



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:50 PM UTC

PDB ID : 8XOD / pdb_00008xod
Title : ThDP-dependent HKA synthase
Authors : Yu, J.H.; Liu, T.
Deposited on : 2024-01-01
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

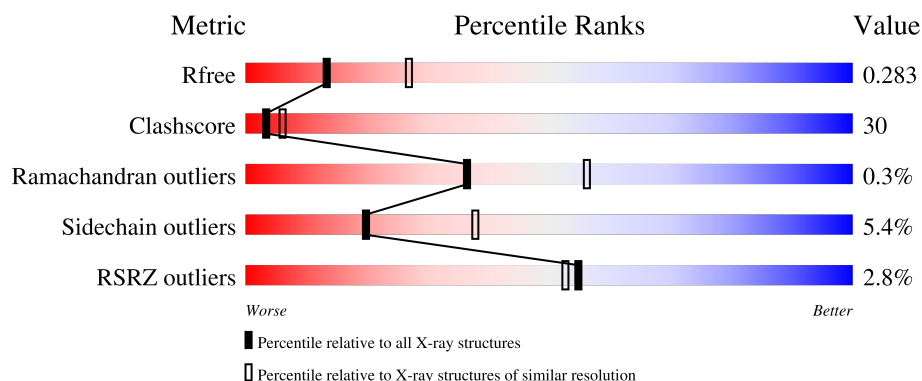
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	584	5% 50% 37% 9%
1	B	584	2% 51% 37% 9%
1	C	584	0% 49% 38% 9%
1	D	584	2% 51% 36% 9%

2 Entry composition [i](#)

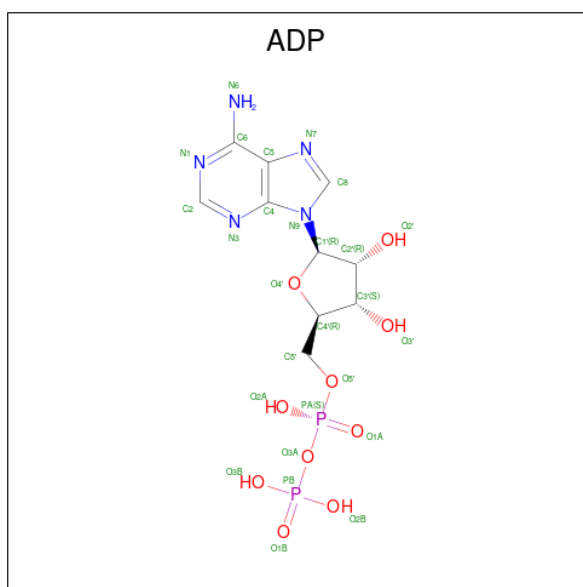
There are 6 unique types of molecules in this entry. The entry contains 16228 atoms, of which 142 are hydrogens and 0 are deuteriums.

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 BbmA-G484F complex with CBOA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			3970	2536	673	735	26			
1	B	531	Total	C	N	O	S	0	0	0
			3964	2533	672	733	26			
1	C	530	Total	C	N	O	S	0	0	0
			3956	2529	671	730	26			
1	D	530	Total	C	N	O	S	0	0	0
			3956	2529	671	730	26			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



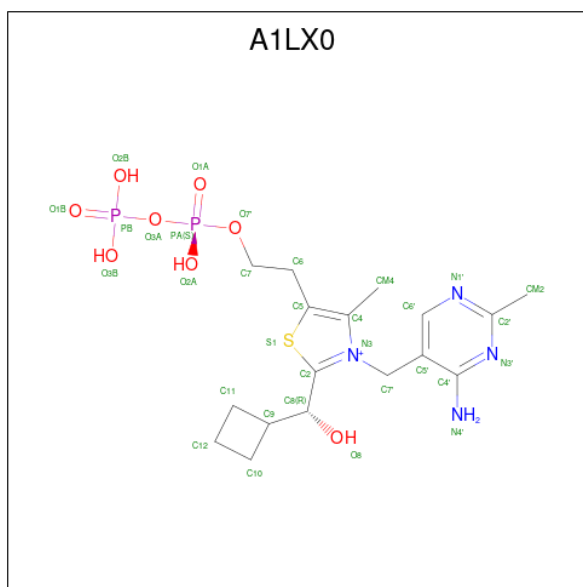
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[({R})-cyclobutyl(oxidanyl)methyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (CCD ID: A1LX0) (formula: C₁₇H₂₇N₄O₈P₂S) (labeled as "Ligand of Interest" by depositor).

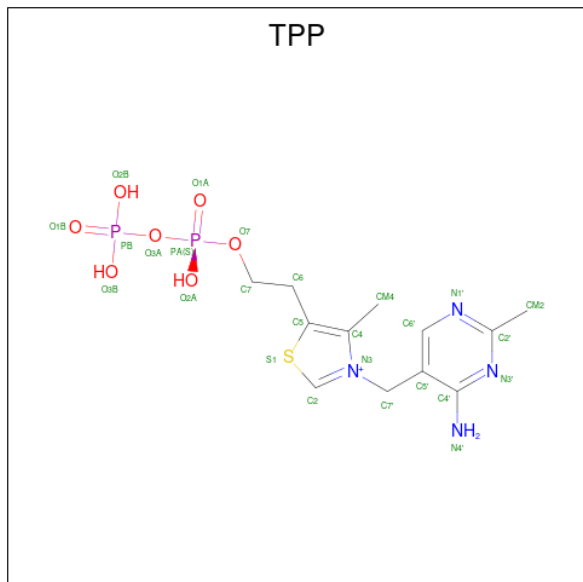


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			58	17	26	4	8	2	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			58	17	26	4	8	2	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			58	17	26	4	8	2	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		

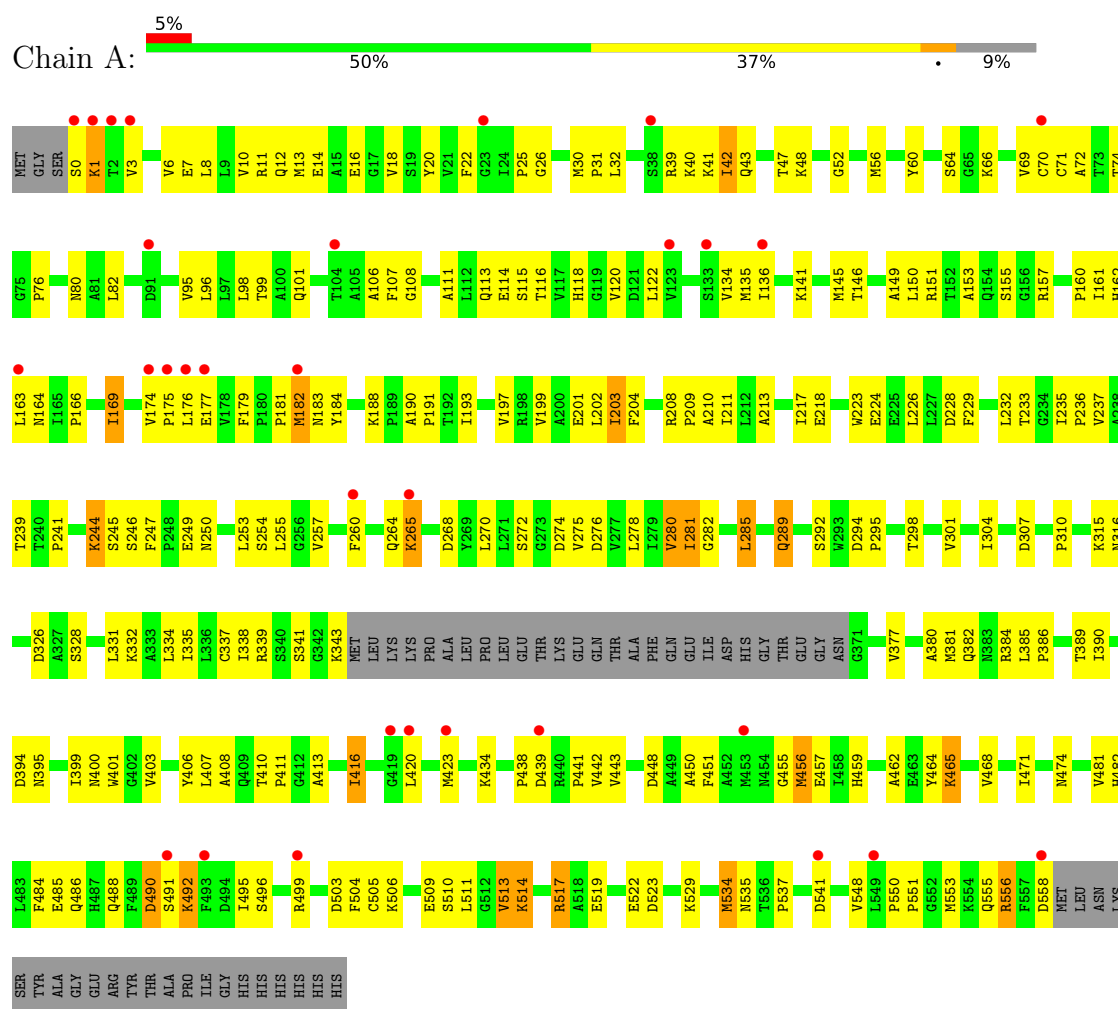
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		

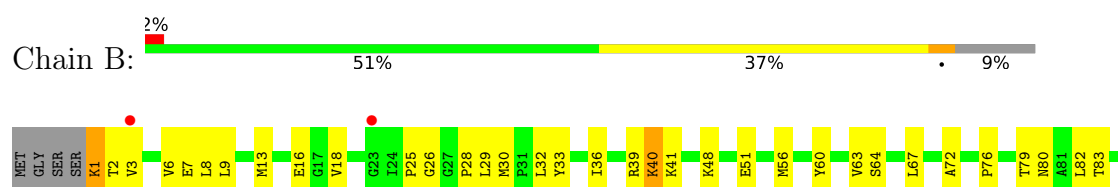
3 Residue-property plots

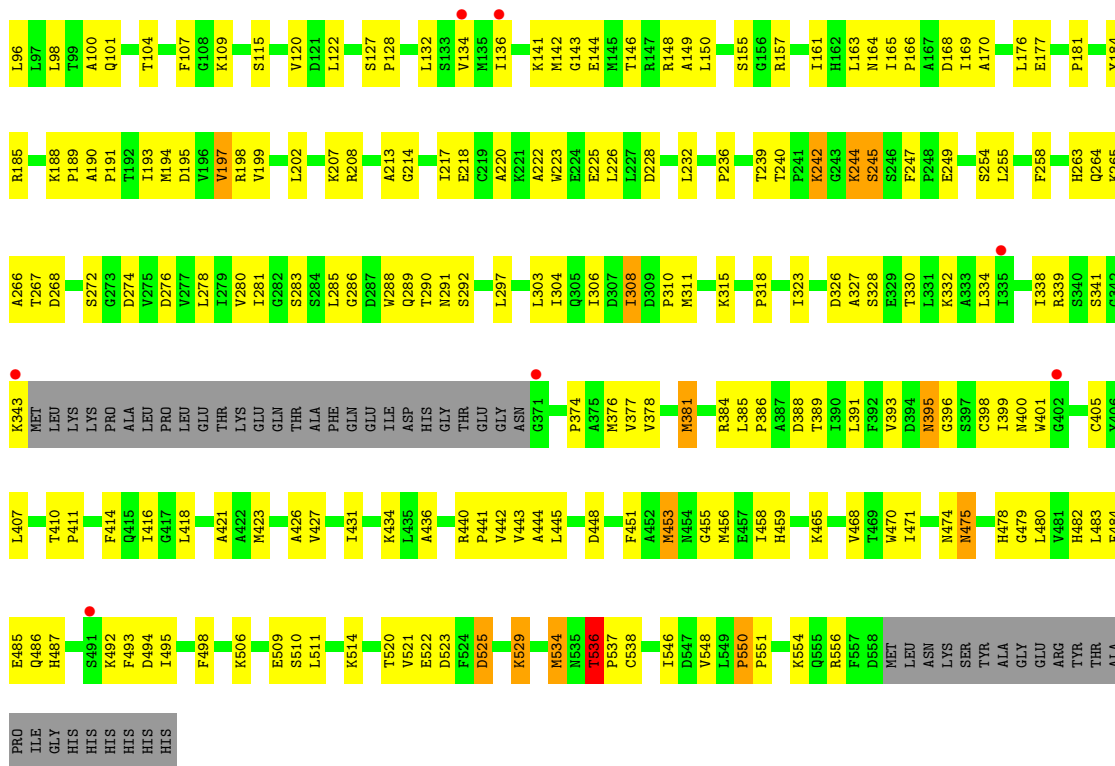
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BbmA-G484F complex with CBOA



• Molecule 1: BbmA-G484F complex with CBOA



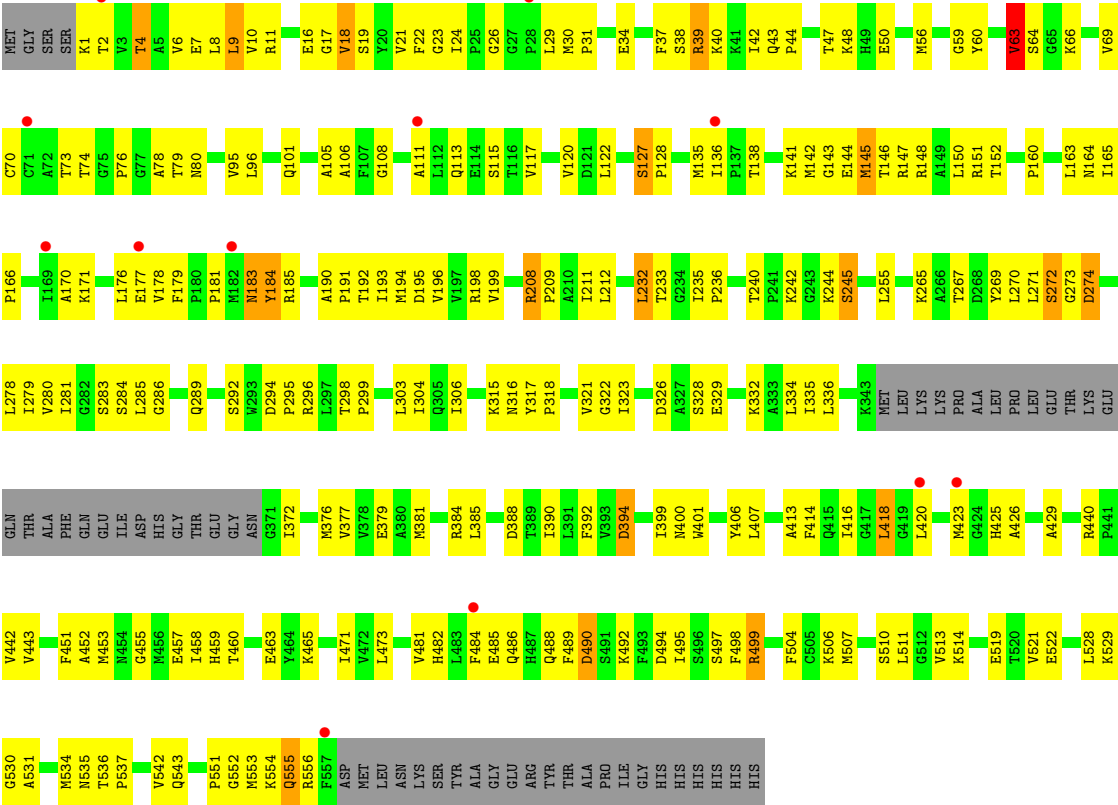


- Molecule 1: BbmA-G484F complex with CBOA



ARG
TYR
THR
ALA
SER
PRO
ILE
GLY
HIS
HIS
HIS
HIS
HIS

● Molecule 1: BbmA-G484F complex with CBOA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.94Å 116.69Å 201.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.75 24.94 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.94-2.75) 98.9 (24.94-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.1.17.3360	Depositor
R, R_{free}	0.203 , 0.286 0.221 , 0.283	Depositor DCC
R_{free} test set	2000 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	1.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16228	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.07 % 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 4.5381e-04. 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: A1LX0, TPP, MG, ADP

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	0.84	4/4058 (0.1%)	0.90	11/5517 (0.2%)
1	B	0.81	0/4052	0.84	14/5509 (0.3%)
1	C	0.83	4/4044 (0.1%)	0.89	14/5498 (0.3%)
1	D	0.81	3/4044 (0.1%)	0.89	10/5498 (0.2%)
All	All	0.82	11/16198 (0.1%)	0.88	49/22022 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	498	PHE	N-CA	-7.83	1.36	1.45
1	D	394	ASP	CA-C	-5.87	1.47	1.53
1	D	184	TYR	CA-C	-5.86	1.46	1.53
1	C	243	GLY	C-O	-5.31	1.17	1.24
1	A	280	VAL	C-O	-5.25	1.18	1.24
1	A	416	ILE	C-O	-5.08	1.19	1.24
1	A	514	LYS	C-O	-5.07	1.17	1.23
1	A	278	LEU	C-O	-5.04	1.18	1.24
1	C	286	GLY	C-O	-5.04	1.18	1.23
1	C	466	ILE	N-CA	-5.04	1.42	1.46
1	C	280	VAL	C-O	-5.02	1.18	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	ASP	N-CA-C	-11.06	98.30	112.23
1	D	499	ARG	N-CA-C	-9.44	101.89	113.41
1	D	38	SER	N-CA-C	-9.41	101.36	113.12
1	B	534	MET	N-CA-C	8.02	123.11	113.16
1	B	2	THR	N-CA-C	7.71	121.94	108.75
1	C	385	LEU	CA-C-N	7.69	127.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	LEU	C-N-CA	7.69	127.74	119.90
1	D	39	ARG	N-CA-C	7.60	121.04	111.69
1	C	294	ASP	CA-C-N	7.47	127.11	119.19
1	C	294	ASP	C-N-CA	7.47	127.11	119.19
1	C	281	ILE	CB-CA-C	-7.23	103.06	111.09
1	A	534	MET	N-CA-C	7.16	121.27	112.54
1	A	523	ASP	N-CA-C	-7.01	103.69	111.82
1	A	492	LYS	N-CA-C	-6.91	104.11	112.54
1	B	244	LYS	CA-C-N	6.85	134.62	121.54
1	B	244	LYS	C-N-CA	6.85	134.62	121.54
1	B	536	THR	CA-C-N	6.85	126.88	119.90
1	B	536	THR	C-N-CA	6.85	126.88	119.90
1	C	534	MET	N-CA-C	6.56	119.43	111.82
1	D	127	SER	CB-CA-C	-6.45	102.53	113.04
1	A	380	ALA	N-CA-C	-6.40	104.38	111.36
1	B	521	VAL	CB-CA-C	-6.33	103.77	111.88
1	A	40	LYS	N-CA-C	6.32	120.58	112.86
1	D	2	THR	N-CA-C	6.19	119.28	109.81
1	B	39	ARG	N-CA-C	6.12	122.13	113.02
1	C	244	LYS	CA-C-N	5.93	132.87	121.54
1	C	244	LYS	C-N-CA	5.93	132.87	121.54
1	A	438	PRO	CA-C-N	-5.86	113.35	122.67
1	A	438	PRO	C-N-CA	-5.86	113.35	122.67
1	C	281	ILE	N-CA-C	5.82	116.96	106.61
1	A	465	LYS	N-CA-CB	-5.74	103.07	112.25
1	A	282	GLY	N-CA-C	5.74	123.73	114.90
1	B	245	SER	N-CA-CB	5.72	120.16	110.49
1	C	279	ILE	CB-CA-C	-5.66	104.81	111.09
1	C	3	VAL	CB-CA-C	-5.60	103.50	111.34
1	D	63	VAL	N-CA-C	-5.60	107.00	111.81
1	A	556	ARG	N-CA-C	5.46	119.69	113.19
1	D	490	ASP	N-CA-C	5.46	122.44	110.80
1	A	265	LYS	CB-CA-C	-5.41	101.81	110.79
1	B	465	LYS	CG-CD-CE	-5.41	98.86	111.30
1	B	550	PRO	N-CA-C	5.38	117.27	110.70
1	D	183	ASN	CB-CA-C	-5.37	101.13	110.09
1	B	521	VAL	N-CA-C	5.26	115.89	110.36
1	C	411	PRO	N-CA-C	5.26	118.75	110.80
1	C	417	GLY	N-CA-C	-5.25	100.74	113.18
1	D	497	SER	O-C-N	5.23	128.92	123.06
1	B	525	ASP	N-CA-C	5.16	117.57	111.33
1	B	40	LYS	N-CA-C	5.11	121.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	SER	N-CA-C	5.04	118.57	111.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3970	0	4008	278	0
1	B	3964	0	4003	231	0
1	C	3956	0	3999	245	0
1	D	3956	0	3999	271	0
2	A	27	12	12	2	0
2	B	27	12	12	3	0
2	C	27	12	12	0	0
2	D	27	12	12	2	0
3	A	32	26	0	5	0
3	C	32	26	0	7	0
3	D	32	26	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	26	16	16	6	0
6	A	3	0	0	3	0
6	B	2	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	16086	142	16073	971	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 30.

All (971) 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:D:145:MET:HE2	1:D:145:MET:HA	1.23	1.13
1:A:237:VAL:HB	1:A:247:PHE:CE2	1.87	1.10
1:A:236:PRO:HB2	1:A:255:LEU:HD11	1.19	1.09
1:D:208:ARG:HD2	1:D:274:ASP:HB3	1.30	1.08
1:C:384:ARG:HH11	1:C:529:LYS:HB2	1.14	1.08
1:A:255:LEU:HA	1:A:265:LYS:CE	1.83	1.07
1:A:213:ALA:HB1	1:A:217:ILE:CD1	1.84	1.07
1:A:236:PRO:CB	1:A:255:LEU:HD11	1.83	1.06
1:A:423:MET:HE1	3:A:602:A1LX0:C4	1.85	1.05
1:C:232:LEU:HD22	1:C:338:ILE:HD13	1.38	1.04
1:D:255:LEU:HD21	1:D:269:TYR:HD2	1.18	1.04
1:A:182:MET:HE2	6:A:702:HOH:O	1.56	1.03
1:A:400:ASN:HD21	1:A:553:MET:CE	1.70	1.03
1:A:204:PHE:CE1	1:A:338:ILE:HD13	1.93	1.03
1:C:267:THR:O	1:C:271:LEU:HB2	1.59	1.02
1:A:255:LEU:CA	1:A:265:LYS:HE2	1.88	1.02
1:B:217:ILE:HD13	1:B:226:LEU:HD22	1.44	1.00
1:B:13:MET:HB3	1:B:18:VAL:HG21	1.42	1.00
1:B:166:PRO:HD2	1:B:169:ILE:HD11	1.42	1.00
1:D:4:THR:CG2	1:D:7:GLU:HB2	1.93	0.98
1:C:400:ASN:HD21	1:C:553:MET:CE	1.78	0.97
1:C:384:ARG:NH1	1:C:529:LYS:HB2	1.77	0.97
1:C:479:GLY:O	1:C:483:LEU:HD12	1.65	0.95
1:D:145:MET:HE1	1:D:148:ARG:HD2	1.49	0.95
1:B:378:VAL:HA	1:B:381:MET:HG3	1.47	0.95
1:A:484:PHE:CZ	1:A:556:ARG:NH2	2.34	0.95
1:C:400:ASN:ND2	1:C:553:MET:CE	2.29	0.95
1:D:208:ARG:HD2	1:D:274:ASP:CB	1.95	0.94
1:C:400:ASN:HD21	1:C:553:MET:HE1	1.31	0.93
1:D:208:ARG:CD	1:D:274:ASP:HB3	1.97	0.93
1:D:332:LYS:O	1:D:336:LEU:HD23	1.67	0.93
1:C:530:GLY:O	1:C:534:MET:HG2	1.67	0.92
1:B:207:LYS:HG2	1:B:276:ASP:OD2	1.70	0.91
1:B:3:VAL:HG21	1:B:7:GLU:HG2	1.50	0.91
1:A:236:PRO:HB2	1:A:255:LEU:CD1	2.00	0.91
1:A:115:SER:HB3	1:A:122:LEU:HG	1.53	0.90
1:D:142:MET:O	1:D:146:THR:HG23	1.71	0.90
1:D:236:PRO:HB2	1:D:255:LEU:HD11	1.53	0.90
1:D:4:THR:HG23	1:D:7:GLU:CB	2.02	0.90
1:D:384:ARG:HD2	1:D:528:LEU:HD22	1.52	0.90
1:A:423:MET:HE1	3:A:602:A1LX0:CM4	2.03	0.89
1:B:213:ALA:HB1	1:B:217:ILE:HD12	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:SER:HB2	1:D:414:PHE:HB3	1.52	0.88
1:C:236:PRO:HG2	1:C:269:TYR:HE2	1.36	0.88
1:D:381:MET:HE3	1:D:471:ILE:HD12	1.54	0.88
1:B:381:MET:O	1:B:385:LEU:HD12	1.74	0.88
1:B:48:LYS:HE3	1:B:459:HIS:ND1	1.88	0.88
1:C:13:MET:HB3	1:C:18:VAL:HG11	1.56	0.88
1:D:554:LYS:O	1:D:554:LYS:NZ	2.07	0.88
1:C:400:ASN:ND2	1:C:553:MET:HE2	1.90	0.87
1:B:310:PRO:HG2	1:B:311:MET:HE2	1.58	0.86
1:D:4:THR:CG2	1:D:7:GLU:CB	2.53	0.86
1:D:145:MET:HA	1:D:145:MET:CE	2.04	0.86
1:A:204:PHE:CZ	1:A:338:ILE:HD13	2.11	0.85
1:A:82:LEU:HD23	1:D:79:THR:HB	1.58	0.84
1:B:149:ALA:HB1	1:B:161:ILE:HG21	1.59	0.84
1:D:255:LEU:HD21	1:D:269:TYR:CD2	2.10	0.84
1:A:237:VAL:HB	1:A:247:PHE:CD2	2.12	0.84
1:A:209:PRO:HG2	1:A:235:ILE:HG12	1.58	0.83
1:A:400:ASN:HD21	1:A:553:MET:HE1	1.43	0.83
1:D:315:LYS:HD2	1:D:316:ASN:ND2	1.91	0.83
1:D:426:ALA:HA	1:D:429:ALA:HB3	1.60	0.83
1:B:236:PRO:HB2	1:B:255:LEU:HD21	1.61	0.83
1:C:304:ILE:HG12	1:C:321:VAL:CG1	2.08	0.83
1:C:395:ASN:HA	1:C:399:ILE:HD11	1.61	0.83
1:D:321:VAL:HG12	1:D:323:ILE:HD11	1.59	0.82
1:C:204:PHE:HB3	1:C:343:LYS:HE3	1.59	0.82
1:D:48:LYS:NZ	1:D:460:THR:HG22	1.93	0.82
1:B:199:VAL:CG2	1:B:334:LEU:HD21	2.10	0.82
1:B:482:HIS:O	1:B:486:GLN:HG3	1.79	0.82
1:A:255:LEU:HA	1:A:265:LYS:HE2	0.92	0.81
1:A:3:VAL:CG2	1:A:7:GLU:CD	2.52	0.81
1:B:377:VAL:O	1:B:381:MET:HG2	1.78	0.81
1:C:400:ASN:ND2	1:C:553:MET:HE1	1.94	0.81
1:B:3:VAL:HG21	1:B:7:GLU:CG	2.10	0.81
1:D:552:GLY:C	1:D:555:GLN:OE1	2.23	0.81
1:D:321:VAL:CG1	1:D:323:ILE:HD11	2.11	0.81
1:B:16:GLU:HG3	1:B:150:LEU:HD13	1.62	0.81
1:C:13:MET:O	1:C:18:VAL:HG12	1.82	0.80
1:D:145:MET:CE	1:D:148:ARG:HD2	2.10	0.80
1:A:400:ASN:ND2	1:A:553:MET:CE	2.43	0.80
1:A:484:PHE:HZ	1:A:556:ARG:NH2	1.75	0.80
1:A:118:HIS:CE1	1:C:145:MET:HE1	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:MET:HE1	3:A:602:A1LX0:C5	2.11	0.80
1:D:177:GLU:O	1:D:177:GLU:HG3	1.81	0.80
1:D:47:THR:HB	1:D:457:GLU:OE2	1.83	0.79
1:D:236:PRO:HG2	1:D:269:TYR:HE2	1.45	0.79
1:C:185:ARG:HG3	1:C:185:ARG:HH11	1.47	0.79
1:A:47:THR:HB	1:A:457:GLU:OE2	1.82	0.79
1:C:388:ASP:O	1:C:440:ARG:CD	2.30	0.79
1:D:255:LEU:CD2	1:D:269:TYR:HD2	1.96	0.79
1:D:514:LYS:HG2	1:D:534:MET:HE1	1.64	0.79
1:A:204:PHE:HE1	1:A:338:ILE:HD13	1.44	0.79
1:B:6:VAL:HG12	1:B:170:ALA:O	1.83	0.79
1:A:188:LYS:HE2	1:A:326:ASP:OD2	1.83	0.79
1:B:217:ILE:CD1	1:B:226:LEU:HD22	2.12	0.78
1:D:267:THR:O	1:D:271:LEU:HB2	1.84	0.78
1:C:451:PHE:HZ	1:C:458:ILE:HD13	1.47	0.78
1:A:1:LYS:HG2	1:A:176:LEU:HD22	1.64	0.78
1:B:459:HIS:HB2	1:B:511:LEU:HD13	1.65	0.78
1:B:132:LEU:HB3	1:B:161:ILE:HD12	1.66	0.78
1:A:3:VAL:HG21	1:A:7:GLU:CD	2.09	0.78
1:D:4:THR:HG23	1:D:7:GLU:HB2	1.65	0.77
1:D:136:ILE:HD13	1:D:142:MET:HE1	1.66	0.77
1:D:236:PRO:CG	1:D:269:TYR:HE2	1.96	0.77
1:B:166:PRO:HD2	1:B:169:ILE:CD1	2.14	0.77
1:A:244:LYS:HE3	1:A:403:VAL:HA	1.66	0.77
1:D:406:TYR:C	1:D:407:LEU:HD23	2.11	0.76
1:C:388:ASP:O	1:C:440:ARG:HD2	1.86	0.76
1:B:242:LYS:HD2	1:B:418:LEU:HB2	1.67	0.76
1:C:548:VAL:O	1:C:550:PRO:HD3	1.86	0.75
1:D:60:TYR:O	1:D:64:SER:HB3	1.85	0.75
1:A:18:VAL:O	1:A:42:ILE:HD13	1.86	0.75
1:C:199:VAL:HG13	1:C:304:ILE:HD13	1.68	0.75
1:A:442:VAL:HG23	1:A:468:VAL:HG22	1.69	0.75
1:A:522:GLU:N	1:A:522:GLU:OE1	2.16	0.75
1:C:60:TYR:O	1:C:64:SER:HB3	1.87	0.75
1:D:209:PRO:HG2	1:D:235:ILE:HG12	1.69	0.75
1:D:514:LYS:HG2	1:D:534:MET:CE	2.17	0.75
1:B:386:PRO:O	1:B:389:THR:HG23	1.87	0.74
1:A:169:ILE:HD12	1:A:169:ILE:O	1.87	0.74
1:B:109:LYS:HE3	1:C:316:ASN:OD1	1.87	0.74
1:A:255:LEU:HG	1:A:265:LYS:HE3	1.69	0.74
1:B:82:LEU:HD13	1:C:82:LEU:HD22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ASP:OD1	1:D:198:ARG:NH2	2.20	0.74
1:D:328:SER:O	1:D:332:LYS:HG2	1.87	0.74
1:A:382:GLN:OE1	1:A:407:LEU:HB3	1.88	0.74
1:B:83:THR:HG21	1:C:80:ASN:OD1	1.88	0.74
1:A:295:PRO:O	1:A:298:THR:HG23	1.88	0.73
1:C:166:PRO:HB2	1:C:169:ILE:CG2	2.19	0.73
1:B:13:MET:O	1:B:18:VAL:HG22	1.88	0.73
1:C:149:ALA:HB1	1:C:161:ILE:HG21	1.70	0.73
1:D:193:ILE:HD12	1:D:193:ILE:N	2.04	0.73
1:D:381:MET:HE3	1:D:471:ILE:CD1	2.18	0.73
1:B:434:LYS:HB2	1:B:442:VAL:HG21	1.71	0.72
1:B:308:ILE:O	1:B:308:ILE:HD12	1.89	0.72
1:C:395:ASN:HD22	1:C:399:ILE:HD11	1.53	0.72
1:C:479:GLY:O	1:C:483:LEU:CD1	2.37	0.72
1:C:135:MET:HE3	1:C:166:PRO:HG2	1.71	0.72
1:D:377:VAL:O	1:D:381:MET:HG3	1.90	0.72
1:A:188:LYS:CE	1:A:326:ASP:OD2	2.36	0.72
1:C:48:LYS:HE2	1:C:459:HIS:ND1	2.05	0.72
1:A:281:ILE:N	1:A:281:ILE:HD12	2.05	0.72
1:D:26:GLY:O	1:D:30:MET:HG2	1.88	0.72
1:C:388:ASP:HB2	1:C:440:ARG:HD3	1.70	0.72
1:B:199:VAL:HG23	1:B:334:LEU:HD21	1.72	0.72
1:D:143:GLY:HA3	1:D:177:GLU:OE2	1.89	0.72
1:A:434:LYS:HB2	1:A:442:VAL:HG21	1.71	0.71
1:B:395:ASN:HA	1:B:399:ILE:HD11	1.70	0.71
1:C:443:VAL:HG22	1:C:469:THR:HB	1.72	0.71
1:B:13:MET:HB3	1:B:18:VAL:CG2	2.20	0.71
1:C:135:MET:HE3	1:C:166:PRO:CG	2.20	0.71
1:C:394:ASP:OD1	1:C:426:ALA:N	2.24	0.71
1:A:386:PRO:O	1:A:389:THR:HG23	1.90	0.71
1:C:434:LYS:NZ	1:C:438:PRO:O	2.23	0.71
1:B:556:ARG:O	1:B:556:ARG:HG3	1.91	0.70
1:B:381:MET:C	1:B:385:LEU:HD12	2.15	0.70
1:D:115:SER:HB3	1:D:122:LEU:HG	1.72	0.70
1:C:132:LEU:HB3	1:C:161:ILE:HD12	1.72	0.70
1:C:334:LEU:O	1:C:338:ILE:HG13	1.91	0.70
1:A:82:LEU:CD2	1:D:79:THR:HB	2.22	0.69
1:A:106:ALA:HB1	1:A:111:ALA:HB2	1.73	0.69
1:A:289:GLN:HE21	1:A:289:GLN:N	1.90	0.69
1:B:381:MET:CB	1:B:385:LEU:HD12	2.22	0.69
1:C:236:PRO:HG2	1:C:269:TYR:CE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:VAL:HG12	1:D:170:ALA:O	1.92	0.69
1:A:14:GLU:OE1	1:A:39:ARG:NH2	2.26	0.69
1:B:381:MET:CB	1:B:385:LEU:CD1	2.71	0.69
1:B:213:ALA:HB1	1:B:217:ILE:CD1	2.23	0.69
1:A:13:MET:HB3	1:A:18:VAL:HG11	1.75	0.68
1:A:401:TRP:CZ3	1:A:551:PRO:HD3	2.28	0.68
1:C:481:VAL:O	1:C:485:GLU:HG3	1.93	0.68
1:D:406:TYR:O	1:D:407:LEU:HD23	1.92	0.68
1:C:399:ILE:HG12	1:C:416:ILE:HD11	1.75	0.68
1:C:244:LYS:HD3	1:C:414:PHE:CD2	2.29	0.68
1:C:386:PRO:O	1:C:389:THR:HG22	1.93	0.68
1:C:185:ARG:HH11	1:C:185:ARG:CG	2.06	0.68
1:D:271:LEU:HB3	1:D:296:ARG:HH12	1.58	0.68
1:A:280:VAL:HG11	1:A:285:LEU:HD21	1.76	0.67
1:C:26:GLY:O	1:C:30:MET:HG2	1.93	0.67
1:C:233:THR:OG1	1:C:235:ILE:HG13	1.94	0.67
1:D:193:ILE:HD12	1:D:193:ILE:H	1.59	0.67
1:A:80:ASN:ND2	1:D:453:MET:HE1	2.10	0.67
1:B:236:PRO:CB	1:B:255:LEU:HD21	2.24	0.67
1:B:381:MET:HB3	1:B:385:LEU:HD11	1.76	0.67
1:C:483:LEU:O	1:C:487:HIS:HD2	1.76	0.67
1:D:536:THR:HB	1:D:537:PRO:HD2	1.76	0.67
1:D:37:PHE:CE1	1:D:44:PRO:HG3	2.29	0.67
1:D:384:ARG:CD	1:D:528:LEU:HD22	2.24	0.67
1:A:141:LYS:HZ1	1:C:105:ALA:HA	1.58	0.67
1:B:400:ASN:HB3	1:B:551:PRO:HD2	1.77	0.67
1:C:29:LEU:HG	1:C:29:LEU:O	1.95	0.67
1:D:198:ARG:NH1	1:D:321:VAL:HG22	2.10	0.67
1:B:389:THR:HG22	1:B:441:PRO:HG2	1.78	0.66
1:C:10:VAL:O	1:C:14:GLU:HG3	1.95	0.66
1:A:529:LYS:O	1:A:529:LYS:HG2	1.94	0.66
1:B:82:LEU:HD23	1:C:79:THR:HB	1.76	0.66
1:A:18:VAL:HG13	1:A:42:ILE:CD1	2.26	0.66
1:A:149:ALA:HB1	1:A:161:ILE:HG21	1.78	0.66
1:A:484:PHE:CE1	1:A:556:ARG:NH2	2.63	0.66
1:B:334:LEU:O	1:B:338:ILE:HG13	1.95	0.66
1:A:232:LEU:HD13	1:A:232:LEU:O	1.95	0.66
1:B:485:GLU:OE2	1:B:495:ILE:HG22	1.96	0.66
1:C:115:SER:HB3	1:C:122:LEU:HG	1.76	0.66
1:B:9:LEU:HD12	1:B:142:MET:CE	2.26	0.66
1:B:289:GLN:N	1:B:289:GLN:OE1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:LYS:O	1:D:336:LEU:CD2	2.43	0.66
1:A:6:VAL:HG21	1:A:32:LEU:HA	1.78	0.65
1:B:378:VAL:HA	1:B:381:MET:CG	2.24	0.65
1:C:479:GLY:CA	3:C:602:A1LX0:O3B	2.44	0.65
1:C:7:GLU:O	1:C:10:VAL:HG22	1.96	0.65
1:D:4:THR:HG23	1:D:7:GLU:HB3	1.77	0.65
1:A:250:ASN:OD1	1:A:250:ASN:N	2.26	0.65
1:B:378:VAL:CA	1:B:381:MET:HG3	2.25	0.65
1:C:489:PHE:O	1:C:492:LYS:HG2	1.95	0.65
1:D:236:PRO:HG2	1:D:269:TYR:CE2	2.30	0.65
1:B:115:SER:HB3	1:B:122:LEU:HG	1.79	0.65
1:C:482:HIS:O	1:C:486:GLN:HG3	1.97	0.65
1:A:48:LYS:HE2	1:A:459:HIS:ND1	2.11	0.65
1:A:60:TYR:O	1:A:64:SER:HB2	1.96	0.65
1:A:213:ALA:HB1	1:A:217:ILE:HD11	1.74	0.65
1:A:213:ALA:HB1	1:A:217:ILE:HD13	1.76	0.65
1:C:185:ARG:HG3	1:C:185:ARG:NH1	2.12	0.65
1:C:479:GLY:HA3	3:C:602:A1LX0:O3B	1.96	0.64
1:D:232:LEU:O	1:D:232:LEU:HD13	1.96	0.64
1:B:3:VAL:HG23	1:B:7:GLU:HB3	1.77	0.64
1:A:174:VAL:HB	1:A:175:PRO:HD2	1.78	0.64
1:B:80:ASN:ND2	1:C:453:MET:HE1	2.12	0.64
1:B:141:LYS:NZ	1:D:105:ALA:HA	2.12	0.64
1:A:169:ILE:HD12	1:A:169:ILE:C	2.23	0.64
1:A:448:ASP:HB3	1:A:474:ASN:HA	1.80	0.64
1:C:232:LEU:O	1:C:232:LEU:HD23	1.97	0.64
1:C:394:ASP:OD1	1:C:426:ALA:HB3	1.97	0.64
1:A:395:ASN:HA	1:A:399:ILE:HD11	1.80	0.64
1:B:244:LYS:HD3	1:B:414:PHE:CG	2.32	0.64
1:A:237:VAL:HG11	1:A:247:PHE:CG	2.33	0.64
1:A:310:PRO:HB2	1:B:155:SER:HB3	1.80	0.64
1:A:553:MET:CA	1:A:553:MET:HE2	2.26	0.64
1:C:384:ARG:NH1	1:C:529:LYS:CB	2.57	0.64
1:C:395:ASN:HA	1:C:399:ILE:CD1	2.27	0.64
1:D:4:THR:HG23	1:D:7:GLU:H	1.63	0.64
1:D:29:LEU:O	1:D:29:LEU:HG	1.97	0.64
1:D:271:LEU:O	1:D:296:ARG:NH1	2.30	0.64
1:C:276:ASP:HA	1:C:300:SER:H	1.63	0.63
1:D:376:MET:HA	1:D:379:GLU:HB2	1.78	0.63
1:A:289:GLN:HE21	1:A:289:GLN:H	1.47	0.63
1:C:529:LYS:O	1:C:529:LYS:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:THR:O	1:D:76:PRO:HD2	1.98	0.63
1:C:76:PRO:HG3	1:C:113:GLN:HE21	1.63	0.63
1:B:374:PRO:HB2	1:B:401:TRP:CE2	2.33	0.63
1:D:146:THR:O	1:D:150:LEU:HG	1.99	0.63
1:C:423:MET:HB2	1:C:453:MET:SD	2.38	0.63
1:D:552:GLY:CA	1:D:555:GLN:OE1	2.46	0.63
1:A:26:GLY:O	1:A:30:MET:HG2	1.99	0.62
1:A:193:ILE:HD12	1:A:193:ILE:H	1.64	0.62
1:C:198:ARG:O	1:C:202:LEU:HD13	1.97	0.62
1:C:388:ASP:O	1:C:440:ARG:HD3	1.99	0.62
1:D:16:GLU:HG3	1:D:150:LEU:HD13	1.79	0.62
1:B:218:GLU:HG3	1:B:223:TRP:HZ2	1.63	0.62
1:D:294:ASP:OD1	1:D:295:PRO:HD2	1.98	0.62
1:B:416:ILE:HG23	1:B:418:LEU:HG	1.82	0.62
1:B:423:MET:HE2	5:B:602:TPP:C6'	2.28	0.62
1:C:311:MET:SD	1:D:152:THR:HA	2.39	0.62
1:D:531:ALA:O	1:D:534:MET:HB2	1.99	0.62
1:C:236:PRO:CG	1:C:269:TYR:HE2	2.12	0.62
1:D:321:VAL:HG12	1:D:323:ILE:CD1	2.30	0.62
1:C:244:LYS:NZ	1:C:403:VAL:O	2.33	0.62
1:A:197:VAL:O	1:A:201:GLU:HG2	1.99	0.62
1:B:485:GLU:OE1	1:B:494:ASP:HA	2.00	0.62
1:A:377:VAL:O	1:A:381:MET:HG3	2.00	0.61
1:A:118:HIS:NE2	1:C:145:MET:HE1	2.14	0.61
1:A:141:LYS:NZ	1:C:105:ALA:HA	2.16	0.61
1:C:552:GLY:HA2	1:C:555:GLN:HE21	1.65	0.61
1:A:218:GLU:HG3	1:A:223:TRP:HZ2	1.65	0.61
1:B:388:ASP:HB2	1:B:440:ARG:HD2	1.82	0.61
1:C:209:PRO:HG2	1:C:235:ILE:HG23	1.82	0.61
1:D:401:TRP:CZ3	1:D:551:PRO:HD3	2.36	0.61
1:B:381:MET:HB3	1:B:385:LEU:CD1	2.30	0.61
1:C:204:PHE:HB3	1:C:343:LYS:CE	2.28	0.61
1:B:134:VAL:HG12	1:D:117:VAL:HG11	1.81	0.61
1:B:32:LEU:O	1:B:36:ILE:HG13	2.00	0.61
1:B:79:THR:HB	1:C:83:THR:OG1	2.00	0.61
1:C:169:ILE:HD13	1:C:169:ILE:C	2.25	0.61
1:D:384:ARG:HD2	1:D:528:LEU:CD2	2.29	0.61
1:A:155:SER:HB3	1:B:310:PRO:HB2	1.81	0.60
1:D:11:ARG:HH21	1:D:39:ARG:NH1	1.97	0.60
1:D:4:THR:HG22	1:D:7:GLU:OE2	2.01	0.60
1:B:207:LYS:HE3	1:B:276:ASP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ILE:HG23	1:D:281:ILE:CD1	2.32	0.60
1:D:552:GLY:HA2	1:D:555:GLN:CD	2.26	0.60
1:B:395:ASN:HA	1:B:399:ILE:CD1	2.31	0.60
1:D:101:GLN:HB3	1:D:166:PRO:HA	1.83	0.60
1:A:213:ALA:HB1	1:A:217:ILE:HD12	1.81	0.60
1:B:82:LEU:CD2	1:C:79:THR:HB	2.32	0.60
1:C:82:LEU:HD12	1:C:129:ILE:HD11	1.83	0.60
1:A:255:LEU:HG	1:A:265:LYS:CE	2.32	0.60
1:A:385:LEU:HB3	1:A:389:THR:HG21	1.83	0.60
1:B:3:VAL:CG2	1:B:7:GLU:HG2	2.29	0.60
1:C:338:ILE:HD12	1:C:339:ARG:N	2.17	0.60
1:D:298:THR:HG23	1:D:317:TYR:HD2	1.67	0.60
1:D:244:LYS:O	1:D:245:SER:CB	2.49	0.59
1:D:23:GLY:C	1:D:24:ILE:HD13	2.26	0.59
1:D:30:MET:N	1:D:31:PRO:CD	2.65	0.59
1:A:8:LEU:HD11	1:A:177:GLU:H	1.66	0.59
1:D:534:MET:O	1:D:535:ASN:HB3	2.01	0.59
1:A:484:PHE:CE2	1:A:488:GLN:OE1	2.55	0.59
1:D:323:ILE:HD13	1:D:323:ILE:N	2.18	0.59
1:A:442:VAL:CG2	1:A:468:VAL:HG22	2.31	0.59
1:B:217:ILE:HD13	1:B:226:LEU:CD2	2.27	0.59
1:B:283:SER:HA	2:B:601:ADP:O2B	2.03	0.59
1:D:48:LYS:HZ2	1:D:460:THR:HG22	1.66	0.59
1:A:13:MET:O	1:A:18:VAL:HG12	2.03	0.59
1:A:382:GLN:HE22	1:A:407:LEU:H	1.49	0.59
1:A:3:VAL:CG2	1:A:7:GLU:OE2	2.51	0.58
1:C:204:PHE:CZ	1:C:338:ILE:HG22	2.38	0.58
1:D:233:THR:HG22	1:D:235:ILE:HG13	1.85	0.58
1:A:16:GLU:HG3	1:A:150:LEU:HD13	1.85	0.58
1:A:182:MET:CE	6:A:702:HOH:O	2.29	0.58
1:A:490:ASP:OD1	1:A:490:ASP:N	2.34	0.58
1:A:245:SER:O	1:A:411:PRO:HA	2.04	0.58
1:A:556:ARG:O	1:A:556:ARG:HG2	2.03	0.58
1:B:247:PHE:CD2	1:B:254:SER:HB2	2.38	0.58
1:C:384:ARG:HH12	1:C:529:LYS:HG3	1.67	0.58
1:D:536:THR:HB	1:D:537:PRO:CD	2.32	0.58
1:C:508:ALA:HB3	1:C:515:SER:HB3	1.86	0.58
1:B:423:MET:HE2	5:B:602:TPP:C2'	2.34	0.58
1:B:442:VAL:CG2	1:B:468:VAL:HG22	2.34	0.58
1:D:48:LYS:HZ3	1:D:460:THR:HG22	1.66	0.58
1:D:145:MET:HE1	1:D:148:ARG:CD	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LEU:HD23	1:D:299:PRO:HD3	1.86	0.58
1:D:296:ARG:HH11	1:D:296:ARG:HB3	1.67	0.58
1:A:64:SER:OG	1:A:66:LYS:HB2	2.04	0.57
1:B:41:LYS:O	1:B:41:LYS:HG3	2.03	0.57
1:B:377:VAL:O	1:B:381:MET:CG	2.50	0.57
1:D:471:ILE:HG22	1:D:473:LEU:CD1	2.34	0.57
1:C:303:LEU:HD23	1:C:318:PRO:O	2.04	0.57
1:D:34:GLU:O	1:D:34:GLU:HG2	2.04	0.57
1:A:423:MET:CE	3:A:602:A1LX0:C4	2.74	0.57
1:B:63:VAL:HG13	1:B:436:ALA:HB3	1.86	0.57
1:A:481:VAL:O	1:A:485:GLU:HG3	2.05	0.57
1:C:141:LYS:HE3	1:C:144:GLU:OE1	2.05	0.57
1:C:424:GLY:HA3	1:C:454:ASN:OD1	2.03	0.57
1:D:212:LEU:HD21	1:D:240:THR:HG23	1.85	0.57
1:D:530:GLY:O	1:D:534:MET:HG3	2.04	0.57
1:A:0:SER:O	1:A:0:SER:OG	2.18	0.57
1:A:276:ASP:O	1:A:301:VAL:HB	2.04	0.57
1:C:423:MET:HG3	3:C:602:A1LX0:N3'	2.19	0.57
1:D:4:THR:OG1	1:D:171:LYS:HA	2.04	0.57
1:D:56:MET:HE1	1:D:457:GLU:OE2	2.05	0.57
1:A:209:PRO:CG	1:A:235:ILE:HG12	2.30	0.57
1:A:434:LYS:HG3	1:A:442:VAL:HG22	1.87	0.57
1:C:372:ILE:HD12	1:C:542:VAL:HG13	1.86	0.57
1:D:4:THR:CG2	1:D:7:GLU:HB3	2.30	0.57
1:D:9:LEU:CD1	1:D:146:THR:HG21	2.35	0.57
1:A:153:ALA:HB2	1:A:161:ILE:HG12	1.87	0.56
1:A:209:PRO:HB2	1:A:235:ILE:HD13	1.86	0.56
1:C:201:GLU:HA	1:C:201:GLU:OE1	2.04	0.56
1:C:530:GLY:O	1:C:534:MET:CG	2.47	0.56
1:B:80:ASN:HD21	1:C:453:MET:HE1	1.68	0.56
1:C:33:TYR:HA	1:C:36:ILE:HD12	1.86	0.56
1:C:169:ILE:HG12	1:C:169:ILE:O	2.04	0.56
1:D:43:GLN:HG2	1:D:44:PRO:HD2	1.86	0.56
1:D:191:PRO:HB3	1:D:323:ILE:CG2	2.35	0.56
1:D:244:LYS:HD3	1:D:414:PHE:CE2	2.39	0.56
1:A:289:GLN:H	1:A:289:GLN:NE2	2.02	0.56
1:B:13:MET:C	1:B:18:VAL:HG22	2.29	0.56
1:B:63:VAL:CG1	1:B:436:ALA:HB3	2.35	0.56
1:B:223:TRP:CG	1:B:411:PRO:HB3	2.41	0.56
1:C:423:MET:CE	1:C:450:ALA:HA	2.35	0.56
1:B:51:GLU:HG3	1:B:83:THR:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ILE:HG23	1:C:418:LEU:HG	1.87	0.56
1:D:136:ILE:HD13	1:D:142:MET:CE	2.33	0.56
1:D:392:PHE:HB3	1:D:426:ALA:HB1	1.88	0.56
1:B:479:GLY:O	1:B:483:LEU:HD13	2.04	0.56
1:C:244:LYS:HE3	1:C:249:GLU:OE1	2.05	0.56
1:D:23:GLY:O	1:D:24:ILE:HD13	2.05	0.56
1:A:423:MET:HG2	1:A:450:ALA:HA	1.86	0.56
1:C:29:LEU:HB2	1:C:100:ALA:HB2	1.86	0.56
1:C:74:THR:HG22	1:C:100:ALA:O	2.05	0.56
1:C:149:ALA:CB	1:C:161:ILE:HG21	2.35	0.56
1:B:199:VAL:HG23	1:B:334:LEU:CD2	2.35	0.56
1:B:268:ASP:O	1:B:272:SER:HB3	2.06	0.56
1:B:107:PHE:O	1:D:141:LYS:NZ	2.31	0.55
1:C:484:PHE:HZ	1:C:556:ARG:HH22	1.52	0.55
1:D:298:THR:HG23	1:D:317:TYR:CD2	2.40	0.55
1:C:267:THR:O	1:C:271:LEU:CB	2.45	0.55
1:D:50:GLU:HB2	1:D:80:ASN:HB3	1.88	0.55
1:A:237:VAL:N	1:A:255:LEU:CD1	2.70	0.55
1:B:197:VAL:HG23	1:B:197:VAL:O	2.04	0.55
1:B:115:SER:HA	1:B:120:VAL:O	2.06	0.55
1:C:3:VAL:HG11	1:C:176:LEU:HD12	1.88	0.55
1:C:13:MET:HB3	1:C:18:VAL:CG1	2.33	0.55
1:A:18:VAL:HG13	1:A:42:ILE:HD12	1.88	0.55
1:A:482:HIS:HB2	1:A:496:SER:HB2	1.88	0.55
1:B:3:VAL:HG21	1:B:7:GLU:CD	2.31	0.55
1:D:485:GLU:OE2	1:D:494:ASP:HA	2.07	0.55
1:A:162:HIS:C	1:A:163:LEU:HD23	2.32	0.55
1:C:22:PHE:O	1:C:70:CYS:HA	2.07	0.55
1:C:423:MET:HE2	1:C:453:MET:SD	2.47	0.55
1:D:326:ASP:OD2	1:D:329:GLU:N	2.39	0.55
1:A:193:ILE:O	1:A:197:VAL:HG22	2.07	0.55
1:B:381:MET:HB2	1:B:385:LEU:HD12	1.89	0.54
1:C:395:ASN:ND2	1:C:399:ILE:HD11	2.21	0.54
1:C:76:PRO:CG	1:C:113:GLN:NE2	2.70	0.54
1:C:115:SER:HA	1:C:120:VAL:O	2.06	0.54
1:D:482:HIS:O	1:D:486:GLN:HG3	2.07	0.54
1:A:505:CYS:SG	1:A:517:ARG:NH2	2.79	0.54
1:B:109:LYS:CE	1:C:316:ASN:OD1	2.56	0.54
1:A:18:VAL:HG21	1:A:69:VAL:CG2	2.38	0.54
1:A:260:PHE:CZ	1:A:553:MET:HE1	2.43	0.54
1:C:483:LEU:O	1:C:487:HIS:CD2	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLU:O	1:D:177:GLU:CG	2.51	0.54
1:B:247:PHE:HD2	1:B:254:SER:HB2	1.73	0.54
1:C:9:LEU:HD21	1:C:98:LEU:HD13	1.88	0.54
1:C:233:THR:CB	1:C:235:ILE:HG13	2.38	0.54
1:A:237:VAL:CB	1:A:247:PHE:CD2	2.88	0.54
1:A:423:MET:CE	3:A:602:A1LX0:C5	2.85	0.54
1:C:236:PRO:HB2	1:C:255:LEU:HD21	1.87	0.54
1:D:199:VAL:HG11	1:D:304:ILE:HG21	1.88	0.54
1:D:280:VAL:HG11	1:D:285:LEU:HD21	1.90	0.54
1:D:193:ILE:H	1:D:193:ILE:CD1	2.21	0.54
1:C:505:CYS:HB3	1:C:515:SER:OG	2.07	0.54
1:C:63:VAL:CG2	1:C:436:ALA:HB3	2.38	0.54
1:C:211:ILE:HG22	1:C:237:VAL:HG23	1.90	0.54
1:A:400:ASN:ND2	1:A:553:MET:HE3	2.19	0.53
1:A:459:HIS:HB2	1:A:511:LEU:HD22	1.88	0.53
1:A:3:VAL:HG22	1:A:7:GLU:HB3	1.91	0.53
1:A:513:VAL:HG22	1:A:537:PRO:HB2	1.91	0.53
1:B:225:GLU:HG2	1:B:332:LYS:HG3	1.89	0.53
1:B:281:ILE:HG12	1:B:306:ILE:HD12	1.89	0.53
1:C:302:ALA:HA	1:C:320:ASP:OD2	2.08	0.53
1:B:141:LYS:HD3	1:B:144:GLU:OE1	2.07	0.53
1:B:193:ILE:O	1:B:197:VAL:HG13	2.08	0.53
1:D:372:ILE:HD12	1:D:542:VAL:HG13	1.90	0.53
1:B:188:LYS:NZ	1:B:326:ASP:CG	2.67	0.53
1:B:214:GLY:HA2	1:B:240:THR:OG1	2.09	0.53
1:D:384:ARG:CD	1:D:528:LEU:CD2	2.86	0.53
1:A:334:LEU:O	1:A:338:ILE:HG22	2.08	0.53
1:A:382:GLN:NE2	1:A:407:LEU:H	2.06	0.53
1:D:303:LEU:HD23	1:D:318:PRO:O	2.09	0.53
1:A:52:GLY:O	1:A:56:MET:HG3	2.08	0.53
1:B:141:LYS:HZ3	1:D:105:ALA:HA	1.73	0.53
1:B:381:MET:HE3	1:B:385:LEU:CD1	2.39	0.53
1:A:199:VAL:HG22	1:A:304:ILE:HG12	1.90	0.53
1:D:18:VAL:HG12	1:D:42:ILE:HD12	1.90	0.53
1:D:232:LEU:HD13	1:D:232:LEU:C	2.33	0.53
1:D:296:ARG:NH1	1:D:296:ARG:CB	2.72	0.53
1:A:213:ALA:CB	1:A:217:ILE:CD1	2.74	0.52
1:A:389:THR:HG22	1:A:441:PRO:HG2	1.90	0.52
1:A:264:GLN:O	1:A:268:ASP:OD1	2.27	0.52
1:A:481:VAL:HG13	1:D:30:MET:CE	2.40	0.52
1:A:553:MET:HE2	1:A:553:MET:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLY:O	1:B:30:MET:HG2	2.09	0.52
1:B:96:LEU:HD21	1:B:98:LEU:HD21	1.92	0.52
1:C:455:GLY:O	1:C:458:ILE:HG12	2.09	0.52
1:C:74:THR:O	1:C:76:PRO:HD2	2.09	0.52
1:A:226:LEU:HD12	1:A:226:LEU:O	2.10	0.52
1:A:381:MET:HB3	1:A:385:LEU:HD12	1.91	0.52
1:A:389:THR:HG22	1:A:441:PRO:HB2	1.92	0.52
1:C:232:LEU:CD2	1:C:338:ILE:HD13	2.25	0.52
1:D:286:GLY:C	1:D:289:GLN:OE1	2.52	0.52
1:B:303:LEU:HD23	1:B:318:PRO:O	2.09	0.52
1:D:504:PHE:HD1	1:D:507:MET:CE	2.23	0.52
1:A:1:LYS:CB	1:A:1:LYS:NZ	2.73	0.52
1:A:7:GLU:O	1:A:10:VAL:HG22	2.09	0.52
1:A:71:CYS:HA	1:A:98:LEU:O	2.09	0.52
1:C:258:PHE:HB2	1:C:266:ALA:HB1	1.92	0.52
1:C:338:ILE:HA	1:C:341:SER:HB3	1.91	0.52
1:A:264:GLN:HG2	1:A:268:ASP:OD1	2.10	0.52
1:A:499:ARG:H	1:D:463:GLU:CD	2.14	0.52
1:A:115:SER:HA	1:A:120:VAL:O	2.10	0.52
1:B:399:ILE:HG12	1:B:416:ILE:HD11	1.92	0.52
1:A:328:SER:O	1:A:332:LYS:CG	2.58	0.52
1:C:76:PRO:CG	1:C:113:GLN:HE21	2.23	0.52
1:C:539:LEU:HD23	1:C:540:ILE:N	2.25	0.52
1:A:244:LYS:CE	1:A:403:VAL:O	2.57	0.51
1:D:212:LEU:C	1:D:212:LEU:HD23	2.35	0.51
1:D:481:VAL:O	1:D:485:GLU:HG3	2.09	0.51
1:A:232:LEU:CD2	1:A:339:ARG:HD3	2.40	0.51
1:B:3:VAL:CG2	1:B:7:GLU:CG	2.84	0.51
1:B:480:LEU:O	1:B:484:PHE:HD1	1.93	0.51
1:A:268:ASP:O	1:A:272:SER:CB	2.58	0.51
1:B:1:LYS:N	1:B:1:LYS:CD	2.73	0.51
1:B:148:ARG:NH2	1:D:108:GLY:O	2.43	0.51
1:B:458:ILE:CG1	1:B:511:LEU:HD12	2.41	0.51
1:D:138:THR:HG23	1:D:141:LYS:H	1.75	0.51
1:D:423:MET:SD	3:D:602:A1LX0:CM4	2.98	0.51
1:A:199:VAL:O	1:A:203:ILE:HG23	2.11	0.51
1:A:247:PHE:HE2	1:A:254:SER:HA	1.76	0.51
1:C:375:ALA:O	1:C:378:VAL:HG12	2.10	0.51
1:D:322:GLY:C	1:D:323:ILE:HD13	2.36	0.51
1:A:241:PRO:HA	1:A:257:VAL:HG11	1.93	0.51
1:B:191:PRO:HB3	1:B:323:ILE:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:MET:HB2	1:B:385:LEU:CD1	2.40	0.51
1:C:127:SER:N	1:C:128:PRO:CD	2.72	0.51
1:C:123:VAL:O	1:C:127:SER:HB2	2.11	0.51
1:D:390:ILE:HB	1:D:442:VAL:HG22	1.93	0.51
1:C:434:LYS:HG3	1:C:442:VAL:CG2	2.41	0.51
1:B:218:GLU:HG3	1:B:223:TRP:CZ2	2.43	0.51
1:D:9:LEU:O	1:D:9:LEU:HG	2.08	0.51
1:D:16:GLU:OE1	1:D:185:ARG:NH1	2.43	0.51
1:D:95:VAL:O	1:D:160:PRO:HA	2.10	0.51
1:D:519:GLU:HB2	1:D:543:GLN:OE1	2.10	0.51
1:A:260:PHE:HZ	1:A:553:MET:HE1	1.76	0.51
1:A:315:LYS:HE2	1:A:316:ASN:HD21	1.76	0.51
1:B:217:ILE:HG23	1:B:222:ALA:HB3	1.93	0.51
1:B:395:ASN:N	1:B:395:ASN:ND2	2.59	0.51
1:D:212:LEU:HD21	1:D:240:THR:CG2	2.41	0.51
1:A:395:ASN:HA	1:A:399:ILE:CD1	2.40	0.51
1:A:505:CYS:H	1:A:517:ARG:NH2	2.09	0.51
1:B:398:CYS:HB2	1:B:445:LEU:HD23	1.92	0.51
1:D:21:VAL:HG13	1:D:69:VAL:HG12	1.93	0.51
1:D:281:ILE:HG12	1:D:306:ILE:HD12	1.92	0.50
1:D:451:PHE:CE1	1:D:455:GLY:HA3	2.46	0.50
1:B:427:VAL:HA	1:B:470:TRP:HE1	1.76	0.50
1:D:283:SER:OG	1:D:285:LEU:HD23	2.12	0.50
1:B:479:GLY:N	5:B:602:TPP:O3B	2.43	0.50
1:D:209:PRO:CG	1:D:235:ILE:HG12	2.40	0.50
1:D:484:PHE:O	1:D:488:GLN:HB2	2.11	0.50
1:A:190:ALA:HB1	1:A:191:PRO:HD2	1.93	0.50
1:B:146:THR:O	1:B:150:LEU:HG	2.11	0.50
1:A:211:ILE:HG23	1:A:281:ILE:CD1	2.40	0.50
1:A:213:ALA:CB	1:A:217:ILE:HD11	2.40	0.50
1:B:98:LEU:HD23	1:B:163:LEU:HB2	1.93	0.50
1:D:59:GLY:O	1:D:63:VAL:HG13	2.12	0.50
1:A:13:MET:HB3	1:A:18:VAL:CG1	2.41	0.50
1:A:211:ILE:HG23	1:A:281:ILE:HD13	1.92	0.50
1:A:328:SER:O	1:A:332:LYS:HG3	2.11	0.50
1:B:189:PRO:CG	1:B:308:ILE:HD11	2.42	0.50
1:D:281:ILE:CG1	1:D:306:ILE:HD12	2.42	0.50
1:A:255:LEU:HD12	1:A:255:LEU:N	2.27	0.50
1:A:499:ARG:N	1:D:463:GLU:OE1	2.34	0.50
1:B:520:THR:HG23	1:B:523:ASP:H	1.77	0.50
1:D:315:LYS:HD2	1:D:316:ASN:HD21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TRP:CD1	1:A:246:SER:HA	2.47	0.50
1:A:244:LYS:NZ	1:A:406:TYR:O	2.44	0.50
1:A:294:ASP:OD1	1:A:295:PRO:HD2	2.12	0.50
1:B:79:THR:HG23	1:C:82:LEU:CD2	2.42	0.50
1:B:448:ASP:OD1	1:B:448:ASP:N	2.44	0.50
1:C:332:LYS:O	1:C:336:LEU:HD13	2.12	0.50
1:D:9:LEU:HD12	1:D:146:THR:HG21	1.94	0.50
1:D:18:VAL:HG12	1:D:42:ILE:CD1	2.42	0.50
1:D:286:GLY:H	1:D:289:GLN:NE2	2.09	0.50
1:A:384:ARG:HD3	1:A:529:LYS:HB2	1.92	0.49
1:C:431:ILE:HD13	1:C:461:ALA:HB2	1.94	0.49
1:D:115:SER:HA	1:D:120:VAL:O	2.10	0.49
1:D:272:SER:O	1:D:274:ASP:N	2.45	0.49
1:A:504:PHE:HB2	1:A:541:ASP:OD2	2.12	0.49
1:C:76:PRO:HG3	1:C:113:GLN:NE2	2.27	0.49
1:C:204:PHE:CE1	1:C:338:ILE:HG22	2.47	0.49
1:C:311:MET:SD	1:D:152:THR:HG23	2.53	0.49
1:D:384:ARG:NH1	1:D:529:LYS:HB3	2.26	0.49
1:A:101:GLN:HB3	1:A:166:PRO:HA	1.93	0.49
1:B:492:LYS:HG3	1:B:493:PHE:HD1	1.76	0.49
1:D:244:LYS:HD3	1:D:414:PHE:CZ	2.47	0.49
1:A:237:VAL:CG1	1:A:247:PHE:CD2	2.95	0.49
1:C:134:VAL:HG21	1:C:145:MET:CE	2.42	0.49
1:C:520:THR:HG22	1:C:521:VAL:H	1.78	0.49
1:A:74:THR:O	1:A:76:PRO:HD2	2.13	0.49
1:C:104:THR:HA	1:C:107:PHE:CE1	2.47	0.49
1:D:199:VAL:HG23	1:D:334:LEU:HD21	1.95	0.49
1:A:237:VAL:N	1:A:255:LEU:HD13	2.28	0.49
1:A:276:ASP:HB2	1:A:301:VAL:CG2	2.43	0.49
1:C:202:LEU:N	1:C:202:LEU:HD12	2.27	0.49
1:D:489:PHE:CD1	1:D:489:PHE:N	2.80	0.49
1:A:3:VAL:HG21	1:A:7:GLU:OE1	2.12	0.49
1:D:30:MET:N	1:D:31:PRO:HD2	2.28	0.49
1:D:208:ARG:HD2	1:D:274:ASP:HB2	1.88	0.49
1:B:244:LYS:HD3	1:B:414:PHE:CD1	2.47	0.49
1:C:199:VAL:HG13	1:C:304:ILE:CD1	2.40	0.49
1:D:384:ARG:HD3	1:D:529:LYS:HB3	1.95	0.49
1:D:504:PHE:CD1	1:D:507:MET:HE1	2.48	0.49
1:A:484:PHE:O	1:A:488:GLN:N	2.44	0.48
1:B:423:MET:HE2	5:B:602:TPP:N1'	2.27	0.48
1:D:9:LEU:HD12	1:D:146:THR:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LEU:C	1:D:232:LEU:CD1	2.85	0.48
1:D:236:PRO:HG3	1:D:269:TYR:HE2	1.74	0.48
1:A:506:LYS:HB2	1:D:510:SER:HB3	1.95	0.48
1:B:393:VAL:O	1:B:426:ALA:HB2	2.12	0.48
1:C:101:GLN:HB3	1:C:166:PRO:HA	1.95	0.48
1:D:458:ILE:HD11	1:D:511:LEU:HD12	1.94	0.48
1:A:151:ARG:HD3	1:A:184:TYR:O	2.13	0.48
1:B:391:LEU:HD12	1:B:443:VAL:O	2.13	0.48
1:D:388:ASP:C	1:D:440:ARG:HH21	2.21	0.48
1:D:504:PHE:CD1	1:D:507:MET:CE	2.97	0.48
1:B:157:ARG:HG3	2:B:601:ADP:H2'	1.95	0.48
1:D:555:GLN:CD	1:D:555:GLN:N	2.72	0.48
1:A:8:LEU:CD1	1:A:177:GLU:H	2.26	0.48
1:B:249:GLU:HB2	1:B:407:LEU:HG	1.95	0.48
1:C:6:VAL:O	1:C:10:VAL:HG13	2.13	0.48
1:A:390:ILE:HB	1:A:442:VAL:HG12	1.96	0.48
1:D:296:ARG:HH11	1:D:296:ARG:CB	2.26	0.48
1:A:1:LYS:HE3	1:A:1:LYS:HB2	1.64	0.48
1:A:20:TYR:HA	1:A:43:GLN:O	2.13	0.48
1:A:307:ASP:OD1	2:A:601:ADP:O2'	2.23	0.48
1:A:338:ILE:O	1:A:338:ILE:HD12	2.13	0.48
1:B:381:MET:HE3	1:B:385:LEU:HD11	1.94	0.48
1:B:381:MET:CA	1:B:385:LEU:HD12	2.43	0.48
1:D:4:THR:HG22	1:D:7:GLU:CB	2.42	0.48
1:D:332:LYS:HA	1:D:335:ILE:HG12	1.94	0.48
1:A:47:THR:CG2	1:A:56:MET:HE3	2.44	0.48
1:B:60:TYR:O	1:B:64:SER:CB	2.62	0.48
1:B:79:THR:HG21	1:C:83:THR:HA	1.95	0.48
1:C:223:TRP:CG	1:C:411:PRO:HB3	2.48	0.48
1:A:11:ARG:HG2	1:A:39:ARG:HH21	1.78	0.48
1:A:510:SER:CB	1:D:506:LYS:HB3	2.44	0.48
1:B:228:ASP:O	1:B:232:LEU:HB2	2.13	0.48
1:C:153:ALA:HB2	1:C:161:ILE:HG12	1.96	0.48
1:C:478:HIS:HB2	1:C:481:VAL:CG2	2.43	0.48
1:D:76:PRO:HA	1:D:79:THR:OG1	2.13	0.48
1:A:76:PRO:HD3	1:A:113:GLN:HG2	1.94	0.48
1:B:242:LYS:CD	1:B:418:LEU:HB2	2.39	0.48
1:D:184:TYR:CD1	1:D:184:TYR:C	2.92	0.48
1:A:338:ILE:O	1:A:341:SER:HB3	2.14	0.47
1:B:142:MET:HE1	1:B:165:ILE:HD13	1.95	0.47
1:B:258:PHE:HB2	1:B:266:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLY:C	1:B:480:LEU:HD11	2.39	0.47
1:B:459:HIS:HB2	1:B:511:LEU:HB3	1.96	0.47
1:C:51:GLU:HG2	1:C:55:PHE:CE2	2.49	0.47
1:D:298:THR:CG2	1:D:317:TYR:HD2	2.28	0.47
1:A:107:PHE:CD1	1:A:116:THR:HG21	2.49	0.47
1:D:184:TYR:O	1:D:184:TYR:HD1	1.96	0.47
1:D:372:ILE:HG23	1:D:521:VAL:HG22	1.96	0.47
1:D:514:LYS:CG	1:D:534:MET:HE1	2.40	0.47
1:B:8:LEU:HD21	1:B:143:GLY:CA	2.44	0.47
1:B:28:PRO:HB2	1:B:100:ALA:HB1	1.95	0.47
1:B:326:ASP:OD1	1:B:327:ALA:N	2.48	0.47
1:C:207:LYS:O	1:C:208:ARG:HD3	2.14	0.47
1:A:12:GLN:NE2	1:A:179:PHE:O	2.48	0.47
1:B:207:LYS:HE3	1:B:276:ASP:CB	2.42	0.47
1:B:213:ALA:O	1:B:239:THR:HA	2.14	0.47
1:C:397:SER:N	1:C:480:LEU:HD11	2.29	0.47
1:D:385:LEU:HD22	1:D:443:VAL:HG21	1.97	0.47
1:A:244:LYS:HE3	1:A:403:VAL:CA	2.40	0.47
1:A:385:LEU:CD2	1:A:443:VAL:HG21	2.45	0.47
1:A:510:SER:HB3	1:D:506:LYS:HB3	1.97	0.47
1:B:25:PRO:HB3	1:B:33:TYR:CE2	2.50	0.47
1:B:208:ARG:HA	1:B:208:ARG:NE	2.29	0.47
1:C:479:GLY:N	3:C:602:A1LXO:O3B	2.47	0.47
1:D:9:LEU:CD1	1:D:146:THR:CG2	2.93	0.47
1:A:423:MET:HE3	1:A:423:MET:HB2	1.79	0.47
1:B:127:SER:N	1:B:128:PRO:CD	2.78	0.47
1:B:141:LYS:HZ1	1:D:105:ALA:HA	1.80	0.47
1:B:188:LYS:HZ2	1:B:326:ASP:CG	2.23	0.47
1:B:498:PHE:HB3	1:C:463:GLU:OE2	2.15	0.47
1:C:22:PHE:HD1	1:C:45:ILE:HB	1.78	0.47
1:C:378:VAL:HG13	1:C:379:GLU:N	2.29	0.47
1:D:56:MET:CE	1:D:457:GLU:OE2	2.63	0.47
1:D:245:SER:HB2	1:D:414:PHE:CB	2.35	0.47
1:D:420:LEU:HD12	1:D:420:LEU:HA	1.72	0.47
1:D:552:GLY:HA2	1:D:555:GLN:OE1	2.13	0.47
1:A:264:GLN:NE2	1:A:268:ASP:OD2	2.48	0.47
1:A:464:TYR:O	1:A:465:LYS:CB	2.63	0.47
1:C:40:LYS:HB2	1:C:40:LYS:HE2	1.38	0.47
1:D:451:PHE:CD1	1:D:455:GLY:HA3	2.49	0.47
1:B:149:ALA:CB	1:B:161:ILE:HG21	2.38	0.46
1:C:304:ILE:HG12	1:C:321:VAL:HG11	1.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:PRO:HB3	1:D:323:ILE:HG21	1.97	0.46
1:D:453:MET:HB3	1:D:453:MET:HE2	1.58	0.46
1:C:394:ASP:OD1	1:C:426:ALA:CB	2.62	0.46
1:D:127:SER:HB2	1:D:128:PRO:HD3	1.96	0.46
1:C:295:PRO:C	1:C:297:LEU:H	2.23	0.46
1:D:48:LYS:HB2	1:D:457:GLU:OE1	2.15	0.46
1:B:56:MET:HE2	1:B:431:ILE:HD12	1.97	0.46
1:B:181:PRO:HA	1:B:184:TYR:CZ	2.51	0.46
1:B:202:LEU:HD13	1:B:304:ILE:HD11	1.98	0.46
1:B:453:MET:HE3	1:C:49:HIS:CD2	2.51	0.46
1:C:396:GLY:C	1:C:480:LEU:HD11	2.40	0.46
1:D:209:PRO:HB2	1:D:235:ILE:HD13	1.98	0.46
1:B:29:LEU:HD13	1:B:100:ALA:HB2	1.97	0.46
1:C:195:ASP:O	1:C:199:VAL:HG23	2.16	0.46
1:C:295:PRO:C	1:C:297:LEU:N	2.72	0.46
1:A:60:TYR:O	1:A:64:SER:CB	2.62	0.46
1:B:191:PRO:HG3	1:B:330:THR:HG23	1.98	0.46
1:B:443:VAL:HG13	1:B:471:ILE:HD12	1.97	0.46
1:B:548:VAL:O	1:B:550:PRO:HD3	2.15	0.46
1:C:536:THR:HB	1:C:537:PRO:HD2	1.98	0.46
1:A:229:PHE:O	1:A:233:THR:HG23	2.16	0.46
1:B:101:GLN:NE2	1:B:164:ASN:OD1	2.43	0.46
1:B:378:VAL:HG21	1:B:405:CYS:HB3	1.97	0.46
1:C:386:PRO:HB2	1:C:441:PRO:HG2	1.98	0.46
1:D:242:LYS:HD3	1:D:418:LEU:HB2	1.97	0.46
1:A:135:MET:HA	1:A:164:ASN:HB3	1.98	0.46
1:A:482:HIS:O	1:A:486:GLN:HG3	2.16	0.46
1:C:25:PRO:HD3	1:C:46:LEU:HD12	1.97	0.46
1:C:318:PRO:HA	1:D:183:ASN:O	2.16	0.46
1:D:184:TYR:CD1	1:D:184:TYR:O	2.69	0.46
1:C:56:MET:HE2	1:C:431:ILE:HD12	1.96	0.46
1:D:208:ARG:NE	1:D:274:ASP:HB3	2.30	0.46
1:B:16:GLU:O	6:B:701:HOH:O	2.21	0.46
1:C:22:PHE:CD1	1:C:45:ILE:HB	2.51	0.46
1:A:439:ASP:OD1	1:A:439:ASP:O	2.34	0.45
1:B:536:THR:HG22	1:B:537:PRO:HD2	1.97	0.45
1:C:202:LEU:HD23	1:C:302:ALA:CB	2.46	0.45
1:D:17:GLY:O	1:D:66:LYS:HD3	2.16	0.45
1:A:3:VAL:HG23	1:A:7:GLU:OE2	2.16	0.45
1:A:209:PRO:HG2	1:A:235:ILE:CG1	2.38	0.45
1:A:420:LEU:O	1:D:113:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PRO:HD3	1:C:420:LEU:CD1	2.47	0.45
1:A:72:ALA:O	1:A:99:THR:HA	2.16	0.45
1:C:30:MET:N	1:C:31:PRO:CD	2.80	0.45
1:A:265:LYS:O	1:A:265:LYS:HG3	2.15	0.45
1:A:503:ASP:OD1	1:A:517:ARG:NH2	2.49	0.45
1:C:384:ARG:NH1	1:C:529:LYS:HG3	2.31	0.45
1:A:48:LYS:HA	1:A:48:LYS:HD3	1.77	0.45
1:A:289:GLN:N	1:A:289:GLN:NE2	2.59	0.45
1:A:385:LEU:HD21	1:A:443:VAL:HG21	1.99	0.45
1:B:190:ALA:HB1	1:B:191:PRO:HD2	1.99	0.45
1:D:9:LEU:HD13	1:D:146:THR:HG21	1.98	0.45
1:D:399:ILE:HG22	1:D:416:ILE:HD11	1.98	0.45
1:B:194:MET:HE3	1:B:198:ARG:HH12	1.80	0.45
1:B:255:LEU:HA	1:B:265:LYS:HD2	1.99	0.45
1:B:315:LYS:HD2	1:C:108:GLY:O	2.16	0.45
1:B:423:MET:HE2	5:B:602:TPP:C5'	2.46	0.45
1:D:106:ALA:HB1	1:D:111:ALA:HB2	1.98	0.45
1:B:444:ALA:HB3	1:B:470:TRP:CD1	2.52	0.45
1:B:483:LEU:HD21	1:B:550:PRO:HD3	1.99	0.45
1:C:448:ASP:HB3	1:C:474:ASN:HA	1.98	0.45
1:D:513:VAL:HG13	1:D:537:PRO:HB2	1.99	0.45
1:B:395:ASN:OD1	1:B:421:ALA:HA	2.16	0.45
1:B:506:LYS:HD2	1:C:509:GLU:HG2	1.99	0.45
1:C:400:ASN:HD21	1:C:553:MET:HE2	1.60	0.45
1:D:151:ARG:HA	1:D:185:ARG:HD2	1.99	0.45
1:D:555:GLN:CD	1:D:555:GLN:H	2.25	0.45
1:A:208:ARG:NE	1:A:274:ASP:O	2.32	0.45
1:B:101:GLN:HB3	1:B:166:PRO:HA	1.99	0.45
1:B:478:HIS:HE2	1:C:46:LEU:HD21	1.82	0.45
1:C:478:HIS:CB	1:C:481:VAL:CG2	2.95	0.45
1:A:22:PHE:O	1:A:70:CYS:HA	2.17	0.44
1:B:67:LEU:HD22	1:B:150:LEU:HD22	1.99	0.44
1:C:459:HIS:O	1:C:463:GLU:N	2.45	0.44
1:A:482:HIS:HB2	1:A:496:SER:CB	2.46	0.44
1:B:410:THR:HG23	1:B:411:PRO:HD2	2.00	0.44
1:C:98:LEU:N	1:C:98:LEU:HD23	2.32	0.44
1:C:326:ASP:OD1	1:C:328:SER:N	2.42	0.44
1:D:8:LEU:HD13	1:D:176:LEU:HA	1.99	0.44
1:D:9:LEU:HD12	1:D:146:THR:HB	1.99	0.44
1:D:278:LEU:CB	1:D:299:PRO:HG3	2.47	0.44
1:D:451:PHE:O	1:D:455:GLY:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:O	1:A:42:ILE:CD1	2.62	0.44
1:A:157:ARG:NH2	2:A:601:ADP:H3'	2.33	0.44
1:A:285:LEU:N	1:A:285:LEU:HD23	2.31	0.44
1:B:79:THR:CG2	1:C:82:LEU:HD23	2.46	0.44
1:B:416:ILE:CG2	1:B:418:LEU:HG	2.48	0.44
1:B:522:GLU:H	1:B:522:GLU:CD	2.16	0.44
1:D:278:LEU:CD2	1:D:299:PRO:HD3	2.46	0.44
1:D:455:GLY:O	1:D:458:ILE:HG12	2.17	0.44
1:A:381:MET:O	1:A:385:LEU:HD12	2.18	0.44
1:B:181:PRO:HB3	1:B:185:ARG:NH2	2.33	0.44
5:B:602:TPP:C2	5:B:602:TPP:HN42	2.31	0.44
1:C:377:VAL:HG13	1:C:524:PHE:CE2	2.53	0.44
1:D:136:ILE:CD1	1:D:165:ILE:HG12	2.47	0.44
1:D:190:ALA:HB1	1:D:191:PRO:HD2	1.99	0.44
1:D:279:ILE:HG12	1:D:304:ILE:HD12	1.98	0.44
1:D:335:ILE:HG13	1:D:336:LEU:N	2.33	0.44
1:B:378:VAL:HG21	1:B:405:CYS:CB	2.48	0.44
1:A:25:PRO:HG3	1:D:495:ILE:HG23	2.00	0.44
1:B:475:ASN:HB2	1:B:546:ILE:HB	2.00	0.44
1:C:82:LEU:CD1	1:C:129:ILE:HD11	2.47	0.44
1:C:294:ASP:HA	1:C:295:PRO:HD2	1.68	0.44
1:D:18:VAL:HG12	1:D:18:VAL:O	2.16	0.44
1:A:6:VAL:O	1:A:10:VAL:HG13	2.18	0.44
1:A:80:ASN:HD21	1:D:453:MET:HE1	1.81	0.44
1:B:400:ASN:CB	1:B:551:PRO:HD2	2.46	0.44
1:B:451:PHE:O	1:B:455:GLY:N	2.46	0.44
1:C:86:ALA:HB2	1:C:129:ILE:HD13	1.99	0.44
1:C:261:ALA:HB3	1:C:403:VAL:CG2	2.48	0.44
1:A:434:LYS:HG3	1:A:442:VAL:CG2	2.47	0.44
1:C:147:ARG:HD2	1:C:184:TYR:CD2	2.52	0.44
1:D:198:ARG:HH11	1:D:321:VAL:HG22	1.80	0.44
1:A:141:LYS:HZ1	1:C:105:ALA:CA	2.29	0.44
1:A:416:ILE:HG21	1:A:416:ILE:HD13	1.69	0.44
1:C:545:ASP:HB3	1:C:548:VAL:HG13	1.99	0.44
1:A:30:MET:N	1:A:31:PRO:CD	2.81	0.43
1:A:237:VAL:C	1:A:255:LEU:HD13	2.43	0.43
1:A:517:ARG:HE	1:A:517:ARG:HB2	1.74	0.43
1:C:381:MET:HB3	1:C:528:LEU:HD11	1.99	0.43
1:C:548:VAL:O	1:C:548:VAL:HG23	2.18	0.43
1:D:178:VAL:C	1:D:179:PHE:HD1	2.25	0.43
1:D:199:VAL:CG1	1:D:304:ILE:HD13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:SER:O	1:D:292:SER:OG	2.30	0.43
1:B:115:SER:CA	1:B:120:VAL:O	2.66	0.43
1:D:236:PRO:HB2	1:D:255:LEU:CD1	2.36	0.43
1:D:267:THR:HG23	1:D:271:LEU:HD12	1.99	0.43
1:D:400:ASN:ND2	1:D:553:MET:HG2	2.33	0.43
1:A:548:VAL:O	1:A:550:PRO:HD3	2.17	0.43
1:B:76:PRO:HD3	1:C:420:LEU:HG	2.00	0.43
1:B:194:MET:HE2	1:B:195:ASP:OD1	2.18	0.43
1:B:339:ARG:NH1	1:B:339:ARG:HG2	2.33	0.43
1:C:294:ASP:OD1	1:C:295:PRO:HD2	2.18	0.43
1:D:40:LYS:HD2	1:D:40:LYS:HA	1.59	0.43
1:A:141:LYS:HZ2	1:A:141:LYS:HG2	1.60	0.43
1:B:79:THR:HG23	1:C:82:LEU:HD23	2.01	0.43
1:B:442:VAL:HG23	1:B:468:VAL:HG22	1.99	0.43
1:B:483:LEU:O	1:B:487:HIS:HB2	2.17	0.43
1:B:546:ILE:HG12	1:B:546:ILE:O	2.18	0.43
1:A:451:PHE:O	1:A:455:GLY:N	2.51	0.43
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.84	0.43
1:C:166:PRO:HB2	1:C:169:ILE:HG22	1.98	0.43
1:C:271:LEU:HD22	1:C:271:LEU:HA	1.43	0.43
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.85	0.43
1:A:183:ASN:O	1:B:318:PRO:HA	2.18	0.43
1:A:245:SER:OG	1:A:410:THR:O	2.37	0.43
1:A:456:MET:HE2	1:D:452:ALA:HB1	1.99	0.43
1:D:255:LEU:CD2	1:D:269:TYR:CD2	2.86	0.43
1:A:213:ALA:O	1:A:239:THR:HA	2.18	0.43
1:A:381:MET:HB3	1:A:385:LEU:CD1	2.49	0.43
1:A:462:ALA:HB2	1:A:513:VAL:HG23	2.01	0.43
1:D:48:LYS:HE2	1:D:459:HIS:ND1	2.33	0.43
1:D:147:ARG:HH12	1:D:177:GLU:CD	2.26	0.43
1:D:233:THR:HG22	1:D:233:THR:O	2.18	0.43
1:A:553:MET:HE3	1:A:553:MET:HB2	1.89	0.43
1:B:29:LEU:HD22	1:B:72:ALA:C	2.44	0.43
1:A:522:GLU:N	1:A:522:GLU:CD	2.73	0.43
1:B:434:LYS:HB2	1:B:442:VAL:CG2	2.45	0.43
1:D:425:HIS:O	1:D:429:ALA:HB2	2.18	0.43
1:A:95:VAL:O	1:A:160:PRO:HA	2.19	0.43
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.81	0.43
1:C:135:MET:HE3	1:C:166:PRO:HG3	1.97	0.43
1:C:458:ILE:HG22	1:C:470:TRP:CH2	2.54	0.43
1:A:237:VAL:CB	1:A:247:PHE:CE2	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:O	1:A:335:ILE:HG13	2.19	0.42
1:C:21:VAL:HG13	1:C:69:VAL:HG12	2.01	0.42
1:C:466:ILE:HG22	1:C:468:VAL:HG23	1.99	0.42
1:A:151:ARG:O	1:A:155:SER:HB2	2.19	0.42
1:A:276:ASP:HB2	1:A:301:VAL:HG23	2.01	0.42
1:C:91:ASP:O	1:C:92:SER:HB2	2.19	0.42
1:C:418:LEU:HD23	1:C:418:LEU:HA	1.77	0.42
1:C:423:MET:HG3	3:C:602:A1LX0:C4'	2.48	0.42
1:D:9:LEU:HD12	1:D:146:THR:CG2	2.49	0.42
1:D:283:SER:HA	2:D:601:ADP:O2B	2.19	0.42
1:B:328:SER:O	1:B:332:LYS:HD3	2.18	0.42
1:C:32:LEU:HG	1:C:36:ILE:HD11	2.00	0.42
1:C:233:THR:HB	1:C:235:ILE:HG13	2.00	0.42
1:C:393:VAL:HB	1:C:416:ILE:HG13	2.01	0.42
1:D:78:ALA:HB3	1:D:122:LEU:CD2	2.48	0.42
1:D:181:PRO:HA	1:D:184:TYR:CZ	2.54	0.42
1:D:284:SER:HB3	2:D:601:ADP:O2A	2.19	0.42
1:B:483:LEU:HD21	1:B:550:PRO:CD	2.50	0.42
1:C:50:GLU:HB2	1:C:80:ASN:HB3	2.01	0.42
1:C:217:ILE:HD11	1:C:281:ILE:HG21	2.01	0.42
1:A:134:VAL:HG11	1:A:145:MET:CE	2.50	0.42
1:A:420:LEU:HA	1:A:420:LEU:HD12	1.75	0.42
1:D:4:THR:HG23	1:D:7:GLU:N	2.31	0.42
1:A:69:VAL:HA	1:A:96:LEU:O	2.19	0.42
1:A:177:GLU:O	1:A:177:GLU:HG3	2.20	0.42
1:B:263:HIS:O	1:B:267:THR:HG23	2.20	0.42
1:D:244:LYS:HD3	1:D:414:PHE:CD2	2.55	0.42
1:A:153:ALA:HB2	1:A:161:ILE:CG1	2.49	0.42
1:A:481:VAL:HG13	1:D:30:MET:HE2	2.01	0.42
1:C:486:GLN:HB2	1:C:487:HIS:CD2	2.55	0.42
1:D:296:ARG:NH1	1:D:296:ARG:HB2	2.35	0.42
1:A:1:LYS:NZ	1:A:1:LYS:HB2	2.24	0.42
1:A:47:THR:HG22	1:A:56:MET:CE	2.49	0.42
1:A:141:LYS:O	1:A:145:MET:HG2	2.20	0.42
1:A:155:SER:HB3	1:B:310:PRO:CB	2.49	0.42
1:B:168:ASP:OD1	1:B:168:ASP:N	2.52	0.42
1:B:492:LYS:HE2	1:C:34:GLU:HG3	2.00	0.42
1:C:232:LEU:HD23	1:C:232:LEU:C	2.44	0.42
1:C:244:LYS:HD3	1:C:414:PHE:CG	2.54	0.42
1:C:377:VAL:O	1:C:381:MET:HG2	2.20	0.42
1:D:265:LYS:HE3	1:D:265:LYS:HB2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HA	1:A:184:TYR:CZ	2.54	0.42
1:B:48:LYS:CE	1:B:459:HIS:ND1	2.73	0.42
1:B:136:ILE:HD11	1:B:163:LEU:HD22	2.02	0.42
1:B:286:GLY:O	1:B:290:THR:OG1	2.35	0.42
1:D:451:PHE:CE1	1:D:507:MET:HE3	2.55	0.42
1:B:199:VAL:CG1	1:B:304:ILE:HD13	2.50	0.41
1:B:514:LYS:O	1:B:538:CYS:HA	2.20	0.41
1:C:384:ARG:NH1	1:C:529:LYS:CG	2.83	0.41
1:C:399:ILE:HG23	1:C:416:ILE:HD11	2.02	0.41
1:C:480:LEU:O	1:C:484:PHE:N	2.53	0.41
1:B:188:LYS:HB3	1:B:189:PRO:HD2	2.01	0.41
1:D:147:ARG:HD2	1:D:184:TYR:CD2	2.55	0.41
1:D:192:THR:O	1:D:196:VAL:HG23	2.20	0.41
1:A:509:GLU:OE2	1:D:506:LYS:NZ	2.46	0.41
1:B:384:ARG:HG3	1:B:529:LYS:HZ2	1.85	0.41
1:B:509:GLU:OE1	1:C:506:LYS:HE3	2.20	0.41
1:C:495:ILE:O	1:C:495:ILE:HG13	2.21	0.41
1:D:522:GLU:CD	1:D:522:GLU:H	2.29	0.41
1:D:553:MET:CA	1:D:553:MET:HE3	2.51	0.41
1:A:328:SER:O	1:A:332:LYS:HG2	2.21	0.41
1:A:343:LYS:HD3	1:A:343:LYS:C	2.45	0.41
1:B:16:GLU:OE1	1:B:185:ARG:NH2	2.52	0.41
1:C:67:LEU:HD12	1:C:94:PRO:O	2.21	0.41
1:D:96:LEU:HD11	1:D:163:LEU:HD12	2.02	0.41
1:A:182:MET:HG2	6:A:702:HOH:O	2.19	0.41
1:B:456:MET:HB3	1:B:456:MET:HE3	1.48	0.41
1:B:514:LYS:HB2	1:B:514:LYS:HE3	1.88	0.41
1:A:48:LYS:CE	1:A:459:HIS:ND1	2.82	0.41
1:A:108:GLY:N	1:A:114:GLU:OE1	2.48	0.41
1:A:197:VAL:HG12	1:A:337:CYS:SG	2.61	0.41
1:C:276:ASP:HA	1:C:300:SER:N	2.34	0.41
1:D:11:ARG:HG2	1:D:178:VAL:HG21	2.02	0.41
1:A:210:ALA:HB1	1:A:270:LEU:HD21	2.02	0.41
1:A:249:GLU:HG3	1:A:408:ALA:O	2.20	0.41
1:A:505:CYS:H	1:A:517:ARG:HH21	1.69	0.41
1:B:220:ALA:HB2	2:B:601:ADP:C6	2.55	0.41
1:D:270:LEU:HA	1:D:270:LEU:HD23	1.79	0.41
1:D:553:MET:HE3	1:D:553:MET:O	2.21	0.41
1:A:6:VAL:CG2	1:A:32:LEU:HA	2.48	0.41
1:A:64:SER:HB3	1:A:66:LYS:H	1.86	0.41
1:A:443:VAL:CG1	1:A:471:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:LYS:O	1:B:1:LYS:HG2	2.21	0.41
1:B:166:PRO:O	1:B:169:ILE:HG12	2.20	0.41
1:B:264:GLN:O	1:B:268:ASP:OD1	2.39	0.41
1:B:297:LEU:O	1:B:297:LEU:HG	2.21	0.41
1:C:9:LEU:HD12	1:C:146:THR:CG2	2.50	0.41
1:C:416:ILE:CG2	1:C:418:LEU:HG	2.49	0.41
1:C:453:MET:HE2	1:C:453:MET:HB3	1.79	0.41
1:D:22:PHE:O	1:D:70:CYS:HA	2.21	0.41
1:A:247:PHE:CE2	1:A:254:SER:HA	2.56	0.41
1:A:268:ASP:O	1:A:272:SER:HB2	2.20	0.41
1:A:495:ILE:O	1:A:495:ILE:HG13	2.21	0.41
1:B:101:GLN:HB2	1:B:164:ASN:OD1	2.21	0.41
1:B:244:LYS:HD3	1:B:414:PHE:CD2	2.56	0.41
1:B:278:LEU:HD13	1:B:280:VAL:HG23	2.03	0.41
1:B:280:VAL:HG11	1:B:285:LEU:HD11	2.02	0.41
1:C:24:ILE:HD12	1:C:50:GLU:CD	2.46	0.41
1:C:191:PRO:HG3	1:C:330:THR:HA	2.02	0.41
1:C:213:ALA:O	1:C:239:THR:HA	2.21	0.41
1:C:458:ILE:HD13	1:C:458:ILE:HG21	1.82	0.41
1:C:480:LEU:O	1:C:483:LEU:N	2.54	0.41
1:C:502:ILE:HG21	1:C:507:MET:CE	2.51	0.41
1:C:553:MET:HE2	1:C:553:MET:HB2	1.78	0.41
1:D:18:VAL:O	1:D:42:ILE:HD13	2.21	0.41
1:D:136:ILE:HD12	1:D:165:ILE:HG12	2.02	0.41
1:D:554:LYS:O	1:D:554:LYS:CG	2.69	0.41
1:A:245:SER:OG	1:A:413:ALA:N	2.52	0.41
1:A:268:ASP:O	1:A:272:SER:OG	2.28	0.41
1:A:281:ILE:N	1:A:281:ILE:CD1	2.76	0.41
1:B:18:VAL:HG12	1:B:67:LEU:O	2.21	0.41
1:B:458:ILE:HG12	1:B:511:LEU:HD12	2.01	0.41
1:C:331:LEU:HD23	1:C:331:LEU:HA	1.83	0.41
1:C:397:SER:H	3:C:602:A1LX0:PB	2.44	0.41
1:D:145:MET:CE	1:D:145:MET:CA	2.88	0.41
1:A:22:PHE:O	1:A:70:CYS:CB	2.70	0.40
1:B:376:MET:HE3	1:B:376:MET:HB2	1.81	0.40
1:C:95:VAL:O	1:C:160:PRO:HA	2.21	0.40
1:C:131:LYS:NZ	1:C:155:SER:O	2.53	0.40
1:D:78:ALA:HB3	1:D:122:LEU:HD21	2.03	0.40
1:D:135:MET:HG3	1:D:164:ASN:OD1	2.22	0.40
1:D:278:LEU:HB2	1:D:299:PRO:HG3	2.02	0.40
1:D:407:LEU:HD23	1:D:407:LEU:N	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:O	1:A:228:ASP:OD1	2.39	0.40
1:A:382:GLN:OE1	1:A:407:LEU:O	2.40	0.40
1:B:104:THR:HA	1:B:107:PHE:CE1	2.56	0.40
1:B:448:ASP:HB3	1:B:474:ASN:HA	2.04	0.40
1:C:232:LEU:CD1	1:C:339:ARG:HG3	2.52	0.40
1:C:244:LYS:NZ	1:C:403:VAL:HA	2.37	0.40
1:D:26:GLY:HA3	1:D:73:THR:OG1	2.21	0.40
1:D:245:SER:OG	1:D:413:ALA:N	2.53	0.40
1:D:426:ALA:HA	1:D:429:ALA:CB	2.41	0.40
1:A:292:SER:O	1:A:292:SER:OG	2.31	0.40
1:D:267:THR:CG2	1:D:271:LEU:HD12	2.52	0.40
1:A:18:VAL:HG21	1:A:69:VAL:HG21	2.03	0.40
1:A:107:PHE:HA	1:A:114:GLU:OE1	2.21	0.40
1:A:146:THR:O	1:A:150:LEU:HG	2.21	0.40
1:A:254:SER:O	1:A:265:LYS:NZ	2.47	0.40
1:A:434:LYS:CB	1:A:442:VAL:HG21	2.47	0.40
1:B:288:TRP:HZ3	1:B:418:LEU:HD22	1.87	0.40
1:C:397:SER:N	3:C:602:A1LXO:O2B	2.45	0.40
1:D:48:LYS:HA	1:D:48:LYS:HD3	1.81	0.40
1:A:136:ILE:HG12	1:A:164:ASN:O	2.22	0.40
1:A:162:HIS:O	1:A:163:LEU:HD23	2.21	0.40
1:A:204:PHE:CE1	1:A:338:ILE:CD1	2.84	0.40
1:A:456:MET:HE3	1:A:456:MET:HB3	1.40	0.40
1:C:60:TYR:CD1	1:C:436:ALA:HB2	2.57	0.40
1:C:399:ILE:HG23	1:C:416:ILE:CD1	2.52	0.40
1:C:465:LYS:O	1:C:467:PRO:HD3	2.20	0.40
1:C:529:LYS:HD3	1:C:529:LYS:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/584 (90%)	507 (96%)	21 (4%)	0	100	100
1	B	527/584 (90%)	507 (96%)	18 (3%)	2 (0%)	30	50
1	C	526/584 (90%)	506 (96%)	18 (3%)	2 (0%)	30	50
1	D	526/584 (90%)	504 (96%)	19 (4%)	3 (1%)	21	38
All	All	2107/2336 (90%)	2024 (96%)	76 (4%)	7 (0%)	36	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	SER
1	D	273	GLY
1	D	490	ASP
1	B	40	LYS
1	C	245	SER
1	D	245	SER
1	C	273	GLY

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	420/463 (91%)	395 (94%)	25 (6%)	17	32
1	B	419/463 (90%)	398 (95%)	21 (5%)	22	42
1	C	418/463 (90%)	394 (94%)	24 (6%)	18	35
1	D	418/463 (90%)	398 (95%)	20 (5%)	23	44
All	All	1675/1852 (90%)	1585 (95%)	90 (5%)	20	38

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	41	LYS
1	A	42	ILE
1	A	169	ILE

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Mol	Chain	Res	Type
1	A	182	MET
1	A	202	LEU
1	A	203	ILE
1	A	244	LYS
1	A	275	VAL
1	A	281	ILE
1	A	285	LEU
1	A	289	GLN
1	A	394	ASP
1	A	456	MET
1	A	490	ASP
1	A	491	SER
1	A	492	LYS
1	A	513	VAL
1	A	514	LYS
1	A	517	ARG
1	A	519	GLU
1	A	534	MET
1	A	535	ASN
1	A	555	GLN
1	A	558	ASP
1	B	1	LYS
1	B	176	LEU
1	B	177	GLU
1	B	197	VAL
1	B	242	LYS
1	B	274	ASP
1	B	291	ASN
1	B	292	SER
1	B	308	ILE
1	B	341	SER
1	B	343	LYS
1	B	381	MET
1	B	395	ASN
1	B	453	MET
1	B	475	ASN
1	B	510	SER
1	B	525	ASP
1	B	529	LYS
1	B	534	MET
1	B	536	THR
1	B	554	LYS

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Mol	Chain	Res	Type
1	C	1	LYS
1	C	38	SER
1	C	40	LYS
1	C	42	ILE
1	C	66	LYS
1	C	112	LEU
1	C	141	LYS
1	C	169	ILE
1	C	185	ARG
1	C	244	LYS
1	C	245	SER
1	C	271	LEU
1	C	278	LEU
1	C	292	SER
1	C	296	ARG
1	C	394	ASP
1	C	416	ILE
1	C	439	ASP
1	C	440	ARG
1	C	446	VAL
1	C	534	MET
1	C	535	ASN
1	C	555	GLN
1	C	556	ARG
1	D	1	LYS
1	D	4	THR
1	D	9	LEU
1	D	10	VAL
1	D	18	VAL
1	D	19	SER
1	D	63	VAL
1	D	144	GLU
1	D	145	MET
1	D	194	MET
1	D	208	ARG
1	D	232	LEU
1	D	272	SER
1	D	394	ASP
1	D	418	LEU
1	D	465	LYS
1	D	492	LYS
1	D	499	ARG

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Mol	Chain	Res	Type
1	D	555	GLN
1	D	556	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	118	HIS
1	A	289	GLN
1	A	400	ASN
1	A	486	GLN
1	B	154	GLN
1	B	250	ASN
1	B	291	ASN
1	B	395	ASN
1	B	425	HIS
1	C	113	GLN
1	C	395	ASN
1	C	400	ASN
1	C	478	HIS
1	C	487	HIS
1	C	535	ASN
1	C	555	GLN
1	D	154	GLN
1	D	305	GLN
1	D	409	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 3 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
2	ADP	B	601	-	28,29,29	1.54	5 (17%)	43,45,45	1.76	9 (20%)
3	A1LX0	A	602	4	31,34,34	2.68	15 (48%)	33,51,51	2.53	10 (30%)
3	A1LX0	D	602	4	31,34,34	2.89	18 (58%)	33,51,51	2.27	9 (27%)
3	A1LX0	C	602	4	31,34,34	2.68	15 (48%)	33,51,51	2.53	10 (30%)
5	TPP	B	602	-	26,27,27	0.72	1 (3%)	38,40,40	0.42	0
2	ADP	D	601	-	28,29,29	1.53	5 (17%)	43,45,45	2.02	13 (30%)
2	ADP	C	601	-	28,29,29	1.53	5 (17%)	43,45,45	1.85	13 (30%)
2	ADP	A	601	-	28,29,29	1.44	6 (21%)	43,45,45	2.08	10 (23%)

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
2	ADP	B	601	-	-	2/16/32/32	0/3/3/3
3	A1LX0	A	602	4	-	3/25/31/31	0/3/3/3
3	A1LX0	D	602	4	-	4/25/31/31	0/3/3/3
3	A1LX0	C	602	4	-	3/25/31/31	0/3/3/3
5	TPP	B	602	-	-	7/17/17/17	0/2/2/2
2	ADP	D	601	-	-	3/16/32/32	0/3/3/3
2	ADP	C	601	-	-	2/16/32/32	0/3/3/3
2	ADP	A	601	-	-	3/16/32/32	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	A1LX0	C5-S1	-5.41	1.63	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	A1LX0	C9-C8	-5.40	1.45	1.53
3	D	602	A1LX0	C5'-C4'	-5.30	1.34	1.42
3	D	602	A1LX0	C4-N3	-5.10	1.33	1.40
3	C	602	A1LX0	C4-N3	-4.97	1.33	1.40
3	A	602	A1LX0	C4-N3	-4.93	1.33	1.40
3	C	602	A1LX0	C5-S1	-4.83	1.64	1.74
3	A	602	A1LX0	C5-S1	-4.81	1.64	1.74
2	D	601	ADP	PA-O3A	4.74	1.64	1.59
3	C	602	A1LX0	C9-C8	-4.58	1.46	1.53
2	A	601	ADP	C5-C4	4.55	1.47	1.39
3	A	602	A1LX0	C9-C8	-4.53	1.47	1.53
3	D	602	A1LX0	C8-C2	4.35	1.58	1.51
3	A	602	A1LX0	C5'-C4'	-4.34	1.35	1.42
3	C	602	A1LX0	C5'-C4'	-4.31	1.35	1.42
3	A	602	A1LX0	C8-C2	4.21	1.58	1.51
3	C	602	A1LX0	C8-C2	4.21	1.58	1.51
2	C	601	ADP	C5-C4	4.20	1.46	1.39
2	B	601	ADP	C4-N3	4.19	1.42	1.34
3	A	602	A1LX0	PB-O1B	-4.19	1.37	1.50
3	C	602	A1LX0	PB-O1B	-4.16	1.37	1.50
3	D	602	A1LX0	C2'-N3'	-3.97	1.27	1.34
3	C	602	A1LX0	C4'-N4'	-3.89	1.24	1.34
3	A	602	A1LX0	C4'-N4'	-3.89	1.24	1.34
2	B	601	ADP	C8-N7	3.68	1.38	1.31
2	D	601	ADP	C5-C4	3.63	1.45	1.39
3	D	602	A1LX0	PB-O1B	-3.61	1.39	1.50
3	C	602	A1LX0	C2'-N3'	-3.55	1.28	1.34
3	A	602	A1LX0	C2'-N3'	-3.54	1.28	1.34
3	D	602	A1LX0	C4'-N4'	-3.52	1.25	1.34
5	B	602	TPP	PA-O3A	-3.43	1.55	1.59
2	C	601	ADP	C5-N7	-3.39	1.32	1.39
2	C	601	ADP	C4-N9	-3.30	1.30	1.37
3	D	602	A1LX0	PB-O2B	-3.17	1.43	1.54
2	B	601	ADP	PA-O3A	3.16	1.62	1.59
3	A	602	A1LX0	PB-O2B	-3.12	1.43	1.54
3	C	602	A1LX0	PB-O2B	-3.12	1.43	1.54
2	C	601	ADP	PA-O3A	3.06	1.62	1.59
2	A	601	ADP	PA-O3A	2.89	1.62	1.59
3	D	602	A1LX0	PA-O2A	-2.87	1.42	1.55
3	A	602	A1LX0	PA-O2A	-2.86	1.42	1.55
3	C	602	A1LX0	PA-O2A	-2.85	1.42	1.55
3	D	602	A1LX0	C10-C9	-2.83	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	ADP	C4-N9	-2.80	1.31	1.37
3	D	602	A1LX0	C5-C4	2.73	1.40	1.35
3	D	602	A1LX0	PA-O1A	-2.72	1.41	1.50
3	C	602	A1LX0	PA-O1A	-2.69	1.41	1.50
3	A	602	A1LX0	PA-O1A	-2.69	1.41	1.50
3	A	602	A1LX0	C4'-N3'	-2.68	1.31	1.35
3	C	602	A1LX0	C4'-N3'	-2.67	1.31	1.35
2	D	601	ADP	C5-N7	-2.64	1.34	1.39
3	C	602	A1LX0	C6-C5	2.58	1.56	1.50
3	A	602	A1LX0	C6-C5	2.55	1.56	1.50
3	D	602	A1LX0	C2'-N1'	-2.49	1.30	1.34
2	B	601	ADP	C5-C6	2.47	1.47	1.41
3	D	602	A1LX0	C6-C5	2.43	1.55	1.50
3	A	602	A1LX0	C10-C9	-2.41	1.49	1.54
3	D	602	A1LX0	C6'-N1'	-2.39	1.29	1.34
3	C	602	A1LX0	C10-C9	-2.37	1.49	1.54
3	A	602	A1LX0	C6'-N1'	-2.34	1.29	1.34
3	C	602	A1LX0	C6'-N1'	-2.32	1.29	1.34
2	A	601	ADP	C8-N7	2.31	1.36	1.31
3	D	602	A1LX0	CM4-C4	2.31	1.54	1.49
2	C	601	ADP	C8-N7	2.28	1.36	1.31
2	B	601	ADP	C1'-N9	2.25	1.52	1.46
2	A	601	ADP	C5-N7	-2.18	1.35	1.39
2	A	601	ADP	C4-N9	-2.16	1.33	1.37
2	D	601	ADP	C8-N7	2.12	1.35	1.31
3	D	602	A1LX0	C7'-C5'	2.04	1.54	1.51
2	A	601	ADP	C5-C6	2.01	1.46	1.41

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	A1LX0	C4-C5-S1	-8.30	101.96	110.56
3	C	602	A1LX0	C4-C5-S1	-8.30	101.97	110.56
3	D	602	A1LX0	C4-C5-S1	-8.25	102.02	110.56
3	A	602	A1LX0	C6-C5-S1	6.31	132.83	119.29
3	C	602	A1LX0	C6-C5-S1	6.28	132.77	119.29
2	B	601	ADP	C5-C4-N3	-5.85	118.67	126.72
2	D	601	ADP	C5-C4-N3	-5.48	119.18	126.72
2	A	601	ADP	C5-C4-N3	-5.47	119.19	126.72
2	A	601	ADP	N3-C4-N9	5.40	136.35	127.17
2	D	601	ADP	N3-C4-N9	5.04	135.74	127.17
2	C	601	ADP	C5-C4-N3	-4.62	120.36	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ADP	N3-C2-N1	-4.12	122.35	128.58
3	C	602	A1LX0	CM4-C4-C5	-4.00	117.49	127.75
3	C	602	A1LX0	O3B-PB-O3A	3.99	118.02	104.64
3	A	602	A1LX0	CM4-C4-C5	-3.99	117.53	127.75
3	A	602	A1LX0	O3B-PB-O3A	3.97	117.95	104.64
2	D	601	ADP	C2-N3-C4	3.97	121.52	111.83
2	A	601	ADP	N3-C2-N1	-3.92	122.64	128.58
3	D	602	A1LX0	C6-C5-S1	3.88	127.62	119.29
2	A	601	ADP	C4-N9-C8	3.87	109.81	105.74
3	A	602	A1LX0	CM2-C2'-N1'	3.77	121.21	117.20
2	C	601	ADP	N3-C2-N1	-3.75	122.91	128.58
3	C	602	A1LX0	CM2-C2'-N1'	3.74	121.19	117.20
2	A	601	ADP	N6-C6-N1	3.73	126.68	118.38
3	D	602	A1LX0	O3B-PB-O3A	3.61	116.73	104.64
2	B	601	ADP	N3-C2-N1	-3.60	123.13	128.58
2	A	601	ADP	C2-N3-C4	3.55	120.50	111.83
2	C	601	ADP	N3-C4-N9	3.35	132.86	127.17
3	D	602	A1LX0	N4'-C4'-N3'	3.33	121.52	117.03
2	C	601	ADP	O4'-C1'-N9	3.33	114.49	108.09
3	A	602	A1LX0	C5'-C6'-N1'	-3.32	118.44	123.83
2	D	601	ADP	C4-N9-C8	3.30	109.21	105.74
3	C	602	A1LX0	C5'-C6'-N1'	-3.29	118.47	123.83
2	C	601	ADP	C2-N3-C4	3.27	119.81	111.83
3	A	602	A1LX0	C6'-N1'-C2'	3.18	121.29	116.07
2	A	601	ADP	C5-C6-N6	-3.17	115.43	123.29
3	C	602	A1LX0	C6'-N1'-C2'	3.15	121.25	116.07
2	B	601	ADP	C2-N3-C4	3.12	119.45	111.83
2	C	601	ADP	O2'-C2'-C1'	3.10	120.78	110.10
2	D	601	ADP	O3'-C3'-C4'	-3.01	102.44	111.08
2	B	601	ADP	C5-C4-N9	3.00	109.08	105.81
3	D	602	A1LX0	C5'-C4'-N4'	-2.89	118.25	122.14
2	B	601	ADP	O2'-C2'-C1'	2.78	119.69	110.10
2	D	601	ADP	C5-C6-N6	-2.76	116.46	123.29
3	A	602	A1LX0	CM4-C4-N3	2.73	125.52	121.95
3	D	602	A1LX0	C6'-N1'-C2'	2.71	120.53	116.07
3	C	602	A1LX0	CM4-C4-N3	2.71	125.49	121.95
3	D	602	A1LX0	C5'-C6'-N1'	-2.68	119.47	123.83
3	D	602	A1LX0	C7'-N3-C4	-2.66	119.50	123.95
2	B	601	ADP	C4-C5-N7	-2.57	107.64	110.58
2	C	601	ADP	N6-C6-N1	2.54	124.03	118.38
2	D	601	ADP	C2'-C3'-C4'	2.47	107.38	102.61
2	B	601	ADP	O3'-C3'-C4'	-2.45	104.04	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	N3-C4-N9	2.43	131.30	127.17
2	C	601	ADP	C2-N1-C6	2.39	122.66	118.73
3	A	602	A1LX0	O2B-PB-O1B	-2.36	101.63	110.83
3	C	602	A1LX0	O2B-PB-O1B	-2.36	101.63	110.83
3	A	602	A1LX0	N1'-C2'-N3'	-2.29	121.72	125.53
3	C	602	A1LX0	N1'-C2'-N3'	-2.26	121.77	125.53
2	C	601	ADP	C2'-C1'-N9	-2.25	107.71	113.30
2	A	601	ADP	N9-C8-N7	-2.24	110.75	113.94
2	C	601	ADP	C2'-C3'-C4'	2.24	106.94	102.61
2	D	601	ADP	N6-C6-N1	2.19	123.25	118.38
2	C	601	ADP	O2A-PA-O1A	2.17	122.55	112.44
3	D	602	A1LX0	CM4-C4-C5	-2.16	122.21	127.75
2	C	601	ADP	C4-C5-N7	-2.16	108.12	110.58
2	A	601	ADP	C2-N1-C6	2.10	122.19	118.73
2	D	601	ADP	O3B-PB-O2B	2.08	115.59	107.80
2	C	601	ADP	O2A-PA-O3A	2.06	112.84	107.27
2	D	601	ADP	O2'-C2'-C1'	2.05	117.15	110.10
2	A	601	ADP	O3B-PB-O2B	2.04	115.45	107.80
2	D	601	ADP	O2A-PA-O3A	2.04	112.79	107.27
2	B	601	ADP	C2'-C3'-C4'	2.03	106.53	102.61
2	D	601	ADP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	A1LX0	C2-C8-C9-C11
3	A	602	A1LX0	C7-O7'-PA-O1A
3	C	602	A1LX0	C2-C8-C9-C11
3	C	602	A1LX0	C7-O7'-PA-O1A
3	D	602	A1LX0	C2-C8-C9-C10
3	D	602	A1LX0	C2-C8-C9-C11
5	B	602	TPP	C5-C6-C7-O7
5	B	602	TPP	C7-O7-PA-O1A
5	B	602	TPP	PA-O3A-PB-O3B
2	A	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	O4'-C4'-C5'-O5'
3	D	602	A1LX0	PA-O3A-PB-O2B
5	B	602	TPP	C7-O7-PA-O2A
5	B	602	TPP	C7-O7-PA-O3A
2	C	601	ADP	O4'-C4'-C5'-O5'
5	B	602	TPP	PA-O3A-PB-O1B

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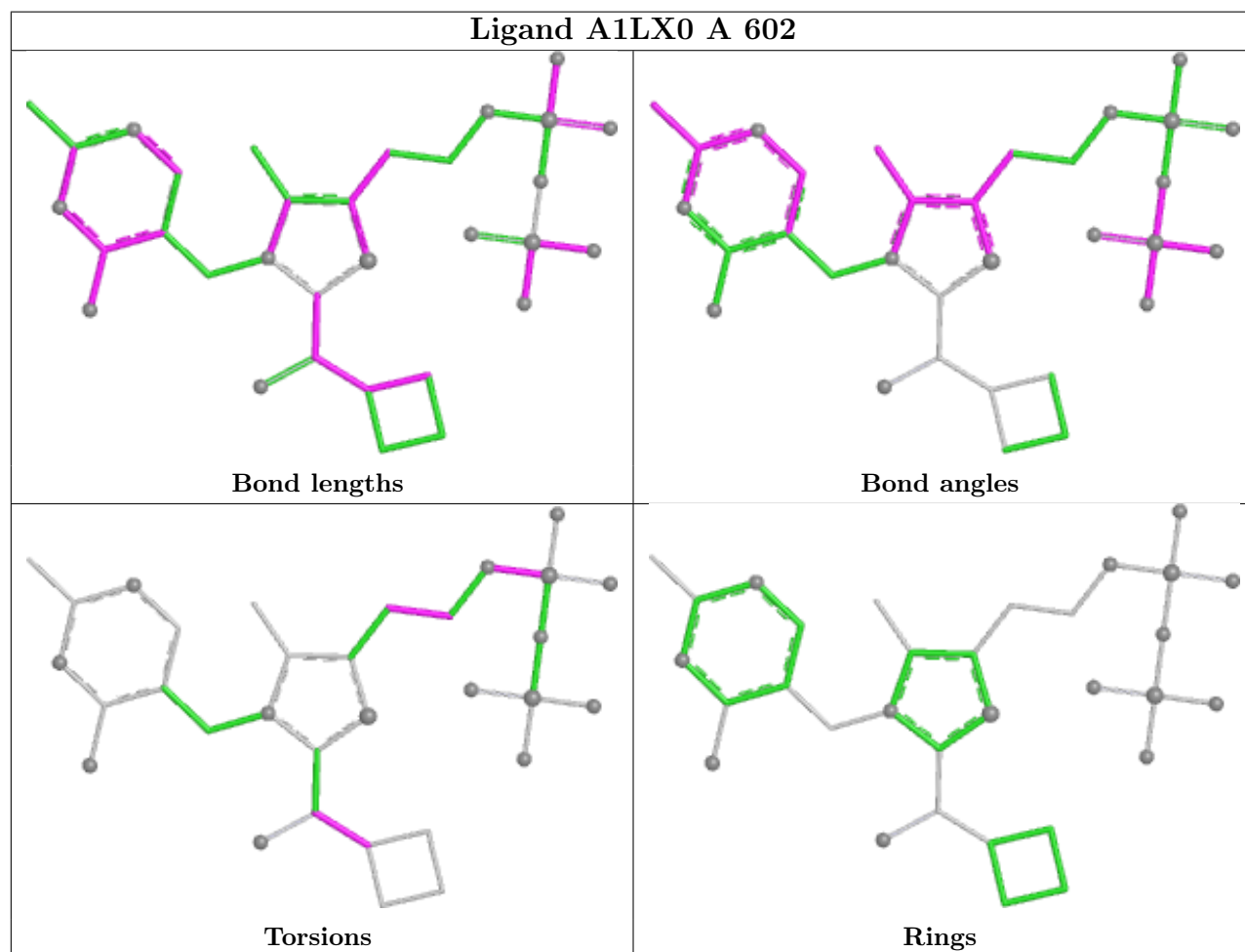
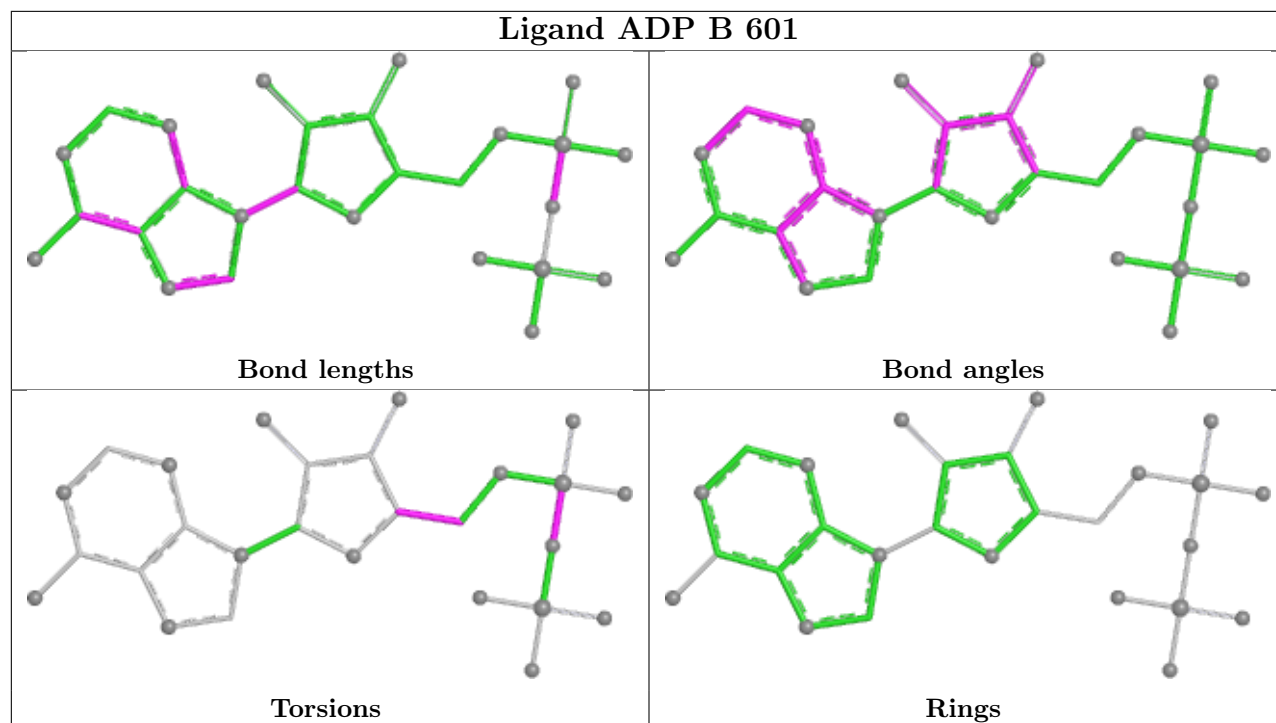
Mol	Chain	Res	Type	Atoms
3	A	602	A1LX0	C5-C6-C7-O7'
3	C	602	A1LX0	C5-C6-C7-O7'
2	D	601	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	PB-O3A-PA-O2A
2	B	601	ADP	PB-O3A-PA-O2A
2	C	601	ADP	PB-O3A-PA-O2A
2	D	601	ADP	PB-O3A-PA-O2A
2	A	601	ADP	C2'-C1'-N9-C8
3	D	602	A1LX0	N3-C2-C8-O8
5	B	602	TPP	C4'-C5'-C7'-N3
2	D	601	ADP	C2'-C1'-N9-C8

There are no ring outliers.

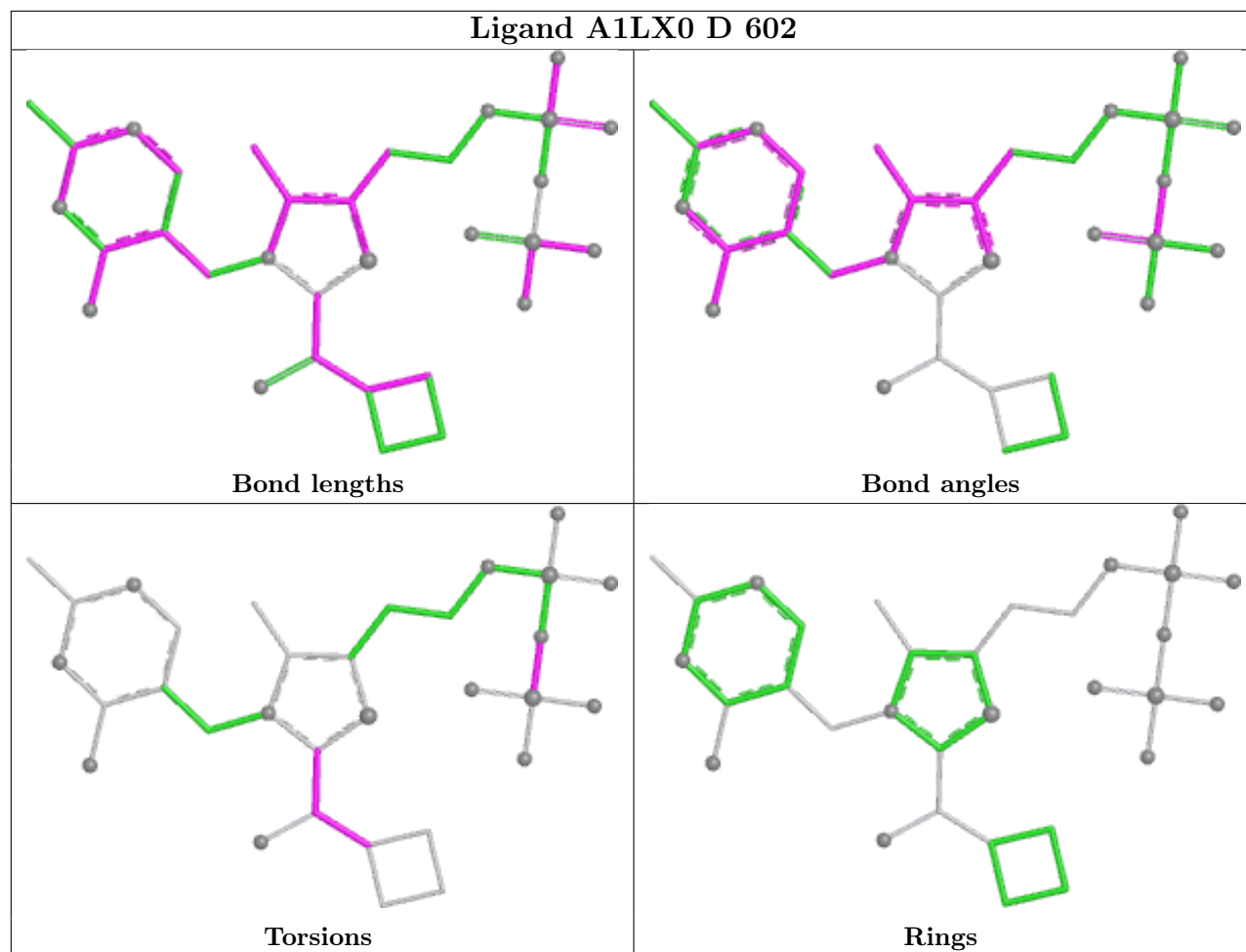
7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ADP	3	0
3	A	602	A1LX0	5	0
3	D	602	A1LX0	1	0
3	C	602	A1LX0	7	0
5	B	602	TPP	6	0
2	D	601	ADP	2	0
2	A	601	ADP	2	0

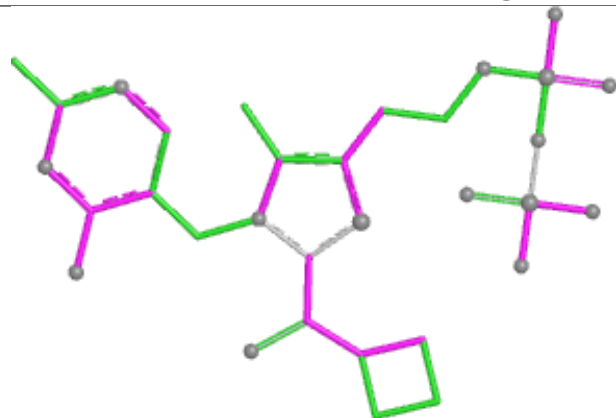
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



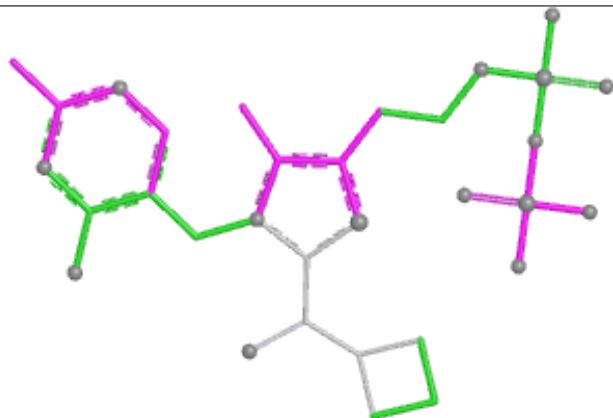
Ligand A1LX0 D 602



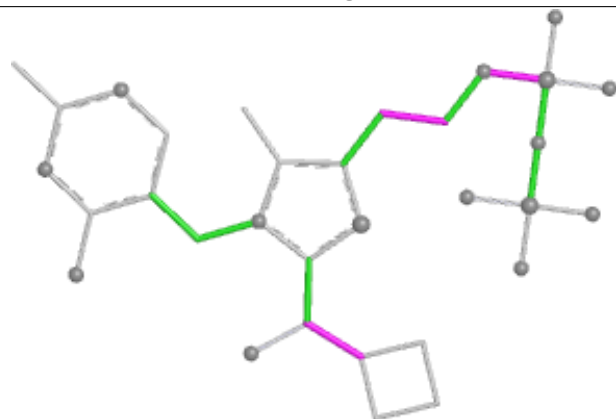
Ligand A1LX0 C 602



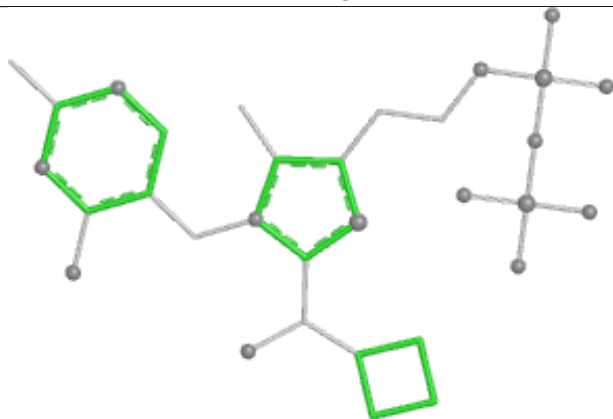
Bond lengths



Bond angles

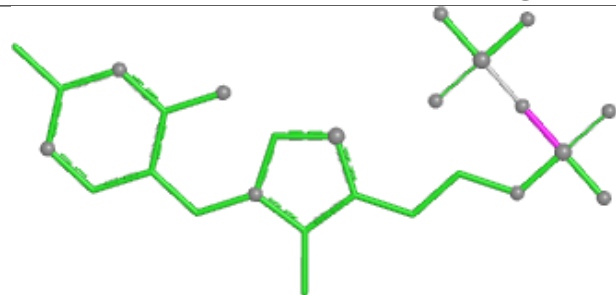


Torsions

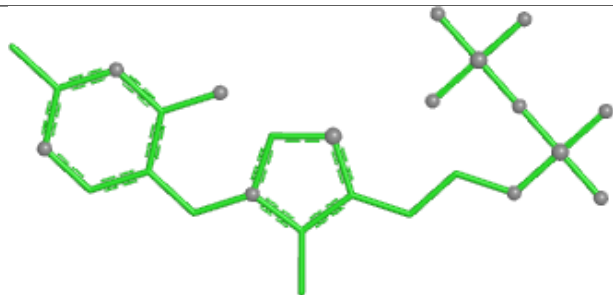


Rings

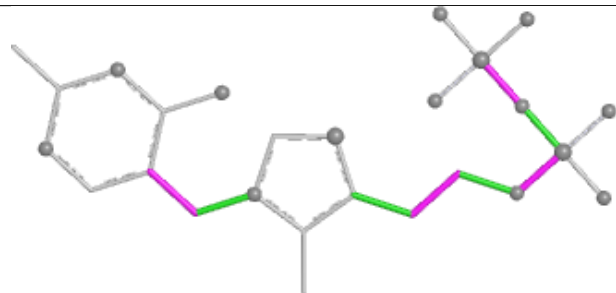
Ligand TPP B 602



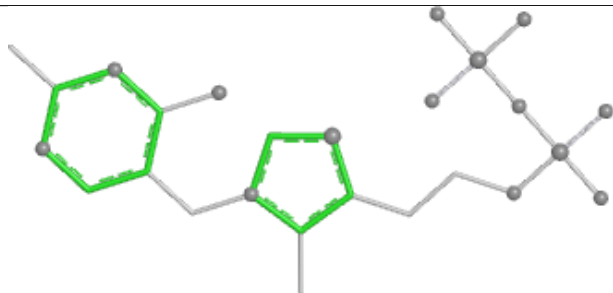
Bond lengths



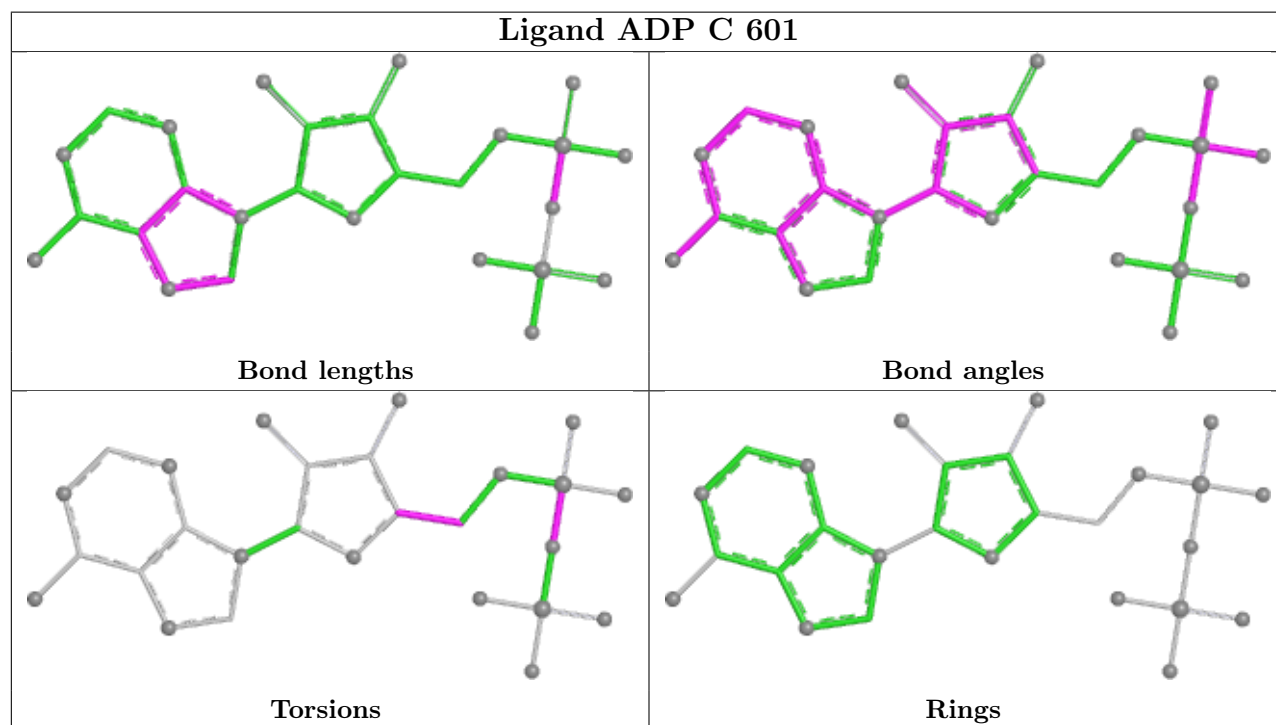
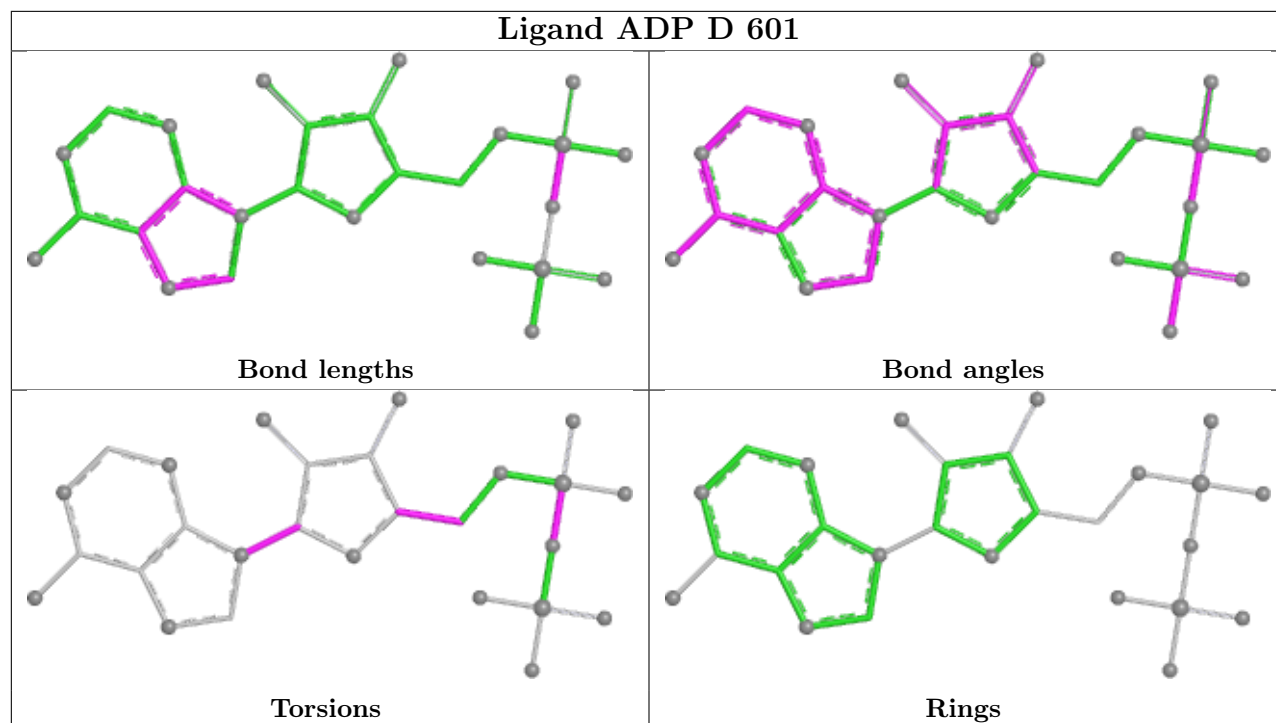
Bond angles

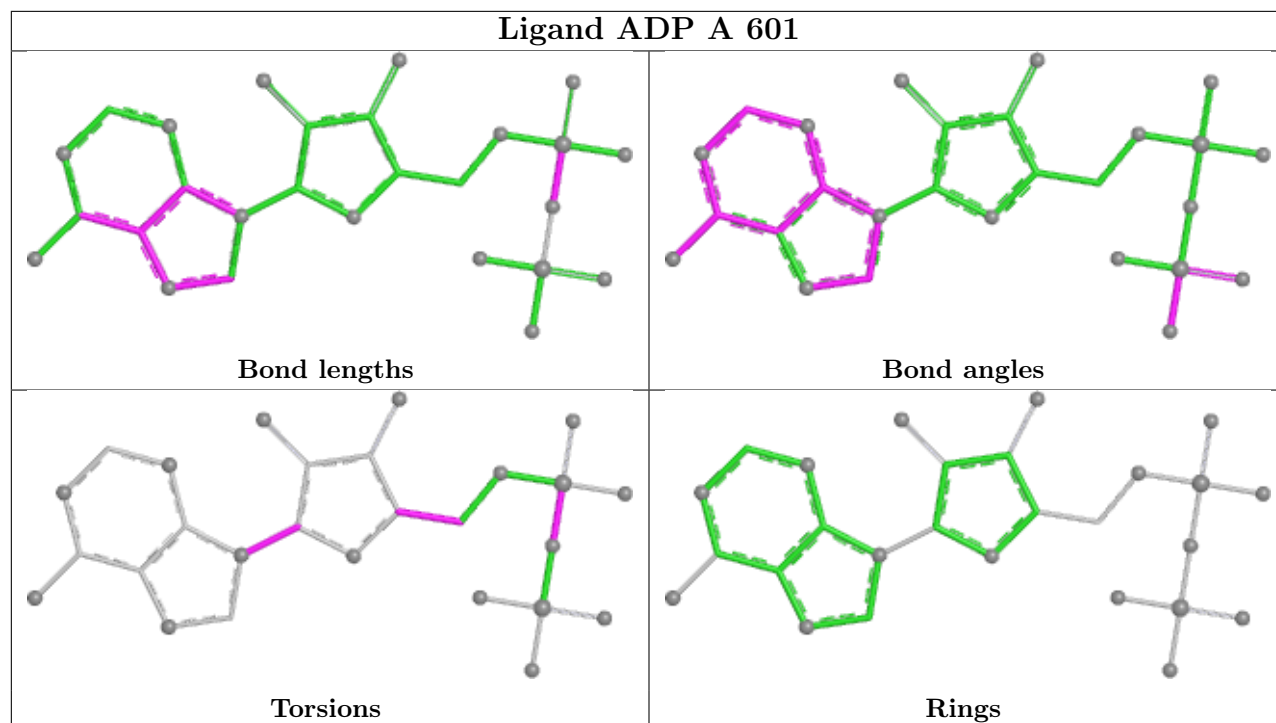


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	532/584 (91%)	0.69	31 (5%) 29 29	30, 67, 101, 138	0
1	B	531/584 (90%)	0.59	9 (1%) 69 67	40, 71, 103, 141	0
1	C	530/584 (90%)	0.52	8 (1%) 72 71	43, 71, 106, 126	0
1	D	530/584 (90%)	0.59	12 (2%) 61 59	38, 67, 100, 141	0
All	All	2123/2336 (90%)	0.60	60 (2%) 55 53	30, 69, 103, 141	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	71	CYS	4.2
1	A	23	GLY	4.0
1	D	177	GLU	4.0
1	A	175	PRO	3.9
1	A	0	SER	3.5
1	D	557	PHE	3.4
1	A	1	LYS	3.4
1	A	136	ILE	3.3
1	A	558	ASP	3.3
1	A	423	MET	3.2
1	C	557	PHE	3.1
1	D	484	PHE	3.0
1	D	423	MET	3.0
1	D	169	ILE	2.8
1	D	182	MET	2.7
1	B	136	ILE	2.6
1	A	176	LEU	2.6
1	A	163	LEU	2.5
1	A	123	VAL	2.5
1	B	491	SER	2.4
1	C	423	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	134	VAL	2.4
1	B	23	GLY	2.4
1	D	420	LEU	2.4
1	A	453	MET	2.4
1	A	491	SER	2.3
1	D	111	ALA	2.3
1	A	177	GLU	2.3
1	A	91	ASP	2.3
1	A	260	PHE	2.3
1	A	265	LYS	2.2
1	A	2	THR	2.2
1	A	541	ASP	2.2
1	C	447	GLY	2.2
1	C	484	PHE	2.2
1	C	556	ARG	2.2
1	A	549	LEU	2.2
1	B	343	LYS	2.2
1	A	3	VAL	2.2
1	D	2	THR	2.2
1	A	182	MET	2.2
1	A	174	VAL	2.2
1	B	335	ILE	2.2
1	A	499	ARG	2.1
1	C	395	ASN	2.1
1	B	402	GLY	2.1
1	B	3	VAL	2.1
1	A	493	PHE	2.1
1	C	298	THR	2.1
1	C	417	GLY	2.1
1	A	38	SER	2.1
1	D	28	PRO	2.1
1	B	371	GLY	2.1
1	A	439	ASP	2.0
1	A	70	CYS	2.0
1	A	133	SER	2.0
1	A	104	THR	2.0
1	A	420	LEU	2.0
1	A	419	GLY	2.0
1	D	136	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

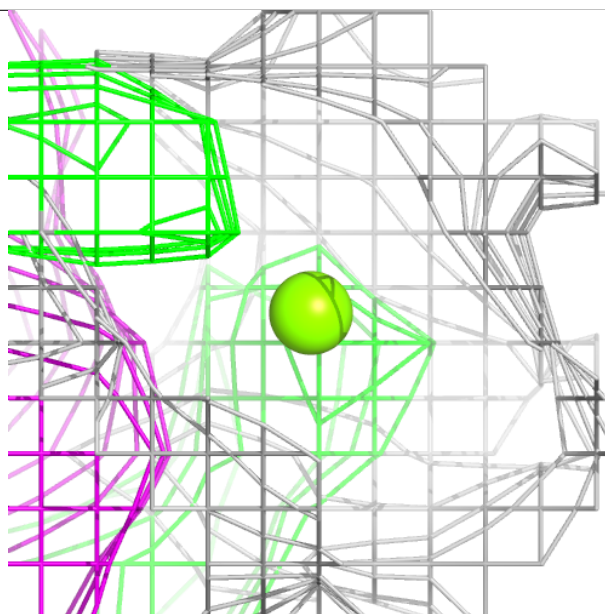
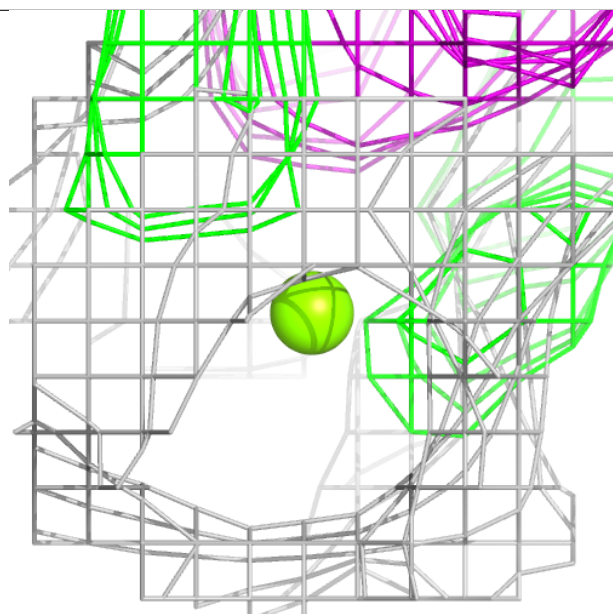
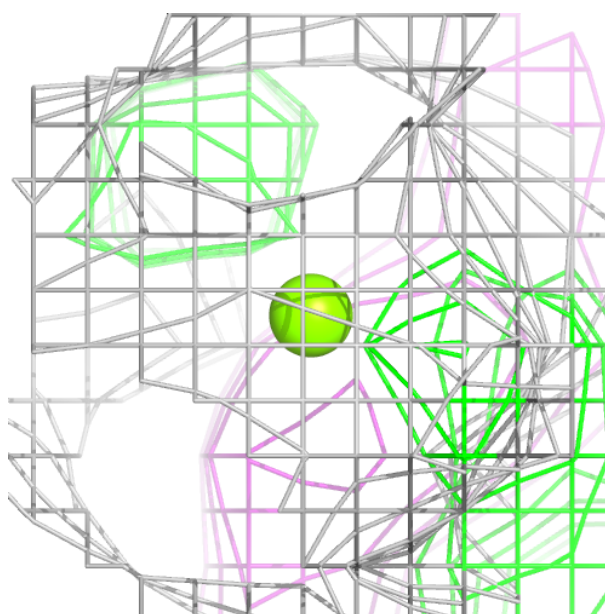
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	603	1/1	0.79	0.15	60,60,60,60	0
4	MG	D	603	1/1	0.80	0.11	69,69,69,69	0
3	A1LX0	A	602	32/32	0.82	0.13	20,20,20,20	0
4	MG	C	603	1/1	0.83	0.08	75,75,75,75	0
3	A1LX0	C	602	32/32	0.84	0.12	20,20,20,20	0
3	A1LX0	D	602	32/32	0.87	0.12	20,20,20,20	0
5	TPP	B	602	26/26	0.89	0.11	42,67,94,108	0
2	ADP	B	601	27/27	0.91	0.10	42,67,87,101	0
2	ADP	C	601	27/27	0.91	0.09	52,65,81,82	0
2	ADP	A	601	27/27	0.91	0.09	44,64,80,87	0
2	ADP	D	601	27/27	0.94	0.07	39,57,79,95	0

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

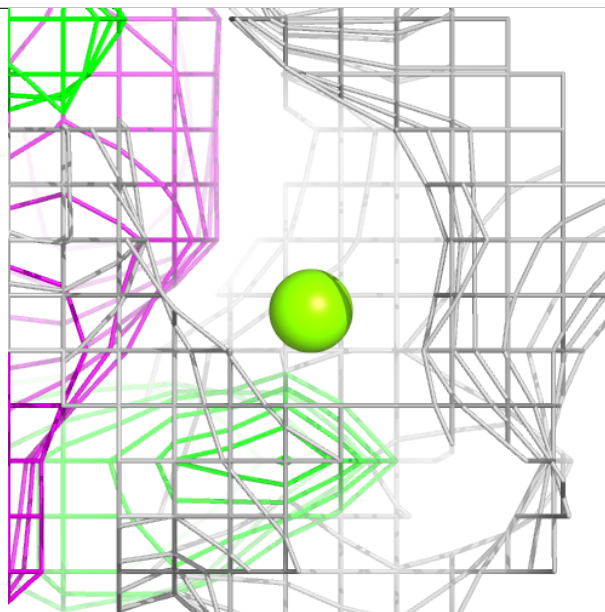
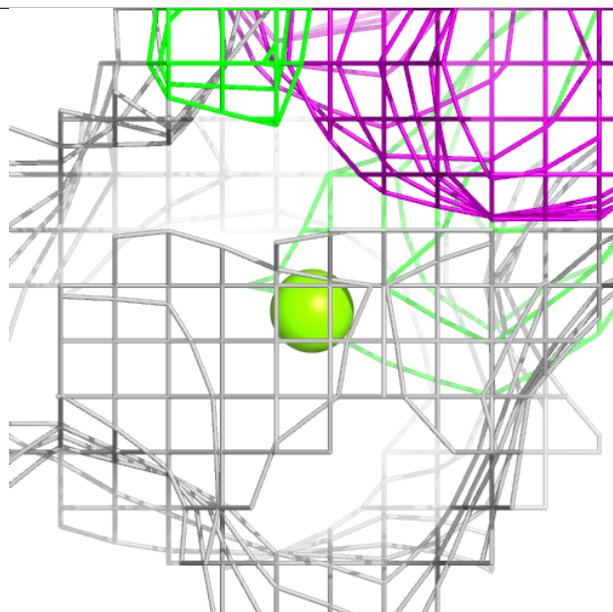
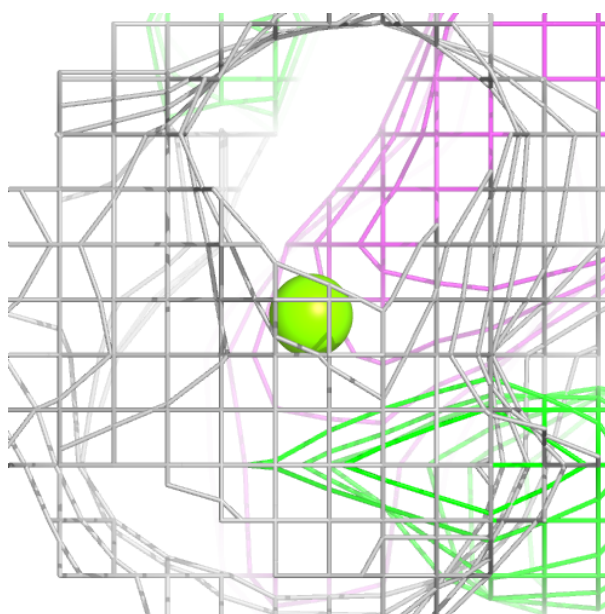
Electron density around MG A 603:

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



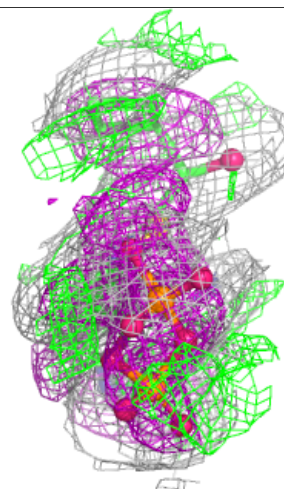
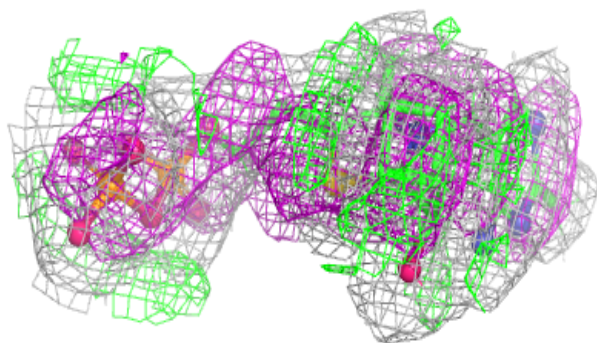
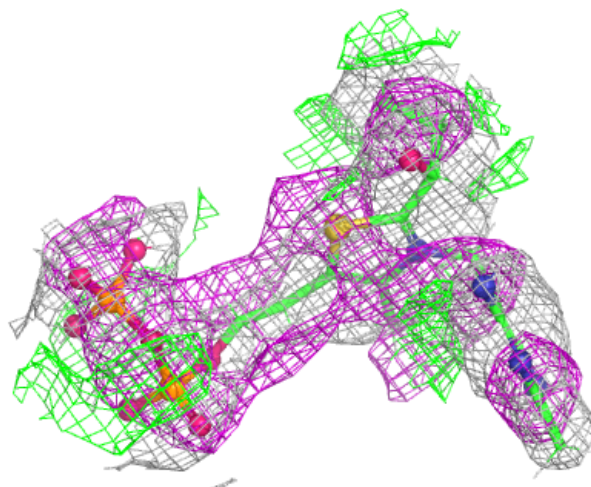
Electron density around MG D 603:

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



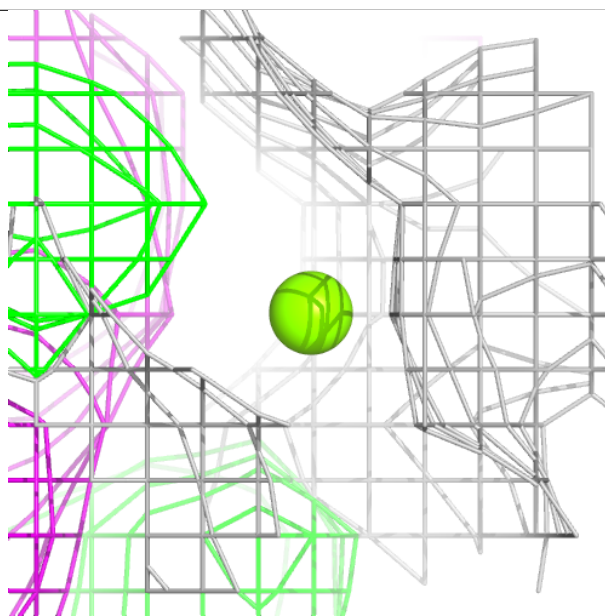
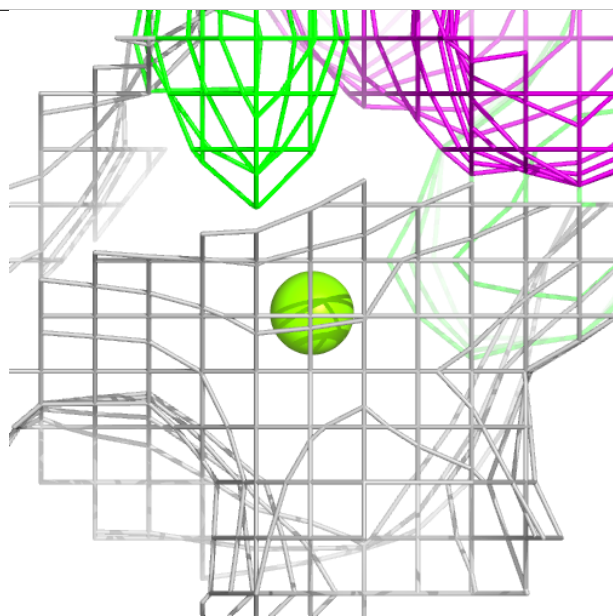
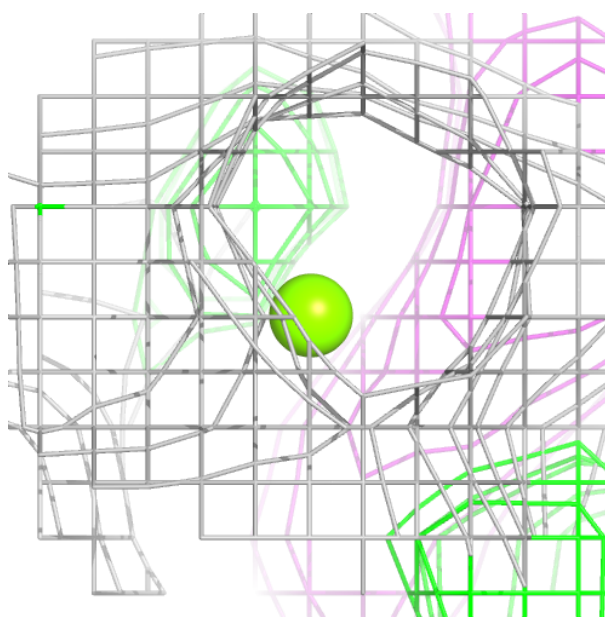
Electron density around A1LX0 A 602:

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



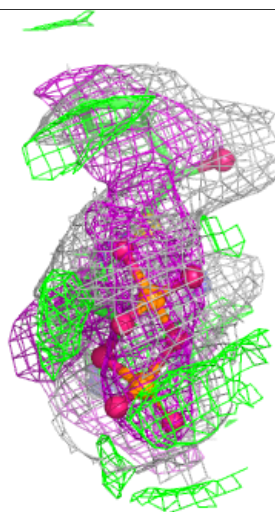
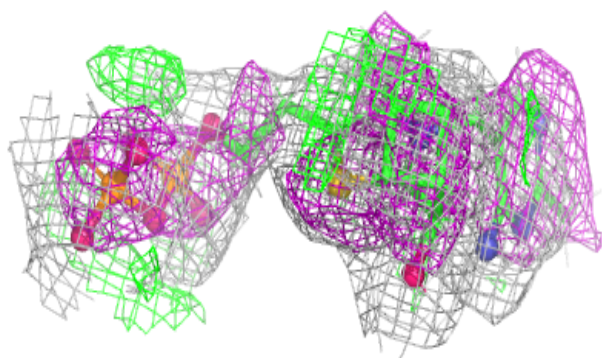
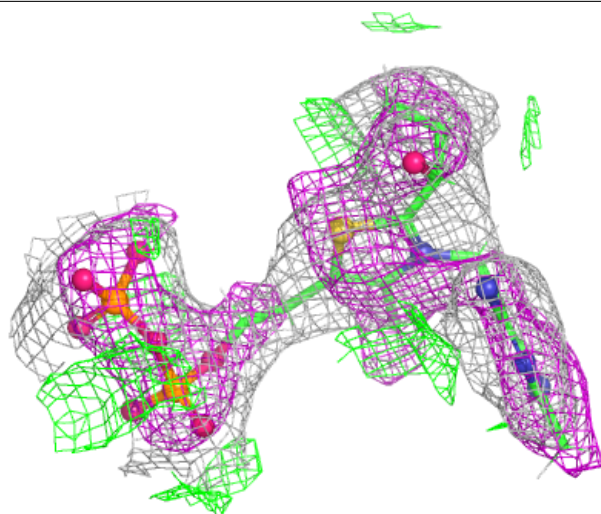
Electron density around MG C 603:

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



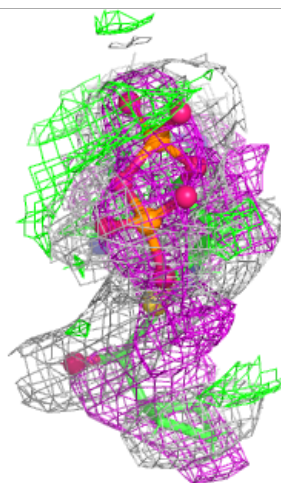
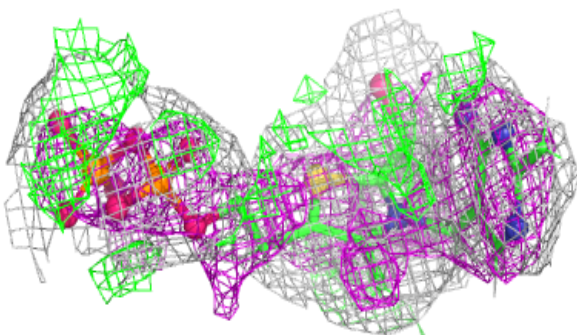
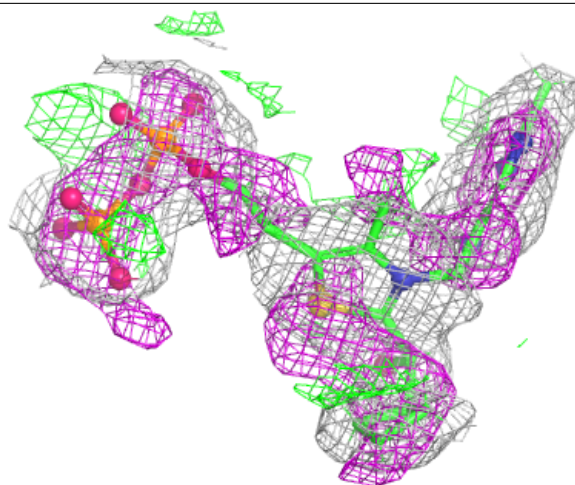
Electron density around A1LX0 C 602:

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



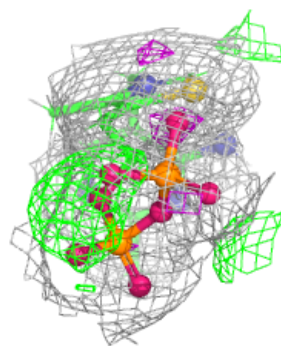
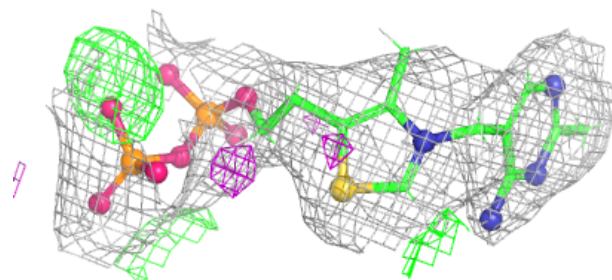
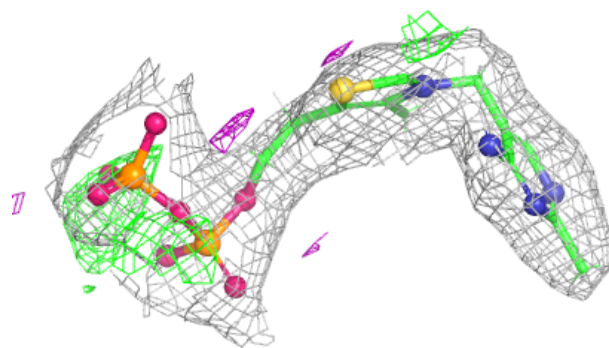
Electron density around A1LX0 D 602:

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

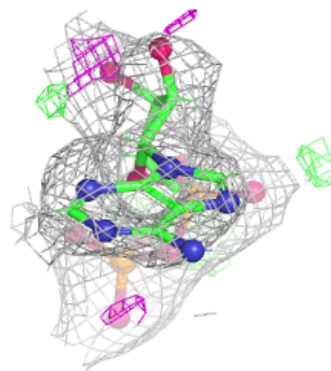
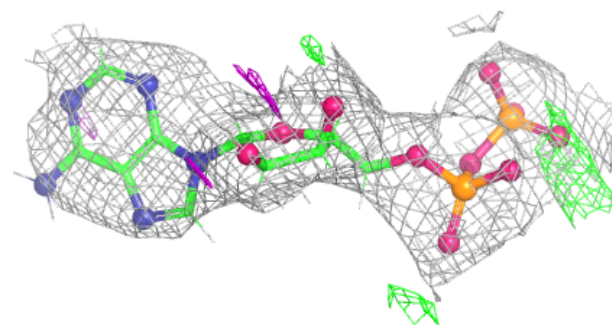
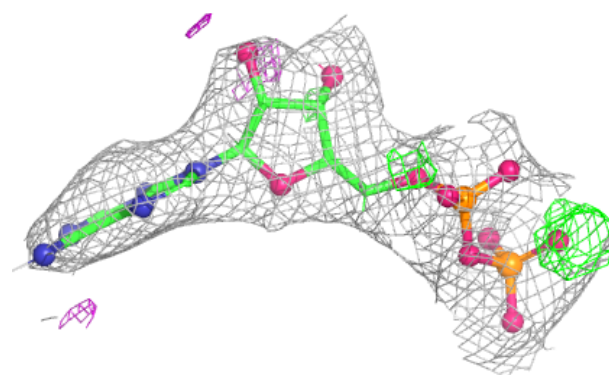


Electron density around TPP B 602:

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

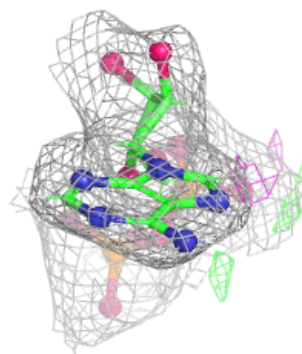
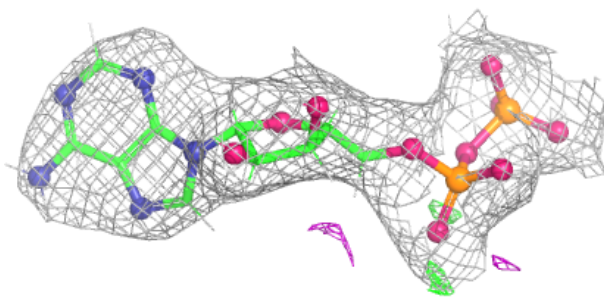
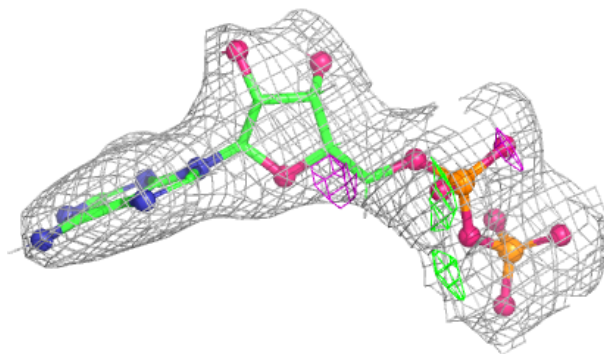
**Electron density around ADP B 601:**

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

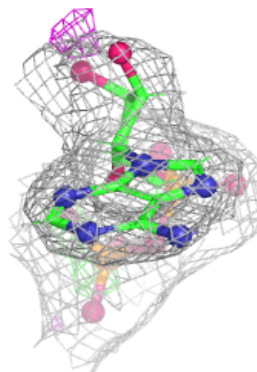
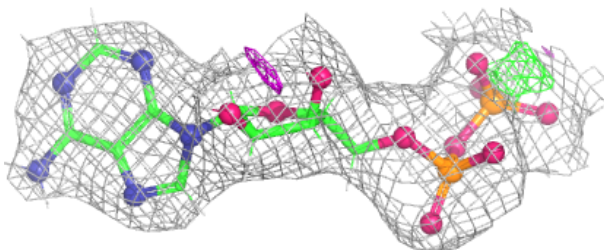
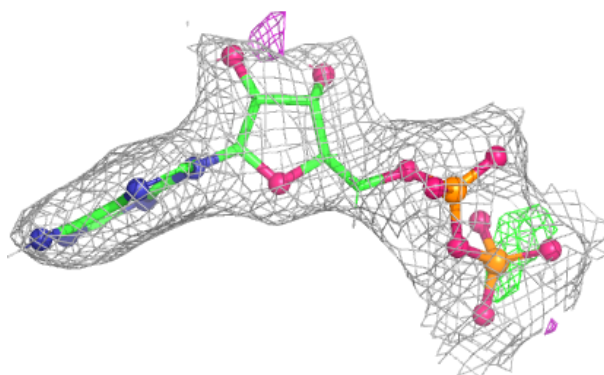


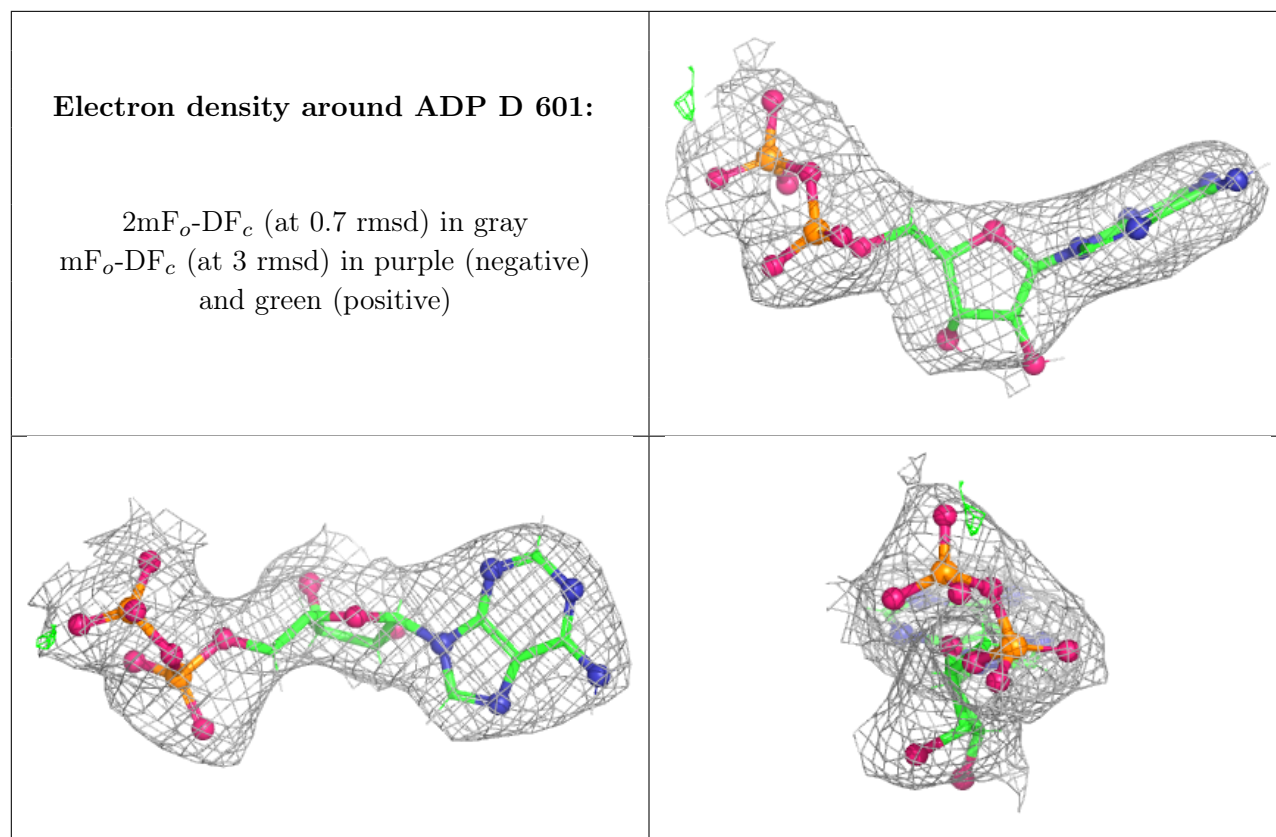
Electron density around ADP C 601:

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

**Electron density around ADP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.