP	CB-CA-C	5.34	121.05	110.42
1	A	101	PRO	CB-CA-C	5.34	118.00	110.20
1	D	300	GLY	N-CA-C	-5.34	107.42	115.32
1	G	292	GLY	N-CA-C	-5.34	107.95	115.32
1	D	336	VAL	N-CA-CB	5.34	118.19	111.46
1	A	155	THR	CA-C-O	5.33	128.02	121.56
1	A	437	HIS	CA-CB-CG	-5.33	108.47	113.80
1	D	494	VAL	O-C-N	5.33	129.23	122.57
1	G	315	ALA	CA-C-N	5.33	130.68	123.11
1	G	315	ALA	C-N-CA	5.33	130.68	123.11
1	A	360	GLN	CB-CA-C	-5.32	101.38	109.89
1	G	365	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	263	ILE	CB-CA-C	5.32	116.99	111.09
1	G	332	PRO	CB-CA-C	-5.31	103.39	110.88
1	A	515	ASP	CB-CA-C	5.31	119.89	111.51
1	J	164	TYR	CA-C-N	-5.30	111.02	121.41
1	J	164	TYR	C-N-CA	-5.30	111.02	121.41
1	J	170	VAL	CB-CA-C	5.30	118.73	110.83
1	D	140	PHE	CA-C-N	5.30	125.60	119.93
1	D	140	PHE	C-N-CA	5.30	125.60	119.93
1	D	155	THR	CA-C-N	5.30	130.55	122.65
1	D	155	THR	C-N-CA	5.30	130.55	122.65
1	J	426	PRO	N-CA-C	-5.30	107.12	114.27
1	D	423	VAL	CA-CB-CG2	5.29	119.40	110.40
1	J	294	GLU	N-CA-C	-5.29	104.92	111.33
1	J	274	ARG	CB-CG-CD	5.29	123.47	111.30
1	G	306	ARG	CA-C-N	5.29	124.92	119.05
1	G	306	ARG	C-N-CA	5.29	124.92	119.05
1	G	278	GLN	N-CA-CB	5.29	118.00	110.44
1	J	522	PRO	CB-CA-C	-5.28	104.85	111.56
1	D	514	THR	CB-CA-C	-5.28	102.46	111.02
1	G	376	VAL	CA-C-N	5.28	129.00	120.82
1	G	376	VAL	C-N-CA	5.28	129.00	120.82
1	J	95	LYS	CB-CA-C	5.27	120.54	111.68
1	A	257	ASP	CA-CB-CG	-5.26	107.34	112.60
1	A	359	PHE	CA-CB-CG	5.26	119.06	113.80
1	J	468	ASN	N-CA-C	-5.25	106.89	113.72
1	J	131	CYS	O-C-N	5.25	127.36	121.32
1	G	257	ASP	CB-CA-C	5.25	120.09	110.11
1	A	193	ARG	CA-C-N	-5.25	115.44	122.42
1	A	193	ARG	C-N-CA	-5.25	115.44	122.42
1	D	322	GLY	CA-C-O	-5.25	116.48	122.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	290	VAL	O-C-N	-5.25	115.12	121.10
1	D	228	GLU	CB-CG-CD	5.24	121.50	112.60
1	G	547	THR	CB-CA-C	-5.23	99.20	110.45
1	A	167	PRO	N-CA-C	-5.23	105.42	112.48
1	A	365	ASP	CA-C-N	5.23	127.81	120.28
1	A	365	ASP	C-N-CA	5.23	127.81	120.28
1	G	355	THR	N-CA-CB	5.22	117.50	110.14
1	D	455	SER	O-C-N	-5.22	115.58	121.43
1	J	107	THR	CA-C-O	-5.21	115.67	121.51
1	G	166	VAL	CA-C-O	5.21	123.74	119.47
1	A	305	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	353	LYS	CA-C-N	5.20	128.65	121.26
1	A	353	LYS	C-N-CA	5.20	128.65	121.26
1	J	231	ARG	CB-CA-C	5.20	120.22	110.70
1	D	268	PRO	N-CA-CB	-5.19	98.83	103.35
1	A	151	PHE	N-CA-C	5.19	117.56	109.52
1	G	159	LYS	CA-C-O	-5.18	114.01	119.97
1	J	324	TRP	CA-C-N	5.18	130.84	122.29
1	J	324	TRP	C-N-CA	5.18	130.84	122.29
1	G	394	PHE	CA-C-N	5.18	129.23	121.72
1	G	394	PHE	C-N-CA	5.18	129.23	121.72
1	J	474	GLU	CB-CG-CD	-5.18	103.80	112.60
1	G	394	PHE	CB-CA-C	-5.18	100.59	109.65
1	A	117	TRP	CA-C-O	-5.17	115.61	121.72
1	J	337	VAL	O-C-N	5.17	128.83	122.83
1	D	89	PHE	CA-CB-CG	-5.17	108.63	113.80
1	D	541	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	G	432	TYR	O-C-N	5.17	125.02	121.71
1	A	272	GLY	CA-C-N	5.17	127.92	120.11
1	A	272	GLY	C-N-CA	5.17	127.92	120.11
1	A	190	ASN	N-CA-CB	5.16	119.11	110.59
1	D	494	VAL	CA-C-O	-5.15	114.35	120.78
1	G	292	GLY	O-C-N	5.15	128.97	122.43
1	G	93	LEU	N-CA-C	5.14	116.97	111.36
1	A	281	LYS	CA-C-N	-5.14	116.14	123.08
1	A	281	LYS	C-N-CA	-5.14	116.14	123.08
1	J	339	ASP	CA-C-N	-5.14	112.12	120.71
1	J	339	ASP	C-N-CA	-5.14	112.12	120.71
1	A	322	GLY	CA-C-O	-5.14	116.06	122.59
1	D	544	ARG	CB-CA-C	5.14	119.89	111.41
1	G	299	ASP	CB-CA-C	-5.14	101.88	110.56
1	A	434	ASN	CA-C-N	5.13	129.98	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ASN	C-N-CA	5.13	129.98	122.85
1	G	399	ARG	CB-CG-CD	5.13	123.09	111.30
1	G	225	ILE	CA-CB-CG2	5.12	119.21	110.50
1	J	418	GLU	CB-CA-C	5.12	119.49	109.35
1	G	242	PHE	CA-C-N	-5.12	112.93	121.94
1	G	242	PHE	C-N-CA	-5.12	112.93	121.94
1	A	136	HIS	CB-CA-C	5.12	118.24	109.80
1	A	363	LYS	CA-C-N	5.12	128.75	120.82
1	A	363	LYS	C-N-CA	5.12	128.75	120.82
1	G	523	SER	CB-CA-C	5.12	117.02	110.98
1	A	265	ARG	CG-CD-NE	5.11	123.25	112.00
1	D	336	VAL	CA-C-N	5.11	128.96	121.80
1	D	336	VAL	C-N-CA	5.11	128.96	121.80
1	G	320	PRO	N-CA-C	-5.11	107.08	114.18
1	A	306	ARG	CB-CG-CD	5.11	123.04	111.30
1	G	205	VAL	CB-CA-C	5.10	119.66	111.29
1	A	482	HIS	CB-CA-C	5.09	124.02	116.53
1	A	126	ASN	CA-C-N	5.09	130.76	122.67
1	A	126	ASN	C-N-CA	5.09	130.76	122.67
1	D	129	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	295	LEU	CA-C-N	5.09	127.56	120.63
1	D	295	LEU	C-N-CA	5.09	127.56	120.63
1	J	159	LYS	N-CA-CB	-5.09	101.47	110.42
1	J	322	GLY	CA-C-N	5.08	131.25	121.54
1	J	322	GLY	C-N-CA	5.08	131.25	121.54
1	A	228	GLU	CA-C-O	-5.08	115.16	120.80
1	D	384	GLY	CA-C-N	5.07	129.34	122.19
1	D	384	GLY	C-N-CA	5.07	129.34	122.19
1	J	368	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	222	GLN	CA-C-N	5.07	130.69	121.92
1	A	222	GLN	C-N-CA	5.07	130.69	121.92
1	D	301	LYS	CB-CA-C	5.07	119.29	110.72
1	J	149	PHE	CB-CA-C	5.06	120.50	110.42
1	A	265	ARG	CA-C-N	-5.06	115.59	122.93
1	A	265	ARG	C-N-CA	-5.06	115.59	122.93
1	J	186	GLY	N-CA-C	-5.06	107.29	115.08
1	A	301	LYS	CB-CA-C	-5.05	100.02	109.72
1	J	131	CYS	CA-C-O	-5.05	113.24	120.16
1	J	91	ASP	CA-CB-CG	-5.05	107.55	112.60
1	G	539	ASP	CB-CA-C	-5.05	102.73	110.81
1	J	269	THR	CA-CB-CG2	5.04	119.08	110.50
1	G	321	ARG	NE-CZ-NH1	-5.04	116.46	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	138	ALA	CB-CA-C	5.04	118.36	109.80
1	A	171	GLU	CB-CA-C	-5.04	102.29	110.85
1	G	231	ARG	CG-CD-NE	5.04	123.08	112.00
1	D	208	THR	CA-C-N	5.03	130.11	122.91
1	D	208	THR	C-N-CA	5.03	130.11	122.91
1	J	171	GLU	CB-CA-C	5.03	118.85	110.90
1	J	321	ARG	CG-CD-NE	5.03	123.07	112.00
1	D	261	MET	N-CA-C	-5.03	102.08	110.17
1	A	193	ARG	CB-CG-CD	-5.02	99.75	111.30
1	A	503	THR	CB-CA-C	5.02	120.41	110.42
1	A	538	GLU	CB-CG-CD	5.02	121.14	112.60
1	J	331	LEU	O-C-N	-5.02	115.55	121.32
1	J	387	PRO	N-CA-CB	5.02	108.81	103.39
1	A	103	LYS	CB-CG-CD	5.01	122.83	111.30
1	D	156	GLN	CB-CG-CD	5.01	121.12	112.60
1	J	136	HIS	CB-CA-C	5.01	118.06	109.80
1	G	421	ALA	CA-C-O	-5.01	115.92	121.28
1	A	291	PRO	CB-CA-C	-5.00	105.21	111.56
1	D	367	ASP	CB-CA-C	-5.00	99.56	110.41

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	171	0
1	D	3644	0	3509	156	0
1	G	3628	0	3491	173	0
1	J	3631	0	3493	189	0
2	A	2	0	0	0	0
2	D	3	0	0	0	0
2	G	3	0	0	0	0
2	J	2	0	0	0	0
3	A	5	0	0	0	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	12	0
4	D	205	0	0	9	0
4	G	194	0	0	4	0
4	J	160	0	0	13	0
All	All	15340	0	14010	678	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 24.

All (678) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:443:ASP:CG	1:D:445:LYS:HE2	1.80	1.06
1:D:465:ASP:HB2	1:D:472:LEU:CD1	1.85	1.06
1:J:99:VAL:HG11	1:J:137:MET:HE1	1.38	1.05
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:465:ASP:HB2	1:D:472:LEU:HD11	1.42	1.01
1:J:99:VAL:CG1	1:J:137:MET:HE1	1.91	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: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
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:D:236:VAL:HG11	1:D:275:TYR:HE1	1.36	0.83
1:G:148:GLU:CD	1:G:183:LYS:HE3	2.04	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:J:97:VAL:HG11	1:J:119:MET:HE1	1.61	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:J:97:VAL:CG1	1:J:119:MET:HE1	2.12	0.80
1:D:205:VAL:HG23	1:D:220:ASP:HA	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:PRO:HB3	1:J:533:VAL:HG11	1.65	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:G:148:GLU:CD	1:G:183:LYS:CE	2.60	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
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: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:G:182:ILE:HG23	1:G:190:ASN:C	2.16	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:G:481:MET:HE3	1:G:496:THR:O	1.92	0.70
1:J:450:THR:HG23	1:J:484:LEU:CD1	2.22	0.70
1:G:82:LYS:HD3	1:G:82:LYS:C	2.17	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:HH11	1:A:265:ARG:CG	1.94	0.69
1:A:214:ASP:OD1	1:A:214:ASP:C	2.36	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: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:A:392:PHE:C	1:A:393:LEU:HD12	2.18	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:A:238:TYR:CD1	1:A:238:TYR:C	2.72	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
1:A:125:TRP:HD1	4:A:815:HOH:O	1.77	0.66
1:G:538:GLU:H	1:G:538:GLU:CD	2.03	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:225:ILE:HG12	1:D:266:LEU:HD11	1.78	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:J:202:GLY:O	1:J:223:LYS:NZ	2.28	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: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
1:D:465:ASP:OD1	1:D:465:ASP:C	2.42	0.61
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:D:122:LEU:C	1:D:122:LEU:HD23	2.25	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:J:99:VAL:CG1	1:J:137:MET:CE	2.76	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:292:GLY:C	1:J:294:GLU:H	2.11	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:311:VAL:CG2	1:G:329:MET:HE3	2.34	0.58
1:G:382:GLN:OE1	1:G:438:MET:HE2	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:A:481:MET:HE2	1:A:484:LEU:HD11	1.85	0.57
1:J:205:VAL:HG23	1:J:220:ASP:HA	1.85	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
1:A:481:MET:HE2	1:A:484:LEU:CD1	2.34	0.57
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:G:395:MET:HE3	1:G:403:ILE:HG12	1.88	0.56
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:456:PRO:O	1:J:457:THR:C	2.42	0.55
1:D:332:PRO:HA	1:D:376:VAL:HG21	1.87	0.55
1:G:124:ALA:HB2	1:G:134:MET:HE1	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:148:GLU:CD	1:G:183:LYS:HE2	2.31	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:D:307:PRO:C	1:D:309:HIS:H	2.15	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:A:286:ASP:OD2	1:A:303:SER:OG	2.23	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: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
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:J:253:ARG:O	1:J:254:ALA:C	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:VAL:HG12	1:J:137:MET:HE1	1.88	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:A:465:ASP:C	1:A:465:ASP:OD1	2.52	0.53
1:G:311:VAL:CG2	1:G:329:MET:CE	2.87	0.53
1:A:339:ASP:CG	1:A:342:ASN:HB2	2.32	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: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:A:510:MET:HE2	1:A:515:ASP:O	2.10	0.52
1:G:163:ILE:HG21	1:G:290:VAL:CG1	2.40	0.52
1:D:382:GLN:C	1:D:382:GLN:NE2	2.67	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:PRO:HA	1:G:108:VAL:HG23	1.92	0.51
1:G:392:PHE:C	1:G:393:LEU:HD12	2.35	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:279:GLY:C	1:D:281:LYS:H	2.18	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:J:173:PRO:C	1:J:174:GLY:O	2.54	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:A:172:ASP:O	1:A:173:PRO:C	2.54	0.51
1:D:377:ILE:HD12	1:D:377:ILE:N	2.25	0.51
1:D:307:PRO:C	1:D:309:HIS:N	2.69	0.51
1:D:383:ALA:HB2	1:D:394:PHE:CD1	2.44	0.51
1:J:173:PRO:O	1:J:174:GLY:C	2.53	0.50
1:J:292:GLY:C	1:J:294:GLU:N	2.67	0.50
1:A:238:TYR:C	1:A:238:TYR:HD1	2.16	0.50
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:481:MET:HG3	1:D:482:HIS:N	2.25	0.50
1:G:430:GLY:C	1:G:432:TYR:N	2.69	0.50
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:312:ALA:O	1:J:313:ASN:C	2.55	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:J:311:VAL:HG23	1:J:329:MET:HE3	1.94	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:404:MET:HG3	1:J:406:TRP:CH2	2.47	0.49
1:D:392:PHE:C	1:D:393:LEU:HD12	2.37	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:D:265:ARG:HG3	1:D:265:ARG:HH11	1.78	0.49
1:G:107:THR:OG1	1:G:525:MET:HE3	2.13	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:A:513:GLU:HA	1:A:513:GLU:OE1	2.13	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:D:207:VAL:HA	1:D:217:ALA:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:185:ASP:OD1	1:A:185:ASP:C	2.55	0.48
1:A:291:PRO:HG2	1:A:452:TRP:CH2	2.49	0.48
1:G:129:ASP:C	1:G:129:ASP:OD1	2.57	0.48
1:J:322:GLY:C	1:J:324:TRP:H	2.21	0.48
1:D:306:ARG:NH2	1:D:309:HIS:CG	2.81	0.48
1:D:530:ASN:C	1:D:531:VAL:CG1	2.85	0.48
1:J:447[A]:ILE:HG12	1:J:449:VAL:HG13	1.95	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: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:G:460:GLY:C	1:G:461:ILE:HG13	2.38	0.47
1:J:193:ARG:HD2	1:J:234:ASP:OD2	2.14	0.47
1:J:273:GLY:N	4:J:718:HOH:O	2.47	0.47
1:A:520:PHE:O	1:D:90:TYR:OH	2.26	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:279:GLY:C	1:D:281:LYS:N	2.73	0.47
1:D:427:ASP:OD2	1:D:471:VAL:HG11	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:PRO:C	1:G:322:GLY:N	2.71	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:G:436:PHE:C	1:G:437:HIS:CG	2.93	0.47
1:A:390:GLN:OE1	1:A:409:SER:HB2	2.15	0.47
1:A:499:GLY:C	1:A:501:GLN:N	2.73	0.47
1:G:200:GLY:HA3	1:G:275:TYR:O	2.15	0.47
1:G:320:PRO:C	1:G:322:GLY:H	2.22	0.47
1:G:387:PRO:HG3	1:G:542:ILE:HG22	1.96	0.47
1:J:479:PRO:O	1:J:479:PRO:CG	2.63	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: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:J:311:VAL:CG2	1:J:329:MET:HE3	2.45	0.46
1:D:407:ASP:OD1	1:D:409:SER:CB	2.56	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: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:A:382:GLN:HB2	1:A:436:PHE:C	2.41	0.46
1:G:206:HIS:O	1:G:218:VAL:HA	2.16	0.46
1:G:311:VAL:HG21	1:G:329:MET:HE1	1.97	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:159:LYS:C	1:G:161:LEU:N	2.73	0.45
1:G:381:HIS:C	1:G:381:HIS:CD2	2.94	0.45
1:J:393:LEU:HD12	1:J:393:LEU:N	2.31	0.45
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:J:307:PRO:C	1:J:309:HIS:H	2.23	0.45
1:G:538:GLU:CD	1:G:538:GLU:N	2.70	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:284:LYS:NZ	1:G:309:HIS:O	2.44	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:A:288:GLU:O	1:A:289:LEU:C	2.59	0.45
1:A:386:SER:OG	1:A:388:ASP:OD1	2.34	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:543:SER:O	1:A:545:SER:N	2.44	0.45
1:G:414:PRO:O	1:G:415:THR:C	2.59	0.45
1:G:475:VAL:HG21	1:G:510:MET:HE2	1.98	0.45
1:A:276:ASP:OD1	1:A:281:LYS:NZ	2.47	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:D:540:LEU:C	1:D:542:ILE:N	2.71	0.45
1:G:202:GLY:C	1:G:203:LEU:HG	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:SER:HA	1:A:426:PRO:HD3	1.83	0.44
1:D:294:GLU:H	1:D:294:GLU:CD	2.24	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:G:214:ASP:C	1:G:214:ASP:OD1	2.59	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: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:150:GLU:OE2	4:J:703:HOH:O	2.20	0.44
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:D:503:THR:HG23	1:D:504:ALA:H	1.83	0.44
1:J:173:PRO:O	1:J:174:GLY:O	2.36	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:A:499:GLY:C	1:A:501:GLN:H	2.25	0.43
1:G:215:GLY:HA2	1:G:231:ARG:HB2	2.00	0.43
1:J:103:LYS:HZ2	1:J:135:HIS:CD2	2.36	0.43
1:J:181:ARG:NH2	4:J:703:HOH:O	2.51	0.43
1:J:313:ASN:HB2	1:J:329:MET:HE1	2.00	0.43
1:J:457:THR:HG22	1:J:458:PRO:O	2.17	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:297:ILE:HG23	1:A:298:GLU:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:HG23	1:A:361:LEU:HD13	2.00	0.43
1:A:212:GLU:H	1:A:212:GLU:CD	2.25	0.43
1:D:457:THR:O	1:D:458:PRO:C	2.60	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:D:332:PRO:O	1:D:333:GLY:C	2.60	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: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
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:242:PHE:CE2	1:A:329:MET:HE1	2.54	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: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:276:ASP:O	1:G:281:LYS:HD3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:348:VAL:O	1:J:358:GLN:HB3	2.20	0.42
1:J:365:ASP:C	1:J:367:ASP:N	2.76	0.42
1:D:122:LEU:C	1:D:122:LEU:CD2	2.91	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:D:176:GLY:HA2	4:D:758:HOH:O	2.18	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: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:A:119:MET:HE3	1:A:146:TYR:CD1	2.55	0.42
1:A:212:GLU:CD	1:A:212:GLU:N	2.77	0.42
1:D:202:GLY:O	1:D:203:LEU:HD23	2.20	0.42
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:119:MET:HE3	1:A:146:TYR:HD1	1.85	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:97:VAL:HG21	1:D:119:MET:HE1	2.02	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:D:433:PRO:HG3	1:D:451:MET:HE3	2.00	0.42
1:G:211:PRO:HD3	1:G:318:PHE:HB3	2.02	0.42
1:J:97:VAL:HG13	1:J:119:MET:HE1	1.96	0.42
1:J:330:ARG:HA	1:J:380:GLY:O	2.20	0.42
1:J:332:PRO:C	1:J:376:VAL:HG13	2.44	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:J:395:MET:HE1	1:J:438:MET:SD	2.60	0.41
1:A:381:HIS:CD2	1:A:381:HIS:C	2.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:ASN:C	1:D:531:VAL:HG13	2.44	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: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: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: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: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:438:MET:HB3	1:G:449:VAL:HG12	2.02	0.41
1:J:292:GLY:CA	1:J:294:GLU:HG2	2.49	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:A:261:MET:HE1	1:A:329:MET:HG3	2.01	0.41
1:D:241:ALA:HB2	1:D:266:LEU:HD21	2.03	0.41
1:D:312:ALA:O	1:D:313:ASN:C	2.60	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: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: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: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:98:LEU:HG	1:G:99:VAL:N	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:HIS:HB3	4:A:733:HOH:O	2.20	0.40
1:A:195:ALA:C	1:A:198:VAL:H	2.29	0.40
1:J:235:MET:HE3	1:J:235:MET:HB3	1.96	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:G:535:ARG:HB2	4:G:721:HOH:O	2.22	0.40
1:J:306:ARG:NH2	1:J:309:HIS:HD1	2.17	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
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:292:GLY:C	1:J:294:GLU:HG2	2.47	0.40
1:J:307:PRO:C	1:J:309:HIS:N	2.80	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%)	6	1
1	D	467/494 (94%)	405 (87%)	51 (11%)	11 (2%)	4	1
1	G	467/494 (94%)	416 (89%)	40 (9%)	11 (2%)	4	1
1	J	467/494 (94%)	411 (88%)	52 (11%)	4 (1%)	14	5
All	All	1867/1976 (94%)	1652 (88%)	180 (10%)	35 (2%)	6	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
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 ⓘ

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%)	352 (90%)	40 (10%)	7	2
1	D	392/415 (94%)	353 (90%)	39 (10%)	7	2
1	G	388/415 (94%)	354 (91%)	34 (9%)	9	2
1	J	389/415 (94%)	349 (90%)	40 (10%)	7	2
All	All	1561/1660 (94%)	1408 (90%)	153 (10%)	8	2

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	137	MET
1	A	150	GLU
1	A	152	VAL
1	A	161	LEU
1	A	171	GLU
1	A	192	GLN
1	A	212	GLU
1	A	223	LYS
1	A	243	ASP
1	A	244	TRP
1	A	249	LYS
1	A	250	ASP
1	A	252	LYS
1	A	262	THR
1	A	265	ARG
1	A	290	VAL
1	A	295	LEU
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	390	GLN
1	A	425	SER
1	A	427	ASP
1	A	434	ASN
1	A	447	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	459	ASN
1	A	471	VAL
1	A	483	THR
1	A	494	VAL
1	A	502	ASN
1	A	505	SER
1	A	523	SER
1	A	525	MET
1	A	527	HIS
1	A	529	ASP
1	D	85	LYS
1	D	92	GLN
1	D	99	VAL
1	D	103	LYS
1	D	122	LEU
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	237	ARG
1	D	249	LYS
1	D	268	PRO
1	D	285	ILE
1	D	294	GLU
1	D	336	VAL
1	D	343	GLN
1	D	393	LEU
1	D	409	SER
1	D	412	ASP
1	D	415	THR
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	505[A]	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	505[B]	SER
1	D	514	THR
1	D	516	GLU
1	D	523	SER
1	D	527	HIS
1	D	530	ASN
1	D	531	VAL
1	G	82	LYS
1	G	85	LYS
1	G	87	GLN
1	G	92	GLN
1	G	98	LEU
1	G	99	VAL
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	232	GLU
1	G	250	ASP
1	G	266	LEU
1	G	270	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	459	ASN
1	G	463	VAL
1	G	464	ILE
1	G	483	THR
1	G	484	LEU
1	G	524	PRO
1	G	527	HIS
1	G	535	ARG
1	G	538	GLU
1	G	545	SER
1	J	85	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	105	SER
1	J	111	THR
1	J	122	LEU
1	J	125	TRP
1	J	137	MET
1	J	143	PRO
1	J	147	LYS
1	J	159	LYS
1	J	161	LEU
1	J	163	ILE
1	J	172	ASP
1	J	179	ILE
1	J	188	ARG
1	J	191	LEU
1	J	218	VAL
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
1	J	376	VAL
1	J	377	ILE
1	J	411	HIS
1	J	422	VAL
1	J	459	ASN
1	J	491	LYS
1	J	514	THR
1	J	521	LEU
1	J	522	PRO
1	J	527	HIS
1	J	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	382	GLN
1	A	396	ASN
1	A	468	ASN
1	D	382	GLN
1	D	401	ASN
1	D	410	ASN
1	G	278	GLN
1	G	309	HIS
1	G	459	ASN
1	J	192	GLN
1	J	342	ASN
1	J	382	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 oligosaccharides 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	603	-	4,4,4	0.71	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	603[A]	-	4,4,4	0.46	0	6,6,6	1.16	0
3	SO4	G	606	-	4,4,4	0.33	0	6,6,6	0.69	0
3	SO4	D	604	-	4,4,4	0.44	0	6,6,6	0.68	0
3	SO4	J	603[A]	-	4,4,4	0.47	0	6,6,6	0.41	0
3	SO4	G	605	-	4,4,4	0.74	0	6,6,6	0.62	0
3	SO4	G	604	-	4,4,4	0.49	0	6,6,6	0.17	0
3	SO4	D	603	-	4,4,4	0.64	0	6,6,6	0.44	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	606	SO4	1	0
3	D	604	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%)	-1.15	0 100 100	9, 19, 28, 42	4 (0%)
1	D	467/494 (94%)	-1.19	0 100 100	8, 17, 26, 37	3 (0%)
1	G	467/494 (94%)	-1.19	0 100 100	8, 17, 25, 38	3 (0%)
1	J	467/494 (94%)	-1.15	0 100 100	10, 19, 30, 37	4 (0%)
All	All	1868/1976 (94%)	-1.17	0 100 100	8, 18, 27, 42	14 (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 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	SO4	D	603	5/5	0.99	0.04	19,20,24,26	5
3	SO4	D	604	5/5	0.99	0.03	9,12,13,14	5
3	SO4	G	603	5/5	0.99	0.04	15,19,22,23	0
3	SO4	G	604	5/5	0.99	0.04	17,17,20,25	5

Continued on next page...

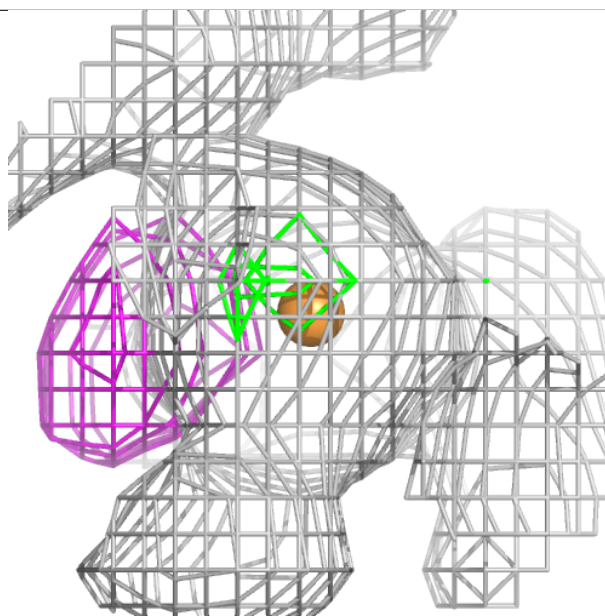
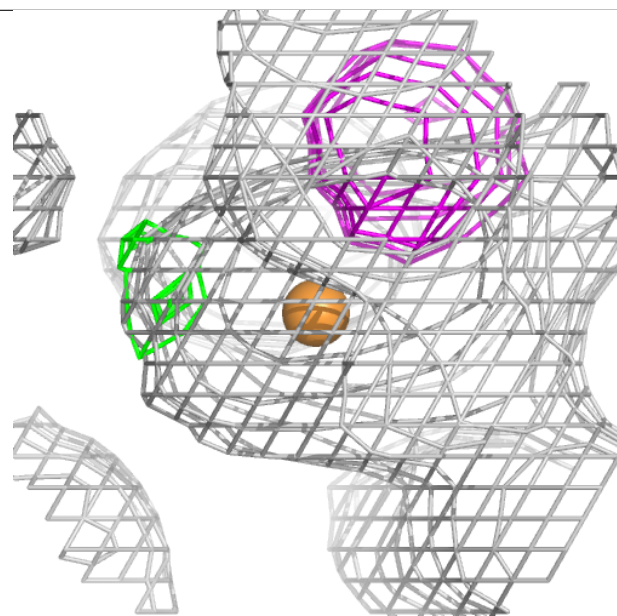
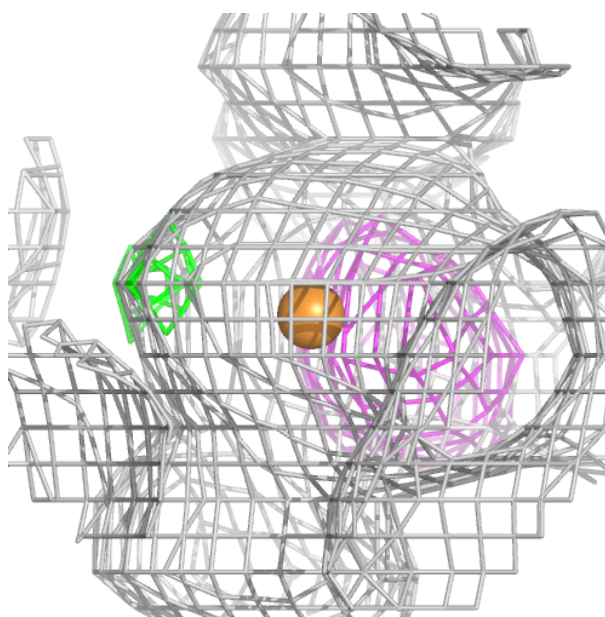
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	G	605	5/5	0.99	0.04	17,18,19,22	5
3	SO4	G	606	5/5	0.99	0.05	18,19,22,23	0
3	SO4	J	603[A]	5/5	0.99	0.04	18,18,19,23	0
2	CU	G	602[B]	1/1	1.00	0.02	15,15,15,15	1
2	CU	J	601	1/1	1.00	0.01	23,23,23,23	0
2	CU	J	602	1/1	1.00	0.02	19,19,19,19	0
3	SO4	A	603[A]	5/5	1.00	0.04	8,8,8,11	5
2	CU	A	601	1/1	1.00	0.03	15,15,15,15	0
2	CU	A	602	1/1	1.00	0.02	22,22,22,22	0
2	CU	D	601	1/1	1.00	0.02	18,18,18,18	0
2	CU	D	602[A]	1/1	1.00	0.02	14,14,14,14	1
2	CU	D	602[B]	1/1	1.00	0.02	6,6,6,6	1
2	CU	G	601	1/1	1.00	0.02	12,12,12,12	0
2	CU	G	602[A]	1/1	1.00	0.02	17,17,17,17	1

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.

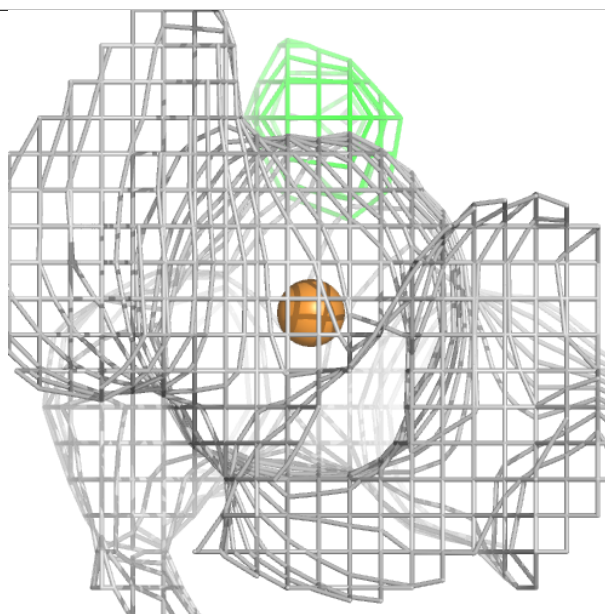
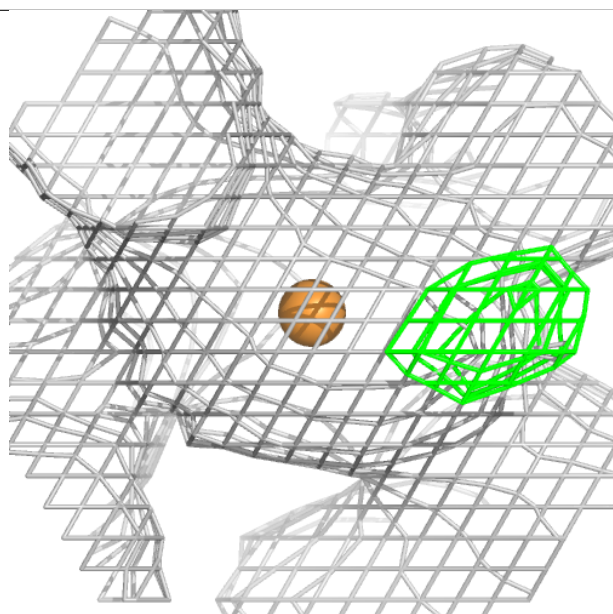
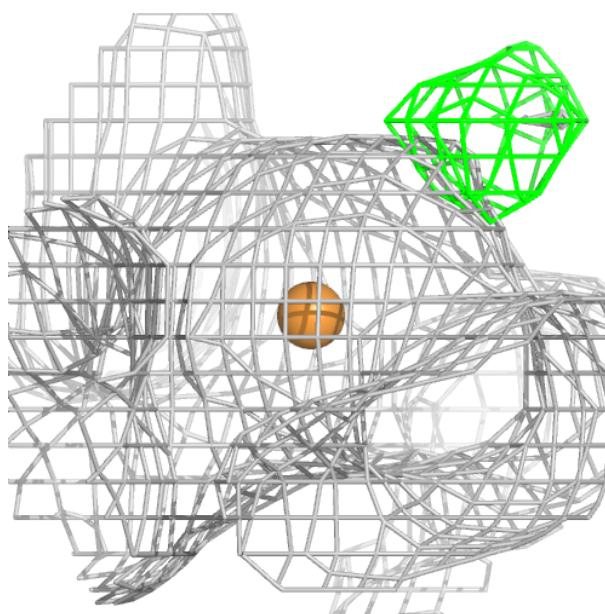
Electron density around CU G 602 (B):

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



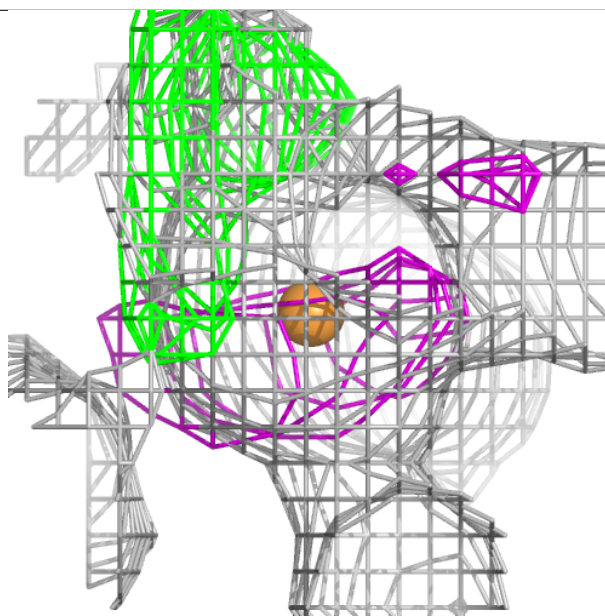
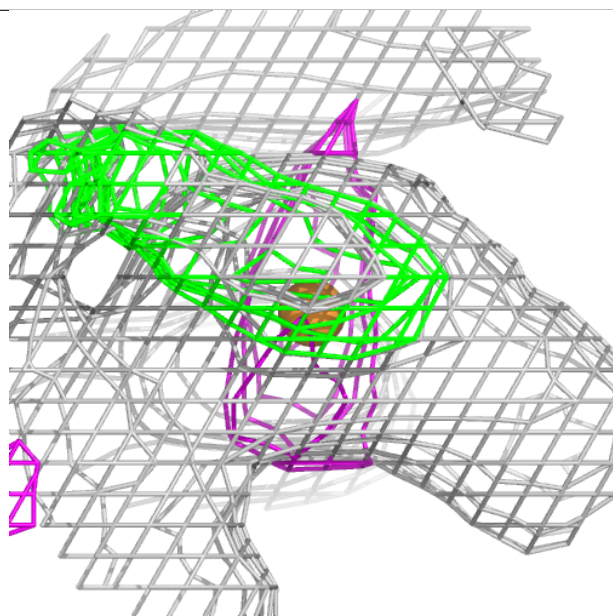
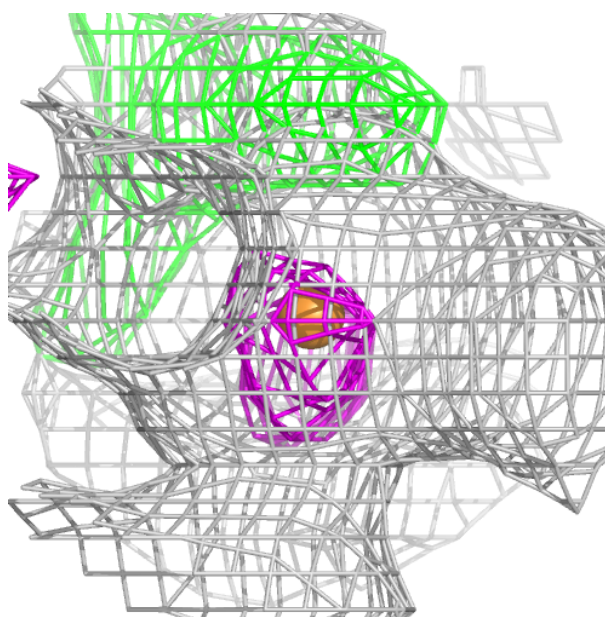
Electron density around CU J 601:

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



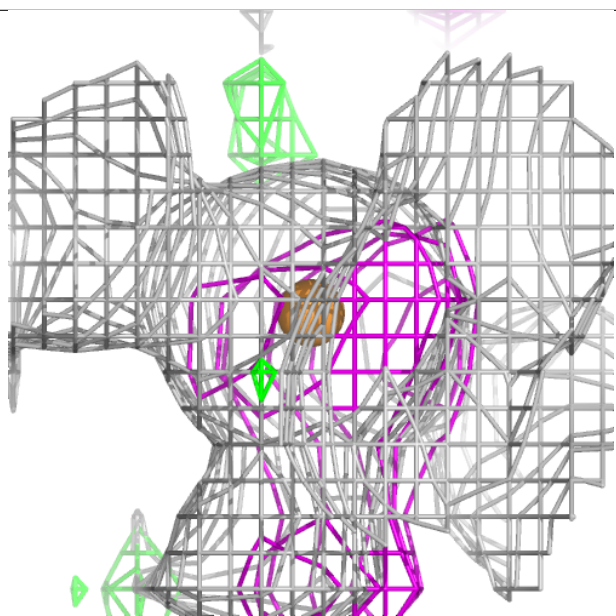
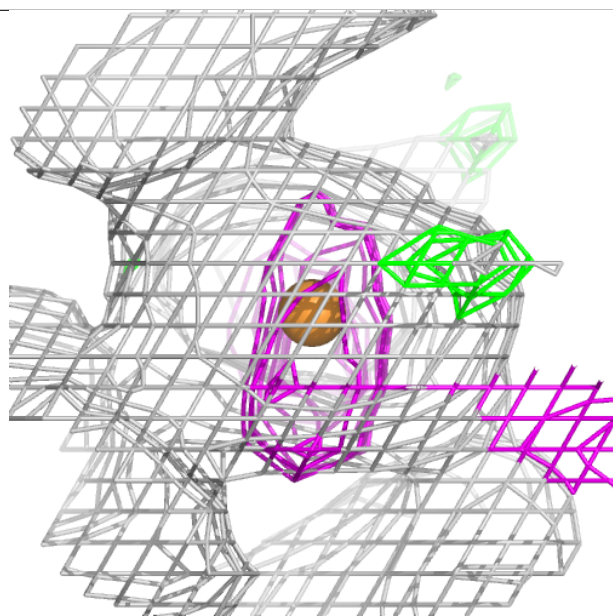
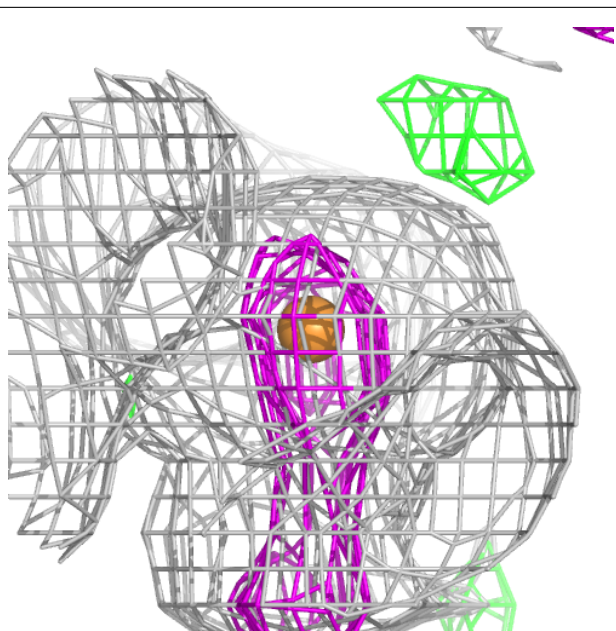
Electron density around CU J 602:

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



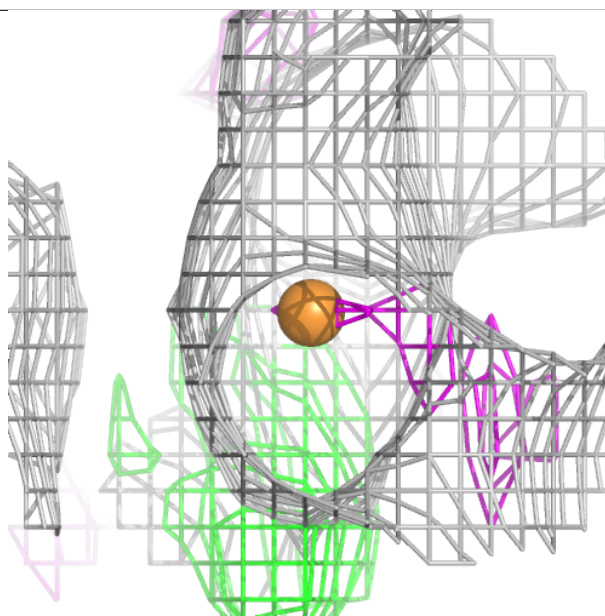
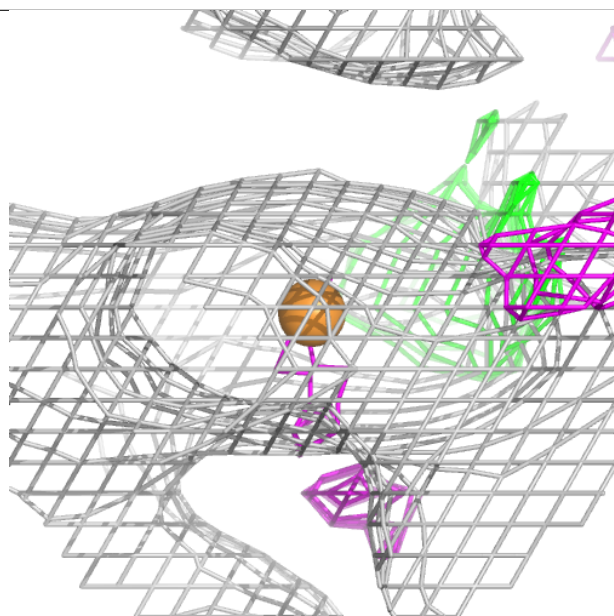
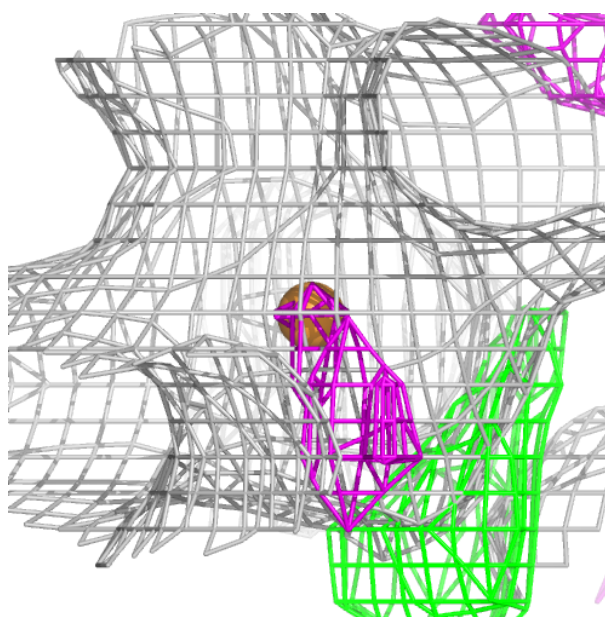
Electron density around CU A 601:

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



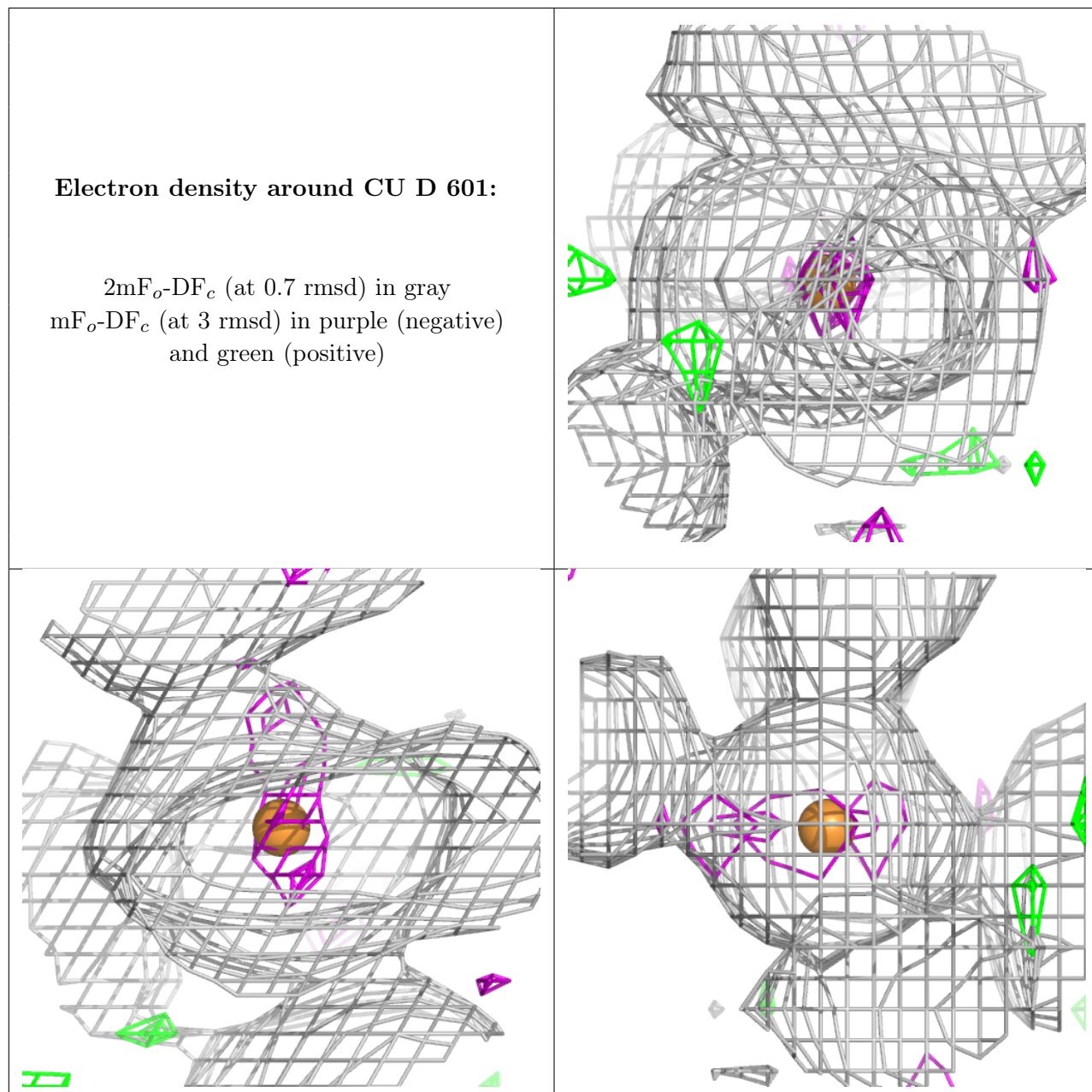
Electron density around CU A 602:

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



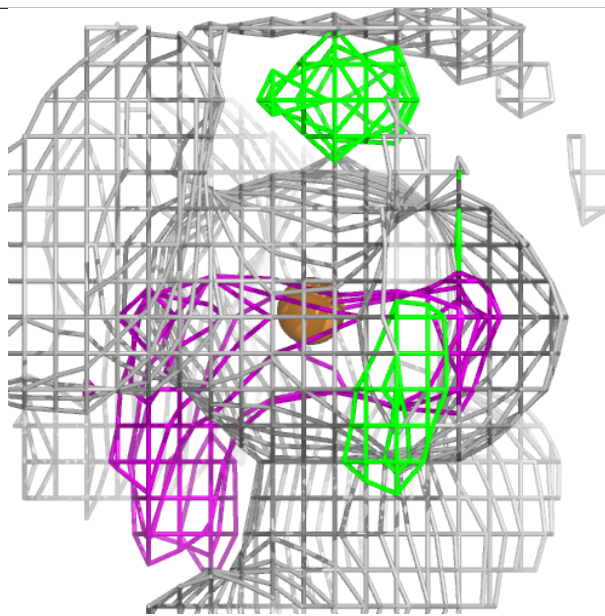
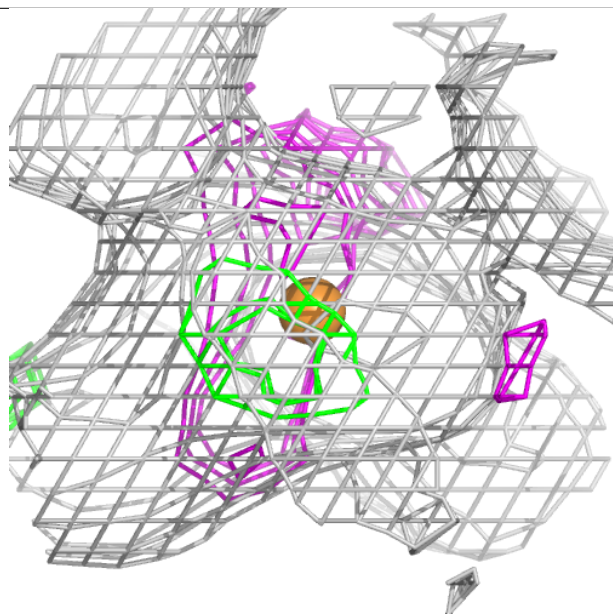
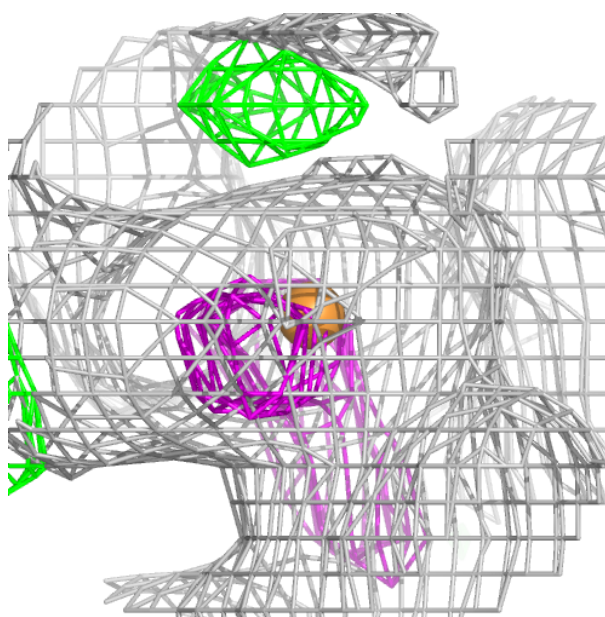
Electron density around CU D 601:

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



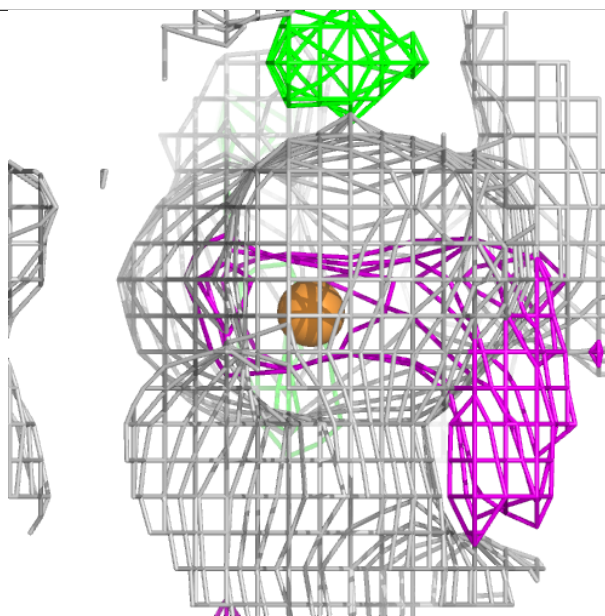
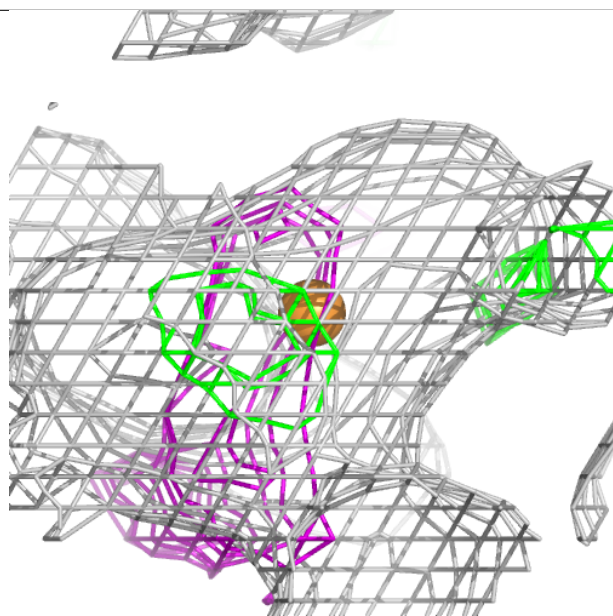
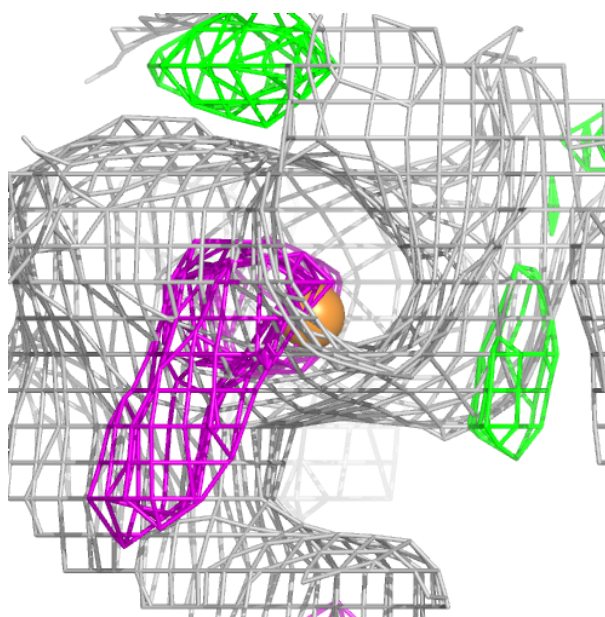
Electron density around CU D 602 (A):

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



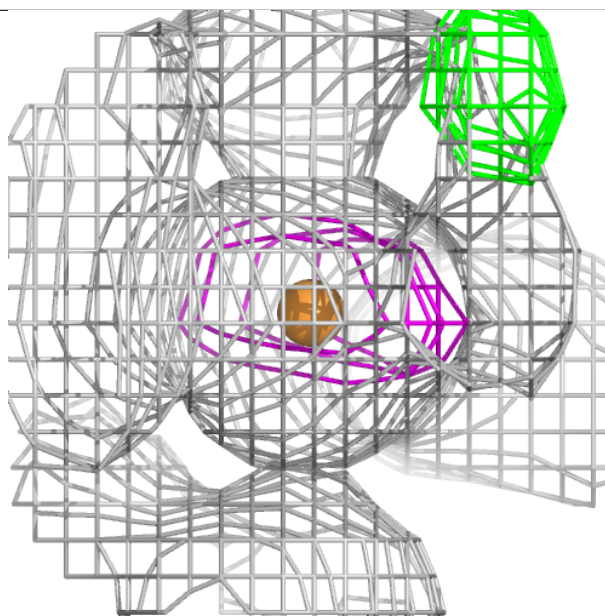
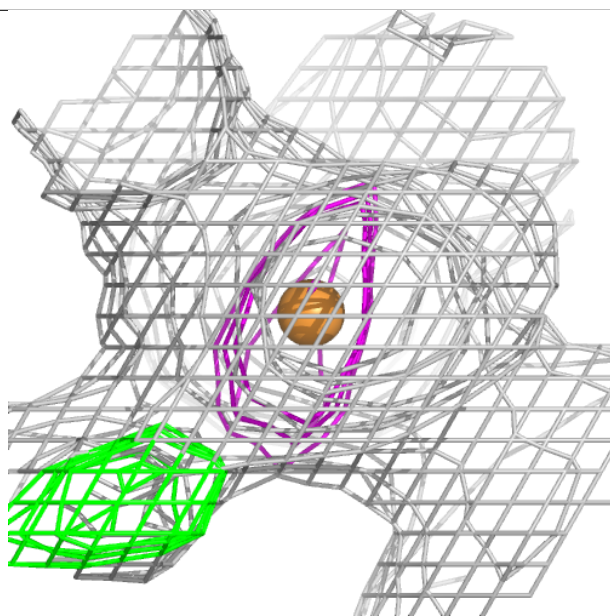
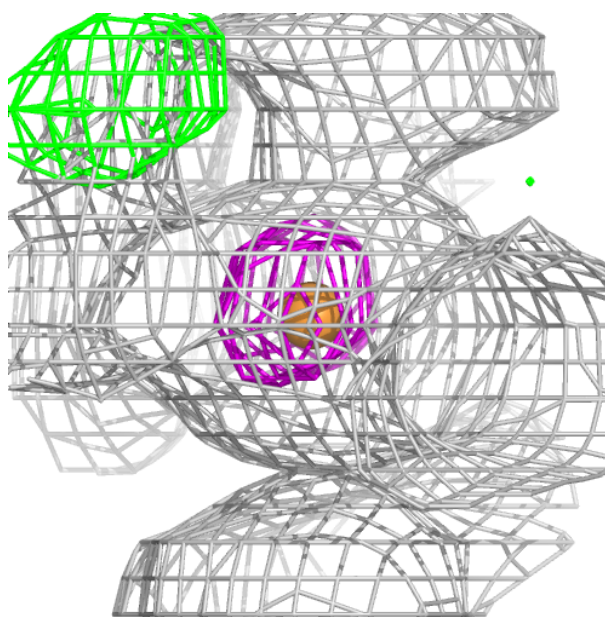
Electron density around CU D 602 (B):

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



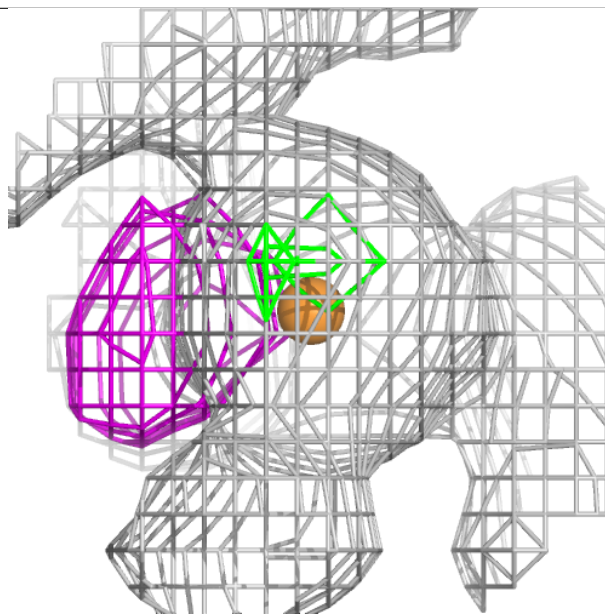
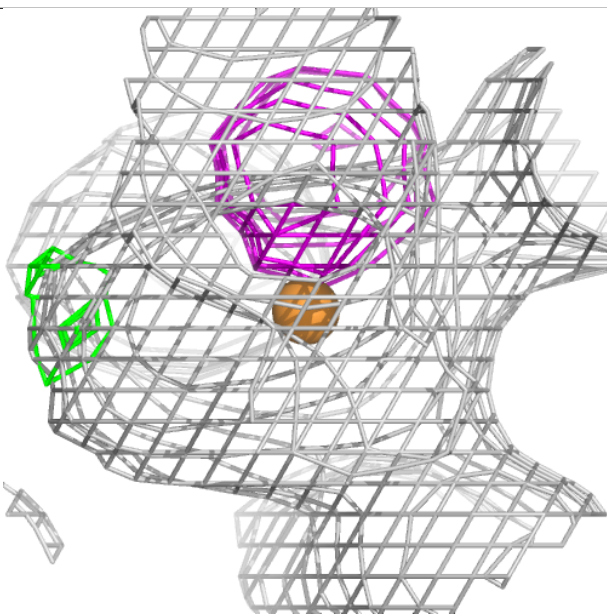
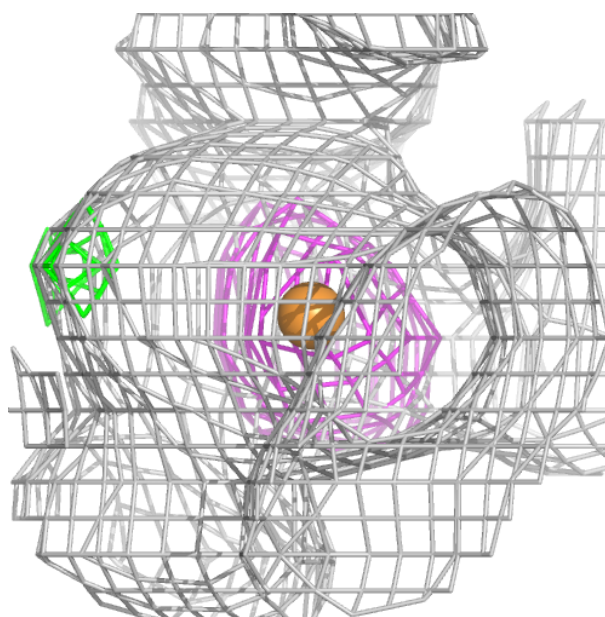
Electron density around CU G 601:

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



Electron density around CU G 602 (A):

$2mF_o-DF_c$ (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.