



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:20 AM UTC

PDB ID : 4GVL / pdb_00004gvl
Title : Crystal Structure of the GsuK RCK domain
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.; Jiang, Y.
Deposited on : 2012-08-30
Resolution : 3.00 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

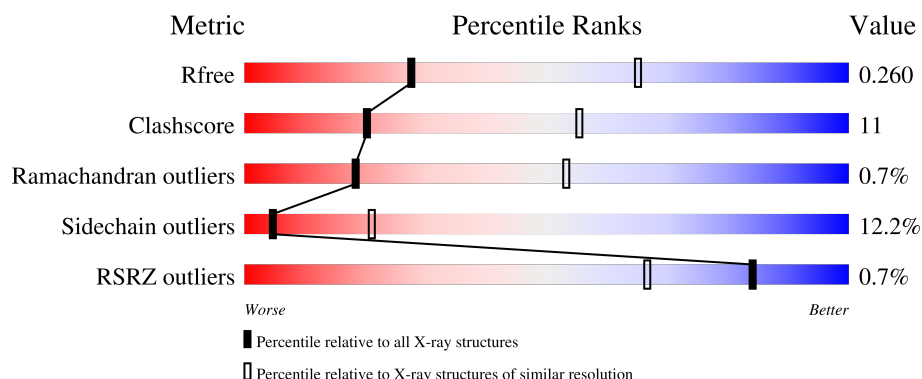
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	462	 66% 27% . . .
1	B	462	 68% 26% . .
1	C	462	 76% 19% . .
1	D	462	 2% 67% 28% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13940 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			
1	B	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			
1	C	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			
1	D	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			

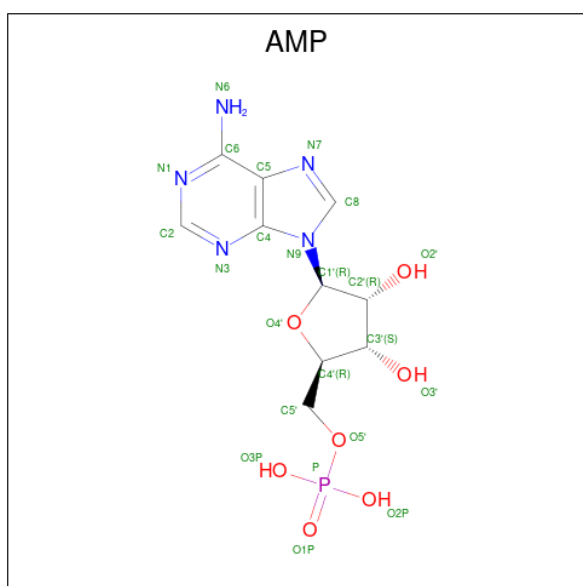
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LEU	-	expression tag	UNP Q74FS9
A	566	VAL	-	expression tag	UNP Q74FS9
A	567	PRO	-	expression tag	UNP Q74FS9
A	568	ARG	-	expression tag	UNP Q74FS9
B	565	LEU	-	expression tag	UNP Q74FS9
B	566	VAL	-	expression tag	UNP Q74FS9
B	567	PRO	-	expression tag	UNP Q74FS9
B	568	ARG	-	expression tag	UNP Q74FS9
C	565	LEU	-	expression tag	UNP Q74FS9
C	566	VAL	-	expression tag	UNP Q74FS9
C	567	PRO	-	expression tag	UNP Q74FS9
C	568	ARG	-	expression tag	UNP Q74FS9
D	565	LEU	-	expression tag	UNP Q74FS9
D	566	VAL	-	expression tag	UNP Q74FS9
D	567	PRO	-	expression tag	UNP Q74FS9
D	568	ARG	-	expression tag	UNP Q74FS9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 23 10 5 7 1	0	0
3	B	1	Total C N O P 23 10 5 7 1	0	0
3	C	1	Total C N O P 23 10 5 7 1	0	0
3	D	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	1	Total Ca 1 1	0	0

Continued on next page...

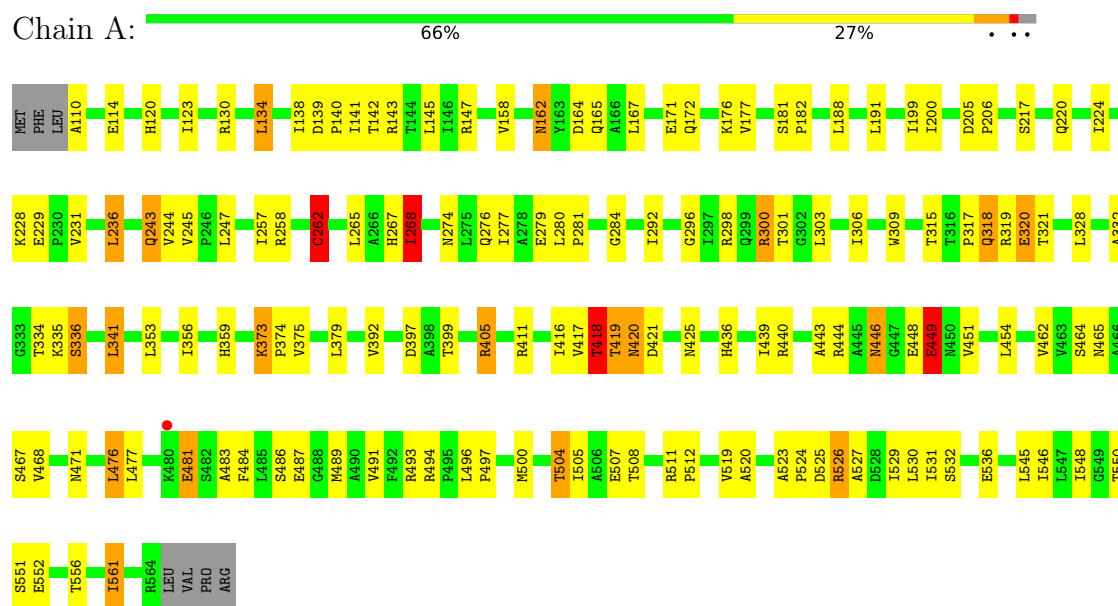
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		

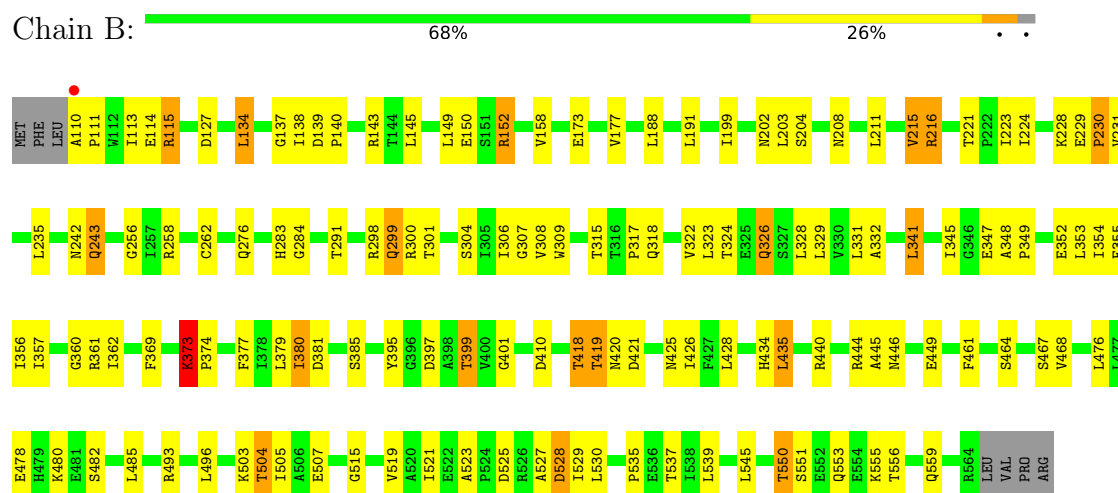
3 Residue-property plots

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: TrkA domain protein

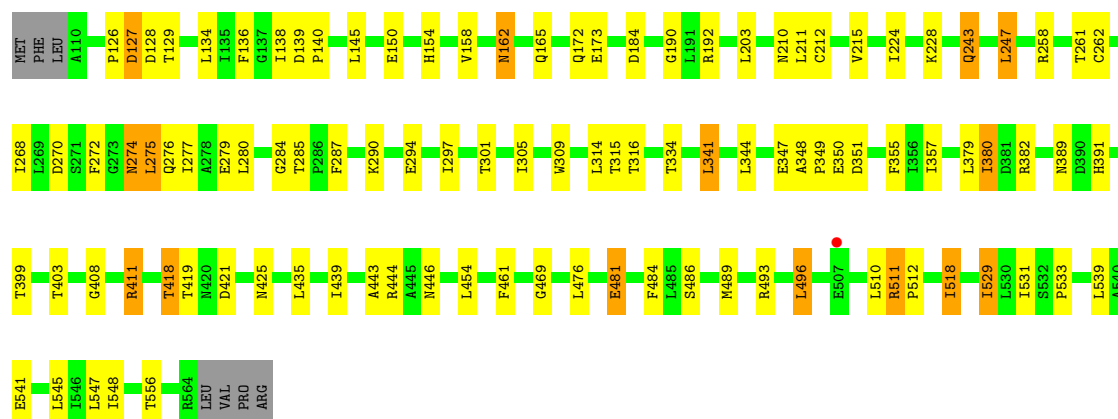


- Molecule 1: TrkA domain protein



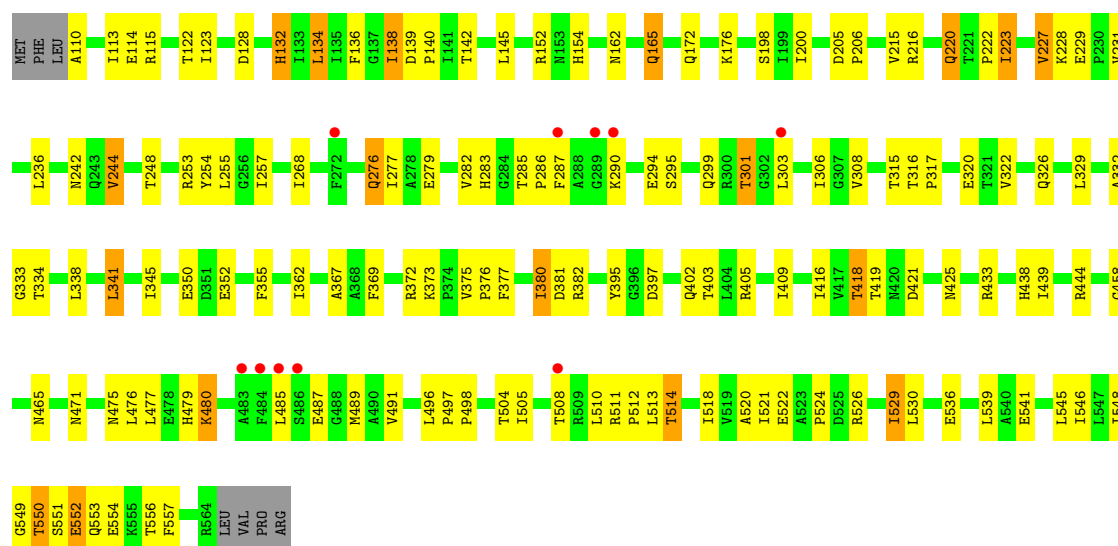
- Molecule 1: TrkA domain protein

Chain C:  76% 19% . .



• Molecule 1: TrkA domain protein

Chain D:  2% 67% 28% . .



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.65Å 161.69Å 310.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 3.00 48.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.45-3.00) 98.7 (48.45-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.262 0.224 , 0.260	Depositor DCC
R_{free} test set	1128 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	100.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13940	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.57	0/3521	0.94	9/4796 (0.2%)
1	B	0.56	0/3521	0.95	3/4796 (0.1%)
1	C	0.65	5/3521 (0.1%)	0.87	5/4796 (0.1%)
1	D	0.68	7/3521 (0.2%)	0.94	9/4796 (0.2%)
All	All	0.62	12/14084 (0.1%)	0.93	26/19184 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	216	ARG	CZ-NH2	15.84	1.54	1.33
1	C	126	PRO	C-N	13.65	1.52	1.33
1	C	190	GLY	C-O	10.53	1.36	1.23
1	C	127	ASP	C-N	10.52	1.47	1.33
1	D	220	GLN	CD-OE1	7.90	1.38	1.23
1	D	220	GLN	C-O	7.67	1.34	1.24
1	C	129	THR	CB-OG1	7.17	1.55	1.43
1	D	216	ARG	CZ-NH1	6.83	1.42	1.32
1	D	220	GLN	CD-NE2	6.46	1.46	1.33
1	C	128	ASP	C-O	-6.42	1.15	1.23
1	D	220	GLN	C-N	6.37	1.43	1.33
1	D	223	ILE	CB-CG1	5.53	1.64	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	385	SER	CA-C-N	11.86	134.66	119.84
1	B	385	SER	C-N-CA	11.86	134.66	119.84
1	D	216	ARG	NE-CZ-NH1	-10.22	111.28	121.50
1	D	220	GLN	OE1-CD-NE2	8.43	131.03	122.60
1	D	552	GLU	N-CA-C	-8.23	102.00	110.97
1	A	245	VAL	N-CA-C	6.39	114.44	107.60
1	D	220	GLN	CG-CD-NE2	-6.29	106.97	116.40
1	A	262	CYS	N-CA-C	6.12	121.63	114.04
1	D	487	GLU	N-CA-C	6.04	117.68	110.19
1	A	497	PRO	CA-C-N	6.02	127.36	119.84
1	A	497	PRO	C-N-CA	6.02	127.36	119.84
1	A	268	ILE	CB-CA-C	-5.94	105.08	110.91
1	D	216	ARG	NH1-CZ-NH2	5.89	126.95	119.30
1	C	533	PRO	CA-C-N	5.60	123.75	119.66
1	C	533	PRO	C-N-CA	5.60	123.75	119.66
1	A	418	THR	CB-CA-C	-5.59	101.89	111.46
1	A	110	ALA	CA-C-N	5.57	125.41	119.28
1	A	110	ALA	C-N-CA	5.57	125.41	119.28
1	D	220	GLN	CA-C-O	5.57	126.52	119.95
1	C	128	ASP	O-C-N	5.50	129.00	122.46
1	B	283	HIS	N-CA-C	5.39	117.59	111.02
1	C	126	PRO	CA-C-N	-5.12	113.03	120.29
1	C	126	PRO	C-N-CA	-5.12	113.03	120.29
1	D	283	HIS	N-CA-C	5.08	116.63	111.14
1	A	519	VAL	CB-CA-C	5.04	115.59	110.65
1	D	480	LYS	N-CA-C	-5.02	105.80	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	LYS	Peptide

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	3460	0	3518	97	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3460	0	3518	82	0
1	C	3460	0	3518	60	0
1	D	3460	0	3518	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	23	0	12	1	0
3	B	23	0	12	2	0
3	C	23	0	12	2	0
3	D	23	0	12	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	13940	0	14120	317	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 11.

All (317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:NH1	1:A:172:GLN:HG2	1.58	1.16
1:B:355:PHE:CZ	1:B:380:ILE:HD11	1.89	1.06
1:A:143:ARG:HH12	1:A:172:GLN:HG2	1.20	1.00
1:D:419:THR:HG22	1:D:421:ASP:H	1.28	0.97
1:A:301:THR:CG2	1:A:303:LEU:HG	1.95	0.97
1:A:419:THR:HG22	1:A:421:ASP:H	1.30	0.96
1:A:436:HIS:HB3	1:A:439:ILE:HD12	1.47	0.96
1:C:418:THR:HG22	1:C:444:ARG:HH11	1.32	0.94
1:C:419:THR:HB	1:C:425:ASN:HD21	1.31	0.92
1:C:419:THR:HB	1:C:425:ASN:ND2	1.87	0.89
1:A:306:ILE:HD11	1:A:332:ALA:HB2	1.58	0.86
1:B:444:ARG:HE	1:B:446:ASN:HD21	1.25	0.85
1:D:553:GLN:HA	1:D:556:THR:HB	1.58	0.85
1:A:301:THR:HG21	1:A:303:LEU:HG	1.60	0.82
1:D:444:ARG:HE	1:D:465:ASN:HD21	1.22	0.82
1:D:551:SER:HA	1:D:554:GLU:HB3	1.60	0.82
1:B:419:THR:HG22	1:B:421:ASP:H	1.44	0.81
1:C:419:THR:HG22	1:C:421:ASP:H	1.46	0.80
1:A:334:THR:HG22	1:A:336:SER:H	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG22	1:A:303:LEU:HG	1.64	0.78
1:B:419:THR:HB	1:B:425:ASN:OD1	1.84	0.78
1:A:258:ARG:O	1:A:440:ARG:NH1	2.16	0.78
1:B:299:GLN:H	1:B:299:GLN:HE21	1.30	0.77
1:D:475:ASN:O	1:D:479:HIS:HB2	1.84	0.77
1:A:138:ILE:HD11	1:A:143:ARG:HG3	1.64	0.76
1:A:486:SER:HA	1:A:489:MET:HE2	1.68	0.75
1:A:143:ARG:HH12	1:A:172:GLN:CG	2.00	0.74
1:A:309:TRP:HB2	1:A:328:LEU:HB3	1.67	0.74
1:A:397:ASP:OD1	1:A:399:THR:HB	1.88	0.74
1:B:550:THR:HG22	1:B:553:GLN:H	1.53	0.74
1:A:268:ILE:HD11	1:A:279:GLU:HG3	1.69	0.74
1:D:308:VAL:HG22	1:D:329:LEU:HD23	1.71	0.73
1:A:134:LEU:CD1	1:A:199:ILE:HG12	2.19	0.72
1:C:268:ILE:HD11	1:C:279:GLU:HG3	1.72	0.71
1:B:262:CYS:HA	1:B:284:GLY:HA3	1.72	0.71
1:D:419:THR:H	1:D:425:ASN:HD21	1.39	0.70
1:A:243:GLN:HE21	1:A:243:GLN:HA	1.57	0.69
1:C:444:ARG:HH21	1:C:446:ASN:HD21	1.39	0.69
1:A:504:THR:HG22	1:A:507:GLU:H	1.58	0.69
1:B:306:ILE:HD11	1:B:332:ALA:HB2	1.74	0.69
1:D:551:SER:HA	1:D:554:GLU:CB	2.22	0.69
1:A:417:VAL:HG12	1:A:425:ASN:HD22	1.57	0.68
1:A:436:HIS:CB	1:A:439:ILE:HD12	2.20	0.68
1:B:111:PRO:HA	1:B:114:GLU:HB3	1.74	0.68
1:A:420:ASN:H	1:A:420:ASN:HD22	1.42	0.68
1:D:419:THR:HB	1:D:425:ASN:ND2	2.08	0.68
1:B:444:ARG:HE	1:B:446:ASN:ND2	1.92	0.67
1:A:520:ALA:HB3	1:A:546:ILE:HB	1.77	0.67
1:A:143:ARG:HH11	1:A:172:GLN:HG2	1.55	0.66
1:D:550:THR:HG22	1:D:552:GLU:H	1.61	0.66
1:A:319:ARG:HG3	1:A:320:GLU:HG3	1.78	0.65
1:D:290:LYS:HB3	1:D:294:GLU:HG3	1.78	0.65
1:D:419:THR:HB	1:D:425:ASN:HD21	1.61	0.65
1:B:523:ALA:HB3	1:B:527:ALA:HB3	1.77	0.65
1:D:306:ILE:HD11	1:D:332:ALA:HB2	1.79	0.65
1:D:529:ILE:HD12	1:D:529:ILE:H	1.60	0.65
1:B:299:GLN:HE21	1:B:299:GLN:N	1.94	0.64
1:B:419:THR:CG2	1:B:421:ASP:H	2.11	0.64
1:D:162:ASN:HD22	1:D:165:GLN:H	1.44	0.64
1:B:360:GLY:HA3	3:B:602:AMP:O5'	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:THR:CB	1:C:425:ASN:HD21	2.07	0.64
1:D:268:ILE:HD12	1:D:277:ILE:HG22	1.80	0.64
1:D:110:ALA:HB1	1:D:113:ILE:HD13	1.78	0.63
1:C:444:ARG:HH21	1:C:446:ASN:ND2	1.96	0.63
1:C:262:CYS:HA	1:C:284:GLY:HA3	1.79	0.63
1:C:211:LEU:O	1:C:215:VAL:HG12	2.00	0.62
1:D:444:ARG:HE	1:D:465:ASN:ND2	1.95	0.62
1:B:354:ILE:O	1:B:377:PHE:HA	1.99	0.62
1:C:270:ASP:HA	1:C:276:GLN:HG2	1.81	0.62
1:A:134:LEU:HD12	1:A:199:ILE:HG12	1.82	0.62
1:A:301:THR:HG21	1:A:303:LEU:CG	2.26	0.62
1:A:296:GLY:O	1:A:300:ARG:HD3	2.00	0.61
1:D:489:MET:HB3	1:D:549:GLY:O	1.99	0.61
1:B:356:ILE:HB	1:B:379:LEU:HD23	1.82	0.60
1:B:418:THR:HG22	1:B:444:ARG:HH11	1.65	0.60
1:B:134:LEU:HD21	1:B:199:ILE:HG12	1.82	0.60
1:A:318:GLN:HB2	1:A:321:THR:HG23	1.83	0.60
1:A:306:ILE:O	1:A:531:ILE:HD11	2.00	0.60
1:B:326:GLN:HE21	1:B:326:GLN:N	1.99	0.60
1:D:132:HIS:H	1:D:132:HIS:CD2	2.20	0.59
1:A:268:ILE:HD12	1:A:277:ILE:HG22	1.84	0.59
1:B:299:GLN:H	1:B:299:GLN:NE2	2.01	0.59
1:C:274:ASN:HD22	1:C:275:LEU:H	1.51	0.59
1:D:418:THR:HG22	1:D:444:ARG:HD2	1.84	0.58
1:A:301:THR:HG21	1:A:303:LEU:CD1	2.33	0.58
1:A:262:CYS:HA	1:A:284:GLY:HA3	1.85	0.58
1:B:152:ARG:H	1:B:152:ARG:HD2	1.68	0.58
1:A:420:ASN:HB3	3:A:602:AMP:H5'1	1.85	0.58
1:C:243:GLN:HA	1:C:243:GLN:HE21	1.69	0.58
1:D:369:PHE:HA	1:D:372:ARG:HH11	1.69	0.57
1:B:138:ILE:HD11	1:B:143:ARG:HG3	1.86	0.57
1:B:309:TRP:HB2	1:B:328:LEU:HB3	1.84	0.57
1:A:267:HIS:HE1	1:A:276:GLN:NE2	2.03	0.57
1:D:205:ASP:HB2	1:D:206:PRO:HD3	1.87	0.57
1:D:496:LEU:HD11	1:D:539:LEU:HB3	1.86	0.56
1:A:243:GLN:HA	1:A:243:GLN:NE2	2.20	0.56
1:C:162:ASN:ND2	1:C:165:GLN:H	2.03	0.56
1:B:258:ARG:O	1:B:440:ARG:NH1	2.38	0.56
1:B:139:ASP:HB2	1:B:140:PRO:CD	2.36	0.56
1:D:489:MET:HB2	1:D:548:ILE:HG22	1.87	0.56
1:D:139:ASP:HB2	1:D:140:PRO:HD2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:THR:H	1:A:425:ASN:HD21	1.54	0.56
1:B:397:ASP:OD1	1:B:399:THR:HB	2.06	0.56
1:B:444:ARG:NE	1:B:446:ASN:HD21	1.97	0.56
1:A:373:LYS:O	1:A:375:VAL:N	2.39	0.55
1:B:152:ARG:HH12	1:B:478:GLU:HG3	1.71	0.55
1:D:200:ILE:HD11	1:D:477:LEU:HD11	1.87	0.55
1:A:257:ILE:HG23	1:A:281:PRO:HG3	1.88	0.55
1:A:550:THR:HG22	1:A:552:GLU:H	1.72	0.55
1:B:355:PHE:CE2	1:B:380:ILE:HD11	2.41	0.54
1:D:491:VAL:HG13	1:D:548:ILE:HG12	1.90	0.54
1:A:265:LEU:HD23	1:A:280:LEU:HB2	1.89	0.54
1:C:444:ARG:NH2	1:C:446:ASN:HD21	2.03	0.54
1:C:408:GLY:O	1:C:411:ARG:HG3	2.07	0.53
1:D:397:ASP:OD1	3:D:602:AMP:N6	2.41	0.53
1:A:529:ILE:HD12	1:A:529:ILE:H	1.72	0.53
1:D:476:LEU:O	1:D:480:LYS:HB2	2.07	0.53
1:A:224:ILE:HD12	1:A:477:LEU:HD23	1.89	0.53
1:C:270:ASP:C	1:C:272:PHE:H	2.17	0.53
1:C:355:PHE:HD2	1:C:380:ILE:HD11	1.74	0.53
1:A:444:ARG:HH21	1:A:446:ASN:HD22	1.57	0.53
1:A:526:ARG:HA	1:A:526:ARG:HH11	1.74	0.53
1:A:444:ARG:NH2	1:A:446:ASN:HD22	2.07	0.53
1:A:139:ASP:HB2	1:A:140:PRO:HD2	1.91	0.53
1:B:224:ILE:HG23	1:B:243:GLN:HB3	1.90	0.53
1:C:136:PHE:HB3	1:C:203:LEU:HD11	1.91	0.52
1:D:553:GLN:O	1:D:557:PHE:HB2	2.08	0.52
1:B:505:ILE:HD12	1:B:537:THR:HB	1.90	0.52
1:C:224:ILE:HG23	1:C:243:GLN:HB3	1.90	0.52
1:A:493:ARG:O	1:A:494:ARG:HD2	2.10	0.52
1:B:326:GLN:HE21	1:B:326:GLN:H	1.58	0.52
1:B:349:PRO:HG2	1:B:352:GLU:HB3	1.92	0.51
1:D:301:THR:HG21	1:D:341:LEU:HB2	1.93	0.51
1:A:419:THR:N	1:A:425:ASN:HD21	2.07	0.51
1:B:529:ILE:HD12	1:B:529:ILE:H	1.75	0.51
1:C:162:ASN:HD22	1:C:165:GLN:H	1.59	0.51
1:B:449:GLU:HG3	1:C:184:ASP:OD2	2.10	0.51
1:B:496:LEU:HD11	1:B:539:LEU:HB3	1.92	0.51
1:A:525:ASP:C	1:A:527:ALA:H	2.18	0.51
1:A:205:ASP:HB2	1:A:206:PRO:HD3	1.93	0.51
1:D:152:ARG:HD3	1:D:154:HIS:CE1	2.46	0.51
1:B:515:GLY:HA3	1:B:553:GLN:NE2	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:HIS:CG	1:A:359:HIS:O	2.63	0.50
1:B:528:ASP:OD1	1:B:528:ASP:N	2.43	0.50
1:B:515:GLY:HA3	1:B:553:GLN:HE22	1.75	0.50
1:A:523:ALA:HB3	1:A:527:ALA:HB3	1.94	0.49
1:B:134:LEU:CD2	1:B:199:ILE:HG12	2.41	0.49
1:C:511:ARG:HB3	1:C:512:PRO:HD3	1.94	0.49
1:C:357:ILE:HG12	1:C:380:ILE:HD12	1.92	0.49
1:A:229:GLU:HG3	1:A:231:VAL:HG22	1.94	0.49
1:B:216:ARG:NH1	1:B:221:THR:O	2.38	0.49
1:C:382:ARG:HG3	3:C:602:AMP:C2	2.47	0.49
1:D:419:THR:HG23	3:D:602:AMP:C8	2.47	0.49
1:A:243:GLN:HE21	1:A:243:GLN:CA	2.20	0.49
1:B:211:LEU:O	1:B:215:VAL:HG13	2.12	0.49
1:B:229:GLU:O	1:B:230:PRO:C	2.55	0.49
1:D:520:ALA:HB3	1:D:546:ILE:HB	1.94	0.49
1:D:419:THR:HG22	1:D:421:ASP:N	2.12	0.49
1:D:405:ARG:HA	1:D:409:ILE:HG22	1.95	0.49
1:D:444:ARG:NE	1:D:465:ASN:HD21	2.02	0.49
1:B:215:VAL:CG2	1:B:223:ILE:HD11	2.43	0.49
1:C:419:THR:HG22	1:C:421:ASP:N	2.20	0.49
1:C:127:ASP:OD2	1:C:192:ARG:NH2	2.46	0.48
1:A:188:LEU:HA	1:A:191:LEU:HD12	1.95	0.48
1:B:308:VAL:HG22	1:B:329:LEU:HD23	1.95	0.48
1:C:341:LEU:HA	1:C:344:LEU:HD12	1.94	0.48
1:A:162:ASN:C	1:A:162:ASN:HD22	2.21	0.48
1:B:426:ILE:HD12	1:C:210:ASN:ND2	2.29	0.48
1:C:139:ASP:HB2	1:C:140:PRO:HD2	1.95	0.48
1:A:334:THR:HG22	1:A:336:SER:N	2.23	0.48
1:D:367:ALA:HB1	1:D:377:PHE:CE1	2.49	0.48
1:C:290:LYS:HB3	1:C:294:GLU:HG3	1.95	0.47
1:B:115:ARG:O	1:B:115:ARG:HG2	2.14	0.47
1:D:255:LEU:HD22	1:D:416:ILE:HG23	1.97	0.47
1:A:471:ASN:C	1:A:471:ASN:OD1	2.57	0.47
1:C:243:GLN:HA	1:C:243:GLN:NE2	2.28	0.47
1:A:224:ILE:HD13	1:A:476:LEU:HB3	1.97	0.47
1:D:162:ASN:ND2	1:D:165:GLN:H	2.10	0.47
1:B:445:ALA:HB3	1:B:464:SER:HA	1.97	0.47
1:D:303:LEU:HD23	1:D:333:GLY:HA3	1.97	0.47
1:C:418:THR:HG22	1:C:444:ARG:HD3	1.97	0.47
1:B:215:VAL:HG21	1:B:223:ILE:HD11	1.96	0.47
1:D:513:LEU:HD23	1:D:514:THR:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:THR:C	1:C:287:PHE:H	2.23	0.46
1:C:309:TRP:CE2	1:C:314:LEU:HD13	2.50	0.46
1:C:529:ILE:H	1:C:529:ILE:HD12	1.80	0.46
1:D:134:LEU:HD13	1:D:136:PHE:CE2	2.49	0.46
1:D:438:HIS:CD2	1:D:439:ILE:HG13	2.50	0.46
1:A:139:ASP:HB2	1:A:140:PRO:CD	2.45	0.46
1:B:381:ASP:O	1:B:395:TYR:HA	2.15	0.46
1:B:496:LEU:CD1	1:B:539:LEU:HB3	2.46	0.46
1:B:355:PHE:HZ	1:B:380:ILE:HD11	1.69	0.46
1:A:162:ASN:ND2	1:A:165:GLN:H	2.13	0.46
1:D:505:ILE:HD11	1:D:521:ILE:HD11	1.98	0.46
1:A:138:ILE:HD12	1:A:142:THR:OG1	2.16	0.46
1:B:188:LEU:HA	1:B:191:LEU:HD12	1.98	0.46
1:C:496:LEU:HD21	1:C:539:LEU:HD13	1.96	0.46
1:A:417:VAL:HG12	1:A:425:ASN:ND2	2.28	0.46
1:B:229:GLU:CG	1:B:361:ARG:HH21	2.28	0.46
1:D:223:ILE:N	1:D:242:ASN:OD1	2.49	0.46
1:B:504:THR:HG22	1:B:507:GLU:H	1.81	0.45
1:D:138:ILE:H	1:D:138:ILE:HG13	1.54	0.45
1:C:272:PHE:C	1:C:274:ASN:H	2.24	0.45
1:D:198:SER:HB3	1:D:222:PRO:HG2	1.98	0.45
1:A:120:HIS:CE1	1:D:115:ARG:HG2	2.50	0.45
1:D:285:THR:HB	1:D:286:PRO:HD2	1.98	0.45
1:D:362:ILE:HG22	1:D:418:THR:HG21	1.99	0.45
1:A:356:ILE:HG12	1:A:416:ILE:HD12	1.98	0.45
1:A:416:ILE:HG22	1:A:418:THR:OG1	2.17	0.45
1:B:110:ALA:HB3	1:B:113:ILE:HD12	1.99	0.45
1:B:341:LEU:HD13	1:B:345:ILE:HD11	1.98	0.45
1:C:315:THR:HG22	1:C:316:THR:H	1.81	0.45
1:A:443:ALA:HB1	1:A:454:LEU:HD22	1.98	0.45
1:B:348:ALA:HB1	1:B:349:PRO:HD2	1.98	0.45
1:C:350:GLU:HG3	1:C:351:ASP:H	1.82	0.45
1:C:510:LEU:HD12	1:C:518:ILE:HD11	1.98	0.45
1:D:227:VAL:HG12	1:D:229:GLU:H	1.81	0.45
1:A:493:ARG:HA	1:A:545:LEU:O	2.17	0.44
1:A:419:THR:CG2	1:A:420:ASN:N	2.80	0.44
1:C:139:ASP:HB2	1:C:140:PRO:CD	2.47	0.44
1:A:267:HIS:CE1	1:A:276:GLN:NE2	2.84	0.44
1:B:307:GLY:HA2	1:B:317:PRO:HD3	1.99	0.44
1:B:551:SER:O	1:B:555:LYS:HG3	2.17	0.44
1:C:493:ARG:HA	1:C:545:LEU:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ILE:HD12	1:B:444:ARG:CZ	2.48	0.44
1:A:523:ALA:HB1	1:A:524:PRO:HD2	2.00	0.44
1:B:229:GLU:HA	1:B:230:PRO:HD2	1.84	0.44
1:B:276:GLN:O	1:B:332:ALA:HA	2.17	0.44
1:C:443:ALA:HB1	1:C:454:LEU:HD22	1.98	0.44
1:B:256:GLY:HA3	1:B:369:PHE:CD2	2.53	0.44
1:D:489:MET:HB3	1:D:549:GLY:C	2.43	0.44
1:D:514:THR:HG21	1:D:557:PHE:CD1	2.53	0.44
1:C:138:ILE:HD13	1:C:158:VAL:HG11	2.00	0.44
1:A:483:ALA:O	1:A:486:SER:HB2	2.18	0.44
1:C:518:ILE:HD13	1:C:545:LEU:HD22	2.00	0.43
1:A:449:GLU:H	1:A:449:GLU:CD	2.26	0.43
1:A:504:THR:HG23	1:A:505:ILE:N	2.33	0.43
1:D:381:ASP:OD2	1:D:382:ARG:N	2.52	0.43
1:B:137:GLY:HA3	1:B:202:ASN:O	2.19	0.43
1:D:306:ILE:CD1	1:D:332:ALA:HB2	2.48	0.43
1:A:418:THR:HG22	1:A:444:ARG:HH11	1.84	0.43
1:C:379:LEU:HD12	1:C:391:HIS:HB3	2.00	0.43
1:C:419:THR:HG23	3:C:602:AMP:C8	2.54	0.43
1:D:491:VAL:HG22	1:D:548:ILE:HG23	2.01	0.43
1:C:247:LEU:HD21	1:C:469:GLY:HA2	1.99	0.43
1:A:500:MET:HE1	1:A:561:ILE:HD11	2.00	0.43
1:C:315:THR:HG22	1:C:316:THR:N	2.34	0.43
1:D:402:GLN:O	1:D:403:THR:C	2.61	0.43
1:B:258:ARG:HG2	1:B:461:PHE:CG	2.54	0.42
1:B:304:SER:OG	1:B:493:ARG:NH1	2.48	0.42
1:B:360:GLY:HA3	3:B:602:AMP:P	2.59	0.42
1:C:258:ARG:HG3	1:C:461:PHE:CD1	2.54	0.42
1:B:203:LEU:HB2	1:B:208:ASN:OD1	2.19	0.42
1:C:481:GLU:HA	1:C:484:PHE:HD2	1.82	0.42
1:A:451:VAL:HG13	1:A:462:VAL:HG11	2.02	0.42
1:B:291:THR:HG22	1:B:322:VAL:HG22	2.01	0.42
1:D:248:THR:HG22	1:D:362:ILE:HG13	2.01	0.42
1:A:292:ILE:HD13	1:A:317:PRO:HB3	2.00	0.42
1:A:334:THR:HG22	1:A:335:LYS:N	2.34	0.42
1:B:258:ARG:HG2	1:B:461:PHE:CD1	2.55	0.42
1:D:253:ARG:HG3	1:D:369:PHE:CE1	2.54	0.42
1:C:481:GLU:HA	1:C:484:PHE:CD2	2.53	0.42
1:D:254:TYR:HA	1:D:257:ILE:HD12	2.01	0.42
1:D:355:PHE:HD2	1:D:380:ILE:HD11	1.83	0.42
1:A:464:SER:O	1:A:465:ASN:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ILE:HG21	1:B:428:LEU:HD13	2.01	0.42
1:D:510:LEU:HD13	1:D:518:ILE:HD11	2.02	0.42
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.92	0.42
1:C:134:LEU:HD13	1:C:136:PHE:CE2	2.55	0.42
1:C:486:SER:HA	1:C:489:MET:HE2	2.02	0.42
1:D:511:ARG:N	1:D:512:PRO:HD2	2.35	0.42
1:A:143:ARG:HH21	1:A:147:ARG:HH21	1.68	0.42
1:A:481:GLU:H	1:A:481:GLU:HG3	1.59	0.42
1:B:204:SER:HA	1:B:228:LYS:HE2	2.00	0.42
1:A:511:ARG:HB3	1:A:512:PRO:HD3	2.02	0.41
1:D:355:PHE:CD2	1:D:380:ILE:HD11	2.54	0.41
1:A:265:LEU:HD21	1:A:341:LEU:CD1	2.50	0.41
1:B:467:SER:O	1:B:468:VAL:C	2.63	0.41
1:B:529:ILE:HD12	1:B:529:ILE:N	2.35	0.41
1:D:352:GLU:O	1:D:376:PRO:HG2	2.19	0.41
1:D:276:GLN:HB2	1:D:338:LEU:HD11	2.02	0.41
1:D:373:LYS:O	1:D:375:VAL:N	2.54	0.41
1:D:550:THR:HB	1:D:552:GLU:HB2	2.02	0.41
1:A:298:ARG:HD3	1:A:526:ARG:HH22	1.86	0.41
1:D:287:PHE:HD2	1:D:295:SER:HB2	1.85	0.41
1:A:318:GLN:HB2	1:A:318:GLN:HE21	1.56	0.41
1:A:448:GLU:O	1:A:451:VAL:HG23	2.21	0.41
1:B:434:HIS:HD2	1:B:435:LEU:HD13	1.85	0.41
1:D:497:PRO:HA	1:D:498:PRO:HD2	1.83	0.41
1:A:405:ARG:HE	1:A:405:ARG:HB2	1.57	0.41
1:B:347:GLU:OE1	1:B:347:GLU:N	2.45	0.41
1:D:282:VAL:O	1:D:282:VAL:HG12	2.21	0.41
1:D:433:ARG:HD2	1:D:458:GLY:O	2.21	0.41
1:B:152:ARG:NH1	1:B:478:GLU:HG3	2.36	0.41
1:C:518:ILE:HG23	1:C:547:LEU:HG	2.01	0.41
1:A:200:ILE:HD11	1:A:477:LEU:HD11	2.03	0.41
1:A:476:LEU:HD12	1:A:476:LEU:HA	1.90	0.41
1:B:134:LEU:HD21	1:B:199:ILE:CG1	2.49	0.41
1:B:434:HIS:HD2	1:B:435:LEU:CD1	2.34	0.41
1:B:505:ILE:HB	1:B:535:PRO:O	2.21	0.41
1:C:301:THR:HG21	1:C:341:LEU:HD12	2.03	0.41
1:D:227:VAL:HG21	1:D:244:VAL:HG13	2.03	0.41
1:D:554:GLU:HA	1:D:557:PHE:HB2	2.01	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.89	0.40
1:A:500:MET:SD	1:A:508:THR:HG23	2.62	0.40
1:D:341:LEU:O	1:D:345:ILE:HG12	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:THR:HA	1:D:317:PRO:HD3	1.88	0.40
1:A:181:SER:HA	1:A:182:PRO:HD2	1.89	0.40
1:C:297:ILE:HB	1:C:305:ILE:HD11	2.03	0.40
1:A:120:HIS:HE1	1:D:115:ARG:O	2.05	0.40
1:B:139:ASP:HB2	1:B:140:PRO:HD3	2.03	0.40
1:C:162:ASN:HD22	1:C:162:ASN:C	2.29	0.40
1:C:348:ALA:HA	1:C:349:PRO:HD3	1.94	0.40
1:D:138:ILE:HD11	1:D:165:GLN:NE2	2.36	0.40
1:A:356:ILE:HB	1:A:379:LEU:HD23	2.03	0.40
1:D:268:ILE:HD11	1:D:279:GLU:HG3	2.03	0.40
1:D:381:ASP:O	1:D:395:TYR:HA	2.22	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	453/462 (98%)	413 (91%)	36 (8%)	4 (1%)	14	48
1	B	453/462 (98%)	414 (91%)	35 (8%)	4 (1%)	14	48
1	C	453/462 (98%)	408 (90%)	44 (10%)	1 (0%)	43	76
1	D	453/462 (98%)	417 (92%)	33 (7%)	3 (1%)	18	53
All	All	1812/1848 (98%)	1652 (91%)	148 (8%)	12 (1%)	18	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	401	GLY
1	A	467	SER
1	B	374	PRO
1	D	350	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	449	GLU
1	B	230	PRO
1	C	541	GLU
1	D	524	PRO
1	A	374	PRO
1	D	541	GLU
1	A	468	VAL
1	B	373	LYS

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	370/378 (98%)	317 (86%)	53 (14%)	3	16
1	B	370/378 (98%)	319 (86%)	51 (14%)	3	17
1	C	370/378 (98%)	335 (90%)	35 (10%)	8	31
1	D	370/378 (98%)	328 (89%)	42 (11%)	5	24
All	All	1480/1512 (98%)	1299 (88%)	181 (12%)	5	21

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	123	ILE
1	A	130	ARG
1	A	134	LEU
1	A	141	ILE
1	A	145	LEU
1	A	158	VAL
1	A	162	ASN
1	A	164	ASP
1	A	167	LEU
1	A	171	GLU
1	A	176	LYS
1	A	177	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	217	SER
1	A	220	GLN
1	A	228	LYS
1	A	236	LEU
1	A	243	GLN
1	A	244	VAL
1	A	262	CYS
1	A	268	ILE
1	A	274	ASN
1	A	300	ARG
1	A	315	THR
1	A	318	GLN
1	A	320	GLU
1	A	336	SER
1	A	341	LEU
1	A	353	LEU
1	A	373	LYS
1	A	392	VAL
1	A	405	ARG
1	A	411	ARG
1	A	418	THR
1	A	419	THR
1	A	420	ASN
1	A	446	ASN
1	A	449	GLU
1	A	476	LEU
1	A	481	GLU
1	A	484	PHE
1	A	487	GLU
1	A	491	VAL
1	A	496	LEU
1	A	504	THR
1	A	526	ARG
1	A	530	LEU
1	A	532	SER
1	A	536	GLU
1	A	548	ILE
1	A	551	SER
1	A	556	THR
1	A	561	ILE
1	B	115	ARG
1	B	127	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	134	LEU
1	B	145	LEU
1	B	149	LEU
1	B	150	GLU
1	B	152	ARG
1	B	158	VAL
1	B	173	GLU
1	B	177	VAL
1	B	215	VAL
1	B	216	ARG
1	B	231	VAL
1	B	235	LEU
1	B	242	ASN
1	B	243	GLN
1	B	298	ARG
1	B	299	GLN
1	B	300	ARG
1	B	301	THR
1	B	315	THR
1	B	318	GLN
1	B	323	LEU
1	B	324	THR
1	B	326	GLN
1	B	331	LEU
1	B	341	LEU
1	B	353	LEU
1	B	373	LYS
1	B	380	ILE
1	B	399	THR
1	B	410	ASP
1	B	418	THR
1	B	419	THR
1	B	420	ASN
1	B	435	LEU
1	B	476	LEU
1	B	480	LYS
1	B	482	SER
1	B	485	LEU
1	B	503	LYS
1	B	504	THR
1	B	519	VAL
1	B	521	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	525	ASP
1	B	528	ASP
1	B	530	LEU
1	B	545	LEU
1	B	550	THR
1	B	556	THR
1	B	559	GLN
1	C	145	LEU
1	C	150	GLU
1	C	154	HIS
1	C	162	ASN
1	C	172	GLN
1	C	173	GLU
1	C	212	CYS
1	C	228	LYS
1	C	243	GLN
1	C	247	LEU
1	C	261	THR
1	C	274	ASN
1	C	275	LEU
1	C	277	ILE
1	C	280	LEU
1	C	334	THR
1	C	341	LEU
1	C	347	GLU
1	C	380	ILE
1	C	389	ASN
1	C	399	THR
1	C	403	THR
1	C	411	ARG
1	C	418	THR
1	C	435	LEU
1	C	439	ILE
1	C	476	LEU
1	C	481	GLU
1	C	496	LEU
1	C	511	ARG
1	C	518	ILE
1	C	529	ILE
1	C	531	ILE
1	C	548	ILE
1	C	556	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	114	GLU
1	D	122	THR
1	D	123	ILE
1	D	128	ASP
1	D	132	HIS
1	D	134	LEU
1	D	138	ILE
1	D	142	THR
1	D	145	LEU
1	D	165	GLN
1	D	172	GLN
1	D	176	LYS
1	D	215	VAL
1	D	220	GLN
1	D	227	VAL
1	D	228	LYS
1	D	231	VAL
1	D	236	LEU
1	D	244	VAL
1	D	276	GLN
1	D	299	GLN
1	D	301	THR
1	D	315	THR
1	D	320	GLU
1	D	322	VAL
1	D	326	GLN
1	D	334	THR
1	D	341	LEU
1	D	380	ILE
1	D	418	THR
1	D	471	ASN
1	D	485	LEU
1	D	504	THR
1	D	508	THR
1	D	514	THR
1	D	522	GLU
1	D	526	ARG
1	D	529	ILE
1	D	530	LEU
1	D	536	GLU
1	D	545	LEU
1	D	550	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	132	HIS
1	A	162	ASN
1	A	210	ASN
1	A	243	GLN
1	A	267	HIS
1	A	276	GLN
1	A	318	GLN
1	A	326	GLN
1	A	420	ASN
1	A	425	ASN
1	B	120	HIS
1	B	153	ASN
1	B	243	GLN
1	B	276	GLN
1	B	283	HIS
1	B	299	GLN
1	B	318	GLN
1	B	326	GLN
1	B	402	GLN
1	B	406	GLN
1	B	420	ASN
1	B	446	ASN
1	B	475	ASN
1	B	553	GLN
1	B	559	GLN
1	C	162	ASN
1	C	243	GLN
1	C	274	ASN
1	C	389	ASN
1	C	425	ASN
1	C	446	ASN
1	C	450	ASN
1	C	453	GLN
1	D	120	HIS
1	D	132	HIS
1	D	154	HIS
1	D	162	ASN
1	D	243	GLN
1	D	274	ASN
1	D	318	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	326	GLN
1	D	389	ASN
1	D	402	GLN
1	D	425	ASN
1	D	438	HIS
1	D	446	ASN
1	D	453	GLN
1	D	465	ASN
1	D	475	ASN
1	D	553	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AMP	C	602	-	25,25,25	1.53	4 (16%)	37,38,38	1.95	10 (27%)
3	AMP	D	602	-	25,25,25	1.54	4 (16%)	37,38,38	1.99	8 (21%)
3	AMP	A	602	-	25,25,25	1.53	3 (12%)	37,38,38	2.07	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	B	602	-	25,25,25	1.48	4 (16%)	37,38,38	2.04	12 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	C	602	-	-	2/10/26/26	0/3/3/3
3	AMP	D	602	-	-	1/10/26/26	0/3/3/3
3	AMP	A	602	-	-	1/10/26/26	0/3/3/3
3	AMP	B	602	-	-	0/10/26/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	AMP	C5-C4	5.19	1.48	1.39
3	C	602	AMP	C5-C4	5.08	1.48	1.39
3	D	602	AMP	C5-C4	5.01	1.48	1.39
3	B	602	AMP	C5-C4	4.67	1.47	1.39
3	A	602	AMP	C5-C6	3.14	1.49	1.41
3	C	602	AMP	C5-C6	3.13	1.49	1.41
3	D	602	AMP	C5-C6	3.04	1.49	1.41
3	B	602	AMP	C5-C6	2.80	1.48	1.41
3	A	602	AMP	C8-N7	2.72	1.36	1.31
3	D	602	AMP	C8-N7	2.64	1.36	1.31
3	C	602	AMP	C8-N7	2.47	1.36	1.31
3	B	602	AMP	C8-N7	2.45	1.36	1.31
3	D	602	AMP	C5-N7	-2.32	1.34	1.39
3	B	602	AMP	C5-N7	-2.13	1.35	1.39
3	C	602	AMP	C5-N7	-2.02	1.35	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	AMP	C5-C4-N3	-6.40	117.90	126.72
3	A	602	AMP	C5-C4-N3	-6.27	118.08	126.72
3	C	602	AMP	C5-C4-N3	-5.70	118.87	126.72
3	B	602	AMP	C5-C4-N3	-5.29	119.43	126.72
3	D	602	AMP	N3-C4-N9	4.69	135.15	127.17
3	A	602	AMP	N3-C4-N9	4.66	135.10	127.17
3	C	602	AMP	N3-C4-N9	4.46	134.75	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	AMP	N3-C4-N9	4.36	134.58	127.17
3	D	602	AMP	C2-N3-C4	3.98	121.56	111.83
3	A	602	AMP	C2-N3-C4	3.93	121.43	111.83
3	A	602	AMP	C4-C5-N7	-3.90	106.13	110.58
3	B	602	AMP	C4-C5-N7	-3.85	106.19	110.58
3	C	602	AMP	C2-N3-C4	3.80	121.12	111.83
3	D	602	AMP	C4-C5-N7	-3.74	106.31	110.58
3	B	602	AMP	C4-N9-C8	3.68	109.60	105.74
3	C	602	AMP	C4-C5-N7	-3.62	106.44	110.58
3	C	602	AMP	N3-C2-N1	-3.48	123.32	128.58
3	B	602	AMP	C2-N3-C4	3.40	120.12	111.83
3	A	602	AMP	N3-C2-N1	-3.20	123.73	128.58
3	B	602	AMP	N3-C2-N1	-3.16	123.79	128.58
3	D	602	AMP	N3-C2-N1	-3.16	123.80	128.58
3	A	602	AMP	O4'-C1'-N9	3.11	114.07	108.09
3	B	602	AMP	C5-N7-C8	3.09	108.30	103.45
3	B	602	AMP	N9-C8-N7	-2.83	109.92	113.94
3	A	602	AMP	C5-N7-C8	2.74	107.76	103.45
3	C	602	AMP	C4-N9-C8	2.58	108.44	105.74
3	C	602	AMP	C5-N7-C8	2.58	107.50	103.45
3	D	602	AMP	C5-N7-C8	2.54	107.44	103.45
3	B	602	AMP	C6-C5-N7	2.46	136.84	132.09
3	A	602	AMP	O3P-P-O2P	2.44	116.94	107.80
3	C	602	AMP	C6-C5-N7	2.40	136.71	132.09
3	A	602	AMP	C6-C5-N7	2.38	136.67	132.09
3	B	602	AMP	O2P-P-O5'	-2.30	100.67	106.67
3	D	602	AMP	C6-C5-N7	2.26	136.46	132.09
3	D	602	AMP	O4'-C1'-N9	2.24	112.39	108.09
3	B	602	AMP	O3P-P-O2P	2.10	115.68	107.80
3	A	602	AMP	C4-N9-C8	2.09	107.93	105.74
3	C	602	AMP	O3P-P-O2P	2.08	115.61	107.80
3	C	602	AMP	O4'-C1'-N9	2.07	112.07	108.09
3	B	602	AMP	O4'-C1'-N9	2.04	112.00	108.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

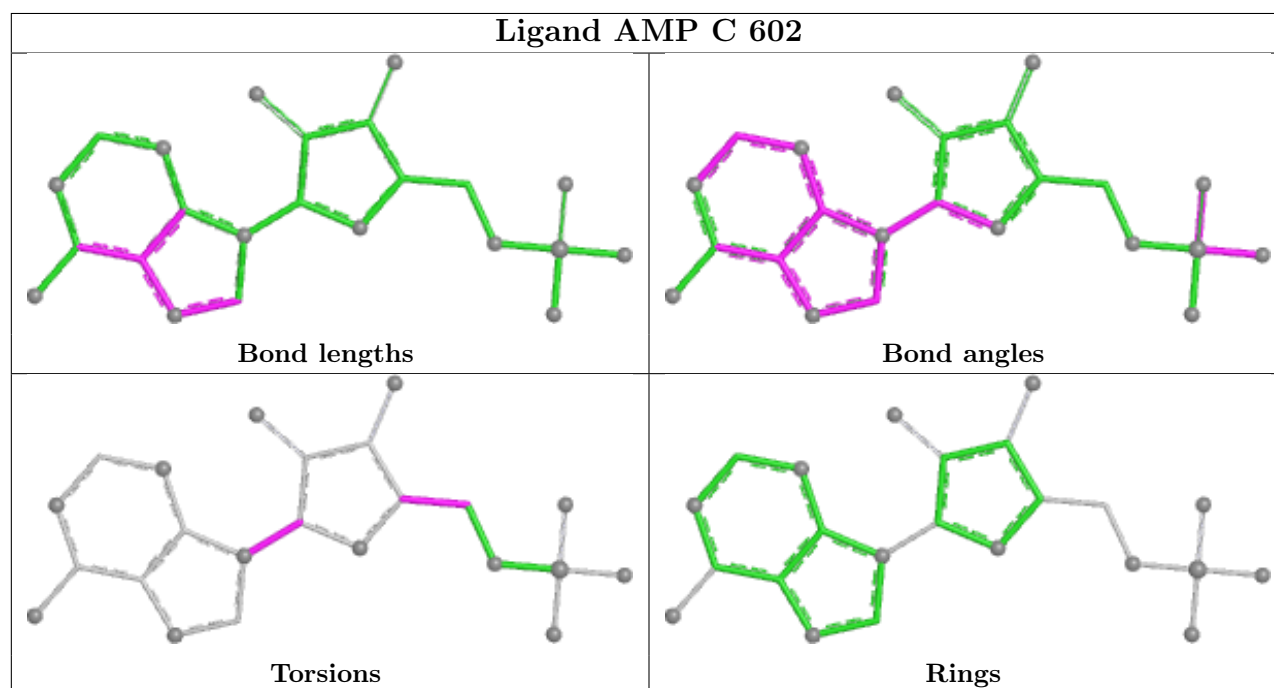
Mol	Chain	Res	Type	Atoms
3	C	602	AMP	O4'-C4'-C5'-O5'
3	C	602	AMP	C2'-C1'-N9-C8
3	A	602	AMP	O4'-C4'-C5'-O5'
3	D	602	AMP	O4'-C4'-C5'-O5'

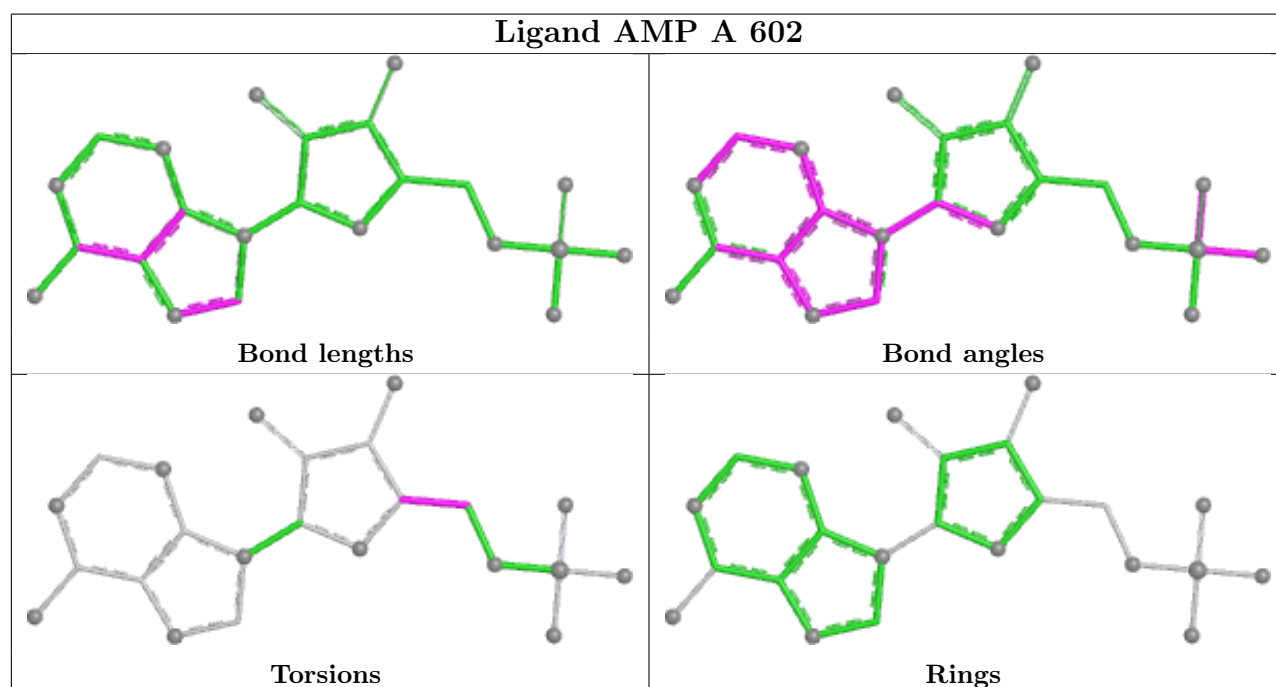
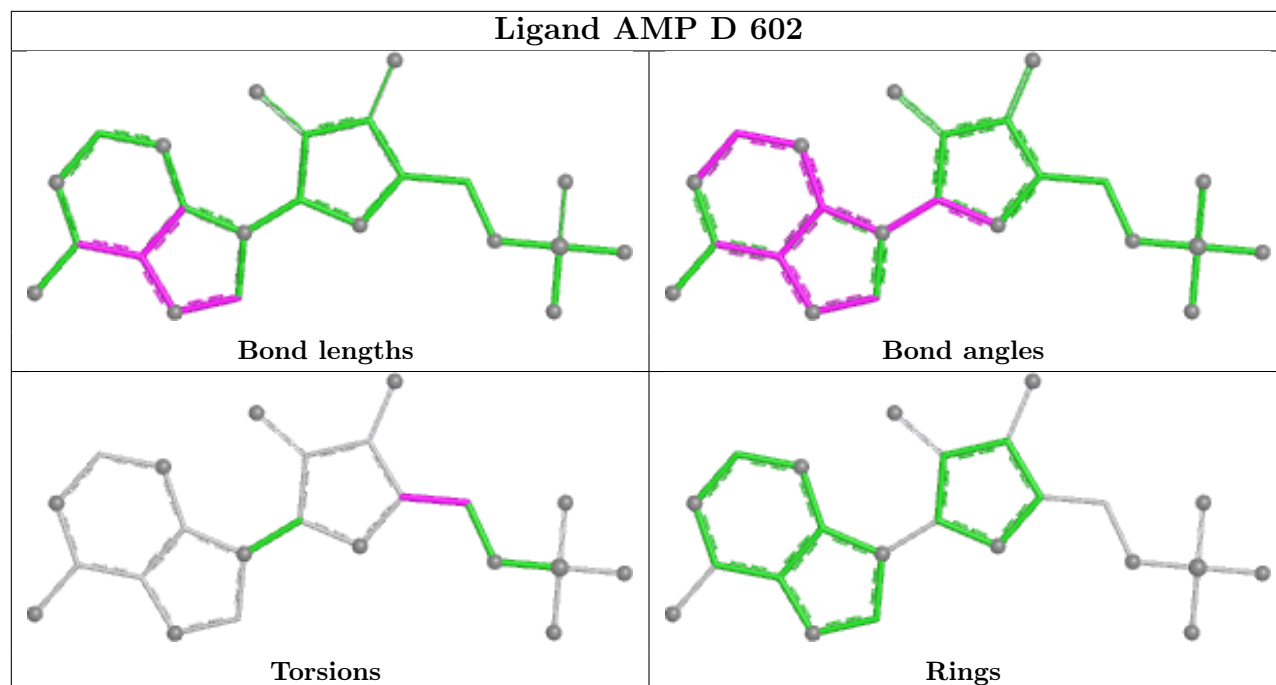
There are no ring outliers.

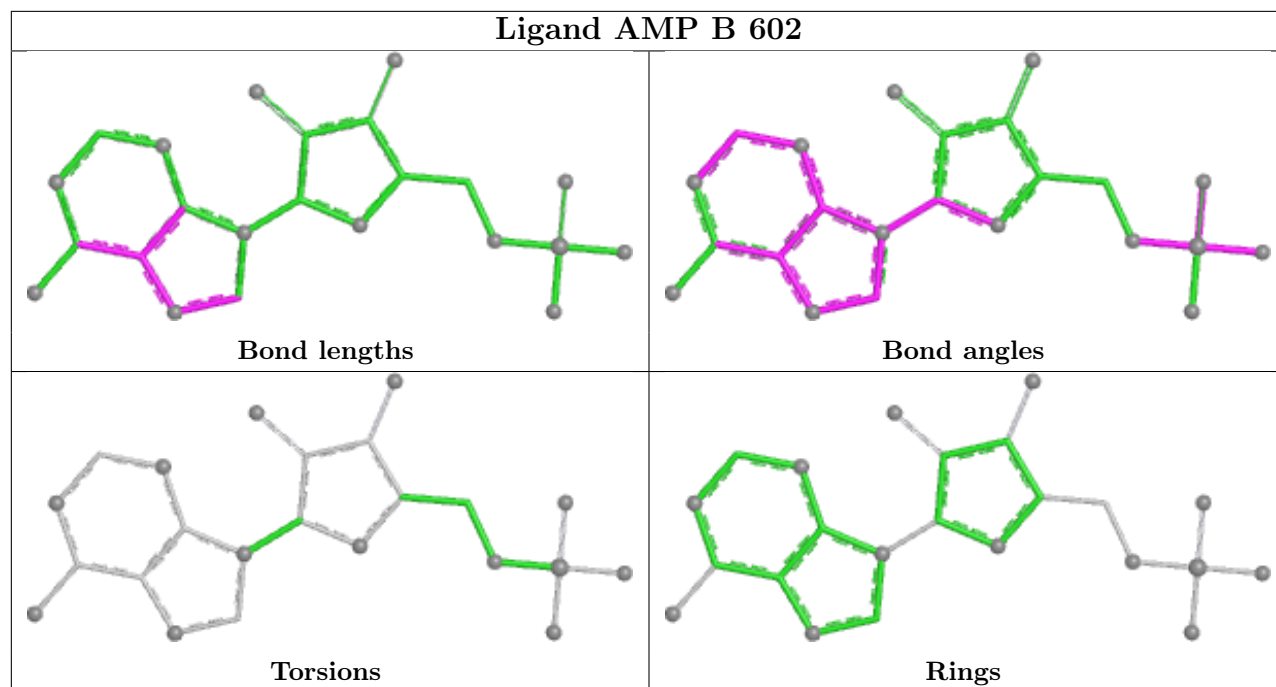
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	AMP	2	0
3	D	602	AMP	2	0
3	A	602	AMP	1	0
3	B	602	AMP	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.







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	455/462 (98%)	-0.34	1 (0%) 91 83	66, 95, 148, 228	0
1	B	455/462 (98%)	-0.40	1 (0%) 91 83	67, 96, 135, 169	0
1	C	455/462 (98%)	-0.04	1 (0%) 91 83	95, 135, 277, 306	0
1	D	455/462 (98%)	-0.07	10 (2%) 62 39	81, 129, 196, 271	0
All	All	1820/1848 (98%)	-0.21	13 (0%) 84 66	66, 113, 226, 306	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	486	SER	3.7
1	D	508	THR	3.1
1	D	483	ALA	3.1
1	A	480	LYS	2.7
1	D	484	PHE	2.5
1	D	289	GLY	2.4
1	C	507	GLU	2.2
1	D	272	PHE	2.2
1	D	290	LYS	2.2
1	D	485	LEU	2.2
1	D	287	PHE	2.2
1	B	110	ALA	2.1
1	D	303	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

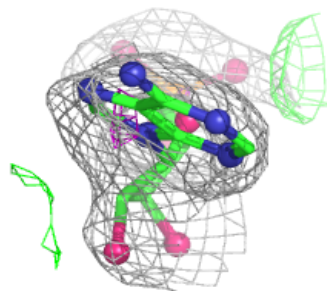
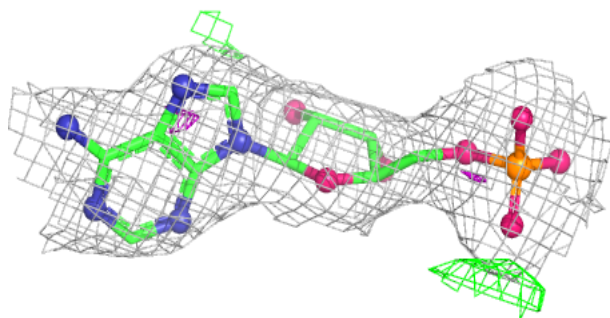
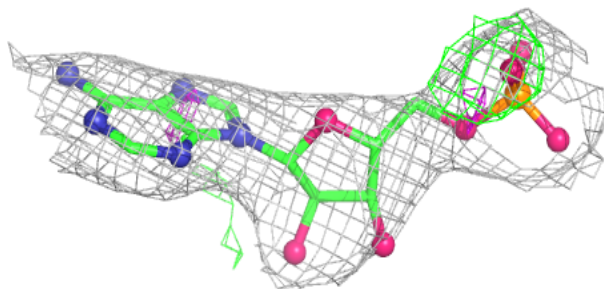
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	A	602	23/23	0.85	0.10	103,105,112,113	0
3	AMP	D	602	23/23	0.86	0.12	123,126,131,134	0
3	AMP	C	602	23/23	0.89	0.10	164,170,172,176	0
3	AMP	B	602	23/23	0.95	0.08	81,83,85,87	0
4	CA	A	604	1/1	0.98	0.04	101,101,101,101	0
4	CA	C	603	1/1	0.98	0.06	121,121,121,121	0
4	CA	B	603	1/1	0.99	0.03	106,106,106,106	0
4	CA	A	603	1/1	0.99	0.05	87,87,87,87	0
2	ZN	A	601	1/1	1.00	0.02	87,87,87,87	0
2	ZN	B	601	1/1	1.00	0.01	76,76,76,76	0
2	ZN	C	601	1/1	1.00	0.01	112,112,112,112	0
2	ZN	D	601	1/1	1.00	0.02	103,103,103,103	0

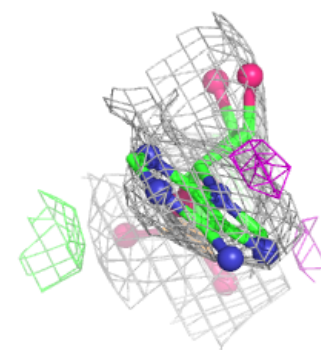
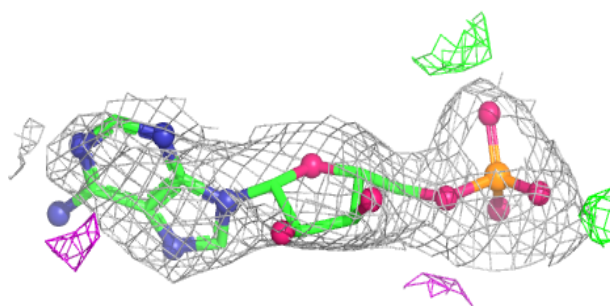
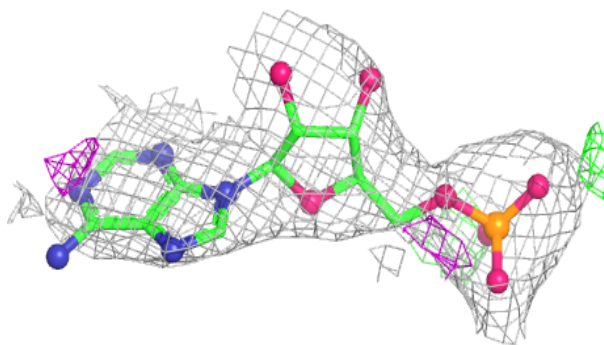
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP 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)

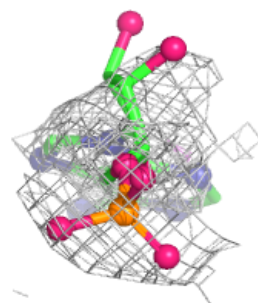
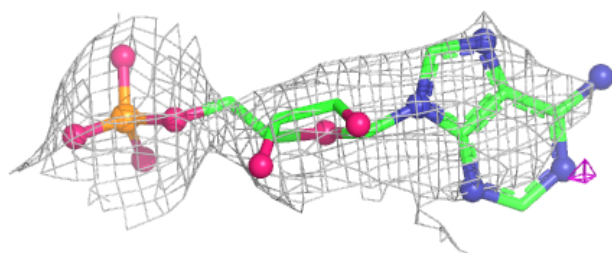
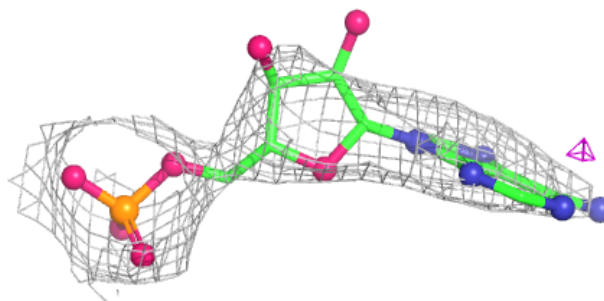
**Electron density around AMP D 602:**

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

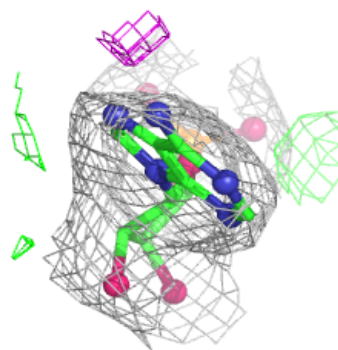
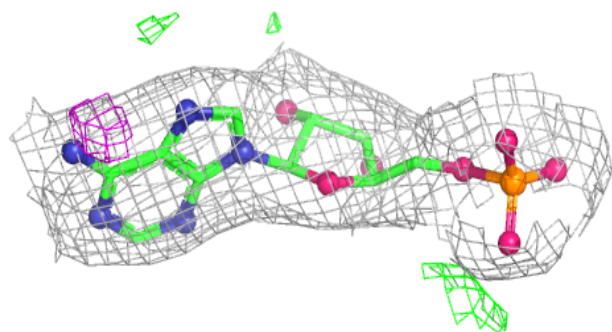
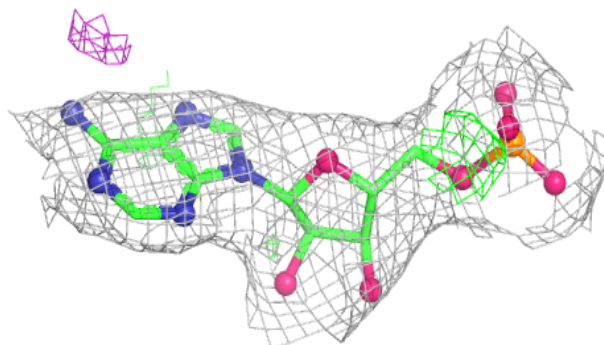


Electron density around AMP C 602:

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

**Electron density around AMP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.