



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:48 PM UTC

PDB ID : 8AR7 / pdb_00008ar7
Title : Bovine glutamate dehydrogenase in ternary complex with the allosteric activators ADP and leucine
Authors : Aleshin, V.A.; Bellinzoni, M.
Deposited on : 2022-08-15
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

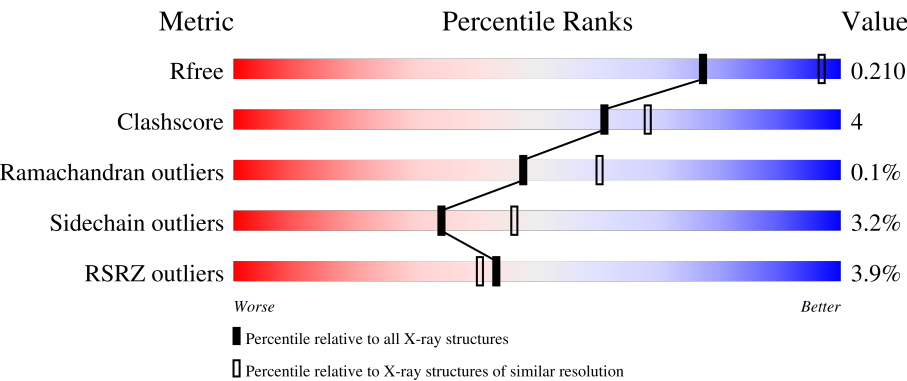
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.45 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	561	5% 77% 11% 12%
1	B	561	3% 78% 10% 11%
1	C	561	5% 79% 8% 12%
1	D	561	5% 77% 10% 11%
1	E	561	% 78% 10% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	561	% 78%11%11%

2 Entry composition [i](#)

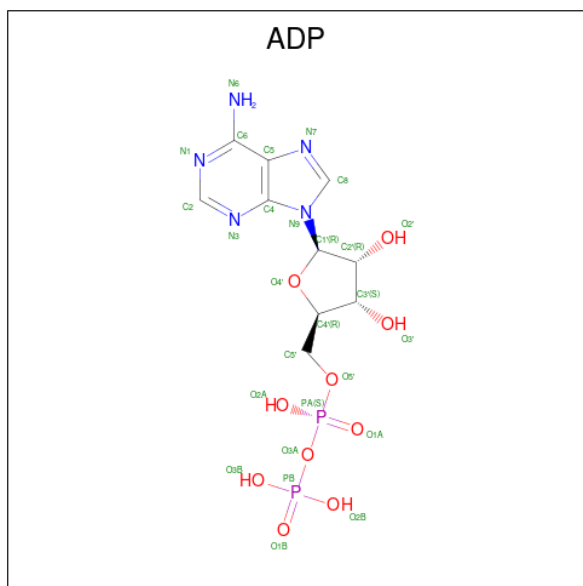
There are 5 unique types of molecules in this entry. The entry contains 23655 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate dehydrogenase (NAD(P)(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3817	2411	668	720	18			
1	B	497	Total	C	N	O	S	0	0	0
			3826	2421	670	717	18			
1	C	494	Total	C	N	O	S	0	0	0
			3804	2408	666	712	18			
1	D	497	Total	C	N	O	S	0	0	0
			3826	2421	670	717	18			
1	E	499	Total	C	N	O	S	0	0	0
			3865	2443	680	724	18			
1	F	499	Total	C	N	O	S	0	0	0
			3856	2437	677	724	18			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

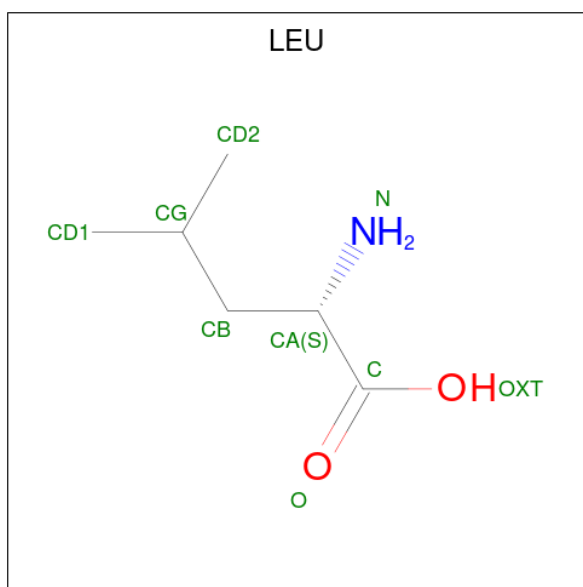


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		

- Molecule 4 is LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	B	1	Total	C	N	O	0	0
			9	6	1	2		
4	C	1	Total	C	N	O	0	0
			9	6	1	2		
4	D	1	Total	C	N	O	0	0
			9	6	1	2		
4	E	1	Total	C	N	O	0	0
			9	6	1	2		

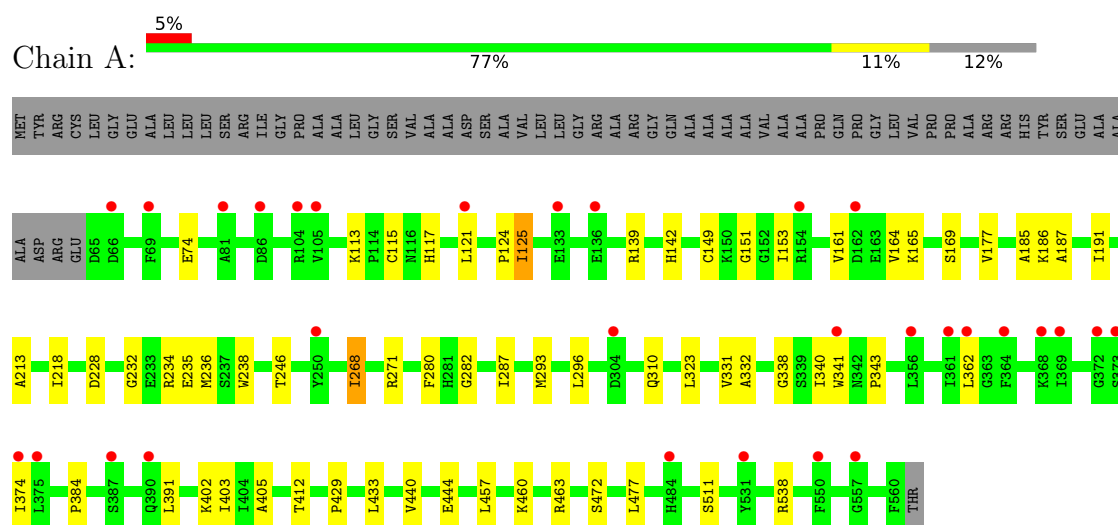
- Molecule 5 is water.

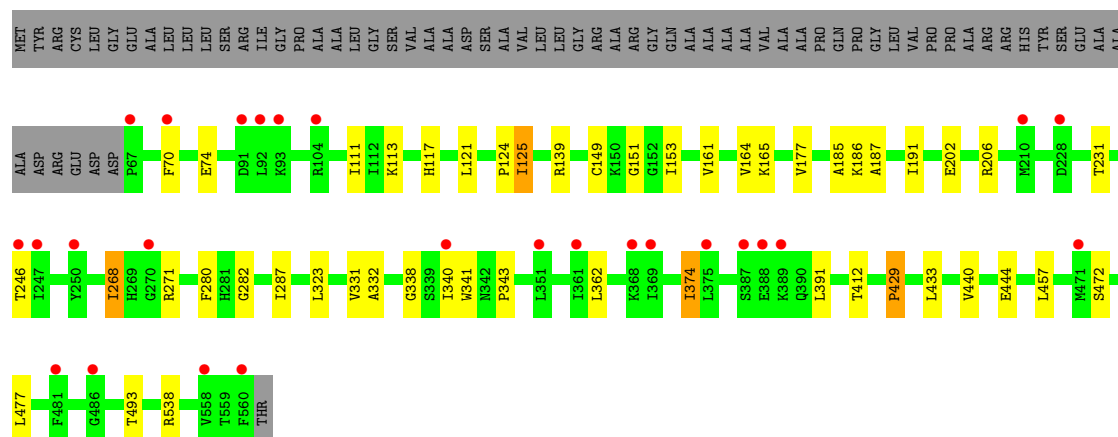
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	60	Total	O	0	0
			60	60		
5	C	73	Total	O	0	0
			73	73		
5	D	77	Total	O	0	0
			77	77		
5	E	87	Total	O	0	0
			87	87		
5	F	71	Total	O	0	0
			71	71		

3 Residue-property plots [i](#)

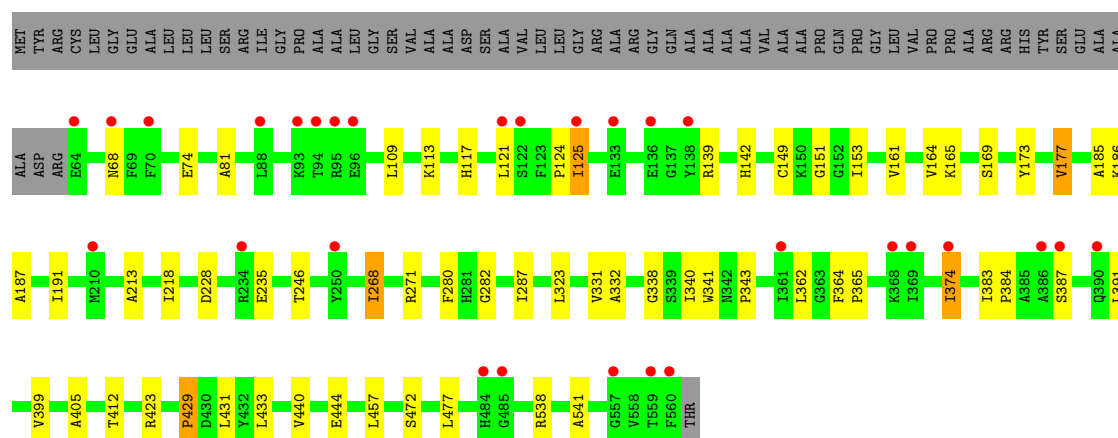
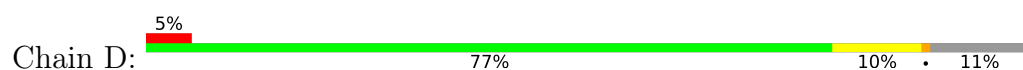
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

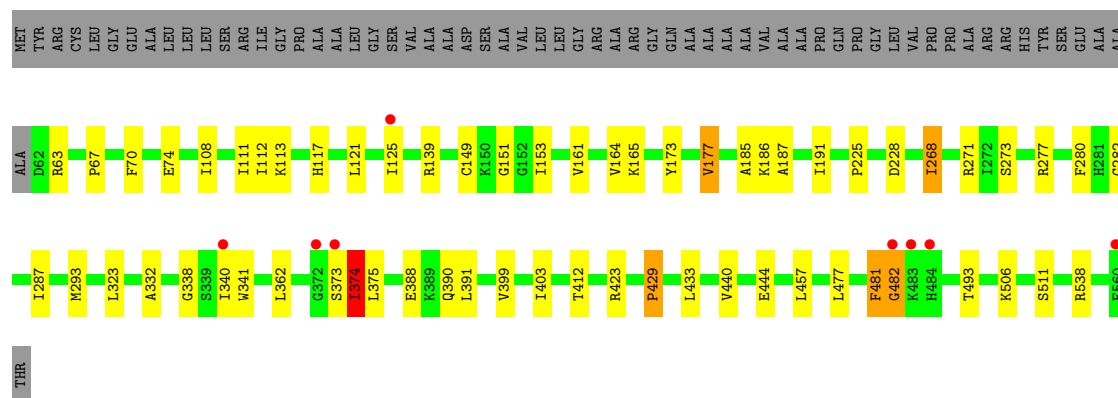
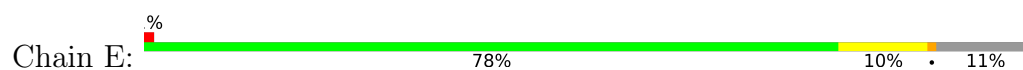




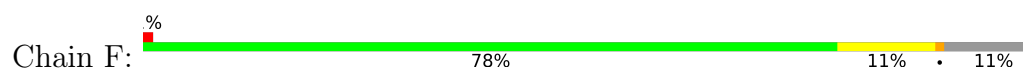
• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))

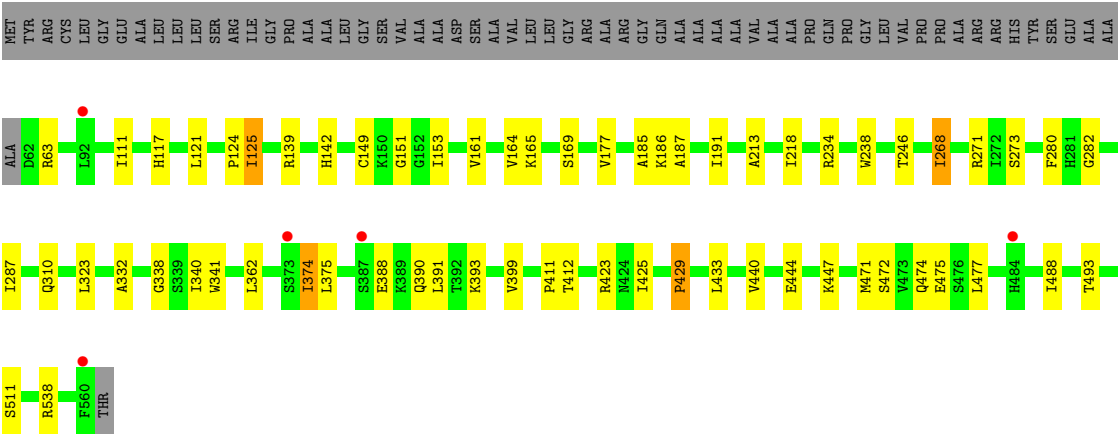


• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))



• Molecule 1: Glutamate dehydrogenase (NAD(P)(+))





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 178.71Å 123.88Å 90.00° 104.00° 90.00°	Depositor
Resolution (Å)	120.20 – 2.45 120.20 – 2.45	Depositor EDS
% Data completeness (in resolution range)	59.0 (120.20-2.45) 59.0 (120.20-2.45)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.4 (8-JUN-2022)	Depositor
R, R_{free}	0.192 , 0.214 0.187 , 0.210	Depositor DCC
R_{free} test set	4196 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23655	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.61	1/3898 (0.0%)	0.98	1/5275 (0.0%)
1	B	0.63	1/3908 (0.0%)	0.98	3/5287 (0.1%)
1	C	0.64	1/3886 (0.0%)	0.98	2/5257 (0.0%)
1	D	0.63	1/3908 (0.0%)	0.99	3/5287 (0.1%)
1	E	0.63	0/3948	1.01	4/5337 (0.1%)
1	F	0.64	1/3938 (0.0%)	0.99	4/5325 (0.1%)
All	All	0.63	5/23486 (0.0%)	0.99	17/31768 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	THR	CA-C	12.18	1.58	1.52
1	B	246	THR	CA-C	10.42	1.57	1.52
1	D	246	THR	CA-C	9.91	1.57	1.52
1	F	246	THR	CA-C	8.72	1.56	1.52
1	A	246	THR	CA-C	7.35	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	228	ASP	CA-CB-CG	6.13	118.73	112.60
1	E	374	ILE	CA-C-N	5.39	127.77	120.38
1	E	374	ILE	C-N-CA	5.39	127.77	120.38
1	B	228	ASP	CA-CB-CG	5.29	117.89	112.60
1	F	429	PRO	CA-C-N	5.29	127.37	120.28
1	F	429	PRO	C-N-CA	5.29	127.37	120.28
1	D	429	PRO	CA-C-N	5.24	127.30	120.28
1	D	429	PRO	C-N-CA	5.24	127.30	120.28
1	F	273	SER	CA-C-N	5.17	127.52	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	273	SER	C-N-CA	5.17	127.52	120.54
1	C	429	PRO	CA-C-N	5.13	127.16	120.28
1	C	429	PRO	C-N-CA	5.13	127.16	120.28
1	B	429	PRO	CA-C-N	5.09	127.10	120.28
1	B	429	PRO	C-N-CA	5.09	127.10	120.28
1	E	429	PRO	CA-C-N	5.08	127.09	120.28
1	E	429	PRO	C-N-CA	5.08	127.09	120.28

There are no chirality outliers.

There are no planarity outliers.

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	3817	0	3720	36	0
1	B	3826	0	3736	35	0
1	C	3804	0	3718	30	0
1	D	3826	0	3736	37	0
1	E	3865	0	3788	36	0
1	F	3856	0	3772	43	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	1	0
2	F	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	18	0	20	0	0
4	B	9	0	10	0	0
4	C	9	0	10	0	0
4	D	9	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	9	0	10	0	0
5	A	71	0	0	0	0
5	B	60	0	0	0	0
5	C	73	0	0	0	0
5	D	77	0	0	0	0
5	E	87	0	0	0	0
5	F	71	0	0	0	0
All	All	23655	0	22602	193	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 4.

All (193) 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:F:139:ARG:HD2	1:F:187:ALA:HB2	1.69	0.74
1:F:332:ALA:HB2	1:F:341:TRP:HD1	1.52	0.73
1:A:460:LYS:HZ2	1:A:463:ARG:HD2	1.58	0.66
1:E:481:PHE:O	1:E:482:GLY:O	2.15	0.64
1:B:139:ARG:HD2	1:B:187:ALA:HB2	1.80	0.64
1:E:373:SER:HB2	1:E:375:LEU:HG	1.81	0.62
1:A:139:ARG:HD2	1:A:187:ALA:HB2	1.82	0.61
1:D:139:ARG:HD2	1:D:187:ALA:HB2	1.83	0.61
1:A:332:ALA:HB1	1:A:374:ILE:HD12	1.83	0.59
1:F:474:GLN:HG3	1:F:488:ILE:O	2.03	0.59
1:C:139:ARG:HD2	1:C:187:ALA:HB2	1.85	0.59
1:B:213:ALA:HA	1:B:218:ILE:HG22	1.86	0.57
1:E:282:GLY:HA3	1:E:433:LEU:HD12	1.86	0.57
1:D:213:ALA:HA	1:D:218:ILE:HG22	1.86	0.57
1:B:151:GLY:HA3	1:B:185:ALA:O	2.05	0.57
1:A:296:LEU:HB3	1:A:402:LYS:HG3	1.88	0.56
1:E:151:GLY:HA3	1:E:185:ALA:O	2.05	0.56
1:A:151:GLY:HA3	1:A:185:ALA:O	2.05	0.56
1:D:139:ARG:CD	1:D:187:ALA:HB2	2.36	0.56
1:C:391:LEU:HB2	1:C:412:THR:HG22	1.88	0.56
1:E:139:ARG:HD2	1:E:187:ALA:HB2	1.87	0.56
1:F:375:LEU:HD11	1:F:390:GLN:HB3	1.87	0.56
1:E:391:LEU:HB2	1:E:412:THR:HG22	1.88	0.56
1:F:282:GLY:HA3	1:F:433:LEU:HD12	1.89	0.55
1:C:282:GLY:HA3	1:C:433:LEU:HD12	1.88	0.55
1:F:151:GLY:HA3	1:F:185:ALA:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLY:HA3	1:A:433:LEU:HD12	1.88	0.54
1:C:74:GLU:HG3	1:C:113:LYS:HE3	1.89	0.54
1:C:151:GLY:HA3	1:C:185:ALA:O	2.06	0.54
1:D:173:TYR:O	1:D:177:VAL:HG13	2.06	0.54
1:D:151:GLY:HA3	1:D:185:ALA:O	2.07	0.54
1:D:282:GLY:HA3	1:D:433:LEU:HD12	1.89	0.54
1:B:282:GLY:HA3	1:B:433:LEU:HD12	1.89	0.54
1:B:391:LEU:HB2	1:B:412:THR:HG22	1.89	0.54
1:F:391:LEU:HB2	1:F:412:THR:HG22	1.90	0.53
1:A:117:HIS:HD2	1:E:121:LEU:CD2	2.22	0.53
1:B:121:LEU:CD2	1:D:117:HIS:HD2	2.22	0.52
1:D:383:ILE:HG12	1:D:405:ALA:HB3	1.92	0.51
1:E:338:GLY:HA3	1:E:362:LEU:HD11	1.93	0.51
1:C:117:HIS:HD2	1:F:121:LEU:CD2	2.23	0.51
1:A:477:LEU:HD21	1:C:477:LEU:HD13	1.92	0.51
1:D:74:GLU:HG3	1:D:113:LYS:HE3	1.93	0.51
1:E:391:LEU:HD12	1:E:412:THR:HG22	1.91	0.51
1:A:293:MET:HE1	1:A:403:ILE:HD11	1.92	0.51
1:E:139:ARG:HH11	1:E:187:ALA:HB2	1.76	0.50
1:A:117:HIS:CD2	1:E:121:LEU:CD2	2.95	0.49
1:D:173:TYR:HB2	1:D:431:LEU:HD11	1.95	0.49
1:E:273:SER:O	1:E:277:ARG:HG3	2.12	0.49
1:C:161:VAL:HG12	1:C:165:LYS:HE2	1.95	0.49
1:D:384:PRO:HD2	1:D:405:ALA:O	2.13	0.49
1:C:332:ALA:HB2	1:C:341:TRP:HD1	1.78	0.49
1:C:139:ARG:HH11	1:C:187:ALA:HB2	1.77	0.49
1:E:63:ARG:HB2	1:E:388:GLU:HA	1.94	0.49
1:F:161:VAL:HG12	1:F:165:LYS:HE2	1.95	0.48
1:A:472:SER:HA	1:C:493:THR:HG23	1.95	0.48
1:C:121:LEU:CD2	1:F:117:HIS:HD2	2.26	0.48
1:D:268:ILE:CG1	1:D:444:GLU:HB2	2.43	0.48
1:E:74:GLU:HG3	1:E:113:LYS:HE3	1.94	0.48
1:B:332:ALA:HB2	1:B:341:TRP:HD1	1.79	0.48
1:D:431:LEU:HD23	1:D:541:ALA:HB1	1.95	0.48
1:F:268:ILE:CG1	1:F:444:GLU:HB2	2.44	0.48
1:B:121:LEU:CD2	1:D:117:HIS:CD2	2.96	0.48
1:A:268:ILE:CG1	1:A:444:GLU:HB2	2.43	0.48
1:F:338:GLY:HA3	1:F:362:LEU:HD11	1.95	0.48
1:A:121:LEU:CD2	1:E:117:HIS:HD2	2.27	0.48
1:C:331:VAL:HG13	1:C:343:PRO:HA	1.96	0.47
1:D:268:ILE:HG13	1:D:444:GLU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HB2	1:A:412:THR:HG22	1.97	0.47
1:E:161:VAL:HG12	1:E:165:LYS:HE2	1.97	0.47
1:E:332:ALA:HB2	1:E:341:TRP:HD1	1.79	0.47
1:A:338:GLY:HA3	1:A:362:LEU:HD11	1.97	0.47
1:D:161:VAL:HG12	1:D:165:LYS:HE2	1.95	0.47
1:B:117:HIS:HD2	1:D:121:LEU:CD2	2.26	0.47
1:C:268:ILE:CG1	1:C:444:GLU:HB2	2.45	0.47
1:D:332:ALA:HB2	1:D:341:TRP:HD1	1.78	0.47
1:A:268:ILE:HG13	1:A:444:GLU:HB2	1.97	0.47
1:D:331:VAL:HG13	1:D:343:PRO:HA	1.97	0.47
1:B:268:ILE:CG1	1:B:444:GLU:HB2	2.44	0.47
1:C:117:HIS:CD2	1:F:121:LEU:CD2	2.97	0.47
1:C:338:GLY:HA3	1:C:362:LEU:HD11	1.96	0.47
1:D:338:GLY:HA3	1:D:362:LEU:HD11	1.97	0.47
2:E:602:ADP:O1A	1:F:447:LYS:NZ	2.46	0.47
1:A:121:LEU:CD2	1:E:117:HIS:CD2	2.98	0.46
1:A:391:LEU:HD13	1:A:412:THR:HG22	1.98	0.46
1:C:121:LEU:CD2	1:F:117:HIS:CD2	2.98	0.46
1:E:268:ILE:CG1	1:E:444:GLU:HB2	2.45	0.46
1:F:149:CYS:HB3	1:F:185:ALA:HB2	1.98	0.46
1:D:391:LEU:HB2	1:D:412:THR:HG22	1.97	0.46
1:A:142:HIS:CG	1:A:169:SER:HA	2.51	0.46
1:C:268:ILE:HG13	1:C:444:GLU:HB2	1.98	0.46
1:A:332:ALA:HB2	1:A:341:TRP:HD1	1.80	0.46
1:E:477:LEU:HD13	1:F:477:LEU:HD21	1.98	0.46
1:F:471:MET:HE3	1:F:475:GLU:HG3	1.98	0.46
1:B:280:PHE:HD1	1:B:323:LEU:HD23	1.81	0.46
1:B:331:VAL:HG13	1:B:343:PRO:HA	1.97	0.46
1:A:310:GLN:HB3	1:A:384:PRO:HA	1.97	0.46
1:B:117:HIS:CD2	1:D:121:LEU:CD2	2.98	0.46
1:D:332:ALA:HB1	1:D:374:ILE:HD11	1.98	0.46
1:F:393:LYS:O	1:F:393:LYS:HG2	2.15	0.46
1:B:268:ILE:HG13	1:B:444:GLU:HB2	1.98	0.45
1:E:280:PHE:HD1	1:E:323:LEU:HD23	1.81	0.45
1:F:280:PHE:HD1	1:F:323:LEU:HD23	1.81	0.45
1:F:423:ARG:HE	1:F:425:ILE:CD1	2.29	0.45
1:B:493:THR:HG23	1:C:472:SER:HA	1.97	0.45
1:F:268:ILE:HG13	1:F:444:GLU:HB2	1.97	0.45
1:B:149:CYS:HB3	1:B:185:ALA:HB2	1.98	0.45
1:E:149:CYS:HB3	1:E:185:ALA:HB2	1.98	0.45
1:F:388:GLU:HB2	1:F:390:GLN:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:HG12	1:F:124:PRO:HB3	1.96	0.45
1:C:332:ALA:HB1	1:C:374:ILE:HD11	1.99	0.45
1:F:268:ILE:HD12	1:F:271:ARG:HB2	1.99	0.45
1:A:331:VAL:HG13	1:A:343:PRO:HA	1.98	0.45
1:C:280:PHE:HD1	1:C:323:LEU:HD23	1.81	0.45
1:A:149:CYS:HB3	1:A:185:ALA:HB2	1.99	0.45
1:B:111:ILE:HG12	1:D:124:PRO:HB3	1.97	0.45
1:B:338:GLY:HA3	1:B:362:LEU:HD11	1.98	0.45
1:D:81:ALA:HB1	1:D:109:LEU:HD13	1.99	0.45
1:D:280:PHE:HD1	1:D:323:LEU:HD23	1.82	0.45
1:E:108:ILE:O	1:E:112:ILE:HG13	2.17	0.45
1:F:429:PRO:HG3	1:F:538:ARG:HA	1.99	0.45
1:C:149:CYS:HB3	1:C:185:ALA:HB2	1.99	0.45
1:D:149:CYS:HB3	1:D:185:ALA:HB2	1.99	0.45
1:F:399:VAL:O	1:F:423:ARG:NH2	2.50	0.45
1:A:280:PHE:HD1	1:A:323:LEU:HD23	1.81	0.44
1:A:384:PRO:HD2	1:A:405:ALA:O	2.16	0.44
1:E:268:ILE:HG13	1:E:444:GLU:HB2	1.99	0.44
1:F:125:ILE:HD13	1:F:125:ILE:HA	1.87	0.44
1:E:493:THR:HG23	1:F:472:SER:HA	1.99	0.44
1:D:268:ILE:HD12	1:D:271:ARG:HB2	1.99	0.44
1:B:391:LEU:HD12	1:B:412:THR:HG22	1.99	0.44
1:E:429:PRO:HG3	1:E:538:ARG:HA	2.00	0.44
1:A:161:VAL:HG12	1:A:165:LYS:HE2	1.98	0.44
1:A:232:GLY:O	1:A:236:MET:HG2	2.18	0.44
1:A:268:ILE:HD12	1:A:271:ARG:HB2	1.99	0.44
1:B:173:TYR:HB2	1:B:431:LEU:HD11	1.98	0.44
1:A:124:PRO:HB3	1:E:111:ILE:HG12	1.99	0.44
1:C:124:PRO:HB3	1:F:111:ILE:HG12	2.00	0.44
1:C:268:ILE:HD12	1:C:271:ARG:HB2	2.00	0.44
1:B:74:GLU:HG3	1:B:113:LYS:HE3	2.00	0.43
1:D:429:PRO:HG3	1:D:538:ARG:HA	2.00	0.43
1:E:268:ILE:HD12	1:E:271:ARG:HB2	2.00	0.43
1:B:268:ILE:HD12	1:B:271:ARG:HB2	2.00	0.43
1:C:153:ILE:HG12	1:C:187:ALA:HB3	2.00	0.43
1:C:429:PRO:HG3	1:C:538:ARG:HA	2.00	0.43
1:F:310:GLN:HB2	1:F:374:ILE:HG22	2.00	0.43
1:B:161:VAL:HG12	1:B:165:LYS:HE2	1.99	0.43
1:F:332:ALA:HB1	1:F:374:ILE:HD11	2.00	0.43
1:F:153:ILE:HG12	1:F:187:ALA:HB3	2.00	0.43
1:A:213:ALA:HA	1:A:218:ILE:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ARG:HB2	1:F:388:GLU:HA	2.01	0.43
1:A:429:PRO:HG3	1:A:538:ARG:HA	1.99	0.43
1:B:429:PRO:HG3	1:B:538:ARG:HA	2.00	0.43
1:B:332:ALA:HB1	1:B:374:ILE:HD11	2.00	0.43
1:F:268:ILE:HG13	1:F:268:ILE:H	1.71	0.43
1:E:477:LEU:HD22	1:E:481:PHE:HE2	1.84	0.43
1:B:77:PHE:CE2	1:B:113:LYS:HB2	2.54	0.42
1:E:173:TYR:O	1:E:177:VAL:HG13	2.19	0.42
1:F:388:GLU:O	1:F:411:PRO:HA	2.19	0.42
1:F:139:ARG:HH11	1:F:187:ALA:HB2	1.83	0.42
1:F:234:ARG:HH11	1:F:238:TRP:HH2	1.65	0.42
1:A:115:CYS:HA	1:A:142:HIS:HA	2.01	0.42
1:B:125:ILE:HD13	1:B:125:ILE:HA	1.88	0.42
1:B:72:MET:HE3	1:B:414:PRO:HD3	2.01	0.42
1:B:139:ARG:HH11	1:B:187:ALA:HB2	1.85	0.42
1:B:526:ARG:HA	1:B:529:MET:HE2	2.02	0.42
1:F:213:ALA:HA	1:F:218:ILE:HG22	2.01	0.42
1:A:234:ARG:HH11	1:A:238:TRP:HH2	1.66	0.41
1:C:202:GLU:O	1:C:206:ARG:HG3	2.19	0.41
1:D:399:VAL:O	1:D:423:ARG:NH2	2.52	0.41
1:B:399:VAL:O	1:B:423:ARG:NH2	2.53	0.41
1:D:125:ILE:HD13	1:D:125:ILE:HA	1.89	0.41
1:D:153:ILE:HG12	1:D:187:ALA:HB3	2.02	0.41
1:E:67:PRO:HA	1:E:70:PHE:CD2	2.55	0.41
1:B:153:ILE:HG12	1:B:187:ALA:HB3	2.02	0.41
1:E:151:GLY:O	1:E:225:PRO:HA	2.21	0.41
1:A:153:ILE:HG12	1:A:187:ALA:HB3	2.02	0.41
1:D:142:HIS:CG	1:D:169:SER:HA	2.55	0.41
1:A:74:GLU:HG3	1:A:113:LYS:HE3	2.02	0.41
1:D:477:LEU:HD21	1:F:477:LEU:HD13	2.02	0.41
1:E:399:VAL:O	1:E:423:ARG:NH2	2.52	0.41
1:B:213:ALA:CA	1:B:218:ILE:HG22	2.51	0.41
1:E:153:ILE:HG12	1:E:187:ALA:HB3	2.02	0.41
1:C:125:ILE:HD13	1:C:125:ILE:HA	1.88	0.41
1:D:364:PHE:HA	1:D:365:PRO:HD3	1.97	0.41
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.88	0.41
1:D:472:SER:HA	1:F:493:THR:HG23	2.03	0.41
1:E:293:MET:HE1	1:E:403:ILE:HD11	2.03	0.41
1:E:332:ALA:HB1	1:E:374:ILE:CG1	2.51	0.41
1:B:477:LEU:HD13	1:C:477:LEU:HD21	2.02	0.41
1:F:332:ALA:HB2	1:F:341:TRP:CD1	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ALA:CA	1:D:218:ILE:HG22	2.52	0.40
1:B:384:PRO:HD2	1:B:405:ALA:O	2.21	0.40
1:F:142:HIS:CG	1:F:169:SER:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/561 (88%)	482 (98%)	12 (2%)	0	100	100
1	B	495/561 (88%)	482 (97%)	13 (3%)	0	100	100
1	C	492/561 (88%)	480 (98%)	12 (2%)	0	100	100
1	D	495/561 (88%)	484 (98%)	10 (2%)	1 (0%)	43	53
1	E	497/561 (89%)	481 (97%)	15 (3%)	1 (0%)	43	53
1	F	497/561 (89%)	484 (97%)	13 (3%)	0	100	100
All	All	2970/3366 (88%)	2893 (97%)	75 (2%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	387	SER
1	E	482	GLY

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	398/455 (88%)	386 (97%)	12 (3%)	36	48
1	B	398/455 (88%)	385 (97%)	13 (3%)	33	45
1	C	396/455 (87%)	383 (97%)	13 (3%)	33	45
1	D	398/455 (88%)	385 (97%)	13 (3%)	33	45
1	E	405/455 (89%)	389 (96%)	16 (4%)	28	39
1	F	403/455 (89%)	392 (97%)	11 (3%)	39	52
All	All	2398/2730 (88%)	2320 (97%)	78 (3%)	34	45

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ILE
1	A	164	VAL
1	A	177	VAL
1	A	186	LYS
1	A	191	ILE
1	A	235	GLU
1	A	268	ILE
1	A	287	ILE
1	A	340	ILE
1	A	440	VAL
1	A	457	LEU
1	A	511	SER
1	B	99	GLU
1	B	125	ILE
1	B	164	VAL
1	B	177	VAL
1	B	186	LYS
1	B	191	ILE
1	B	268	ILE
1	B	287	ILE
1	B	340	ILE
1	B	374	ILE
1	B	440	VAL
1	B	457	LEU
1	B	511	SER
1	C	70	PHE
1	C	125	ILE
1	C	164	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	177	VAL
1	C	186	LYS
1	C	191	ILE
1	C	231	THR
1	C	268	ILE
1	C	287	ILE
1	C	340	ILE
1	C	374	ILE
1	C	440	VAL
1	C	457	LEU
1	D	68	ASN
1	D	125	ILE
1	D	164	VAL
1	D	177	VAL
1	D	186	LYS
1	D	191	ILE
1	D	235	GLU
1	D	268	ILE
1	D	287	ILE
1	D	340	ILE
1	D	374	ILE
1	D	440	VAL
1	D	457	LEU
1	E	125	ILE
1	E	164	VAL
1	E	177	VAL
1	E	186	LYS
1	E	191	ILE
1	E	228	ASP
1	E	268	ILE
1	E	287	ILE
1	E	340	ILE
1	E	374	ILE
1	E	390	GLN
1	E	440	VAL
1	E	457	LEU
1	E	481	PHE
1	E	506	LYS
1	E	511	SER
1	F	125	ILE
1	F	164	VAL
1	F	177	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	186	LYS
1	F	191	ILE
1	F	268	ILE
1	F	287	ILE
1	F	340	ILE
1	F	374	ILE
1	F	440	VAL
1	F	511	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	310	GLN
1	A	314	ASN
1	A	434	ASN
1	A	554	ASN
1	B	192	ASN
1	B	249	HIS
1	B	310	GLN
1	B	314	ASN
1	B	358	HIS
1	B	510	HIS
1	C	192	ASN
1	C	314	ASN
1	C	358	HIS
1	D	192	ASN
1	D	249	HIS
1	D	310	GLN
1	D	314	ASN
1	D	358	HIS
1	D	510	HIS
1	E	314	ASN
1	E	554	ASN
1	F	68	ASN
1	F	192	ASN
1	F	249	HIS
1	F	314	ASN
1	F	358	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	D	602	-	28,29,29	0.42	0	43,45,45	0.46	0
2	ADP	B	601	-	28,29,29	0.41	0	43,45,45	0.46	0
4	LEU	A	604	-	6,8,8	0.82	0	5,10,10	0.31	0
2	ADP	F	601	-	28,29,29	0.41	0	43,45,45	0.48	0
4	LEU	A	603	-	6,8,8	0.84	0	5,10,10	0.39	0
4	LEU	B	603	-	6,8,8	0.81	0	5,10,10	0.36	0
2	ADP	C	601	-	28,29,29	0.42	0	43,45,45	0.47	0
4	LEU	D	601	-	6,8,8	0.84	0	5,10,10	0.37	0
4	LEU	C	603	-	6,8,8	0.79	0	5,10,10	0.31	0
4	LEU	E	601	-	6,8,8	0.84	0	5,10,10	0.37	0
2	ADP	E	602	-	28,29,29	0.40	0	43,45,45	0.47	0
2	ADP	A	601	-	28,29,29	0.41	0	43,45,45	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	D	602	-	-	8/16/32/32	0/3/3/3
2	ADP	B	601	-	-	6/16/32/32	0/3/3/3
4	LEU	A	604	-	-	0/8/8/8	-
2	ADP	F	601	-	-	7/16/32/32	0/3/3/3
4	LEU	A	603	-	-	1/8/8/8	-
4	LEU	B	603	-	-	0/8/8/8	-
2	ADP	C	601	-	-	6/16/32/32	0/3/3/3
4	LEU	D	601	-	-	1/8/8/8	-
4	LEU	C	603	-	-	0/8/8/8	-
4	LEU	E	601	-	-	1/8/8/8	-
2	ADP	E	602	-	-	8/16/32/32	0/3/3/3
2	ADP	A	601	-	-	7/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	PA-O3A-PB-O3B
2	A	601	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	C5'-O5'-PA-O3A
2	C	601	ADP	PA-O3A-PB-O3B
2	C	601	ADP	C5'-O5'-PA-O2A
2	C	601	ADP	C5'-O5'-PA-O3A
2	D	602	ADP	PA-O3A-PB-O2B
2	D	602	ADP	PA-O3A-PB-O3B
2	D	602	ADP	C5'-O5'-PA-O1A
2	D	602	ADP	C5'-O5'-PA-O3A
2	E	602	ADP	PA-O3A-PB-O3B
2	E	602	ADP	C5'-O5'-PA-O1A
2	E	602	ADP	C5'-O5'-PA-O3A
2	F	601	ADP	PA-O3A-PB-O2B
2	F	601	ADP	PA-O3A-PB-O3B
2	F	601	ADP	C5'-O5'-PA-O1A
2	F	601	ADP	C5'-O5'-PA-O3A
2	A	601	ADP	C2'-C1'-N9-C8
2	D	602	ADP	C2'-C1'-N9-C8
2	B	601	ADP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	601	ADP	C2'-C1'-N9-C8
2	E	602	ADP	C2'-C1'-N9-C8
2	F	601	ADP	C2'-C1'-N9-C8
2	A	601	ADP	C5'-O5'-PA-O1A
2	A	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	C	601	ADP	C5'-O5'-PA-O1A
2	D	602	ADP	C5'-O5'-PA-O2A
2	E	602	ADP	C5'-O5'-PA-O2A
2	E	602	ADP	PA-O3A-PB-O1B
4	A	603	LEU	O-C-CA-N
4	D	601	LEU	O-C-CA-N
4	E	601	LEU	O-C-CA-N
2	B	601	ADP	O4'-C1'-N9-C8
2	F	601	ADP	O4'-C1'-N9-C8
2	E	602	ADP	PB-O3A-PA-O1A
2	F	601	ADP	PB-O3A-PA-O1A
2	E	602	ADP	O4'-C1'-N9-C8
2	A	601	ADP	O4'-C1'-N9-C8
2	C	601	ADP	O4'-C1'-N9-C8
2	D	602	ADP	O4'-C1'-N9-C8
2	A	601	ADP	PB-O3A-PA-O2A
2	D	602	ADP	PB-O3A-PA-O1A

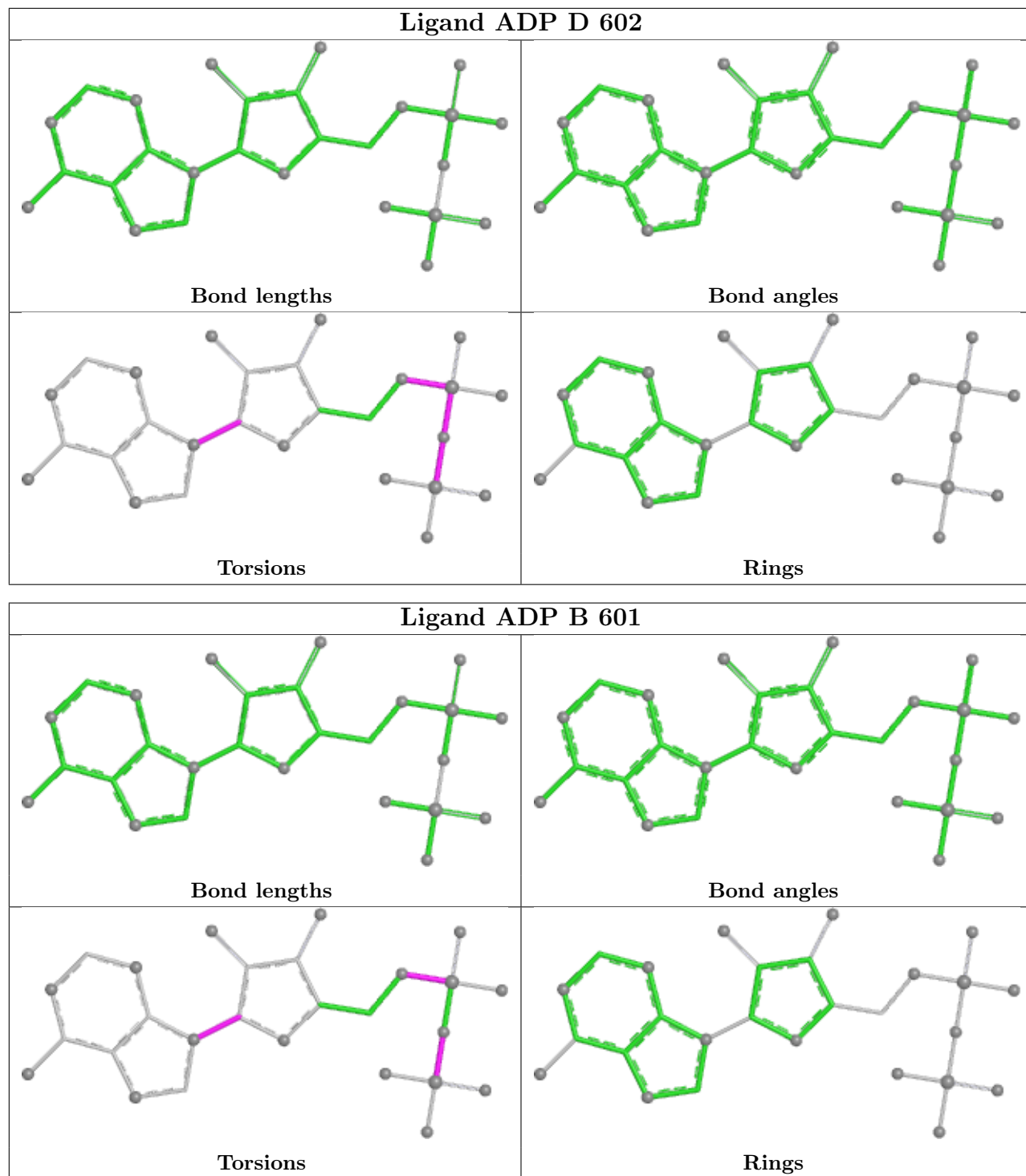
There are no ring outliers.

1 monomer is involved in 1 short contact:

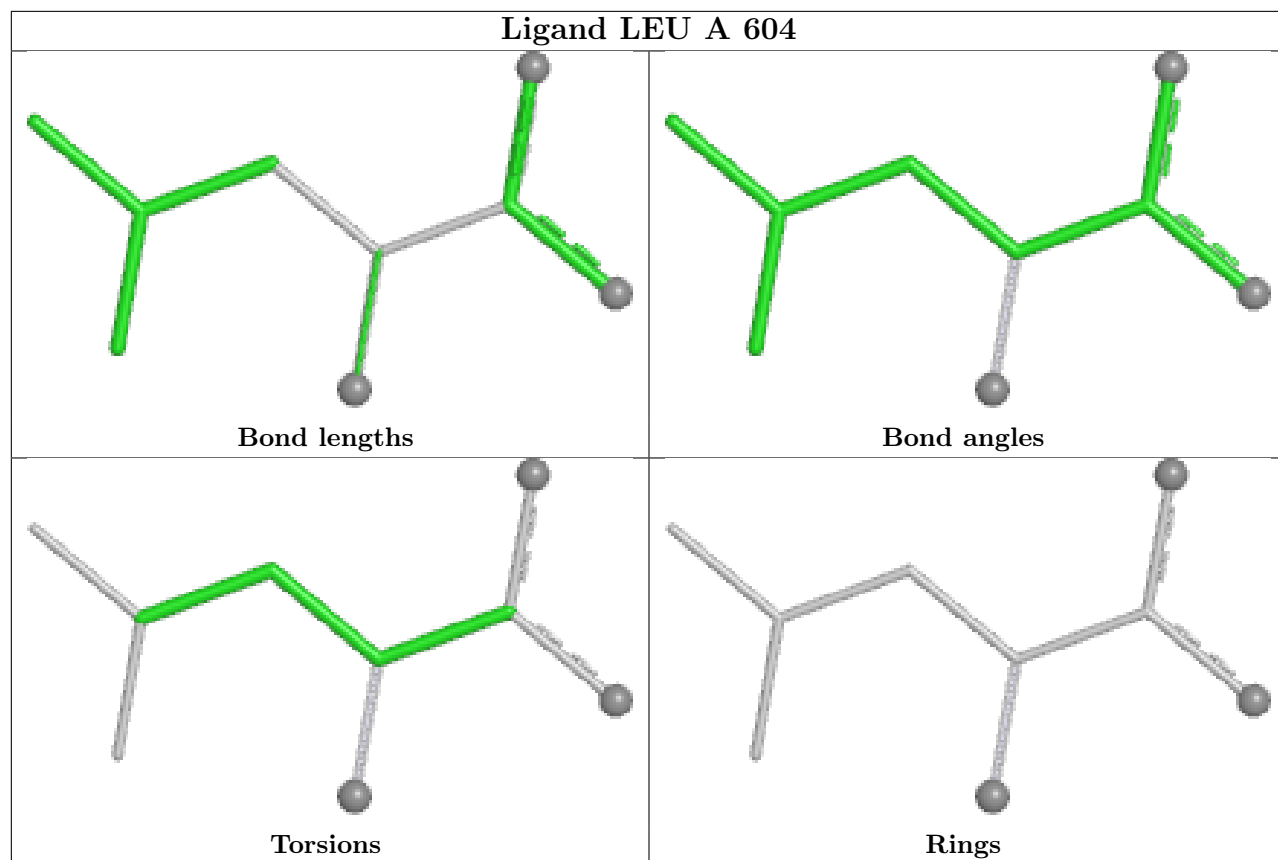
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	602	ADP	1	0

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

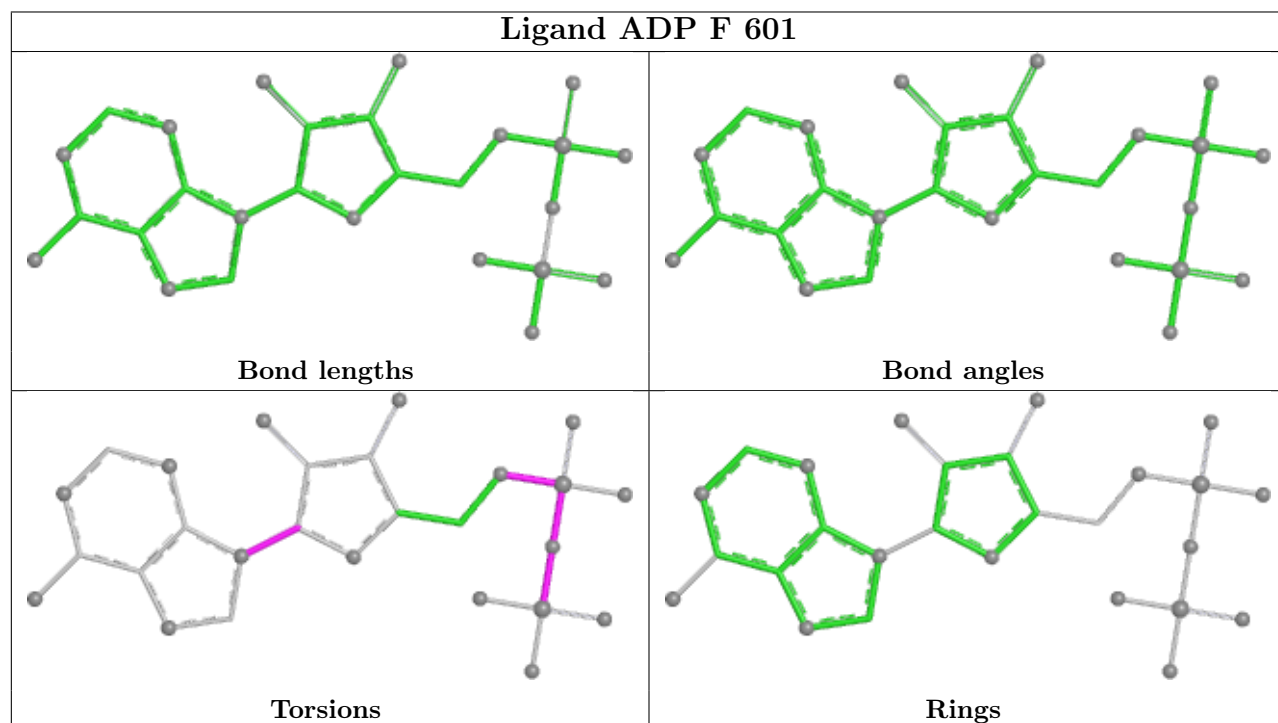
equivalents in the CSD to analyse the geometry.



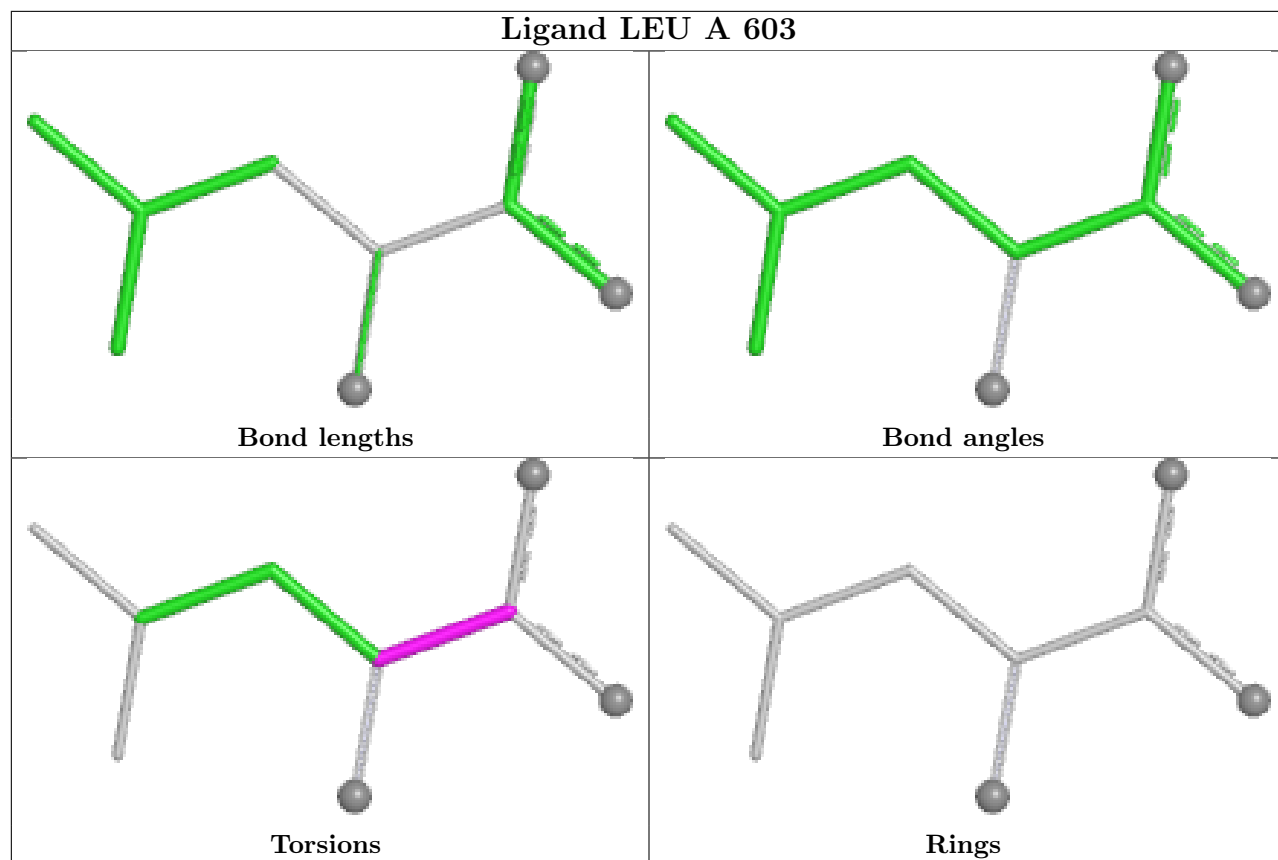
Ligand LEU A 604



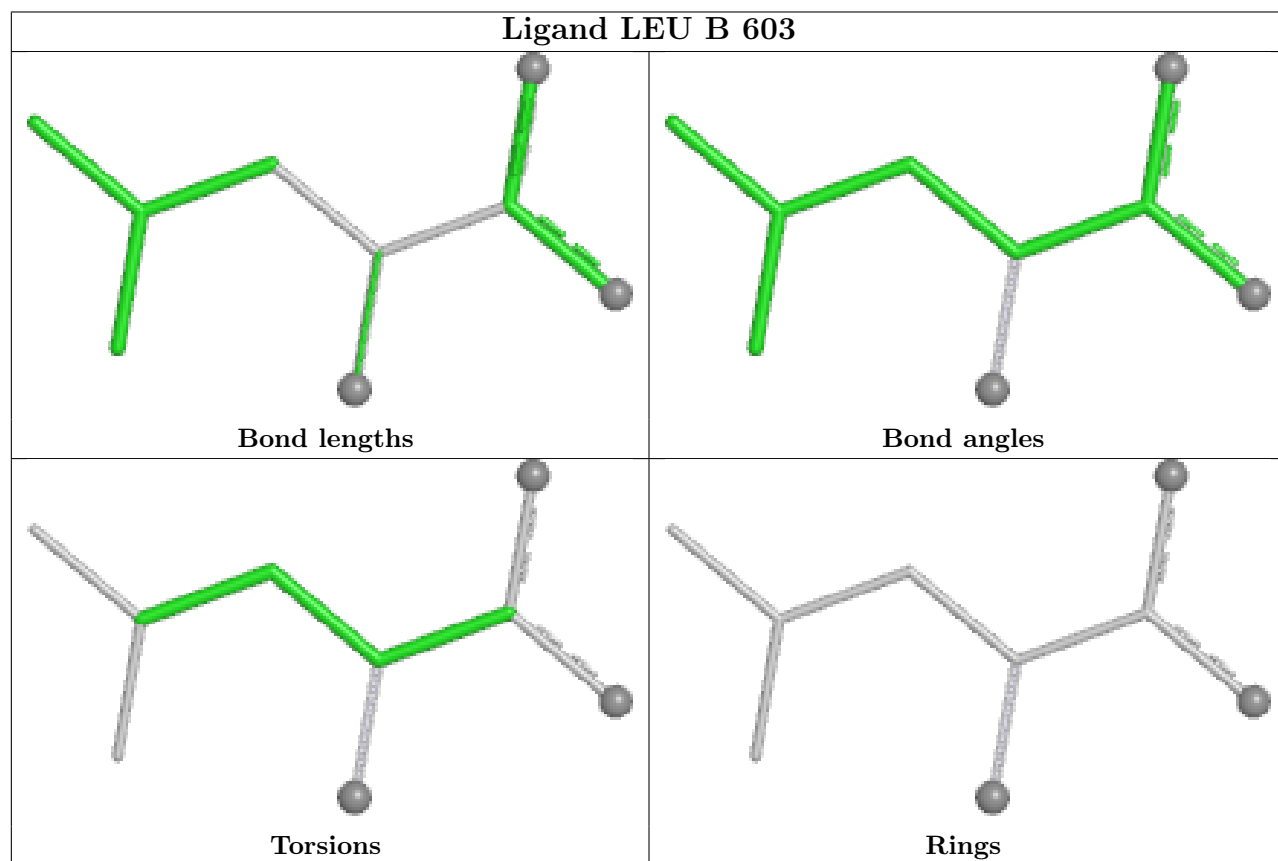
Ligand ADP F 601

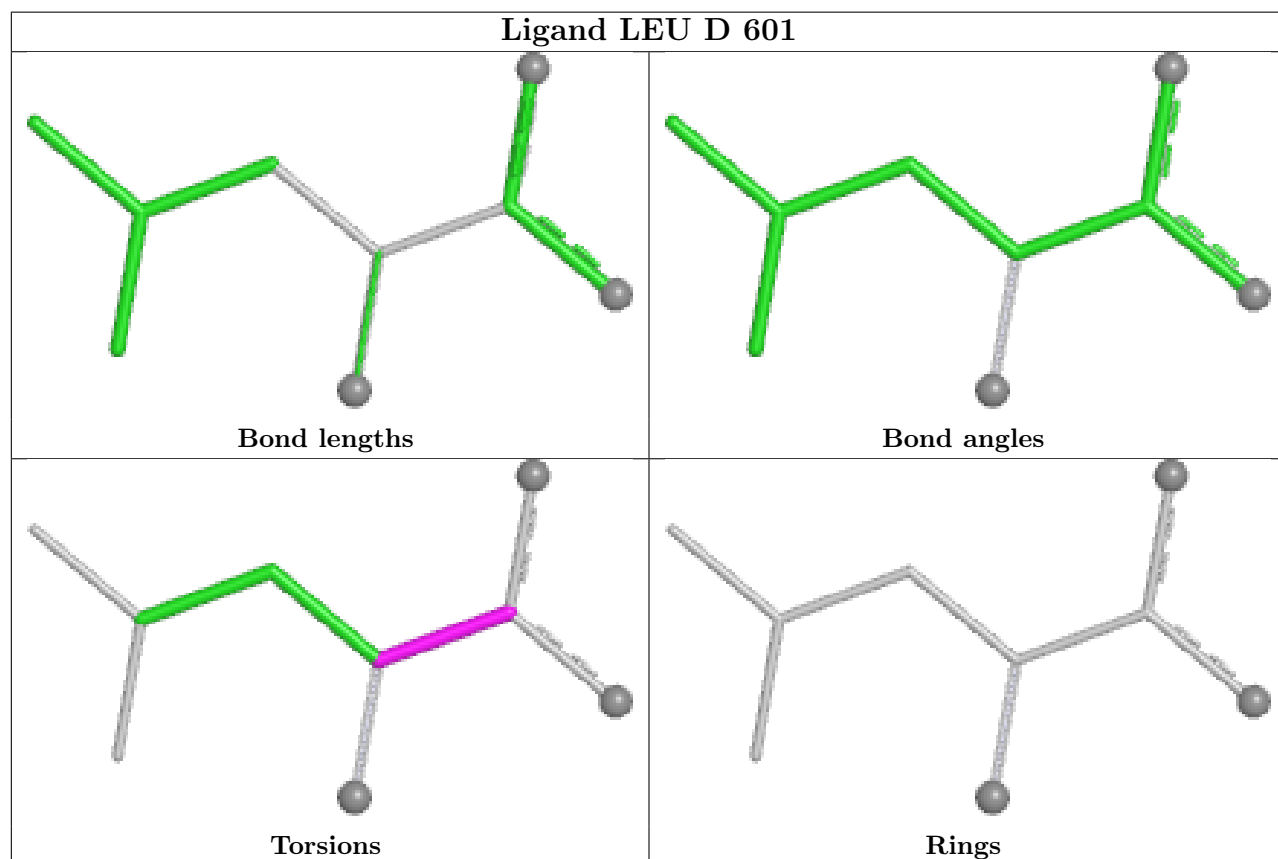
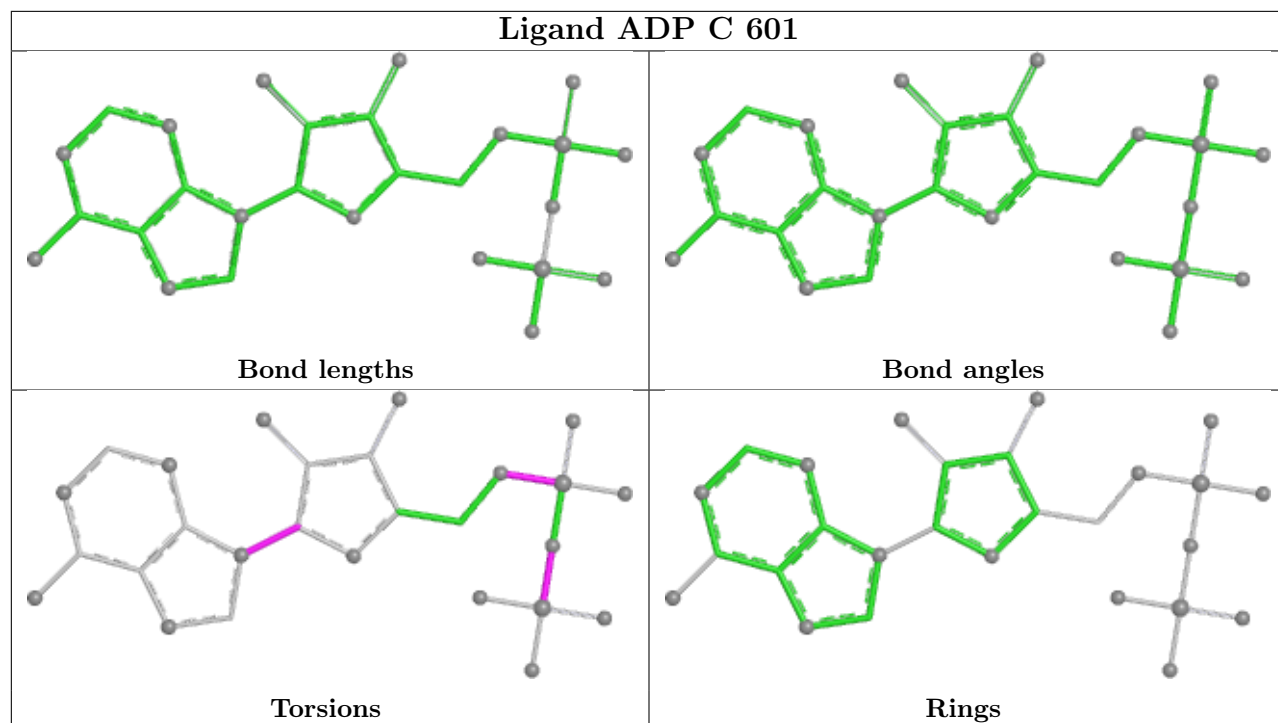


Ligand LEU A 603

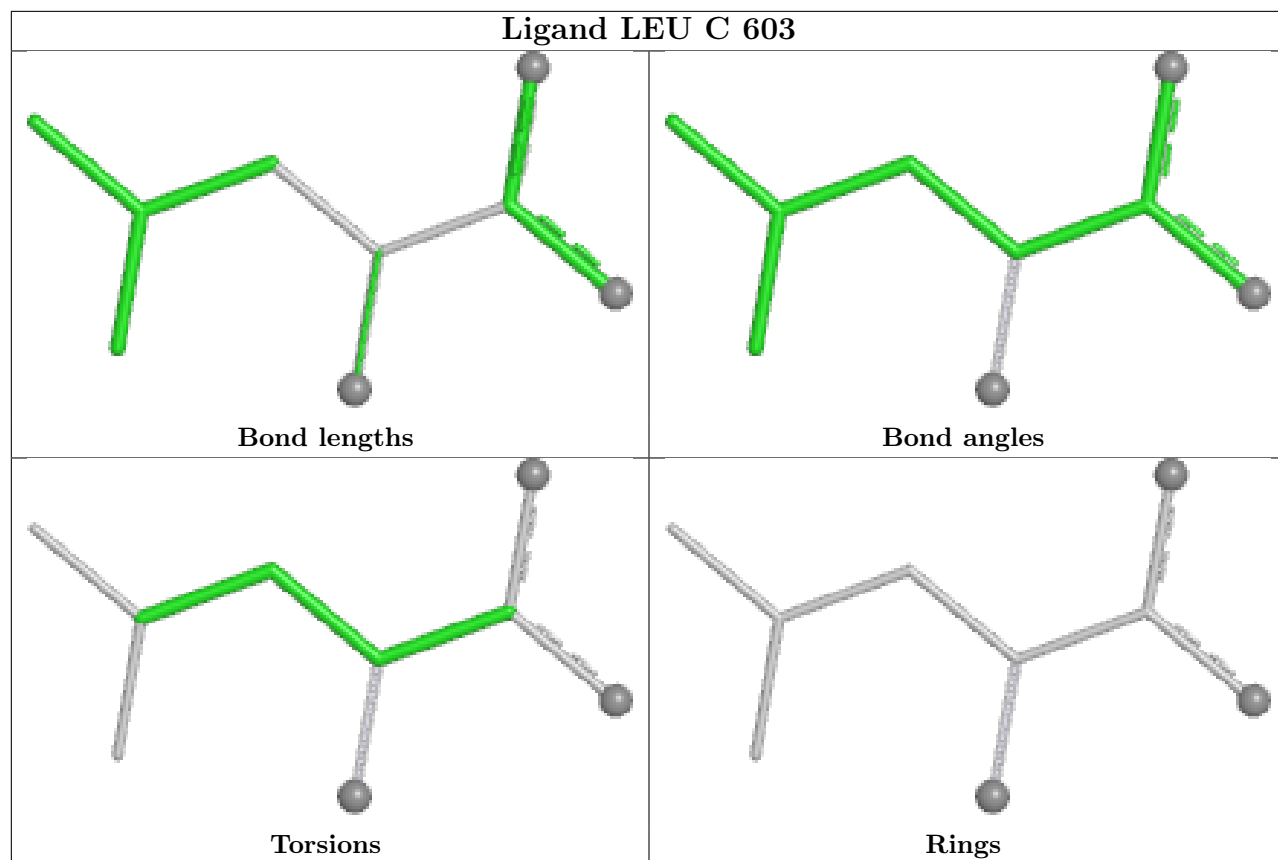


Ligand LEU B 603

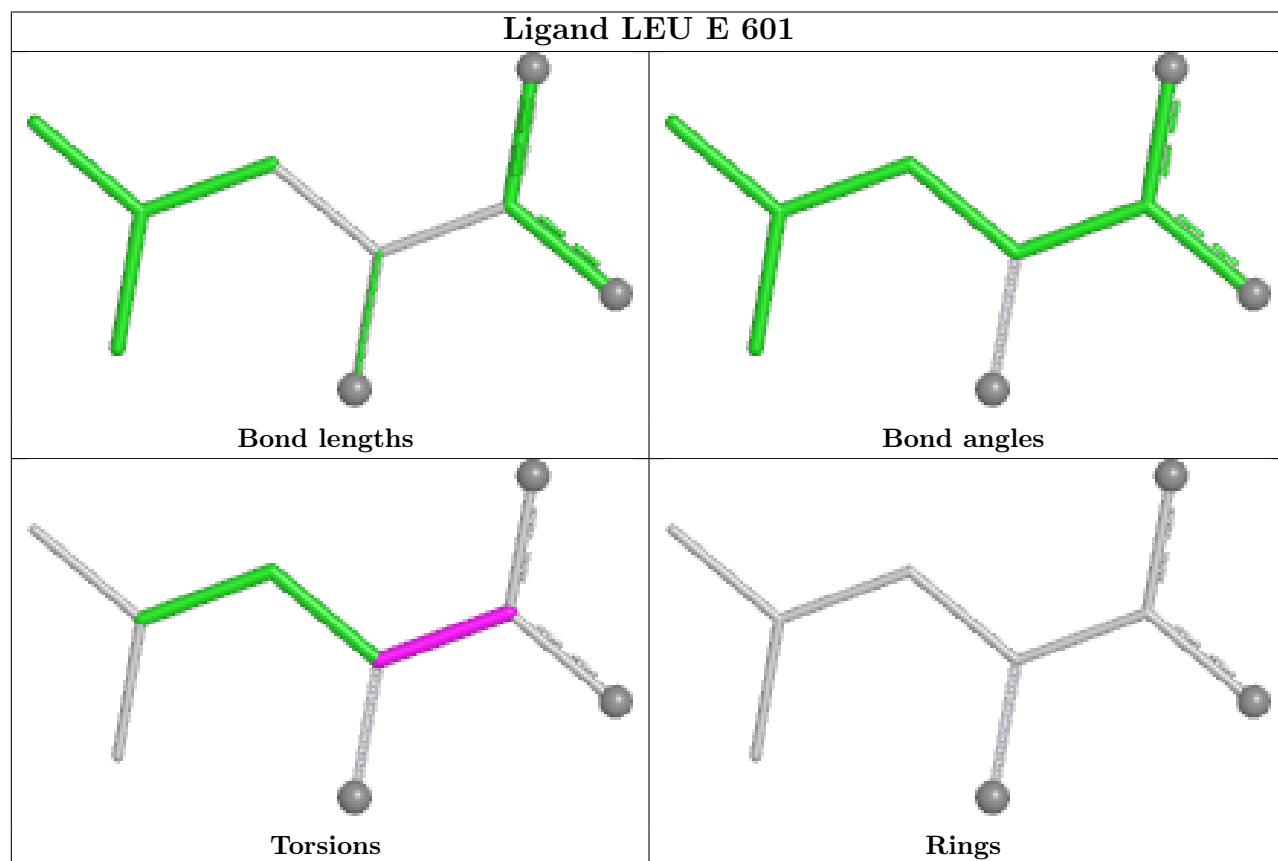


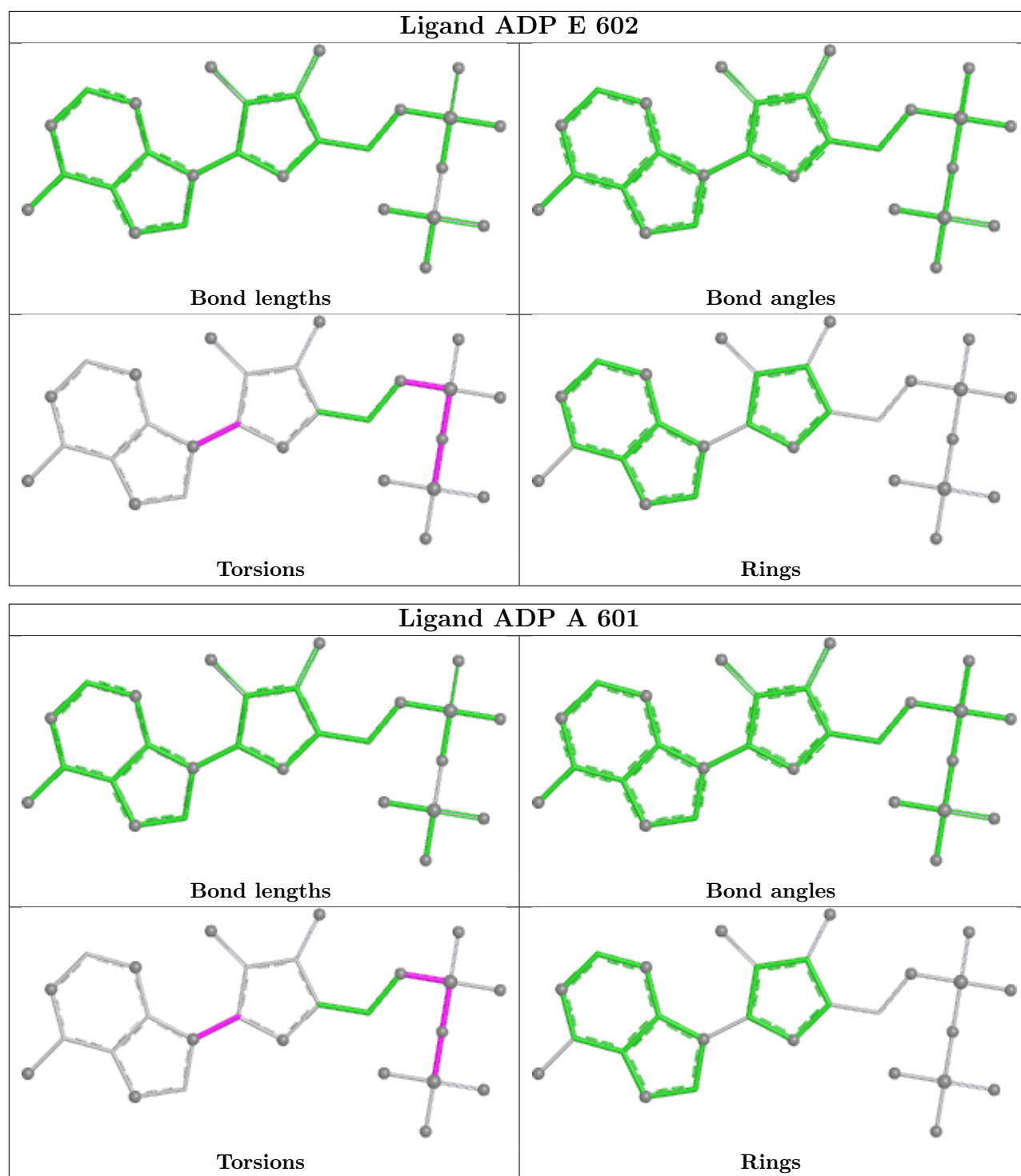


Ligand LEU C 603



Ligand LEU E 601





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	496/561 (88%)	0.48	30 (6%) 27 24	37, 66, 151, 169	0
1	B	497/561 (88%)	0.22	19 (3%) 44 42	37, 68, 120, 141	0
1	C	494/561 (88%)	0.40	26 (5%) 32 29	35, 64, 121, 137	0
1	D	497/561 (88%)	0.42	29 (5%) 29 25	38, 67, 119, 134	0
1	E	499/561 (88%)	0.15	8 (1%) 70 72	33, 58, 87, 101	0
1	F	499/561 (88%)	-0.01	5 (1%) 79 81	34, 58, 97, 132	0
All	All	2982/3366 (88%)	0.27	117 (3%) 43 40	33, 63, 120, 169	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	64	GLU	4.2
1	A	387	SER	3.7
1	C	387	SER	3.7
1	D	136	GLU	3.5
1	F	92	LEU	3.4
1	C	369	ILE	3.4
1	C	93	LYS	3.4
1	B	387	SER	3.4
1	A	250	TYR	3.2
1	D	557	GLY	3.2
1	A	81	ALA	3.1
1	A	105	VAL	3.1
1	D	210	MET	3.1
1	A	369	ILE	3.1
1	A	362	LEU	3.0
1	B	66	ASP	3.0
1	A	372	GLY	3.0
1	C	67	PRO	2.9
1	D	560	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	390	GLN	2.9
1	A	368	LYS	2.9
1	C	375	LEU	2.9
1	C	70	PHE	2.9
1	B	70	PHE	2.8
1	B	560	PHE	2.8
1	C	560	PHE	2.8
1	B	369	ILE	2.8
1	D	368	LYS	2.8
1	E	560	PHE	2.8
1	C	250	TYR	2.7
1	E	484	HIS	2.7
1	A	361	ILE	2.7
1	B	388	GLU	2.7
1	B	65	ASP	2.7
1	C	210	MET	2.7
1	B	64	GLU	2.7
1	D	250	TYR	2.7
1	C	91	ASP	2.6
1	E	372	GLY	2.6
1	A	341	TRP	2.6
1	A	104	ARG	2.6
1	D	122	SER	2.6
1	A	557	GLY	2.5
1	C	361	ILE	2.5
1	A	375	LEU	2.5
1	B	531	TYR	2.5
1	D	68	ASN	2.5
1	A	304	ASP	2.5
1	A	356	LEU	2.5
1	F	387	SER	2.5
1	D	485	GLY	2.4
1	C	104	ARG	2.4
1	C	246	THR	2.4
1	D	93	LYS	2.4
1	D	369	ILE	2.4
1	D	138	TYR	2.4
1	A	364	PHE	2.4
1	C	388	GLU	2.4
1	A	484	HIS	2.4
1	D	121	LEU	2.4
1	B	69	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	374	ILE	2.3
1	A	162	ASP	2.3
1	B	304	ASP	2.3
1	A	550	PHE	2.3
1	D	94	THR	2.3
1	D	88	LEU	2.3
1	B	158	ASP	2.3
1	B	415	GLU	2.3
1	D	234	ARG	2.3
1	C	247	ILE	2.3
1	C	340	ILE	2.3
1	F	560	PHE	2.3
1	D	386	ALA	2.3
1	E	373	SER	2.3
1	E	340	ILE	2.3
1	B	67	PRO	2.3
1	D	559	THR	2.2
1	D	484	HIS	2.2
1	C	92	LEU	2.2
1	D	390	GLN	2.2
1	E	483	LYS	2.2
1	B	386	ALA	2.2
1	C	389	LYS	2.2
1	E	125	ILE	2.2
1	A	373	SER	2.2
1	D	387	SER	2.2
1	B	390	GLN	2.2
1	B	94	THR	2.2
1	A	121	LEU	2.2
1	A	374	ILE	2.2
1	C	228	ASP	2.2
1	D	96	GLU	2.2
1	D	133	GLU	2.2
1	C	351	LEU	2.1
1	F	484	HIS	2.1
1	B	340	ILE	2.1
1	A	154	ARG	2.1
1	D	95	ARG	2.1
1	C	270	GLY	2.1
1	E	482	GLY	2.1
1	A	133	GLU	2.1
1	A	136	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	371	GLU	2.1
1	D	361	ILE	2.1
1	A	531	TYR	2.1
1	A	66	ASP	2.1
1	C	471	MET	2.1
1	A	69	PHE	2.1
1	C	481	PHE	2.1
1	C	558	VAL	2.1
1	C	486	GLY	2.1
1	C	368	LYS	2.0
1	A	86	ASP	2.0
1	D	70	PHE	2.0
1	D	125	ILE	2.0
1	F	373	SER	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	LEU	E	601	9/9	0.90	0.15	58,59,61,61	0
4	LEU	D	601	9/9	0.91	0.16	61,63,63,64	0
4	LEU	C	603	9/9	0.93	0.11	52,54,55,55	0
4	LEU	A	604	9/9	0.93	0.13	59,60,61,62	0
4	LEU	B	603	9/9	0.93	0.14	65,67,68,69	0
4	LEU	A	603	9/9	0.94	0.11	56,57,58,59	0
2	ADP	A	601	27/27	0.95	0.09	65,68,70,70	0
2	ADP	E	602	27/27	0.95	0.09	51,53,60,60	0
2	ADP	F	601	27/27	0.95	0.09	59,61,65,66	0

Continued on next page...

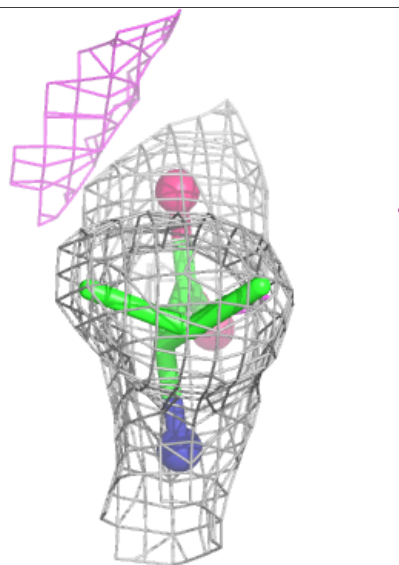
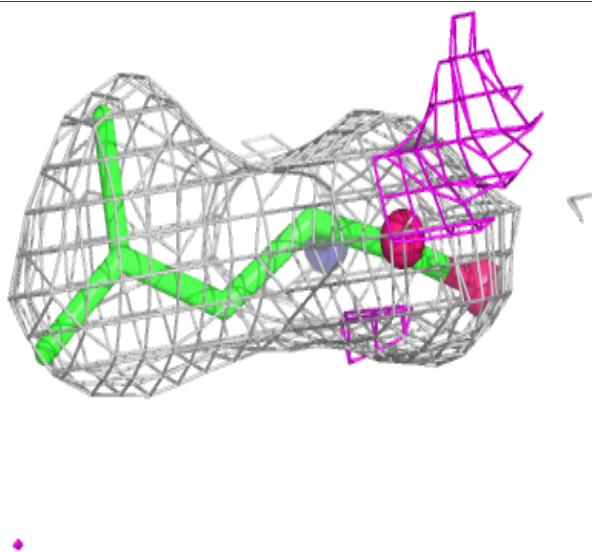
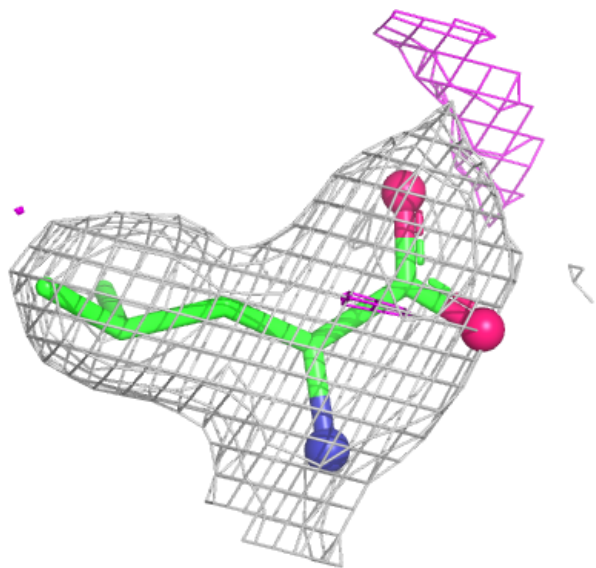
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	B	601	27/27	0.96	0.08	60,62,68,68	0
2	ADP	D	602	27/27	0.96	0.09	63,65,69,69	0
2	ADP	C	601	27/27	0.97	0.07	57,60,65,65	0
3	K	E	603	1/1	0.97	0.04	52,52,52,52	0
3	K	F	602	1/1	0.97	0.05	56,56,56,56	0
3	K	A	602	1/1	0.98	0.06	47,47,47,47	0
3	K	B	602	1/1	0.99	0.07	53,53,53,53	0
3	K	D	603	1/1	0.99	0.03	69,69,69,69	0
3	K	C	602	1/1	1.00	0.06	46,46,46,46	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.

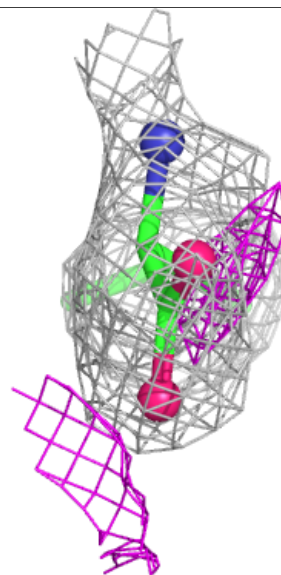
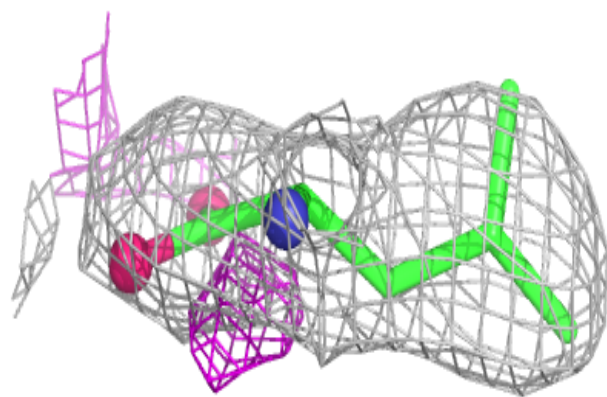
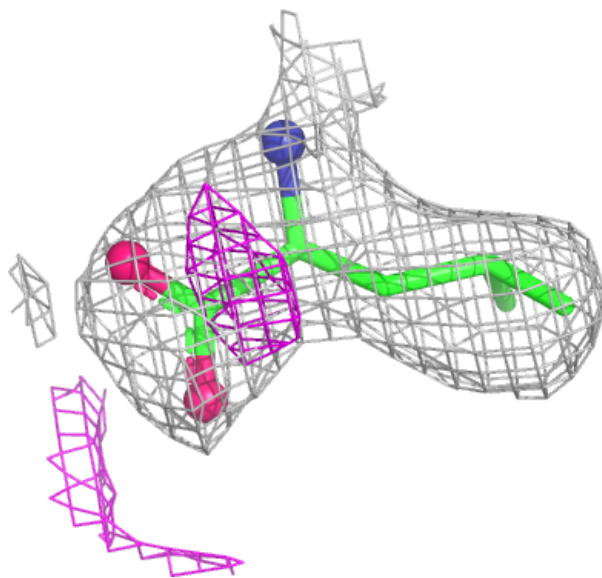
Electron density around LEU E 601:

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



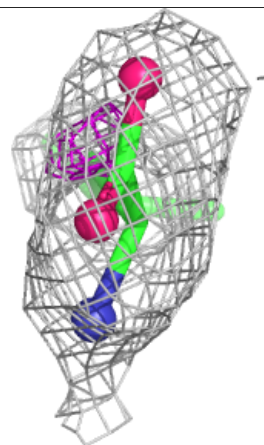
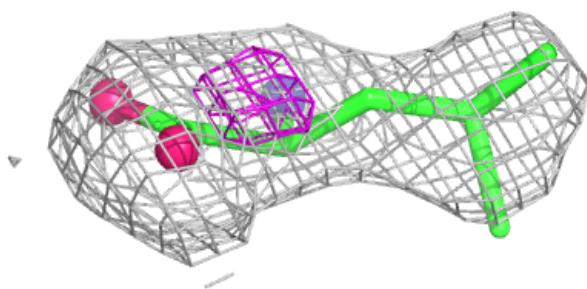
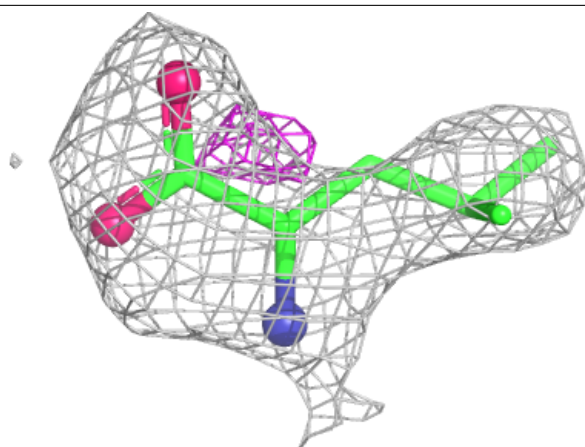
Electron density around LEU D 601:

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



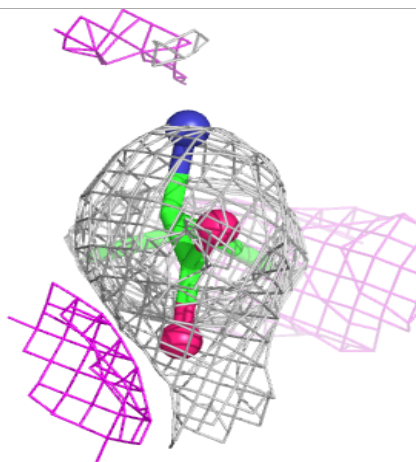
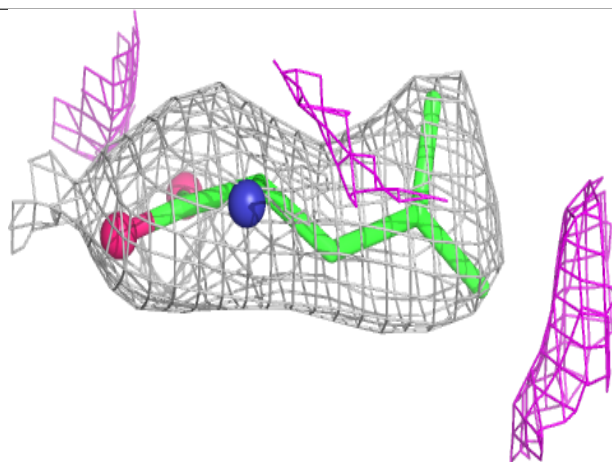
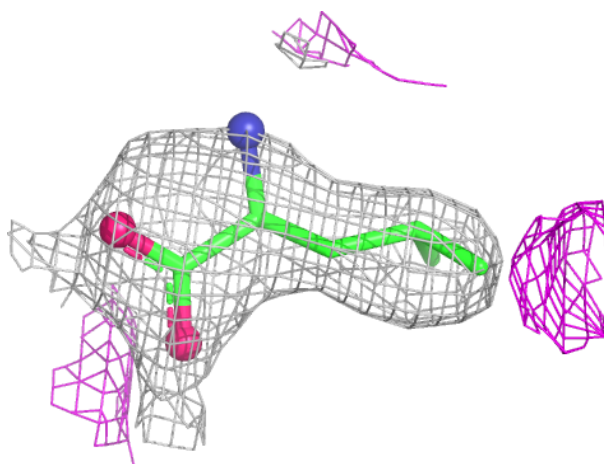
Electron density around LEU C 603:

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



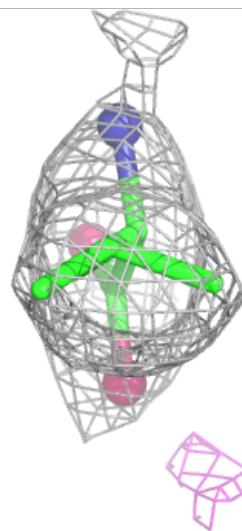
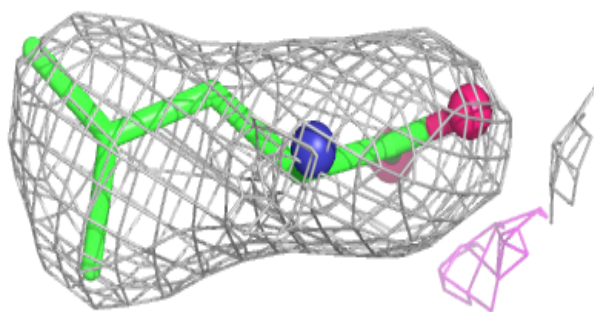
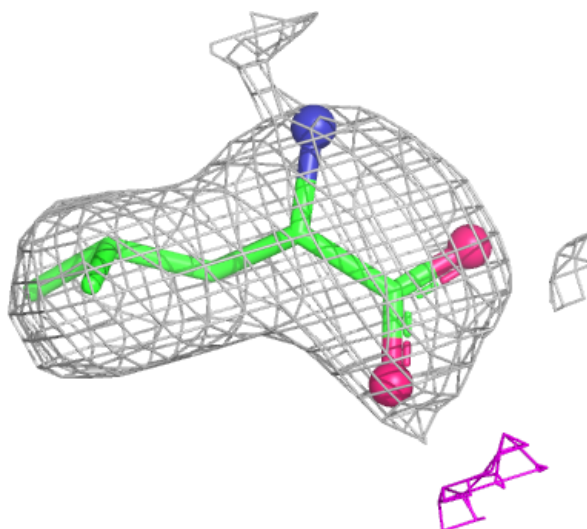
Electron density around LEU A 604:

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



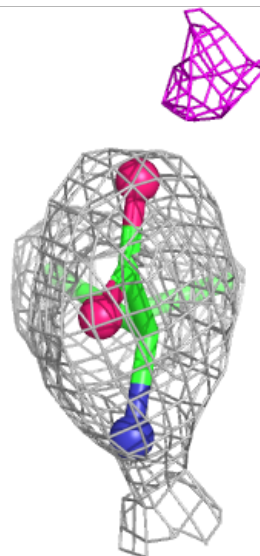
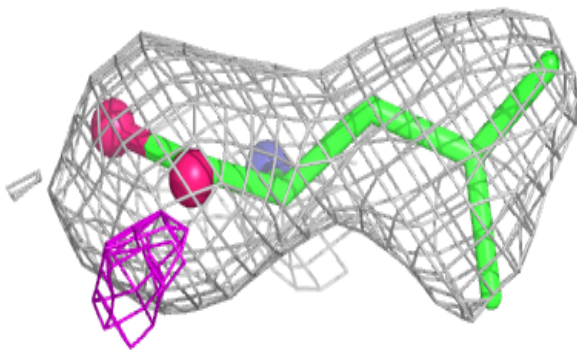
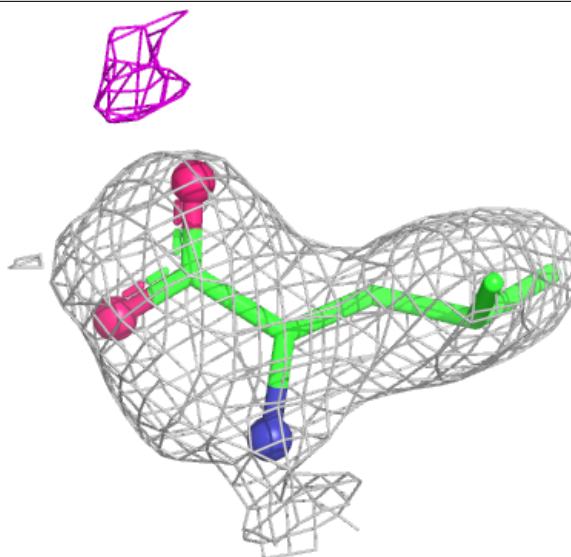
Electron density around LEU B 603:

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



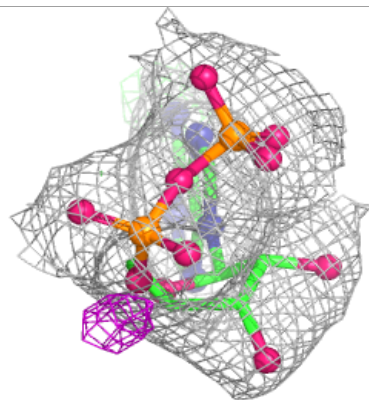
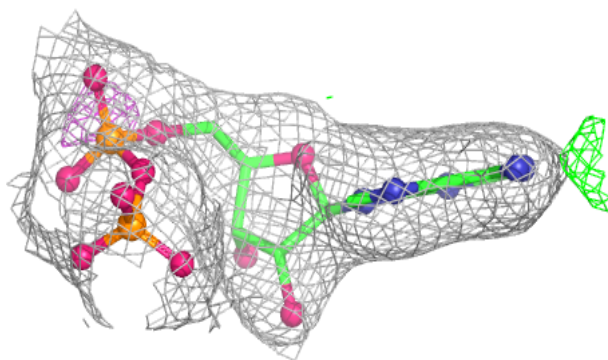
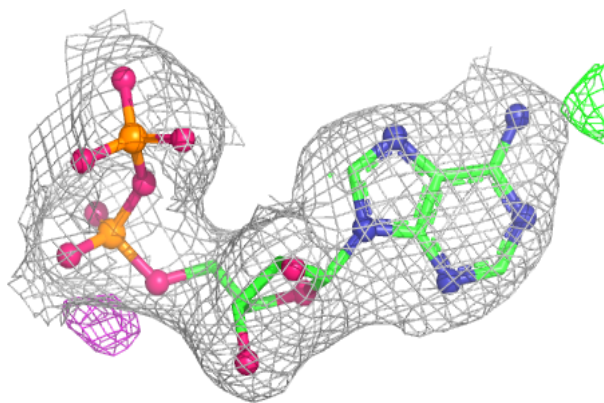
Electron density around LEU A 603:

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

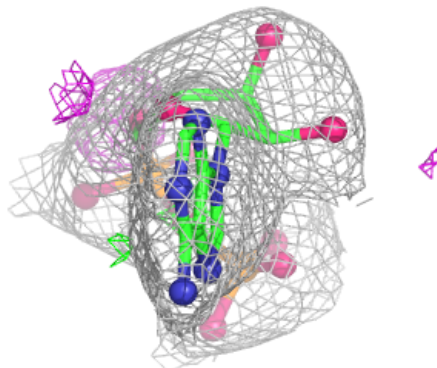
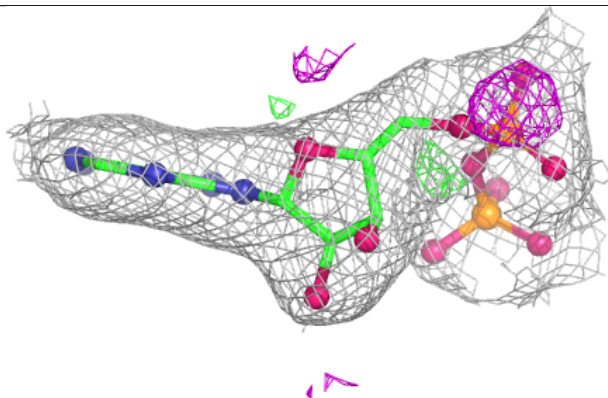
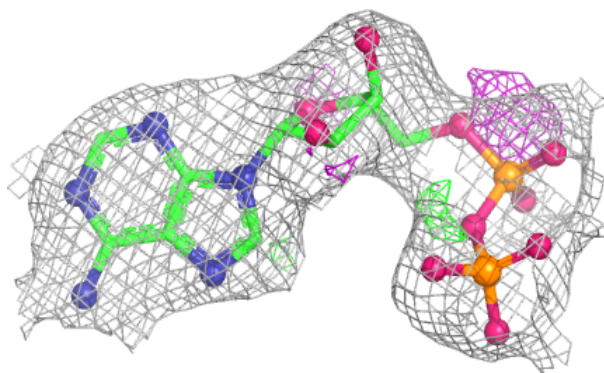


Electron density around ADP A 601:

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

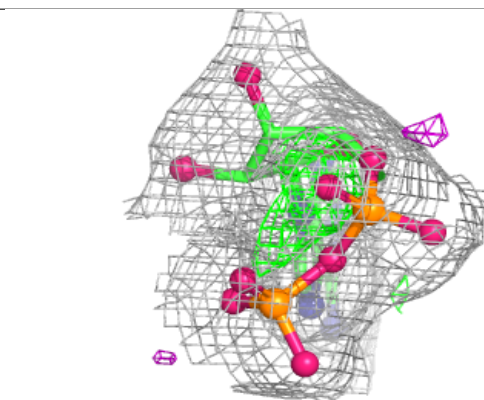
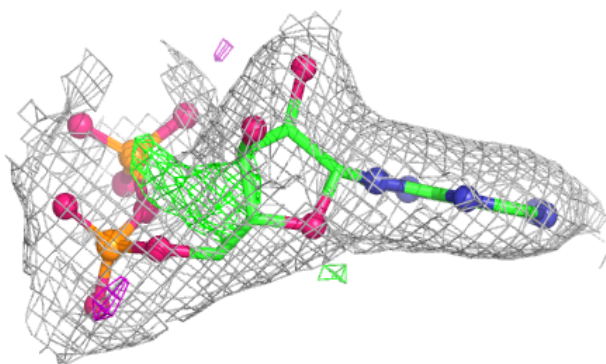
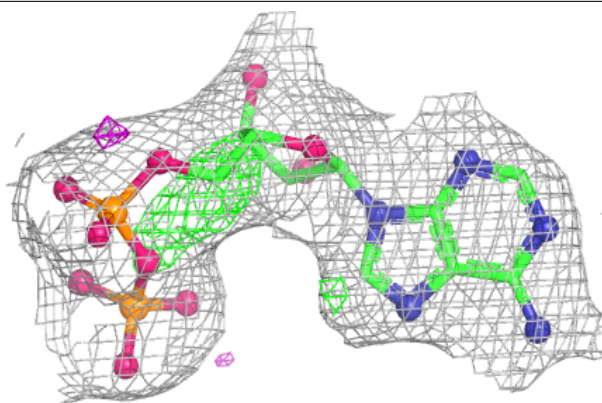
**Electron density around ADP E 602:**

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

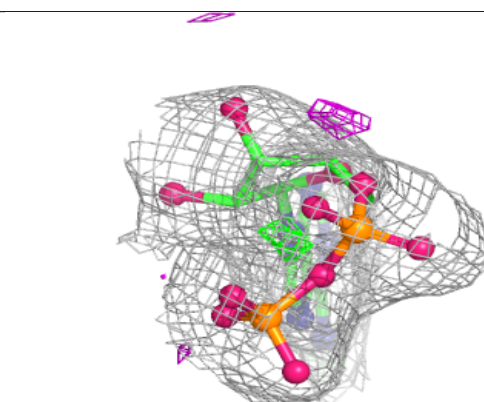
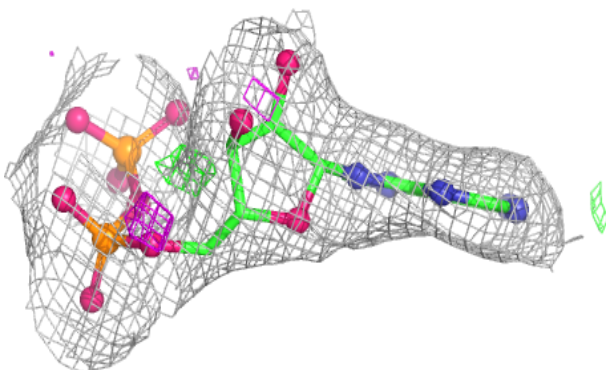
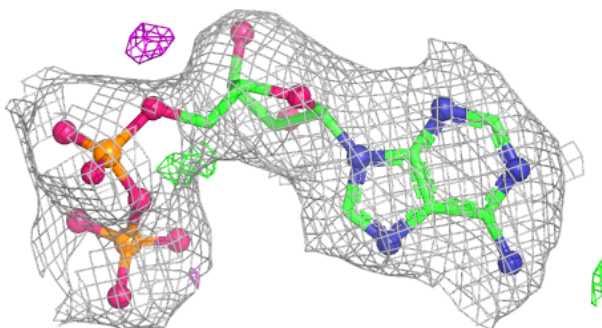


Electron density around ADP F 601:

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

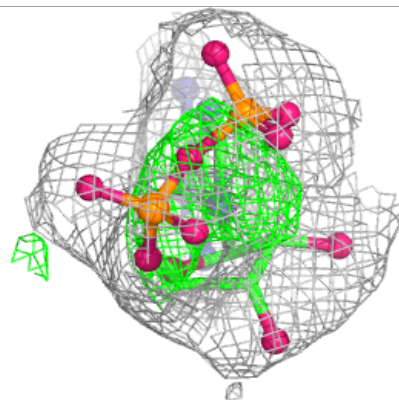
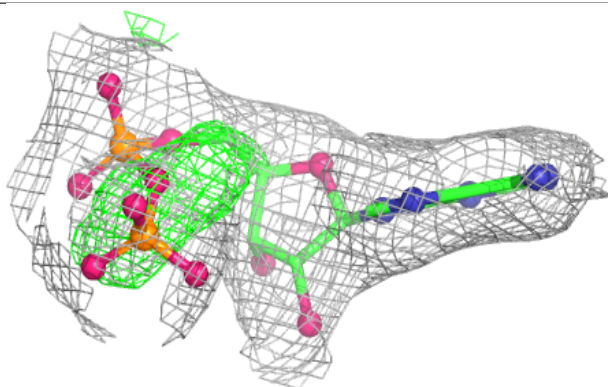
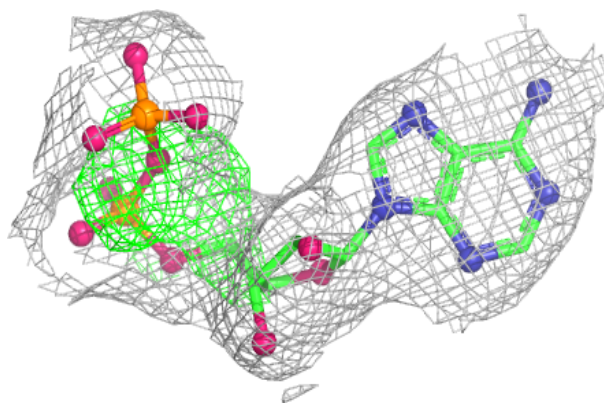
**Electron density around ADP B 601:**

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

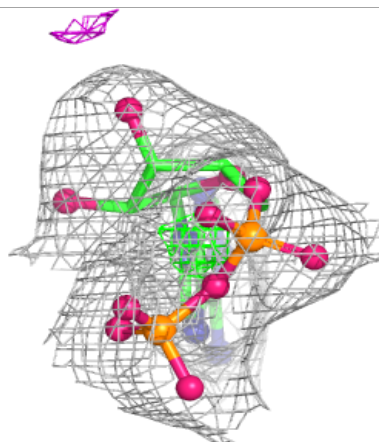
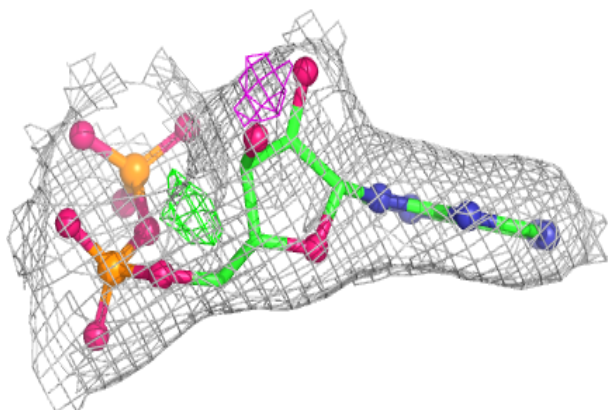
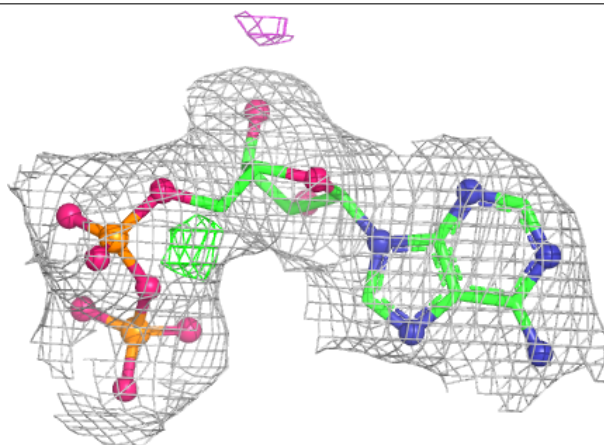


Electron density around ADP D 602:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.