



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:05 AM UTC

PDB ID : 8X77 / pdb_00008x77
Title : Enterovirus proteinase with host factor
Authors : Gao, X.; Cui, S.
Deposited on : 2023-11-23
Resolution : 3.52 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

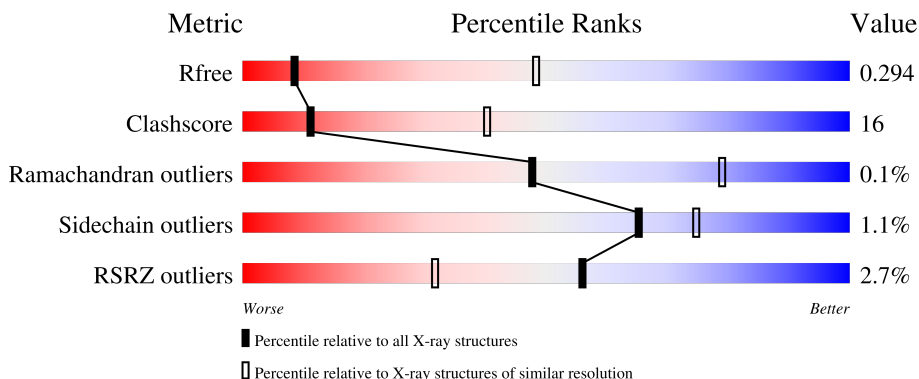
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	594	
1	B	594	
1	D	594	
1	G	594	
2	C	150	

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Mol	Chain	Length	Quality of chain
2	E	150	<p>%</p> <p>57% 34% 6%</p>
2	F	150	<p>69% 24% 6%</p>
2	H	150	<p>3%</p> <p>63% 29% 6%</p>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SAH	B	601	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20944 atoms, of which 20 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 Actin-histidine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	478	3831	2456	642	717	16	0	0	0
1	D	477	3752	2414	625	696	17	0	1	0
1	G	477	3752	2414	625	696	17	0	1	0
1	A	478	3752	2414	625	697	16	0	1	0

- Molecule 2 is a protein called 2A protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	141	1093	682	198	207	6	0	1	0
2	E	141	1101	686	198	211	6	0	1	0
2	H	141	1095	682	198	209	6	0	1	0
2	C	141	1101	686	198	211	6	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	110	ALA	CYS	engineered mutation	UNP R9YK28
E	110	ALA	CYS	engineered mutation	UNP R9YK28
H	110	ALA	CYS	engineered mutation	UNP R9YK28
C	110	ALA	CYS	engineered mutation	UNP R9YK28

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

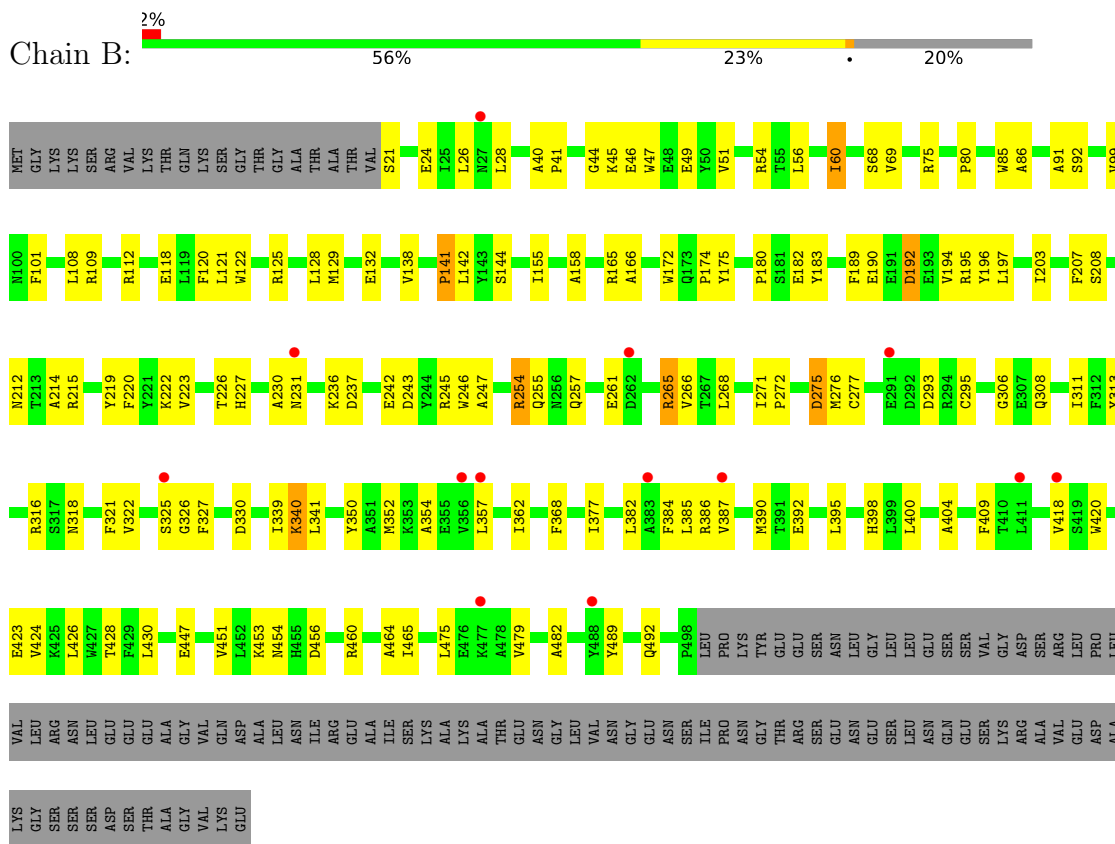
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	289	Total 289	O 289	0	0
5	H	49	Total 49	O 49	0	0
5	A	287	Total 287	O 287	0	0
5	C	38	Total 38	O 38	0	0

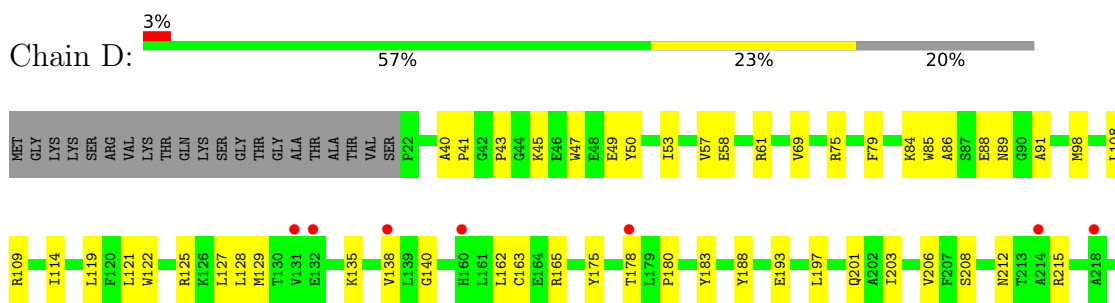
3 Residue-property plots

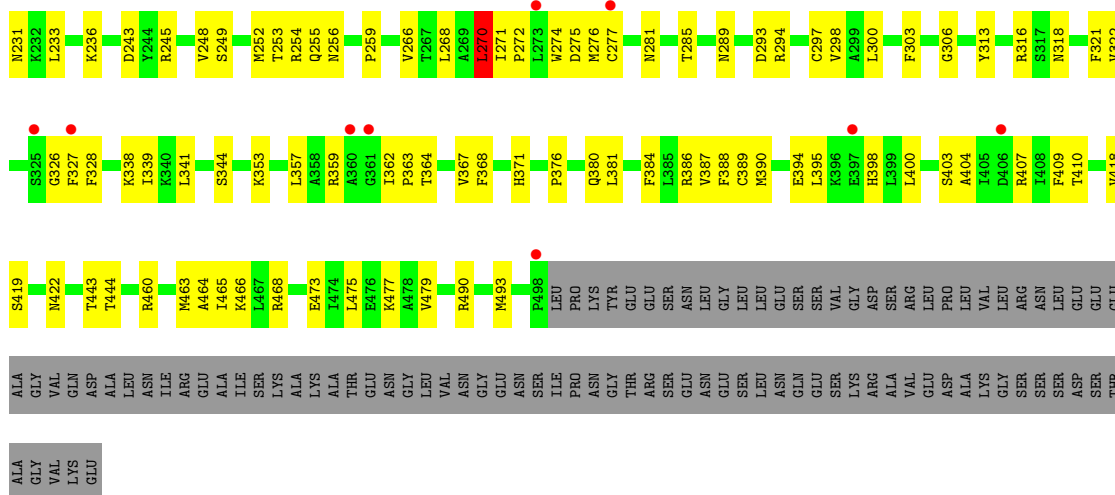
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

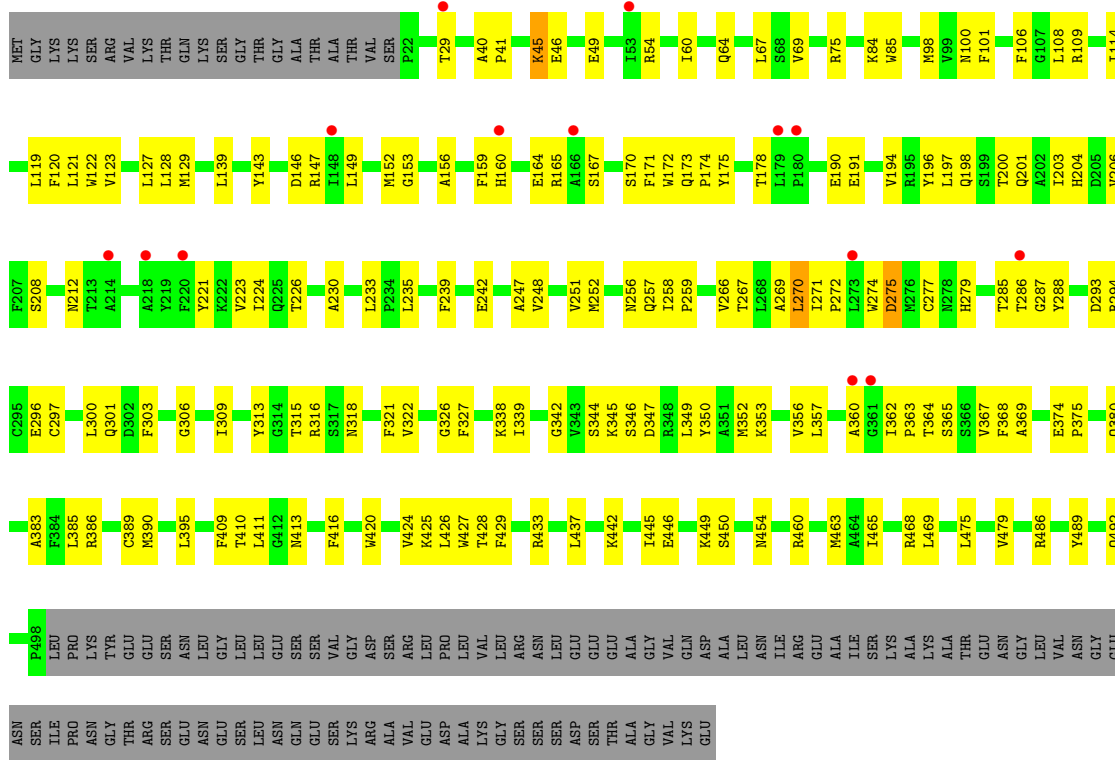


- Molecule 1: Actin-histidine N-methyltransferase

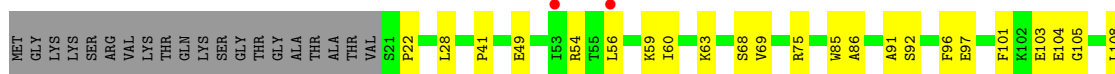




• Molecule 1: Actin-histidine N-methyltransferase

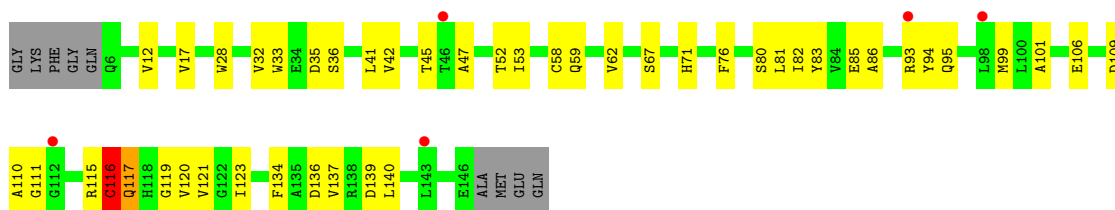


• Molecule 1: Actin-histidine N-methyltransferase



● Molecule 2: 2A protein

Chain C:  3% 63% 29% 6%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	148.95Å 57.48Å 198.62Å 90.00° 110.88° 90.00°	Depositor
Resolution (Å)	19.99 – 3.52 19.99 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-3.52) 98.9 (19.99-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.52Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.274 , 0.291 0.282 , 0.294	Depositor DCC
R_{free} test set	1988 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtrriage
Reported twinning fraction	0.090 for h,-k,-h-l	Depositor
Outliers	2 of 39534 reflections (0.005%)	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20944	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8866e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAH

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	0.23	0/3842	0.47	2/5219 (0.0%)
1	B	0.46	2/3921 (0.1%)	0.79	7/5312 (0.1%)
1	D	0.54	1/3841 (0.0%)	0.62	5/5214 (0.1%)
1	G	0.81	3/3841 (0.1%)	0.51	5/5214 (0.1%)
2	C	0.25	0/1130	1.01	4/1537 (0.3%)
2	E	0.22	0/1130	0.49	1/1537 (0.1%)
2	F	0.39	1/1122 (0.1%)	0.58	0/1527
2	H	0.19	0/1121	0.45	0/1524
All	All	0.50	7/19948 (0.0%)	0.63	24/27084 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	4
1	D	0	1
1	G	0	1
2	E	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	45	LYS	C-N	39.16	1.83	1.33
1	D	400	LEU	C-N	-30.36	0.89	1.33
1	G	275	ASP	C-N	-23.31	0.96	1.33
1	G	270	LEU	C-N	-17.80	1.13	1.33
1	B	275	ASP	C-N	-12.66	1.15	1.33
1	B	40	ALA	C-N	6.65	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	140	LEU	C-O	-5.48	1.18	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	116	CYS	N-CA-C	29.38	149.65	113.23
1	D	400	LEU	O-C-N	20.37	148.12	123.27
1	B	400	LEU	O-C-N	-18.99	101.05	123.27
1	B	40	ALA	O-C-N	-17.40	105.81	121.30
2	C	117	GLN	N-CA-CB	16.73	138.76	110.49
1	D	400	LEU	CA-C-N	-15.56	90.91	121.41
1	D	400	LEU	C-N-CA	-15.56	90.91	121.41
1	G	270	LEU	O-C-N	-11.95	109.30	123.16
1	G	275	ASP	O-C-N	-10.19	106.02	122.42
1	G	275	ASP	CA-C-N	8.15	135.02	122.23
1	G	275	ASP	C-N-CA	8.15	135.02	122.23
1	G	45	LYS	O-C-N	-8.05	112.98	122.15
2	C	117	GLN	N-CA-C	-7.94	93.89	110.80
2	C	116	CYS	CB-CA-C	-7.88	93.56	109.55
1	A	22	PRO	N-CA-C	-7.63	102.93	113.53
1	B	24	GLU	N-CA-C	-7.60	103.00	111.28
1	D	270	LEU	O-C-N	-6.77	115.31	123.16
1	B	400	LEU	CA-C-N	6.21	133.58	121.41
1	B	400	LEU	C-N-CA	6.21	133.58	121.41
2	E	141	LEU	N-CA-C	-5.80	106.29	113.19
1	D	388	PHE	CA-C-O	-5.77	114.30	120.42
1	B	60	ILE	N-CA-C	-5.31	105.54	110.53
1	B	275	ASP	O-C-N	-5.25	114.77	122.43
1	A	346	SER	N-CA-C	-5.19	104.33	111.81

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	21	SER	Peptide
1	B	275	ASP	Mainchain
1	B	295	CYS	Mainchain
1	B	44	GLY	Mainchain
1	D	270	LEU	Mainchain
2	E	137	VAL	Mainchain
1	G	270	LEU	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3752	0	3583	118	0
1	B	3831	0	3733	124	0
1	D	3752	0	3583	96	0
1	G	3752	0	3581	137	0
2	C	1101	0	1039	37	0
2	E	1101	0	1039	41	0
2	F	1093	0	1031	45	0
2	H	1095	0	1033	41	0
3	B	26	20	17	12	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	A	287	0	0	1	1
5	B	324	0	0	13	2
5	C	38	0	0	2	0
5	D	297	0	0	4	4
5	E	61	0	0	2	0
5	F	72	0	0	0	1
5	G	289	0	0	2	2
5	H	49	0	0	4	0
All	All	20924	20	18639	621	6

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 16.

All (621) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:MET:HE3	1:B:395:LEU:CD1	1.27	1.57
1:B:352:MET:CE	1:B:395:LEU:HD12	1.47	1.43
1:G:45:LYS:C	1:G:46:GLU:N	1.83	1.35
1:D:256:ASN:ND2	1:D:274:TRP:CH2	2.08	1.21
2:F:137:VAL:O	2:F:140:LEU:HD22	1.41	1.21
1:G:175:TYR:OH	1:G:275:ASP:OD2	1.65	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:MET:HE1	1:B:418:VAL:HG11	1.31	1.10
1:D:390:MET:HE1	1:D:418:VAL:HG11	1.29	1.09
2:F:140:LEU:HD23	2:F:140:LEU:O	1.54	1.06
1:B:352:MET:HG2	1:B:395:LEU:HD13	1.38	1.01
1:B:352:MET:CE	1:B:395:LEU:CD1	2.17	1.01
1:G:256:ASN:ND2	1:G:274:TRP:CH2	2.29	1.01
1:B:237:ASP:HB2	5:B:732:HOH:O	1.57	1.00
1:D:256:ASN:ND2	1:D:274:TRP:HH2	1.47	0.99
1:D:256:ASN:OD1	1:D:274:TRP:CZ3	2.15	0.98
1:G:41:PRO:HG3	1:G:49:GLU:HG3	1.48	0.96
1:D:183:TYR:O	1:D:460:ARG:NH2	1.99	0.95
2:H:6:GLN:HE21	2:H:6:GLN:N	1.65	0.95
1:G:256:ASN:ND2	1:G:274:TRP:HH2	1.64	0.94
1:D:389:CYS:HB2	1:D:422:ASN:OD1	1.68	0.92
1:D:40:ALA:C	1:D:41:PRO:N	2.29	0.91
1:G:256:ASN:OD1	1:G:274:TRP:CZ3	2.24	0.91
1:G:256:ASN:HD21	1:G:274:TRP:HH2	0.93	0.91
1:A:390:MET:O	5:A:601:HOH:O	1.90	0.88
2:E:140:LEU:HD12	2:E:142:TRP:CE2	2.10	0.87
1:G:175:TYR:OH	1:G:275:ASP:CG	2.18	0.86
1:B:231:ASN:OD1	1:B:236:LYS:NZ	2.08	0.86
1:D:465:ILE:HG12	1:D:468:ARG:HH21	1.42	0.85
1:A:104:GLU:OE2	1:A:308:GLN:NE2	2.10	0.85
1:D:409:PHE:CZ	2:E:83:TYR:HB2	2.12	0.84
1:B:390:MET:CE	1:B:418:VAL:HG11	2.06	0.84
1:B:276:MET:O	3:B:601:SAH:HB2	1.76	0.84
1:G:173:GLN:HG3	1:G:174:PRO:HD3	1.60	0.84
2:C:12:VAL:HG21	2:C:53:ILE:HD11	1.60	0.84
1:D:175:TYR:OH	1:D:275:ASP:OD2	1.95	0.83
1:B:352:MET:HE3	1:B:395:LEU:HD13	1.57	0.83
1:G:121:LEU:HB2	1:G:297:CYS:HB3	1.61	0.82
1:A:430:LEU:HD23	1:A:482:ALA:HB2	1.60	0.82
1:D:357:LEU:HD11	1:D:364:THR:HA	1.60	0.82
1:B:69:VAL:HB	5:B:704:HOH:O	1.79	0.81
1:B:222:LYS:NZ	5:B:703:HOH:O	2.14	0.81
1:G:175:TYR:HH	1:G:275:ASP:CG	1.89	0.81
1:B:352:MET:CG	1:B:395:LEU:HD13	2.10	0.80
1:B:352:MET:HE1	1:B:392:GLU:HA	1.62	0.80
1:D:253:THR:HG23	1:D:254:ARG:HG3	1.61	0.80
1:A:443:THR:OG1	1:A:468:ARG:NH1	2.14	0.79
1:D:256:ASN:CG	1:D:274:TRP:CH2	2.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ALA:HB1	1:D:91:ALA:HB3	1.64	0.78
1:G:224:ILE:HD12	1:G:230:ALA:HB1	1.66	0.78
1:B:316:ARG:NH2	1:B:325:SER:OG	2.17	0.76
1:G:40:ALA:C	1:G:41:PRO:N	2.44	0.76
1:D:254:ARG:NH2	1:D:276:MET:SD	2.59	0.76
1:D:398:HIS:O	1:D:404:ALA:HB1	1.85	0.76
1:B:352:MET:CE	1:B:395:LEU:HD13	2.15	0.75
1:B:386:ARG:HA	1:B:426:LEU:HD21	1.69	0.75
1:G:128:LEU:HD22	1:G:271:ILE:HG12	1.70	0.74
1:A:69:VAL:O	1:A:165:ARG:NH2	2.18	0.74
2:C:12:VAL:HG21	2:C:53:ILE:CD1	2.17	0.74
1:A:390:MET:SD	1:A:422:ASN:ND2	2.61	0.74
1:D:122:TRP:HB2	1:D:294:ARG:HD2	1.70	0.72
1:D:313:TYR:O	1:D:316:ARG:NH1	2.22	0.72
1:A:170:SER:HB3	1:A:173:GLN:HG2	1.70	0.72
1:D:201:GLN:NE2	1:D:338:LYS:O	2.19	0.71
1:G:198:GLN:HE22	1:G:442:LYS:HB3	1.55	0.71
1:B:327:PHE:CD2	3:B:601:SAH:C6	2.73	0.71
1:G:338:LYS:HB3	1:G:367:VAL:HG12	1.73	0.71
2:E:20:ARG:NH1	2:E:34:GLU:OE1	2.23	0.70
2:H:30:ASN:HB3	2:H:44:SER:HB3	1.73	0.70
1:A:212:ASN:OD1	1:A:215:ARG:NH2	2.20	0.70
2:F:12:VAL:HG11	2:F:53:ILE:HD11	1.73	0.70
1:B:128:LEU:HD22	1:B:271:ILE:HA	1.75	0.69
1:D:121:LEU:HB2	1:D:297:CYS:HB3	1.72	0.69
1:B:276:MET:HA	3:B:601:SAH:HB1	1.74	0.69
1:G:256:ASN:CG	1:G:274:TRP:CH2	2.71	0.69
1:A:203:ILE:HA	1:A:206:VAL:HG12	1.76	0.68
1:B:266:VAL:HG13	2:F:115:ARG:HB2	1.76	0.68
1:G:301:GLN:HG3	1:G:303:PHE:HE1	1.58	0.68
1:G:223:VAL:HA	1:G:226:THR:HG22	1.75	0.68
1:D:208:SER:O	1:D:212:ASN:ND2	2.26	0.68
1:A:97:GLU:OE2	1:A:109:ARG:NH2	2.27	0.68
1:B:75:ARG:HH22	3:B:601:SAH:C	2.07	0.68
1:A:254:ARG:NH2	1:A:313:TYR:OH	2.27	0.67
2:C:17:VAL:HG22	2:C:42:VAL:HG23	1.75	0.67
1:G:208:SER:O	1:G:212:ASN:ND2	2.26	0.67
1:D:390:MET:HE1	1:D:418:VAL:CG1	2.17	0.67
1:G:230:ALA:HA	1:G:233:LEU:HD13	1.77	0.66
1:B:316:ARG:HH21	1:B:325:SER:HG	1.39	0.66
2:F:140:LEU:O	2:F:140:LEU:CD2	2.37	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:PHE:O	1:D:326:GLY:N	2.26	0.66
1:G:321:PHE:O	1:G:326:GLY:N	2.27	0.66
1:B:69:VAL:N	5:B:704:HOH:O	2.20	0.66
1:A:409:PHE:CE1	2:C:83:TYR:HA	2.30	0.66
1:B:99:VAL:HG21	1:B:109:ARG:HD3	1.78	0.65
1:A:75:ARG:NE	1:A:178:THR:O	2.29	0.65
1:A:208:SER:O	1:A:212:ASN:ND2	2.30	0.65
1:D:256:ASN:OD1	1:D:274:TRP:HZ3	1.77	0.65
1:B:327:PHE:CE2	3:B:601:SAH:N6	2.65	0.65
2:F:137:VAL:CG2	2:F:140:LEU:HD11	2.26	0.65
1:G:409:PHE:CE1	2:H:94:TYR:HA	2.31	0.65
1:B:409:PHE:CD1	2:F:94:TYR:HA	2.32	0.65
1:D:58:GLU:OE1	1:D:61:ARG:NE	2.27	0.65
1:D:327:PHE:HA	1:D:463:MET:SD	2.37	0.64
1:A:233:LEU:HD13	1:A:235:LEU:HB2	1.79	0.64
1:D:384:PHE:O	1:D:387:VAL:HG22	1.96	0.64
2:H:78:LYS:HE2	2:H:79:PRO:HD2	1.79	0.64
2:F:140:LEU:HD23	2:F:140:LEU:C	2.21	0.64
2:H:20:ARG:NH1	2:H:34:GLU:OE1	2.29	0.64
1:G:41:PRO:HD3	1:G:49:GLU:CD	2.22	0.64
1:B:385:LEU:O	1:B:426:LEU:HD11	1.98	0.63
1:G:313:TYR:HB3	1:G:316:ARG:NH2	2.13	0.63
1:D:114:ILE:HB	1:D:303:PHE:HB2	1.78	0.63
1:D:256:ASN:HD21	1:D:274:TRP:HH2	0.72	0.63
1:B:386:ARG:CA	1:B:426:LEU:HD21	2.28	0.63
2:F:16:ARG:NH1	2:F:27:ASP:OD1	2.31	0.63
1:D:125:ARG:NH2	1:D:259:PRO:O	2.28	0.63
1:A:182:GLU:OE1	1:A:460:ARG:NH2	2.31	0.63
1:G:109:ARG:NH1	1:G:306:GLY:O	2.31	0.63
1:B:430:LEU:HD23	1:B:482:ALA:HB2	1.80	0.63
1:B:182:GLU:OE1	1:B:460:ARG:NH2	2.31	0.62
1:D:357:LEU:HD12	1:D:362:ILE:HG22	1.80	0.62
1:A:356:VAL:O	1:A:360:ALA:N	2.31	0.62
1:D:256:ASN:CG	1:D:274:TRP:CZ3	2.76	0.62
1:A:389:CYS:SG	1:A:425:LYS:HG2	2.39	0.62
1:G:129:MET:HE2	1:G:172:TRP:HB3	1.81	0.62
2:E:39:ASP:OD1	2:E:90:TYR:OH	2.13	0.62
1:D:79:PHE:HB3	1:D:98:MET:HE3	1.81	0.62
2:H:38:ARG:NH1	2:H:139:ASP:OD2	2.24	0.62
2:H:46:THR:HG23	5:H:309:HOH:O	1.98	0.62
2:H:58:CYS:SG	2:H:117:GLN:NE2	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:PHE:CD1	2:C:94:TYR:HA	2.34	0.62
1:B:352:MET:SD	1:B:395:LEU:HB3	2.40	0.61
1:G:122:TRP:HB2	1:G:294:ARG:HD2	1.82	0.61
1:G:197:LEU:HB3	1:G:203:ILE:HD13	1.82	0.61
1:G:313:TYR:HB3	1:G:316:ARG:HH22	1.66	0.61
1:B:208:SER:O	1:B:212:ASN:ND2	2.33	0.61
2:C:76:PHE:HB3	2:C:101:ALA:HB2	1.83	0.61
1:B:377:ILE:HD12	1:B:382:LEU:HB2	1.83	0.61
1:D:109:ARG:NE	1:D:306:GLY:O	2.30	0.61
2:E:38:ARG:NH2	2:E:136:ASP:O	2.34	0.60
1:A:263:GLY:O	2:C:115:ARG:NH1	2.34	0.60
1:B:352:MET:SD	1:B:395:LEU:CB	2.90	0.60
1:B:276:MET:HA	3:B:601:SAH:CB	2.31	0.60
1:A:254:ARG:NE	1:A:275:ASP:O	2.34	0.60
1:B:125:ARG:NH2	1:B:293:ASP:OD2	2.35	0.60
2:E:36:SER:O	2:E:95:GLN:NE2	2.35	0.60
2:E:140:LEU:HD12	2:E:142:TRP:NE1	2.17	0.60
1:B:129:MET:HE3	1:B:175:TYR:HD2	1.67	0.60
1:D:89:ASN:HB2	1:D:127:LEU:HD21	1.82	0.60
1:G:175:TYR:CZ	1:G:272:PRO:HA	2.36	0.60
1:B:321:PHE:O	1:B:326:GLY:N	2.33	0.59
1:G:353:LYS:HG3	1:G:395:LEU:HD11	1.84	0.59
1:G:69:VAL:H	1:G:165:ARG:HH22	1.50	0.59
1:A:386:ARG:NH1	1:A:411:LEU:O	2.36	0.59
2:C:45:THR:HG22	2:C:47:ALA:H	1.68	0.59
1:B:197:LEU:HG	1:B:464:ALA:HB1	1.85	0.59
1:G:285:THR:HG21	1:G:300:LEU:HA	1.82	0.59
1:B:129:MET:HE2	1:B:172:TRP:HB3	1.85	0.59
1:D:398:HIS:C	1:D:404:ALA:HB1	2.28	0.59
1:A:101:PHE:CE2	1:A:308:GLN:HB2	2.37	0.59
1:A:128:LEU:HD22	1:A:271:ILE:HA	1.83	0.59
1:A:119:LEU:HA	1:A:298:VAL:HA	1.85	0.59
1:G:259:PRO:HA	1:G:266:VAL:HA	1.84	0.59
1:G:327:PHE:HA	1:G:463:MET:HE3	1.84	0.59
2:H:6:GLN:N	2:H:6:GLN:NE2	2.45	0.59
1:A:487:GLU:HA	1:A:490:ARG:HG2	1.85	0.59
2:C:81:LEU:HD11	2:C:94:TYR:HB2	1.85	0.58
1:G:303:PHE:CE2	1:G:309:ILE:HG13	2.38	0.58
1:B:189:PHE:CE1	1:B:460:ARG:HB3	2.37	0.58
1:A:175:TYR:OH	1:A:275:ASP:OD2	2.14	0.58
2:E:82:ILE:HG13	2:E:100:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:PHE:CD1	2:H:94:TYR:HA	2.38	0.58
2:F:140:LEU:HG	2:F:143:LEU:HB2	1.85	0.58
1:G:349:LEU:HD23	1:G:395:LEU:HD12	1.86	0.58
2:E:21:HIS:HB3	2:E:90:TYR:CE2	2.38	0.58
1:D:197:LEU:HG	1:D:203:ILE:HD12	1.86	0.58
1:D:398:HIS:CE1	1:D:407:ARG:HB3	2.39	0.58
1:D:390:MET:CE	1:D:418:VAL:HG11	2.20	0.58
2:E:37:SER:O	2:E:96:SER:N	2.29	0.58
2:E:21:HIS:HB3	2:E:90:TYR:CZ	2.40	0.57
1:G:288:TYR:OH	1:G:293:ASP:OD1	2.22	0.57
1:G:203:ILE:HA	1:G:206:VAL:HG12	1.86	0.57
1:A:380:GLN:OE1	1:A:380:GLN:N	2.37	0.57
1:G:201:GLN:HE22	1:G:338:LYS:HB2	1.70	0.57
1:B:80:PRO:HD3	5:B:817:HOH:O	2.04	0.56
2:E:82:ILE:HG13	2:E:100:LEU:HD11	1.87	0.56
2:H:25:HIS:HA	2:H:28:TRP:HE3	1.70	0.56
3:B:601:SAH:O4'	3:B:601:SAH:HG2	2.06	0.56
1:A:103:GLU:HB3	1:A:104:GLU:OE1	2.05	0.56
1:A:109:ARG:HD2	1:A:306:GLY:HA2	1.86	0.56
1:B:390:MET:HE1	1:B:418:VAL:CG1	2.22	0.56
1:B:420:TRP:CE3	1:B:492:GLN:HB3	2.40	0.56
2:F:19:ASN:ND2	2:F:124:VAL:O	2.36	0.56
1:A:96:PHE:CE1	1:A:273:LEU:HD11	2.40	0.56
1:A:328:PHE:HE2	1:A:467:LEU:HA	1.70	0.56
1:D:41:PRO:HD3	1:D:49:GLU:OE1	2.06	0.56
1:G:128:LEU:CD2	1:G:271:ILE:HG12	2.35	0.56
1:G:196:TYR:O	1:G:468:ARG:NH1	2.38	0.56
1:G:200:THR:O	1:G:203:ILE:HG22	2.05	0.56
1:D:339:ILE:N	1:D:368:PHE:O	2.34	0.55
1:G:67:LEU:HG	1:G:242:GLU:HG3	1.87	0.55
2:F:81:LEU:HA	2:F:96:SER:HA	1.87	0.55
2:E:67:SER:N	2:E:109:ASP:OD1	2.39	0.55
2:E:81:LEU:HG	2:E:96:SER:HA	1.88	0.55
1:G:274:TRP:NE1	1:G:286:THR:HG21	2.22	0.55
1:A:419:SER:OG	1:A:422:ASN:HB2	2.07	0.55
2:F:12:VAL:HG21	2:F:53:ILE:CD1	2.36	0.55
2:E:12:VAL:HG11	2:E:53:ILE:HD11	1.88	0.55
1:D:255:GLN:HB2	1:D:268:LEU:HD22	1.89	0.55
2:F:12:VAL:HG21	2:F:53:ILE:HD11	1.89	0.55
2:F:137:VAL:HG22	2:F:140:LEU:HD11	1.87	0.55
1:G:175:TYR:O	1:G:178:THR:OG1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:MET:HE1	2:C:121:VAL:HG12	1.89	0.55
1:B:424:VAL:O	1:B:428:THR:OG1	2.21	0.54
1:G:287:GLY:O	1:G:296:GLU:N	2.40	0.54
1:B:125:ARG:NH1	1:B:261:GLU:OE2	2.40	0.54
1:B:112:ARG:NH2	1:B:118:GLU:OE2	2.28	0.54
1:G:460:ARG:H	1:G:460:ARG:HD2	1.73	0.54
2:C:67:SER:N	2:C:109:ASP:OD1	2.35	0.54
1:A:321:PHE:O	1:A:326:GLY:N	2.37	0.54
1:D:138:VAL:HB	5:D:641:HOH:O	2.07	0.54
2:E:145:GLU:OE1	2:E:146:GLU:N	2.37	0.53
1:A:86:ALA:HB1	1:A:91:ALA:HB3	1.89	0.53
1:B:352:MET:HE3	1:B:395:LEU:HD12	0.55	0.53
1:A:158:ALA:HB1	1:A:247:ALA:HB1	1.89	0.53
1:D:53:ILE:O	1:D:57:VAL:HG23	2.09	0.53
1:D:69:VAL:HG13	1:D:165:ARG:HE	1.74	0.53
1:A:352:MET:HG2	1:A:395:LEU:HD13	1.91	0.53
1:G:353:LYS:NZ	1:G:390:MET:O	2.39	0.53
1:B:86:ALA:HB1	1:B:91:ALA:HB3	1.91	0.53
1:B:142:LEU:HD12	1:B:227:HIS:CD2	2.44	0.53
1:G:149:LEU:HD11	1:G:159:PHE:HD2	1.73	0.52
2:F:141:LEU:C	2:F:143:LEU:N	2.66	0.52
2:E:84:VAL:HG12	2:E:126:THR:HG21	1.89	0.52
1:A:129:MET:HE1	1:A:176:ILE:HD11	1.91	0.52
2:H:144:ASP:HB3	5:H:308:HOH:O	2.09	0.52
1:B:313:TYR:HE2	3:B:601:SAH:H8	1.73	0.52
1:D:75:ARG:NH2	1:D:180:PRO:HG3	2.24	0.52
1:A:112:ARG:NH2	1:A:118:GLU:OE1	2.41	0.52
1:B:41:PRO:HD3	1:B:49:GLU:OE1	2.09	0.52
1:B:277:CYS:O	1:B:313:TYR:OH	2.22	0.52
1:G:120:PHE:CZ	1:G:309:ILE:HD11	2.45	0.52
1:G:256:ASN:O	1:G:269:ALA:N	2.42	0.52
1:G:201:GLN:HA	1:G:204:HIS:HD1	1.75	0.52
1:D:163:CYS:SG	1:D:233:LEU:HD12	2.49	0.52
2:E:136:ASP:OD1	2:E:137:VAL:N	2.42	0.52
1:G:203:ILE:HD12	1:G:206:VAL:HG11	1.92	0.52
1:B:75:ARG:NH2	3:B:601:SAH:O	2.40	0.52
2:E:59:GLN:HG3	2:E:76:PHE:O	2.10	0.52
1:G:41:PRO:HD3	1:G:49:GLU:OE2	2.10	0.52
1:G:29:THR:HG21	1:G:221:TYR:CD2	2.44	0.51
2:E:10:ILE:HB	2:E:17:VAL:HB	1.93	0.51
2:E:55:ARG:NH2	2:E:141:LEU:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:PHE:O	1:G:433:ARG:N	2.29	0.51
1:A:252:MET:HE2	1:A:324:HIS:HA	1.91	0.51
2:H:21:HIS:HB3	2:H:90:TYR:CE2	2.45	0.51
1:B:56:LEU:O	1:B:60:ILE:HG13	2.10	0.51
1:B:475:LEU:O	1:B:479:VAL:HG23	2.10	0.51
1:G:69:VAL:O	1:G:165:ARG:NH1	2.39	0.51
1:A:322:VAL:HG13	1:A:463:MET:SD	2.50	0.51
1:A:355:GLU:OE2	1:A:359:ARG:NE	2.42	0.51
1:A:390:MET:HE1	1:A:418:VAL:HG11	1.92	0.51
1:B:47:TRP:HH2	1:B:194:VAL:HG23	1.76	0.51
1:B:68:SER:OG	1:B:243:ASP:OD2	2.25	0.51
2:C:32:VAL:CG2	2:C:42:VAL:HG13	2.41	0.51
1:B:420:TRP:CZ3	1:B:492:GLN:HB3	2.46	0.50
1:G:338:LYS:HB3	1:G:367:VAL:CG1	2.40	0.50
1:B:276:MET:C	3:B:601:SAH:HB2	2.36	0.50
1:D:353:LYS:CE	1:D:395:LEU:HD11	2.41	0.50
1:G:173:GLN:HG3	1:G:174:PRO:CD	2.37	0.50
1:B:350:TYR:O	1:B:354:ALA:N	2.44	0.50
1:B:409:PHE:CE1	2:F:83:TYR:HA	2.46	0.50
1:G:190:GLU:O	1:G:194:VAL:HG23	2.11	0.50
1:G:344:SER:C	1:G:346:SER:N	2.67	0.50
1:G:427:TRP:CD1	1:G:489:TYR:HE2	2.29	0.50
2:C:116:CYS:N	2:C:119:GLY:O	2.42	0.50
1:B:158:ALA:HB1	1:B:247:ALA:HB1	1.92	0.50
2:F:67:SER:N	2:F:109:ASP:OD1	2.44	0.50
1:G:60:ILE:O	1:G:64:GLN:OE1	2.29	0.50
1:B:92:SER:OG	1:B:121:LEU:HA	2.12	0.50
2:F:76:PHE:CE2	2:F:114:LEU:HD21	2.47	0.50
2:F:137:VAL:CG2	2:F:140:LEU:CD1	2.89	0.50
1:A:96:PHE:HE1	1:A:273:LEU:HD11	1.77	0.50
1:A:116:ALA:N	1:A:302:ASP:OD1	2.43	0.50
1:A:327:PHE:HA	1:A:463:MET:HE2	1.94	0.50
1:B:386:ARG:N	1:B:426:LEU:HD21	2.27	0.50
2:C:111:GLY:HA2	2:C:123:ILE:HD11	1.94	0.50
1:G:465:ILE:HG23	1:G:468:ARG:HE	1.76	0.50
1:G:356:VAL:O	1:G:360:ALA:N	2.40	0.49
1:A:54:ARG:NH2	1:A:190:GLU:HA	2.27	0.49
1:B:155:ILE:HG21	1:B:220:PHE:HE2	1.77	0.49
1:G:175:TYR:OH	1:G:275:ASP:OD1	2.30	0.49
1:G:175:TYR:CD1	1:G:272:PRO:HB3	2.48	0.49
1:G:256:ASN:OD1	1:G:274:TRP:HZ3	1.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLN:NE2	2:F:117:GLN:OE1	2.46	0.49
1:G:409:PHE:CZ	2:H:94:TYR:HA	2.47	0.49
1:A:377:ILE:HD12	1:A:382:LEU:HB2	1.94	0.49
1:B:142:LEU:HD12	1:B:227:HIS:HD2	1.78	0.49
1:G:338:LYS:HA	1:G:369:ALA:HA	1.94	0.49
2:F:137:VAL:O	2:F:140:LEU:CD2	2.34	0.49
1:D:357:LEU:HD12	1:D:363:PRO:O	2.13	0.49
1:G:100:ASN:HA	1:G:106:PHE:HA	1.93	0.49
2:H:117:GLN:CD	2:H:117:GLN:H	2.21	0.49
2:F:140:LEU:HG	2:F:143:LEU:CB	2.43	0.49
1:G:123:VAL:HG13	1:G:127:LEU:HD12	1.94	0.49
1:A:248:VAL:O	1:A:252:MET:HG2	2.13	0.49
1:A:255:GLN:HB2	1:A:268:LEU:HD22	1.93	0.49
2:E:140:LEU:HD12	2:E:142:TRP:CZ2	2.47	0.49
1:B:108:LEU:HD12	1:B:277:CYS:SG	2.53	0.49
1:B:125:ARG:NH2	5:B:713:HOH:O	2.46	0.49
2:C:59:GLN:HG3	2:C:76:PHE:O	2.13	0.49
1:B:219:TYR:O	1:B:223:VAL:HG23	2.13	0.48
1:G:380:GLN:HA	1:G:383:ALA:HB3	1.94	0.48
1:A:216:GLN:OE1	1:A:244:TYR:OH	2.19	0.48
2:C:116:CYS:N	2:C:121:VAL:HG23	2.28	0.48
1:B:129:MET:HE3	1:B:175:TYR:CD2	2.46	0.48
2:F:66:ASN:HB2	2:F:109:ASP:HA	1.95	0.48
1:G:119:LEU:HD11	1:G:296:GLU:HB3	1.95	0.48
1:G:413:ASN:HB3	1:G:416:PHE:HB3	1.95	0.48
2:H:37:SER:O	2:H:95:GLN:HA	2.13	0.48
2:F:141:LEU:O	2:F:143:LEU:N	2.46	0.48
1:D:212:ASN:OD1	1:D:215:ARG:NH2	2.33	0.48
1:A:56:LEU:O	1:A:60:ILE:HG13	2.13	0.48
1:A:92:SER:HB3	1:A:122:TRP:CD2	2.49	0.48
1:D:289:ASN:O	1:D:293:ASP:N	2.47	0.48
1:D:359:ARG:HD2	5:D:711:HOH:O	2.14	0.48
1:D:443:THR:OG1	1:D:444:THR:N	2.46	0.48
1:G:200:THR:O	1:G:204:HIS:ND1	2.45	0.48
2:F:81:LEU:HD11	2:F:94:TYR:HD2	1.79	0.48
2:E:135:ALA:C	5:E:305:HOH:O	2.56	0.48
1:A:277:CYS:O	1:A:313:TYR:OH	2.22	0.48
1:A:188:TYR:O	1:A:460:ARG:NH1	2.47	0.48
1:A:189:PHE:CE1	1:A:460:ARG:HB3	2.48	0.48
2:E:55:ARG:CZ	2:E:141:LEU:HA	2.43	0.48
2:E:12:VAL:HG11	2:E:143:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:ASN:HB2	2:H:109:ASP:HA	1.96	0.48
1:B:92:SER:HB3	1:B:122:TRP:CD2	2.49	0.47
1:B:196:TYR:CD1	1:B:465:ILE:HD11	2.49	0.47
1:D:272:PRO:O	1:D:274:TRP:N	2.44	0.47
1:A:283:LEU:HD13	5:C:310:HOH:O	2.14	0.47
1:A:322:VAL:HG21	1:A:467:LEU:HD22	1.95	0.47
1:B:479:VAL:HA	5:B:790:HOH:O	2.14	0.47
1:D:248:VAL:O	1:D:252:MET:HG2	2.13	0.47
1:D:318:ASN:O	1:D:322:VAL:HG23	2.15	0.47
1:D:339:ILE:HG12	1:D:341:LEU:HD22	1.96	0.47
1:G:386:ARG:NH1	1:G:411:LEU:O	2.48	0.47
1:A:279:HIS:HB2	1:A:313:TYR:CD2	2.48	0.47
1:A:294:ARG:NE	1:A:296:GLU:OE2	2.33	0.47
1:D:475:LEU:O	1:D:479:VAL:HG23	2.14	0.47
1:G:389:CYS:O	1:G:425:LYS:NZ	2.31	0.47
1:A:327:PHE:HE2	1:A:329:PHE:HB2	1.80	0.47
1:B:128:LEU:HD23	1:B:272:PRO:HD2	1.96	0.47
1:A:368:PHE:CG	1:A:381:LEU:HD13	2.50	0.47
2:C:136:ASP:OD1	2:C:137:VAL:N	2.48	0.47
1:B:138:VAL:O	1:B:141:PRO:HD2	2.14	0.47
2:C:32:VAL:HG23	2:C:42:VAL:HG13	1.97	0.47
2:C:140:LEU:N	2:C:140:LEU:HD22	2.29	0.47
2:F:68:ARG:HH12	2:F:104:HIS:CG	2.33	0.47
1:G:347:ASP:O	1:G:350:TYR:HB2	2.14	0.47
1:G:349:LEU:HA	1:G:352:MET:HE3	1.96	0.47
1:G:475:LEU:O	1:G:479:VAL:HG23	2.15	0.47
2:H:99:MET:HE1	2:H:121:VAL:HG12	1.97	0.47
2:C:85:GLU:HG2	2:C:86:ALA:N	2.29	0.47
1:D:175:TYR:O	1:D:178:THR:OG1	2.26	0.47
1:G:301:GLN:HG3	1:G:303:PHE:CE1	2.45	0.47
1:G:344:SER:O	1:G:345:LYS:C	2.57	0.47
1:B:352:MET:HE3	1:B:395:LEU:CG	2.28	0.47
1:B:398:HIS:O	1:B:404:ALA:HB1	2.15	0.47
1:G:139:LEU:O	1:G:143:TYR:N	2.25	0.47
1:G:446:GLU:O	1:G:449:LYS:HG3	2.15	0.47
1:A:441:TYR:OH	1:A:471:GLU:OE1	2.32	0.47
1:A:445:ILE:O	1:A:449:LYS:HG3	2.15	0.47
2:F:62:VAL:HG12	2:F:71:HIS:HB3	1.97	0.47
1:D:193:GLU:OE2	1:D:460:ARG:HB2	2.14	0.47
2:E:25:HIS:O	2:E:29:ALA:N	2.48	0.47
1:B:80:PRO:HG3	5:B:817:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:HA	2:F:115:ARG:HD3	1.98	0.46
2:H:116:CYS:HB3	2:H:121:VAL:CG2	2.45	0.46
2:F:58:CYS:HB2	2:F:116:CYS:HB2	1.68	0.46
2:E:122:GLY:HA3	5:E:305:HOH:O	2.15	0.46
2:H:55:ARG:NH1	2:H:141:LEU:HD23	2.30	0.46
2:F:137:VAL:HG22	2:F:140:LEU:CD1	2.44	0.46
2:F:141:LEU:C	2:F:143:LEU:H	2.22	0.46
1:G:357:LEU:HB2	1:G:362:ILE:O	2.15	0.46
1:A:159:PHE:HE2	1:A:224:ILE:HD11	1.80	0.46
1:B:142:LEU:HD13	1:B:230:ALA:HB2	1.97	0.46
1:B:447:GLU:O	1:B:451:VAL:HG23	2.15	0.46
1:B:101:PHE:CE2	1:B:308:GLN:HB2	2.49	0.46
1:D:473:GLU:O	1:D:477:LYS:HG3	2.15	0.46
2:H:21:HIS:HB3	2:H:90:TYR:CZ	2.50	0.46
2:H:56:CYS:O	2:H:138:ARG:NH1	2.49	0.46
1:A:54:ARG:NH1	1:A:189:PHE:O	2.31	0.46
2:C:33:TRP:CH2	2:C:35:ASP:HB2	2.51	0.46
1:G:98:MET:SD	1:G:98:MET:N	2.89	0.46
2:H:55:ARG:NH1	2:H:138:ARG:O	2.49	0.46
1:A:357:LEU:HB3	1:A:362:ILE:O	2.15	0.46
1:B:69:VAL:O	1:B:165:ARG:NH2	2.39	0.46
1:D:43:PRO:C	1:D:45:LYS:H	2.24	0.46
1:G:146:ASP:CG	1:G:149:LEU:HD23	2.41	0.46
1:G:258:ILE:O	1:G:267:THR:N	2.41	0.46
1:G:279:HIS:HB2	1:G:313:TYR:CD1	2.49	0.46
1:A:54:ARG:HH22	1:A:190:GLU:HA	1.81	0.46
1:G:54:ARG:NH1	1:G:191:GLU:OE1	2.49	0.46
1:G:128:LEU:HD22	1:G:271:ILE:CG1	2.41	0.46
1:A:41:PRO:HG3	1:A:49:GLU:HB2	1.98	0.46
1:A:408:ILE:HD12	1:A:408:ILE:H	1.81	0.46
1:A:436:LEU:O	1:A:440:THR:HG23	2.16	0.46
1:A:188:TYR:HB3	1:A:460:ARG:NH1	2.31	0.46
1:B:340:LYS:HB3	1:B:340:LYS:HE2	1.44	0.45
1:D:403:SER:O	1:D:407:ARG:HG3	2.16	0.45
2:F:76:PHE:HB3	2:F:101:ALA:HB2	1.98	0.45
1:D:135:LYS:HA	1:D:140:GLY:HA2	1.97	0.45
2:H:121:VAL:O	2:H:137:VAL:HG22	2.17	0.45
1:A:224:ILE:HG23	1:A:233:LEU:HD11	1.98	0.45
2:E:23:ALA:HB3	2:E:28:TRP:HE1	1.81	0.45
1:G:114:ILE:HD12	1:G:303:PHE:HB2	1.98	0.45
1:A:68:SER:OG	1:A:243:ASP:OD2	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LYS:NZ	1:A:144:SER:HB3	2.31	0.45
1:A:473:GLU:O	1:A:477:LYS:HG3	2.15	0.45
1:B:69:VAL:CB	5:B:704:HOH:O	2.51	0.45
1:B:69:VAL:HG21	1:B:166:ALA:HA	1.98	0.45
1:B:327:PHE:CD2	3:B:601:SAH:N6	2.84	0.45
1:D:197:LEU:HD22	1:D:464:ALA:HB1	1.99	0.45
1:G:465:ILE:HA	1:G:468:ARG:HG2	1.98	0.45
1:A:129:MET:HE3	1:A:172:TRP:HB2	1.98	0.45
2:C:58:CYS:HB2	2:C:116:CYS:HB2	1.66	0.45
2:C:139:ASP:OD1	2:C:139:ASP:N	2.49	0.45
1:D:188:TYR:HB2	1:D:460:ARG:NH2	2.32	0.45
1:G:409:PHE:CG	2:H:94:TYR:HB3	2.52	0.45
1:A:125:ARG:NH1	1:A:293:ASP:OD1	2.49	0.45
1:A:272:PRO:O	1:A:274:TRP:N	2.44	0.45
1:G:420:TRP:HZ3	1:G:492:GLN:HB3	1.82	0.45
1:B:339:ILE:N	1:B:368:PHE:O	2.49	0.45
1:D:465:ILE:HG12	1:D:468:ARG:NH2	2.22	0.45
2:H:139:ASP:OD1	2:H:139:ASP:N	2.50	0.45
1:A:328:PHE:CE2	1:A:466:LYS:HG3	2.51	0.45
1:B:120:PHE:CD2	1:B:121:LEU:HG	2.52	0.45
1:D:394:GLU:OE2	1:D:419:SER:CB	2.65	0.45
1:G:84:LYS:HG3	1:G:85:TRP:H	1.81	0.45
1:A:173:GLN:O	1:A:177:GLN:HG3	2.17	0.45
2:C:28:TRP:HE1	2:C:41:LEU:HD13	1.81	0.45
2:C:101:ALA:HB3	2:C:134:PHE:HE2	1.82	0.45
1:D:490:ARG:O	1:D:493:MET:HG3	2.17	0.45
2:E:140:LEU:CD1	2:E:142:TRP:NE1	2.80	0.45
1:G:318:ASN:HA	1:G:321:PHE:HB2	1.98	0.45
2:C:80:SER:O	2:C:82:ILE:HG12	2.16	0.45
2:F:136:ASP:OD1	2:F:137:VAL:N	2.50	0.44
2:E:16:ARG:N	2:E:43:SER:O	2.40	0.44
2:H:136:ASP:OD1	2:H:137:VAL:N	2.49	0.44
1:A:317:SER:OG	1:A:320:GLU:HG3	2.18	0.44
1:A:437:LEU:O	1:A:440:THR:OG1	2.33	0.44
1:B:41:PRO:HD3	1:B:49:GLU:CD	2.42	0.44
1:B:311:ILE:HD11	1:B:313:TYR:HE1	1.83	0.44
1:D:108:LEU:HD12	1:D:277:CYS:SG	2.57	0.44
1:A:162:LEU:HD13	1:A:165:ARG:HD3	1.98	0.44
1:G:109:ARG:HA	1:G:109:ARG:HD3	1.81	0.44
1:G:201:GLN:NE2	1:G:338:LYS:HB2	2.31	0.44
2:H:20:ARG:CZ	2:H:36:SER:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TRP:CG	1:A:174:PRO:HG2	2.52	0.44
1:A:112:ARG:NH1	1:A:113:ASP:O	2.50	0.44
1:B:352:MET:SD	1:B:395:LEU:HB2	2.56	0.44
1:G:362:ILE:HD12	1:G:363:PRO:HD2	1.98	0.44
1:B:203:ILE:HG12	1:B:207:PHE:CZ	2.53	0.44
1:B:222:LYS:O	1:B:226:THR:HG23	2.17	0.44
1:A:465:ILE:O	1:A:468:ARG:HG2	2.17	0.44
1:B:456:ASP:OD1	1:A:109:ARG:HD3	2.17	0.44
1:D:344:SER:HB3	5:D:621:HOH:O	2.17	0.44
2:E:85:GLU:OE1	2:E:85:GLU:N	2.40	0.44
1:G:272:PRO:O	1:G:274:TRP:N	2.44	0.44
1:A:289:ASN:O	1:A:293:ASP:N	2.50	0.44
1:G:128:LEU:HD22	1:G:271:ILE:HA	1.99	0.44
1:G:318:ASN:O	1:G:322:VAL:HG23	2.18	0.44
1:G:357:LEU:HD22	1:G:364:THR:HA	2.00	0.44
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.83	0.44
2:F:17:VAL:HG21	2:F:143:LEU:HD21	1.99	0.44
1:D:338:LYS:HG2	1:D:367:VAL:CG1	2.47	0.44
2:E:58:CYS:SG	2:E:118:HIS:ND1	2.88	0.44
1:B:318:ASN:O	1:B:322:VAL:HG23	2.18	0.44
2:F:137:VAL:HG23	2:F:140:LEU:HD11	1.99	0.44
1:D:84:LYS:O	1:D:88:GLU:N	2.47	0.44
2:E:116:CYS:HB3	2:E:121:VAL:CG2	2.48	0.44
1:G:54:ARG:CZ	1:G:191:GLU:HB2	2.48	0.44
1:G:347:ASP:HB3	1:G:350:TYR:HB2	2.00	0.44
1:G:385:LEU:HB3	1:G:426:LEU:HB2	2.00	0.44
2:F:116:CYS:N	2:F:119:GLY:O	2.49	0.43
1:D:285:THR:HG21	1:D:300:LEU:HA	1.99	0.43
1:B:47:TRP:O	1:B:51:VAL:HG23	2.18	0.43
1:B:109:ARG:HE	1:B:306:GLY:HA2	1.83	0.43
1:B:327:PHE:CE2	3:B:601:SAH:C6	3.01	0.43
1:B:453:LYS:HB2	5:B:722:HOH:O	2.19	0.43
2:F:116:CYS:SG	2:F:118:HIS:ND1	2.79	0.43
1:A:222:LYS:O	1:A:226:THR:HG23	2.18	0.43
2:F:116:CYS:N	2:F:121:VAL:HG23	2.33	0.43
1:B:318:ASN:HA	1:B:321:PHE:HB2	2.01	0.43
1:B:453:LYS:N	5:B:722:HOH:O	2.51	0.43
1:G:352:MET:HG3	1:G:395:LEU:HD13	1.99	0.43
2:H:54:ALA:HB2	2:H:119:GLY:C	2.43	0.43
1:G:147:ARG:HB2	1:G:147:ARG:NH1	2.33	0.43
1:D:231:ASN:HA	1:D:236:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:ASN:ND2	2:E:124:VAL:O	2.50	0.43
2:E:37:SER:HA	2:E:94:TYR:O	2.18	0.43
2:E:112:GLY:O	2:E:124:VAL:HG23	2.19	0.43
1:G:152:MET:HE1	2:H:118:HIS:NE2	2.34	0.43
2:H:33:TRP:CZ2	2:H:35:ASP:HB2	2.54	0.43
1:D:353:LYS:HE2	1:D:395:LEU:HD11	1.99	0.43
1:D:381:LEU:HA	1:D:381:LEU:HD23	1.73	0.43
2:H:144:ASP:CG	5:H:308:HOH:O	2.61	0.43
1:A:28:LEU:HB3	1:A:60:ILE:HG12	2.01	0.43
1:B:85:TRP:CG	1:B:174:PRO:HG2	2.53	0.43
1:D:259:PRO:HA	1:D:266:VAL:HA	2.01	0.43
1:A:328:PHE:CE2	1:A:467:LEU:HA	2.53	0.43
2:E:63:TYR:CE1	2:E:72:TYR:HB2	2.54	0.43
1:G:45:LYS:C	1:G:46:GLU:CA	2.84	0.43
1:G:108:LEU:HD12	1:G:277:CYS:SG	2.59	0.43
1:G:171:PHE:HD2	1:G:172:TRP:CE2	2.37	0.43
2:H:99:MET:HE3	2:H:134:PHE:HB2	2.01	0.43
1:A:328:PHE:HD1	1:A:329:PHE:N	2.16	0.43
1:B:255:GLN:HB2	1:B:268:LEU:HD22	2.00	0.43
1:G:153:GLY:HA2	1:G:156:ALA:HB3	2.01	0.43
1:G:167:SER:HB2	1:G:170:SER:HB2	2.01	0.43
1:G:374:GLU:HA	1:G:375:PRO:HA	1.83	0.43
1:B:385:LEU:HB3	1:B:426:LEU:HG	2.00	0.42
1:D:122:TRP:HB2	1:D:294:ARG:CD	2.43	0.42
1:G:120:PHE:CE2	1:G:309:ILE:HD11	2.54	0.42
1:A:101:PHE:N	1:A:105:GLY:O	2.47	0.42
1:B:330:ASP:HA	5:B:724:HOH:O	2.18	0.42
1:B:423:GLU:HG3	1:B:489:TYR:CE1	2.54	0.42
1:B:454:ASN:N	1:B:454:ASN:ND2	2.65	0.42
1:D:58:GLU:HA	1:D:61:ARG:HG2	2.02	0.42
1:G:160:HIS:O	1:G:164:GLU:HG2	2.19	0.42
1:G:339:ILE:N	1:G:368:PHE:O	2.47	0.42
2:C:121:VAL:O	2:C:137:VAL:HG12	2.19	0.42
1:B:183:TYR:HE1	1:B:246:TRP:CD1	2.37	0.42
1:A:386:ARG:O	1:A:390:MET:HG2	2.18	0.42
1:B:357:LEU:HB3	1:B:362:ILE:O	2.19	0.42
2:F:137:VAL:HG23	2:F:140:LEU:CD1	2.49	0.42
1:D:89:ASN:CB	1:D:127:LEU:HD21	2.49	0.42
2:H:140:LEU:N	2:H:140:LEU:HD22	2.34	0.42
1:A:120:PHE:CD2	1:A:121:LEU:HG	2.54	0.42
1:A:266:VAL:HG13	2:C:115:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLU:HA	1:A:375:PRO:HA	1.78	0.42
1:A:468:ARG:O	1:A:472:LYS:NZ	2.44	0.42
2:C:53:ILE:HA	2:C:120:VAL:HG12	2.01	0.42
2:F:116:CYS:HB3	2:F:121:VAL:CG2	2.50	0.42
1:B:192:ASP:O	1:B:195:ARG:HB3	2.20	0.42
1:B:242:GLU:OE1	1:B:245:ARG:NH2	2.34	0.42
1:D:128:LEU:HD22	1:D:271:ILE:HA	2.01	0.42
1:D:245:ARG:O	1:D:249:SER:OG	2.23	0.42
1:G:101:PHE:HE1	1:G:109:ARG:HE	1.68	0.42
1:G:342:GLY:HA2	1:G:365:SER:HB2	2.01	0.42
1:A:224:ILE:O	1:A:236:LYS:HE2	2.19	0.42
2:E:84:VAL:HG11	2:E:95:GLN:HG3	2.00	0.42
1:G:75:ARG:NE	1:G:178:THR:O	2.41	0.42
1:A:108:LEU:HD12	1:A:277:CYS:SG	2.59	0.42
2:F:23:ALA:CB	2:F:41:LEU:HD23	2.49	0.42
1:D:203:ILE:HA	1:D:206:VAL:HB	2.01	0.42
1:G:437:LEU:HD12	5:G:679:HOH:O	2.19	0.42
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.88	0.42
1:D:386:ARG:NH1	1:D:410:THR:O	2.53	0.42
2:C:110:ALA:N	5:C:301:HOH:O	2.48	0.42
1:B:384:PHE:O	1:B:387:VAL:HG22	2.19	0.41
1:G:248:VAL:O	1:G:252:MET:HG2	2.19	0.41
1:A:167:SER:O	1:A:173:GLN:NE2	2.52	0.41
1:B:180:PRO:HD3	1:B:254:ARG:HH12	1.85	0.41
1:D:371:HIS:O	1:D:376:PRO:HA	2.20	0.41
1:A:318:ASN:HB2	1:A:335:ASP:OD1	2.21	0.41
1:A:318:ASN:O	1:A:322:VAL:HG23	2.20	0.41
2:C:36:SER:O	2:C:93:ARG:NH2	2.53	0.41
1:B:54:ARG:NH2	1:B:190:GLU:HA	2.35	0.41
1:G:315:THR:OG1	2:H:75:SER:OG	2.38	0.41
2:H:137:VAL:O	2:H:140:LEU:HB2	2.21	0.41
2:C:52:THR:O	2:C:120:VAL:HG12	2.21	0.41
2:H:117:GLN:HG2	2:H:118:HIS:CE1	2.56	0.41
2:E:121:VAL:O	2:E:137:VAL:HG22	2.21	0.41
1:A:119:LEU:HD11	1:A:296:GLU:HB3	2.03	0.41
1:A:270:LEU:O	1:A:272:PRO:HD3	2.21	0.41
1:D:85:TRP:CH2	1:D:127:LEU:HD22	2.56	0.41
1:D:128:LEU:HD22	1:D:271:ILE:HG12	2.02	0.41
1:D:162:LEU:HD13	1:D:243:ASP:HB3	2.03	0.41
1:B:341:LEU:HD13	1:B:385:LEU:HD21	2.02	0.41
1:D:129:MET:HE3	1:D:270:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:GLN:NE2	5:D:610:HOH:O	2.53	0.41
1:G:450:SER:OG	1:G:454:ASN:OD1	2.25	0.41
1:A:341:LEU:HD11	1:A:429:PHE:HE2	1.85	0.41
1:B:390:MET:SD	1:B:418:VAL:HG11	2.61	0.41
1:D:281:ASN:N	1:D:281:ASN:OD1	2.53	0.41
1:D:328:PHE:CD2	1:D:466:LYS:HB3	2.56	0.41
1:G:235:LEU:HB3	1:G:239:PHE:HB2	2.01	0.41
1:G:410:THR:HG21	5:G:725:HOH:O	2.20	0.41
1:G:428:THR:HG23	1:G:486:ARG:HE	1.84	0.41
1:G:445:ILE:HG23	1:G:469:LEU:HD11	2.01	0.41
2:H:64:TYR:HD1	2:H:71:HIS:CE1	2.39	0.41
1:A:59:LYS:O	1:A:63:LYS:HG2	2.21	0.41
1:A:398:HIS:CE1	1:A:407:ARG:HB3	2.56	0.41
1:A:409:PHE:CE1	2:C:94:TYR:HA	2.56	0.41
1:A:420:TRP:CD1	1:A:492:GLN:HG2	2.55	0.41
2:C:93:ARG:NH1	2:C:95:GLN:OE1	2.38	0.41
2:F:140:LEU:CD2	2:F:140:LEU:C	2.90	0.41
1:D:316:ARG:HB2	1:D:321:PHE:CE1	2.56	0.41
2:H:76:PHE:HB3	2:H:101:ALA:HB2	2.03	0.41
2:H:131:LEU:HD21	5:H:314:HOH:O	2.21	0.41
1:A:69:VAL:HG21	1:A:166:ALA:HA	2.03	0.40
1:A:247:ALA:O	1:A:251:VAL:HG23	2.20	0.40
2:C:116:CYS:HB3	2:C:121:VAL:CG2	2.51	0.40
1:D:119:LEU:HA	1:D:298:VAL:HA	2.02	0.40
1:G:424:VAL:O	1:G:428:THR:OG1	2.20	0.40
1:B:214:ALA:HB2	5:B:731:HOH:O	2.21	0.40
1:B:409:PHE:CZ	2:F:83:TYR:HD1	2.39	0.40
2:F:65:CYS:O	2:F:69:ARG:N	2.55	0.40
1:D:47:TRP:CZ3	1:D:50:TYR:CD2	3.09	0.40
2:E:80:SER:O	2:E:98:LEU:HB2	2.21	0.40
2:E:99:MET:HE2	2:E:136:ASP:HB2	2.04	0.40
2:H:67:SER:N	2:H:109:ASP:OD1	2.53	0.40
1:A:164:GLU:HB3	1:A:170:SER:OG	2.22	0.40
1:A:203:ILE:HA	1:A:206:VAL:CG1	2.46	0.40
1:A:260:THR:OG1	1:A:261:GLU:N	2.54	0.40
2:C:62:VAL:CG1	2:C:71:HIS:HB3	2.51	0.40
1:B:215:ARG:HH11	1:B:215:ARG:HD2	1.77	0.40
1:G:120:PHE:CD2	1:G:121:LEU:HG	2.56	0.40
1:G:247:ALA:O	1:G:251:VAL:HG23	2.21	0.40
1:B:180:PRO:HD3	1:B:254:ARG:NH1	2.36	0.40
2:C:12:VAL:HG21	2:C:53:ILE:HD12	2.00	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:904:HOH:O	5:F:354:HOH:O[1_545]	1.76	0.44
5:D:882:HOH:O	5:G:870:HOH:O[1_645]	1.84	0.36
5:D:852:HOH:O	5:D:876:HOH:O[1_545]	1.87	0.33
5:B:918:HOH:O	5:A:786:HOH:O[1_565]	2.05	0.15
5:D:868:HOH:O	5:G:831:HOH:O[1_655]	2.12	0.08
5:D:675:HOH:O	5:D:724:HOH:O[1_545]	2.19	0.01

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	476/594 (80%)	466 (98%)	10 (2%)	0	100	100
1	B	476/594 (80%)	465 (98%)	11 (2%)	0	100	100
1	D	474/594 (80%)	463 (98%)	11 (2%)	0	100	100
1	G	474/594 (80%)	461 (97%)	13 (3%)	0	100	100
2	C	140/150 (93%)	130 (93%)	9 (6%)	1 (1%)	18	52
2	E	140/150 (93%)	125 (89%)	15 (11%)	0	100	100
2	F	140/150 (93%)	131 (94%)	9 (6%)	0	100	100
2	H	139/150 (93%)	127 (91%)	11 (8%)	1 (1%)	18	52
All	All	2459/2976 (83%)	2368 (96%)	89 (4%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	117	GLN
2	H	91	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	383/518 (74%)	383 (100%)	0	100	100
1	B	406/518 (78%)	395 (97%)	11 (3%)	39	62
1	D	383/518 (74%)	383 (100%)	0	100	100
1	G	383/518 (74%)	382 (100%)	1 (0%)	86	83
2	C	118/123 (96%)	115 (98%)	3 (2%)	42	64
2	E	118/123 (96%)	116 (98%)	2 (2%)	53	70
2	F	116/123 (94%)	113 (97%)	3 (3%)	40	63
2	H	117/123 (95%)	114 (97%)	3 (3%)	40	63
All	All	2024/2564 (79%)	2001 (99%)	23 (1%)	65	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	LEU
1	B	28	LEU
1	B	45	LYS
1	B	46	GLU
1	B	132	GLU
1	B	141	PRO
1	B	144	SER
1	B	192	ASP
1	B	254	ARG
1	B	265	ARG
1	B	340	LYS
2	F	116	CYS
2	F	139	ASP
2	F	140	LEU
2	E	116	CYS
2	E	143	LEU
1	G	257	GLN
2	H	6	GLN
2	H	116	CYS

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Mol	Chain	Res	Type
2	H	144	ASP
2	C	106[A]	GLU
2	C	106[B]	GLU
2	C	116	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
1	B	225	GLN
2	F	95	GLN
2	F	104	HIS
1	D	150	GLN
1	D	255	GLN
1	D	278	ASN
1	D	324	HIS
1	D	334	HIS
1	D	485	ASN
1	G	100	ASN
1	G	150	GLN
1	G	177	GLN
1	G	198	GLN
1	G	225	GLN
1	G	257	GLN
2	H	104	HIS
1	A	64	GLN
1	A	455	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

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SAH	B	601	-	27,28,28	0.89	2 (7%)	36,40,40	1.18	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	B	601	-	-	5/15/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	SAH	O4'-C4'	2.30	1.50	1.45
3	B	601	SAH	OXT-C	-2.10	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	SAH	O4'-C4'-C3'	-4.96	95.30	105.15
3	B	601	SAH	N9-C8-N7	-2.73	110.06	113.94
3	B	601	SAH	C4-N9-C8	2.73	108.60	105.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	SAH	N-CA-CB-CG
3	B	601	SAH	C-CA-CB-CG
3	B	601	SAH	CA-CB-CG-SD

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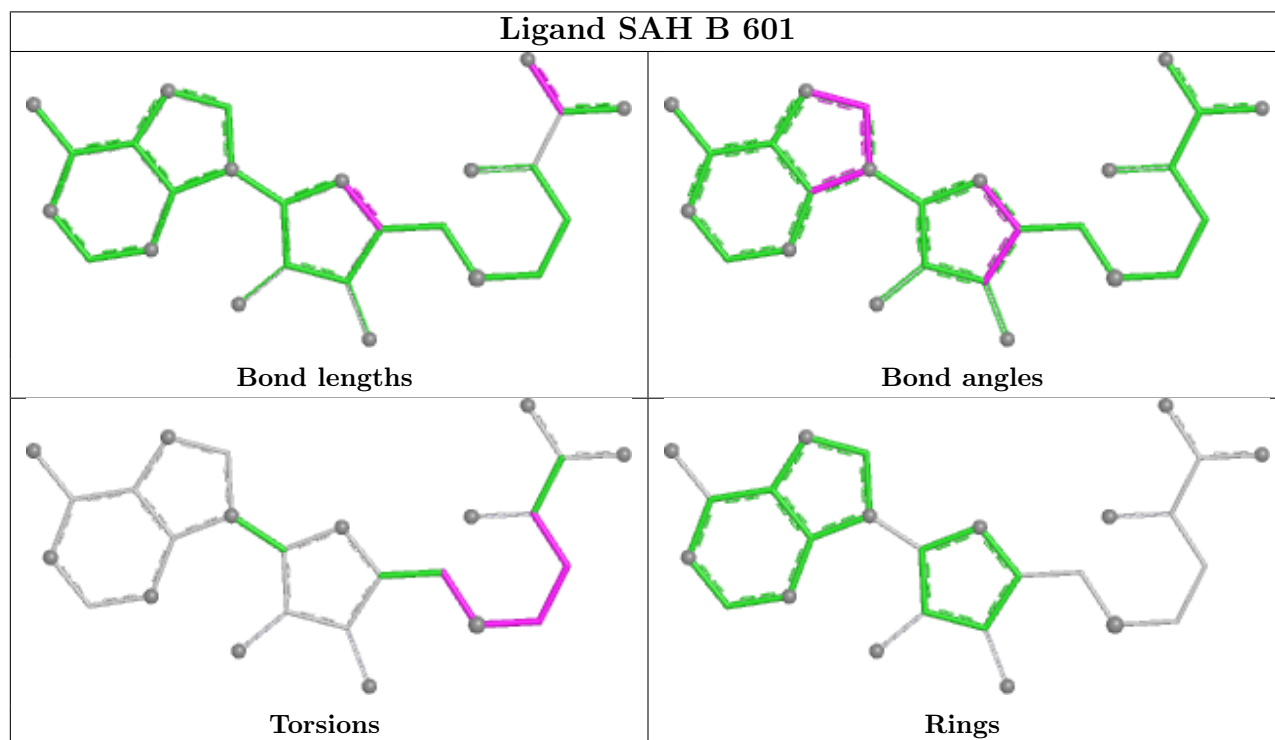
Mol	Chain	Res	Type	Atoms
3	B	601	SAH	CB-CG-SD-C5'
3	B	601	SAH	C4'-C5'-SD-CG

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	SAH	12	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	4
1	D	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	40:ALA	C	41:PRO	N	2.44
1	D	40:ALA	C	41:PRO	N	2.29
1	G	45:LYS	C	46:GLU	N	1.83
1	B	275:ASP	C	276:MET	N	1.15
1	G	270:LEU	C	271:ILE	N	1.13
1	G	275:ASP	C	276:MET	N	0.96
1	D	400:LEU	C	401:GLY	N	0.89

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/594 (80%)	0.42	15 (3%) 51 29	25, 70, 160, 212	0
1	B	478/594 (80%)	0.16	13 (2%) 56 32	8, 40, 151, 207	0
1	D	477/594 (80%)	0.29	16 (3%) 48 27	31, 105, 158, 199	1 (0%)
1	G	477/594 (80%)	0.52	14 (2%) 53 30	66, 130, 170, 211	1 (0%)
2	C	141/150 (94%)	0.59	5 (3%) 47 26	34, 65, 110, 150	1 (0%)
2	E	141/150 (94%)	0.30	1 (0%) 84 61	45, 101, 140, 173	1 (0%)
2	F	141/150 (94%)	-0.08	0 100 100	5, 28, 82, 130	1 (0%)
2	H	141/150 (94%)	0.67	4 (2%) 55 31	109, 150, 175, 202	0
All	All	2474/2976 (83%)	0.35	68 (2%) 56 32	5, 93, 162, 212	5 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	361	GLY	6.2
1	B	383	ALA	5.2
1	D	360	ALA	4.6
1	A	351	ALA	4.5
1	G	214	ALA	4.3
1	G	220	PHE	4.3
1	G	218	ALA	3.7
1	D	325	SER	3.6
1	B	387	VAL	3.4
1	G	180	PRO	3.3
2	C	98	LEU	3.3
1	D	361	GLY	3.1
1	B	291	GLU	3.1
1	A	325	SER	3.1
1	A	343	VAL	3.1
1	B	262	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	112	GLY	2.8
1	B	411	LEU	2.8
1	A	56	LEU	2.7
1	A	255	GLN	2.7
1	G	148	ILE	2.7
1	B	356	VAL	2.7
1	A	494	GLU	2.7
2	H	52	THR	2.7
1	D	160	HIS	2.6
1	D	273	LEU	2.6
1	D	397	GLU	2.6
1	A	418	VAL	2.5
2	C	93	ARG	2.5
1	B	231	ASN	2.4
1	G	360	ALA	2.4
1	B	488	TYR	2.4
1	G	179	LEU	2.4
1	D	214	ALA	2.4
1	A	347	ASP	2.4
1	D	132	GLU	2.4
1	B	477	LYS	2.4
1	B	418	VAL	2.3
2	H	63	TYR	2.3
2	H	35	ASP	2.3
1	D	131	VAL	2.3
1	G	53	ILE	2.3
1	D	498	PRO	2.3
1	D	218	ALA	2.3
1	A	387	VAL	2.2
1	B	357	LEU	2.2
1	D	277	CYS	2.2
2	C	143	LEU	2.2
1	A	53	ILE	2.2
1	A	385	LEU	2.2
1	B	27	ASN	2.1
1	G	166	ALA	2.1
1	A	198	GLN	2.1
1	G	286	THR	2.1
1	A	402	ASP	2.1
1	D	178	THR	2.1
1	D	327	PHE	2.1
1	G	273	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	88	GLU	2.1
1	D	138	VAL	2.1
1	B	325	SER	2.1
1	D	406	ASP	2.0
2	C	46	THR	2.0
2	H	40	LEU	2.0
1	G	160	HIS	2.0
1	G	29	THR	2.0
1	A	120	PHE	2.0
1	A	497	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

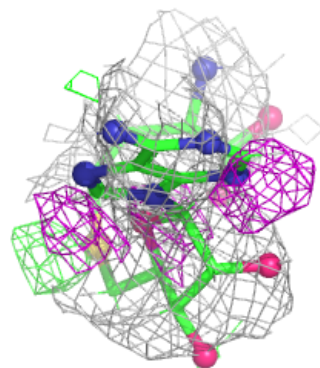
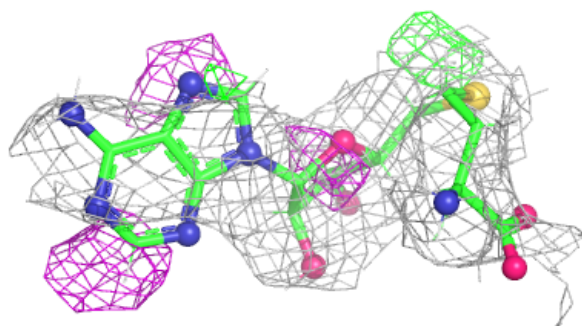
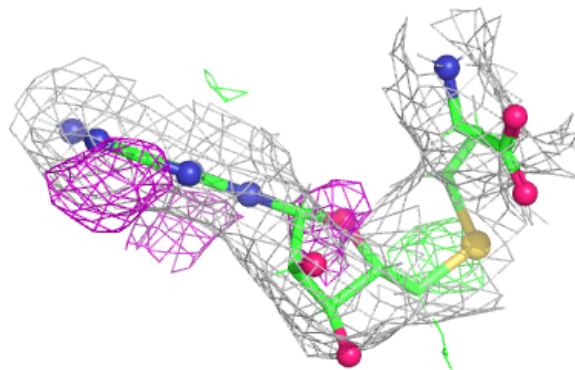
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SAH	B	601	26/26	0.74	0.17	20,63,63,63	0
4	ZN	H	201	1/1	0.88	0.05	162,162,162,162	1
4	ZN	E	201	1/1	0.89	0.05	104,104,104,104	1
4	ZN	F	201	1/1	0.98	0.13	9,9,9,9	1
4	ZN	C	201	1/1	0.99	0.04	68,68,68,68	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.

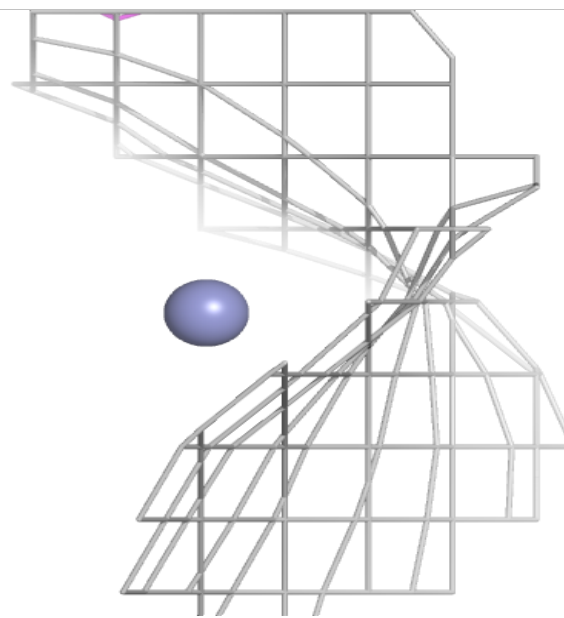
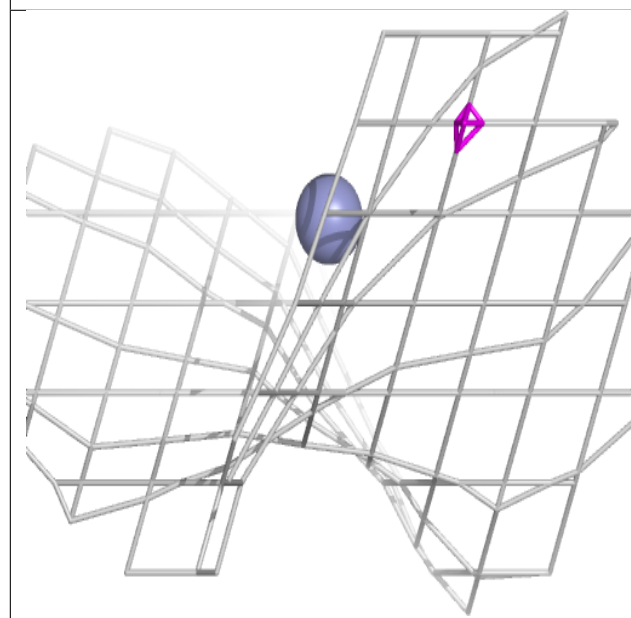
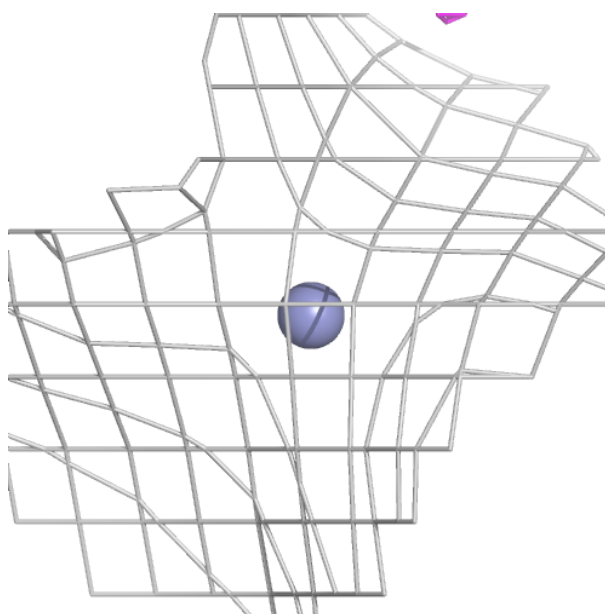
Electron density around SAH B 601:

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



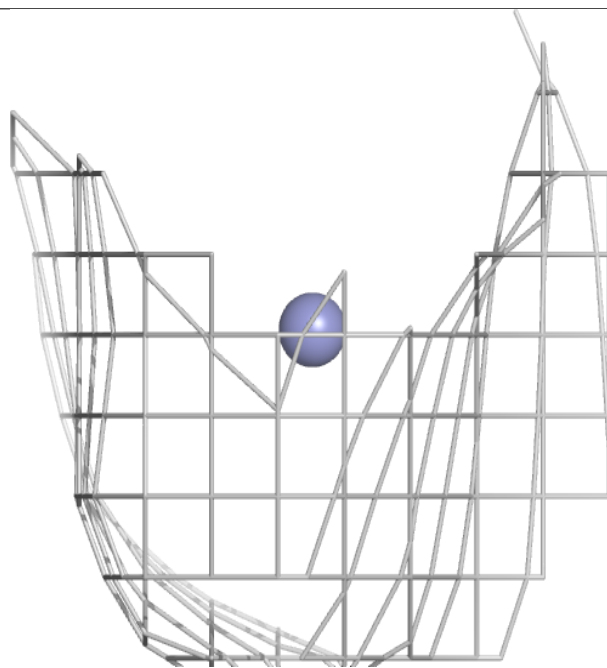
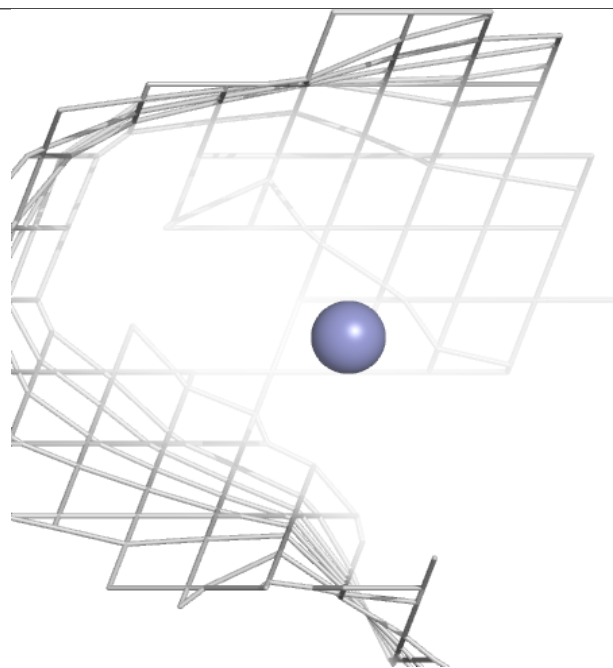
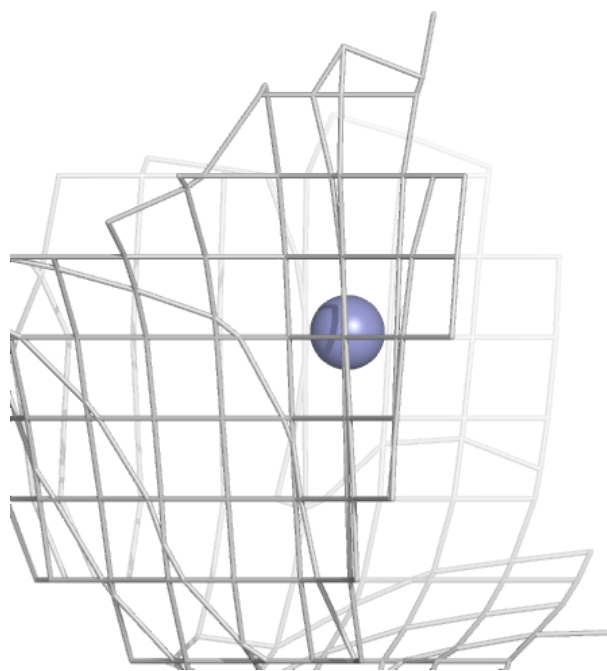
Electron density around ZN H 201:

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



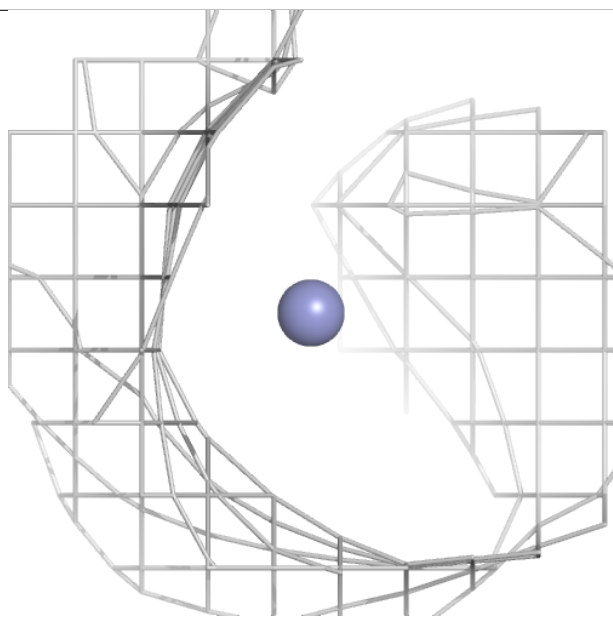
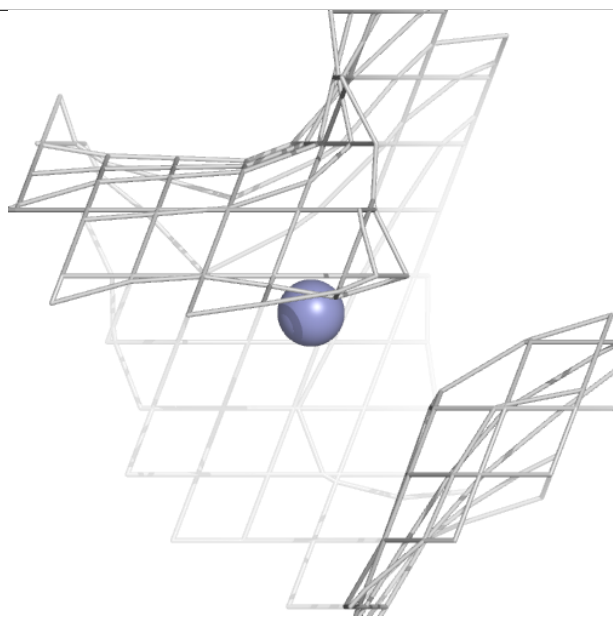
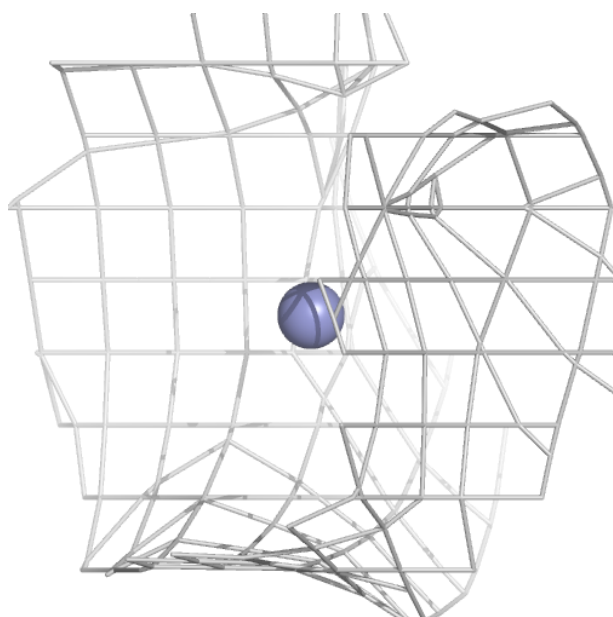
Electron density around ZN E 201:

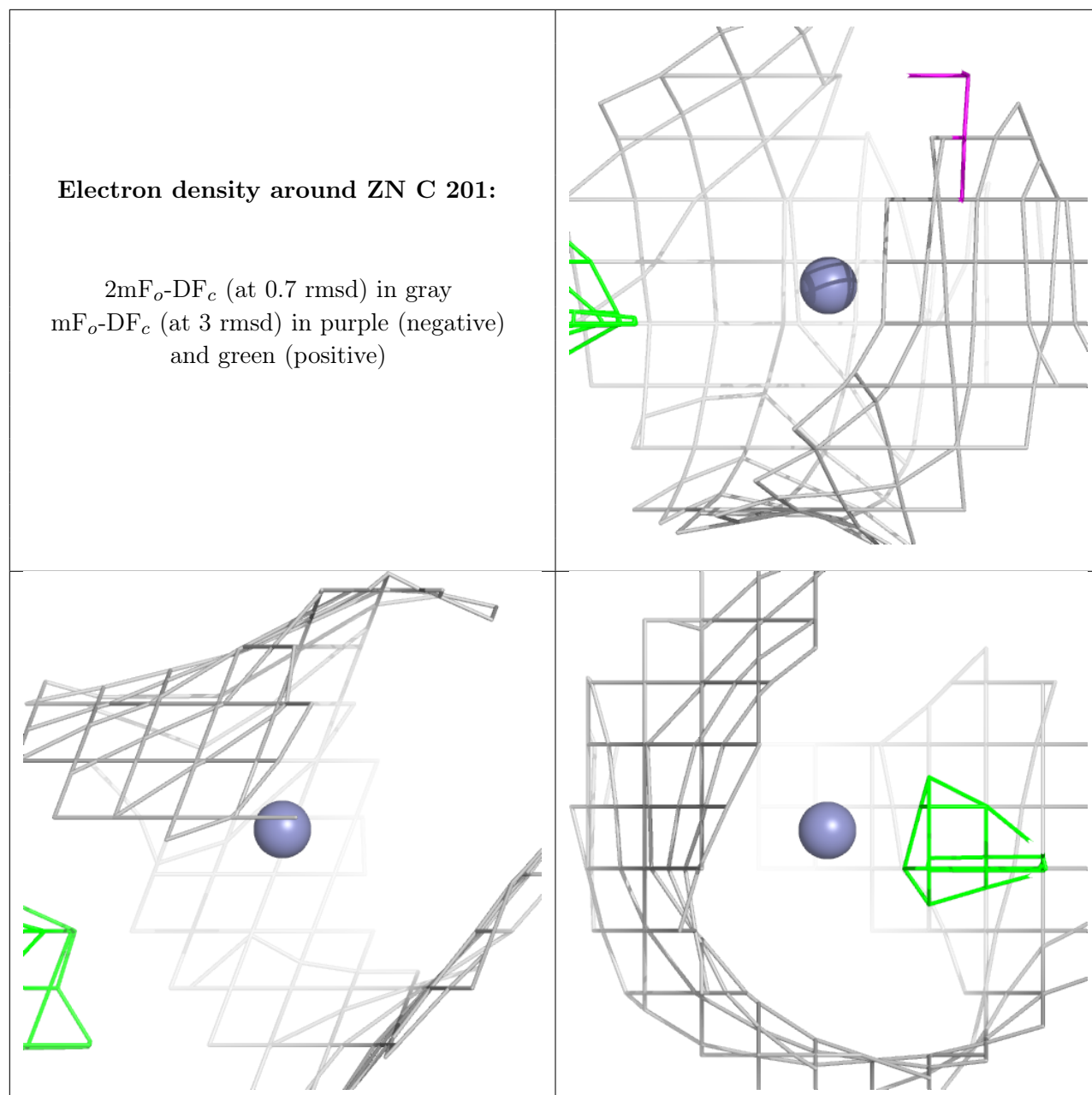
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN F 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.