



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:08 AM UTC

PDB ID : 5UYZ / pdb_00005uyz
Title : Structure of Human T-complex protein 1 subunit epsilon (CCT5) mutant His147Arg
Authors : Pereira, J.H.; McAndrew, R.P.; Sergeeva, O.A.; Ralston, C.Y.; King, J.A.; Adams, P.D.
Deposited on : 2017-02-24
Resolution : 3.60 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

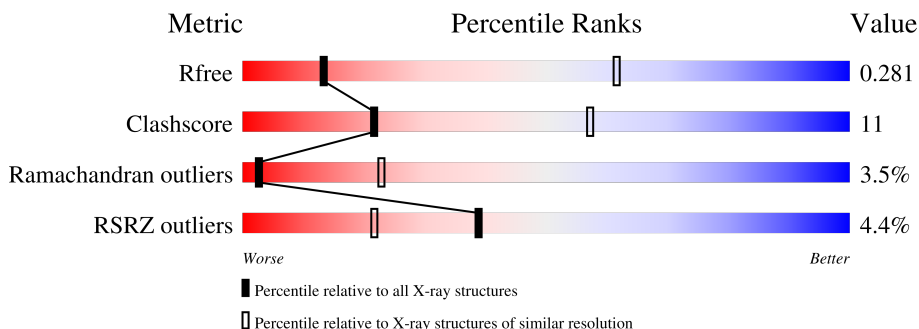
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	541	5% 71% 19% • 9%
1	B	541	3% 64% 24% • 10%
1	C	541	5% 69% 19% • 10%
1	D	541	4% 66% 18% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14962 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.

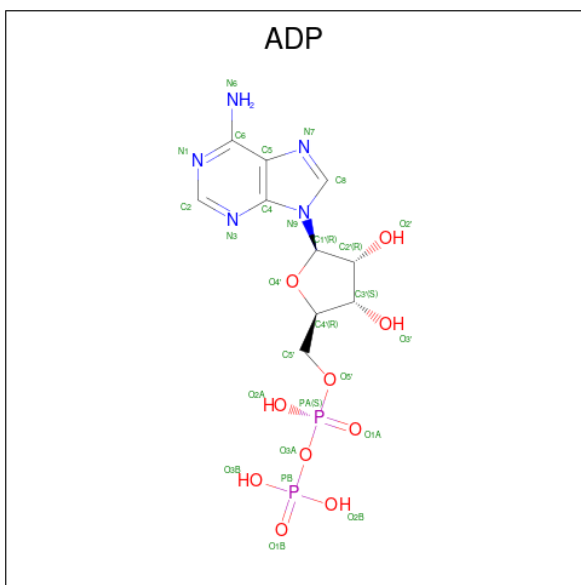
- Molecule 1 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3794	2377	658	730	29			
1	B	488	Total	C	N	O	S	0	0	0
			3758	2353	653	723	29			
1	C	488	Total	C	N	O	S	0	0	0
			3764	2359	652	725	28			
1	D	459	Total	C	N	O	S	0	0	0
			3535	2219	608	681	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ARG	HIS	engineered mutation	UNP P48643
B	147	ARG	HIS	engineered mutation	UNP P48643
C	147	ARG	HIS	engineered mutation	UNP P48643
D	147	ARG	HIS	engineered mutation	UNP P48643

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

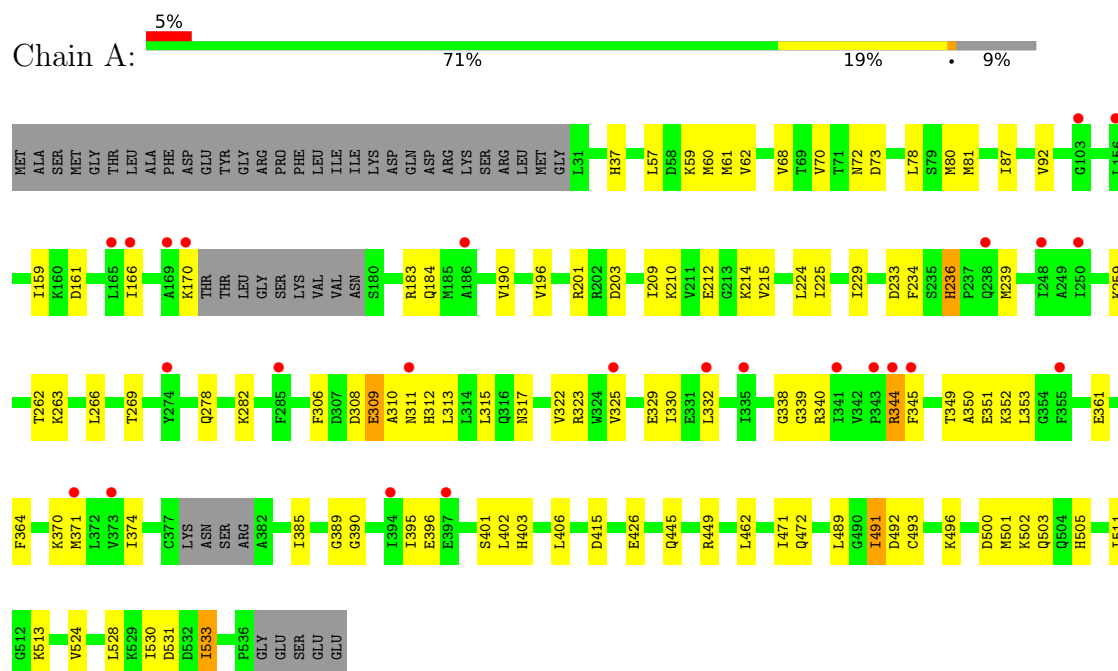
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

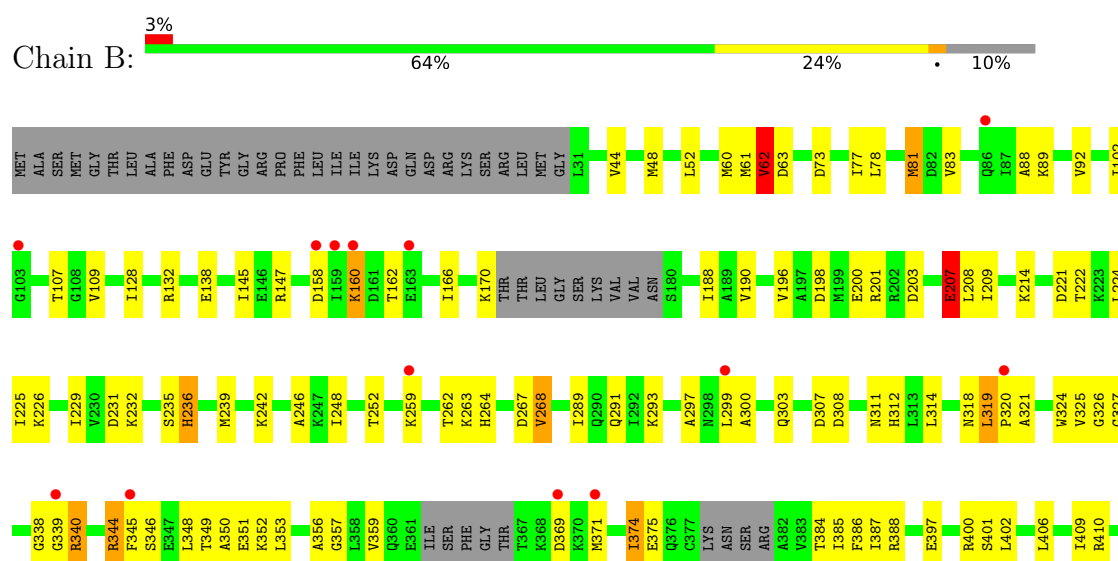
3 Residue-property plots

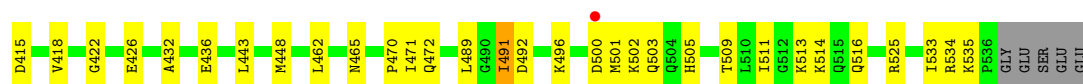
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: T-complex protein 1 subunit epsilon

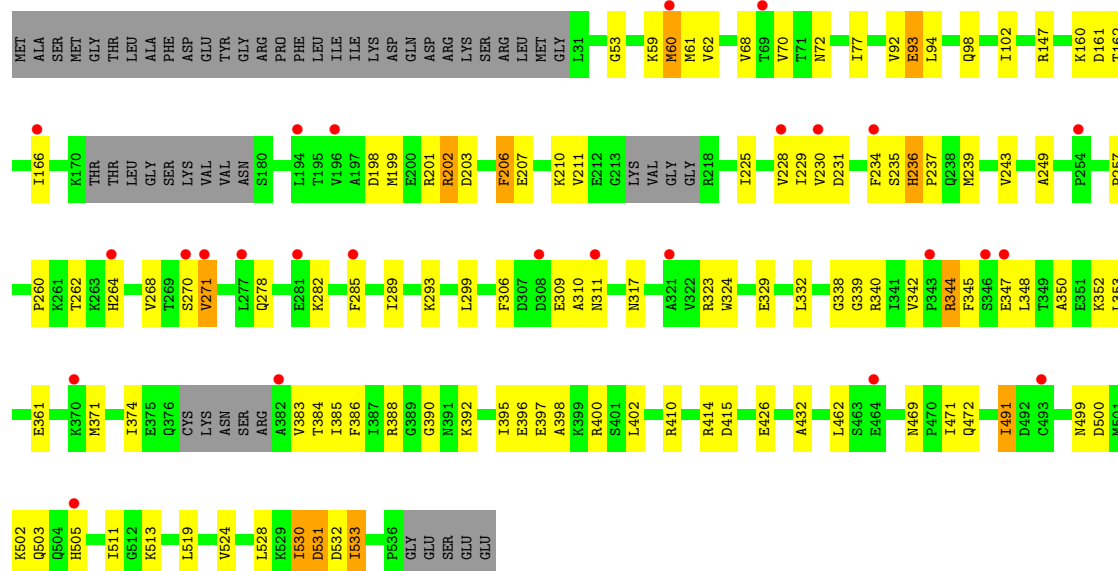


- Molecule 1: T-complex protein 1 subunit epsilon

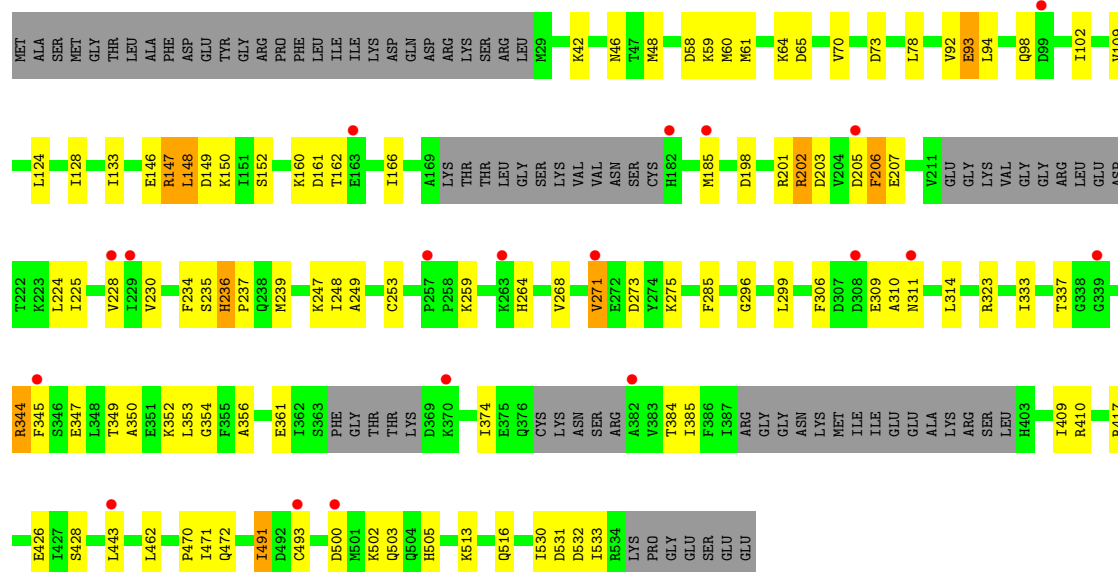




- Molecule 1: T-complex protein 1 subunit epsilon



- Molecule 1: T-complex protein 1 subunit epsilon



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	205.57Å 205.57Å 163.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.42 – 3.60 66.42 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.42-3.60) 99.9 (66.42-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.58Å)	Xtriage
Refinement program	PHENIX (dev_2650: ???)	Depositor
R, R_{free}	0.275 , 0.324 (Not available) , 0.281	Depositor DCC
R_{free} test set	2067 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	115.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 130.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14962	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, MG

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	0.16	0/3837	0.46	3/5169 (0.1%)
1	B	0.20	0/3799	0.54	6/5116 (0.1%)
1	C	0.21	1/3806 (0.0%)	0.50	2/5127 (0.0%)
1	D	0.23	0/3573	0.51	5/4816 (0.1%)
All	All	0.20	1/15015 (0.0%)	0.50	16/20228 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	257	PRO	CA-C	6.11	1.55	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	ARG	CA-C-N	6.86	134.04	121.70
1	C	344	ARG	C-N-CA	6.86	134.04	121.70
1	B	62	VAL	CA-C-N	6.76	133.87	121.70
1	B	62	VAL	C-N-CA	6.76	133.87	121.70
1	D	344	ARG	CA-C-N	6.21	132.88	121.70
1	D	344	ARG	C-N-CA	6.21	132.88	121.70
1	A	344	ARG	CA-C-N	5.97	132.44	121.70
1	A	344	ARG	C-N-CA	5.97	132.44	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ARG	CA-C-N	5.82	132.17	121.70
1	B	344	ARG	C-N-CA	5.82	132.17	121.70
1	D	147	ARG	N-CA-C	-5.77	104.62	111.03
1	A	81	MET	CB-CA-C	-5.30	109.48	115.79
1	B	207	GLU	CA-C-N	5.29	131.22	121.70
1	B	207	GLU	C-N-CA	5.29	131.22	121.70
1	D	146	GLU	CA-C-N	-5.03	113.79	120.63
1	D	146	GLU	C-N-CA	-5.03	113.79	120.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	319	LEU	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	3794	0	3901	74	0
1	B	3758	0	3865	108	0
1	C	3764	0	3867	76	0
1	D	3535	0	3624	76	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
2	D	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
All	All	14962	0	15305	326	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 (326) 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:147:ARG:O	1:D:149:ASP:N	1.96	0.98
1:D:206:PHE:HD1	1:D:207:GLU:HA	1.38	0.89
1:D:426:GLU:OE2	1:D:513:LYS:NZ	2.08	0.86
1:D:147:ARG:O	1:D:150:LYS:N	2.10	0.85
1:A:344:ARG:NH2	1:B:308:ASP:O	2.09	0.85
1:D:147:ARG:NH2	1:D:428:SER:HB3	1.94	0.81
1:B:83:VAL:HA	1:B:89:LYS:HE2	1.64	0.80
1:B:426:GLU:OE2	1:B:513:LYS:NZ	2.16	0.77
1:A:266:LEU:HD23	1:B:268:VAL:HG12	1.67	0.75
1:C:234:PHE:HB2	1:C:239:MET:SD	2.27	0.74
1:D:147:ARG:O	1:D:148:LEU:C	2.32	0.71
1:A:389:GLY:CA	1:A:395:ILE:HD11	2.21	0.71
1:D:160:LYS:O	1:D:162:THR:N	2.24	0.70
1:D:234:PHE:HB2	1:D:239:MET:SD	2.33	0.69
1:D:102:ILE:HA	1:D:410:ARG:HH12	1.57	0.69
1:D:198:ASP:OD2	1:D:202:ARG:NE	2.25	0.68
1:B:344:ARG:HA	1:B:345:PHE:HB3	1.73	0.68
1:B:397:GLU:OE1	1:B:400:ARG:NH1	2.26	0.68
1:D:201:ARG:O	1:D:203:ASP:N	2.24	0.68
1:C:225:ILE:HG21	1:C:385:ILE:HA	1.76	0.67
1:A:389:GLY:H	1:A:395:ILE:HD11	1.60	0.67
1:B:267:ASP:OD1	1:B:268:VAL:N	2.28	0.67
1:D:225:ILE:HD13	1:D:385:ILE:HA	1.75	0.66
1:C:530:ILE:HG22	1:C:531:ASP:H	1.61	0.66
1:A:266:LEU:HD23	1:B:268:VAL:CG1	2.26	0.66
1:D:147:ARG:HH22	1:D:428:SER:HB3	1.59	0.65
1:A:57:LEU:O	1:A:72:ASN:ND2	2.31	0.64
1:C:206:PHE:HD1	1:C:207:GLU:HA	1.62	0.64
1:D:462:LEU:HB3	1:D:491:ILE:HG21	1.78	0.64
1:D:224:LEU:HD23	1:D:225:ILE:H	1.62	0.64
1:C:225:ILE:HD12	1:C:383:VAL:HG12	1.79	0.64
1:C:102:ILE:O	1:C:410:ARG:NH2	2.30	0.63
1:D:225:ILE:HG21	1:D:385:ILE:HA	1.80	0.63
1:A:389:GLY:N	1:A:395:ILE:HD11	2.13	0.63
1:A:344:ARG:HA	1:A:345:PHE:HB3	1.80	0.63
1:B:166:ILE:HD11	1:B:190:VAL:HG23	1.81	0.62
1:A:462:LEU:HB3	1:A:491:ILE:HG21	1.80	0.62
1:A:225:ILE:HG21	1:A:385:ILE:HA	1.82	0.62
1:D:344:ARG:HA	1:D:345:PHE:HB3	1.81	0.61
1:B:52:LEU:O	1:B:465:ASN:ND2	2.33	0.61
1:B:462:LEU:HB3	1:B:491:ILE:HG21	1.83	0.61
1:C:237:PRO:HA	1:C:239:MET:HE2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLN:HA	1:B:324:TRP:HB2	1.81	0.60
1:A:166:ILE:HD11	1:A:190:VAL:HG23	1.82	0.60
1:A:402:LEU:HD22	1:A:406:LEU:HD21	1.84	0.60
1:B:235:SER:O	1:B:311:ASN:ND2	2.33	0.60
1:C:278:GLN:O	1:C:282:LYS:HD3	2.01	0.59
1:D:147:ARG:C	1:D:149:ASP:N	2.57	0.59
1:C:268:VAL:HG12	1:C:270:SER:H	1.66	0.59
1:D:102:ILE:HA	1:D:410:ARG:NH1	2.18	0.59
1:B:226:LYS:NZ	1:B:375:GLU:H	2.01	0.59
1:C:201:ARG:O	1:C:203:ASP:N	2.28	0.59
1:A:224:LEU:HD23	1:A:225:ILE:H	1.68	0.59
1:A:390:GLY:N	1:A:395:ILE:HD11	2.18	0.58
1:C:462:LEU:HB3	1:C:491:ILE:HG21	1.86	0.58
1:A:395:ILE:HD12	1:A:395:ILE:N	2.19	0.58
1:D:185:MET:SD	1:D:185:MET:N	2.77	0.58
1:A:344:ARG:HE	1:B:312:HIS:HB2	1.69	0.57
1:B:102:ILE:O	1:B:410:ARG:NH2	2.34	0.57
1:C:270:SER:OG	1:C:271:VAL:N	2.34	0.57
1:D:249:ALA:HA	1:D:353:LEU:HD22	1.86	0.57
1:B:289:ILE:HG23	1:B:319:LEU:HD12	1.85	0.56
1:B:222:THR:HG22	1:B:388:ARG:H	1.71	0.56
1:D:92:VAL:O	1:D:94:LEU:N	2.34	0.56
1:B:319:LEU:N	1:B:320:PRO:HD3	2.22	0.56
1:A:259:LYS:H	1:A:259:LYS:HD2	1.72	0.54
1:C:225:ILE:HD13	1:C:385:ILE:HA	1.89	0.54
1:A:201:ARG:O	1:A:203:ASP:N	2.33	0.54
1:C:426:GLU:OE2	1:C:513:LYS:NZ	2.21	0.54
1:A:170:LYS:NZ	1:A:401:SER:O	2.39	0.54
1:D:206:PHE:CD1	1:D:207:GLU:HA	2.29	0.54
1:A:210:LYS:NZ	1:A:212:GLU:OE2	2.26	0.54
1:B:188:ILE:HA	1:B:224:LEU:HD12	1.89	0.53
1:A:533:ILE:HG22	1:B:60:MET:HG3	1.89	0.53
1:C:309:GLU:O	1:C:311:ASN:N	2.42	0.53
1:A:395:ILE:HG22	1:A:396:GLU:H	1.73	0.53
1:B:166:ILE:HG12	1:B:409:ILE:HD11	1.91	0.53
1:D:531:ASP:O	1:D:533:ILE:HG23	2.10	0.53
1:A:492:ASP:OD2	1:A:496:LYS:N	2.42	0.52
1:D:268:VAL:HG13	1:D:273:ASP:HB2	1.91	0.52
1:B:357:GLY:N	1:B:374:ILE:O	2.42	0.52
1:B:344:ARG:HA	1:B:345:PHE:CB	2.39	0.52
1:B:503:GLN:C	1:B:505:HIS:H	2.18	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LYS:HZ3	1:B:375:GLU:H	1.58	0.52
1:A:395:ILE:HD12	1:A:395:ILE:H	1.75	0.52
1:D:228:VAL:HA	1:D:384:THR:HB	1.92	0.52
1:B:226:LYS:HZ1	1:B:375:GLU:N	2.08	0.52
1:B:201:ARG:O	1:B:203:ASP:N	2.36	0.52
1:C:293:LYS:NZ	1:C:317:ASN:O	2.43	0.52
1:B:170:LYS:HG2	1:B:401:SER:HB3	1.92	0.51
1:A:62:VAL:HG12	1:A:68:VAL:HG12	1.92	0.51
1:B:259:LYS:HE2	1:B:264:HIS:NE2	2.25	0.51
1:D:471:ILE:HD12	1:D:472:GLN:N	2.26	0.51
1:A:395:ILE:HG22	1:A:396:GLU:N	2.25	0.51
1:C:229:ILE:HG22	1:C:371:MET:HB3	1.93	0.51
1:B:299:LEU:HD21	1:B:359:VAL:HG21	1.93	0.51
1:D:98:GLN:O	1:D:102:ILE:N	2.44	0.51
1:A:350:ALA:HA	1:A:352:LYS:N	2.25	0.51
1:C:61:MET:HE1	1:C:77:ILE:HA	1.92	0.51
1:B:236:HIS:HB3	1:B:239:MET:HE1	1.92	0.50
1:C:92:VAL:O	1:C:94:LEU:N	2.41	0.50
1:B:231:ASP:HA	1:B:369:ASP:HB2	1.93	0.50
1:B:492:ASP:OD2	1:B:496:LYS:N	2.44	0.50
1:C:260:PRO:HG2	1:C:264:HIS:HE1	1.77	0.50
1:C:471:ILE:HD12	1:C:472:GLN:N	2.26	0.50
1:B:225:ILE:HD11	1:B:384:THR:O	2.12	0.50
1:D:306:PHE:HD2	1:D:323:ARG:HG2	1.76	0.50
1:A:306:PHE:HB3	1:A:323:ARG:HD3	1.94	0.50
1:B:226:LYS:NZ	1:B:375:GLU:N	2.59	0.50
1:B:62:VAL:HB	1:B:63:ASP:CA	2.42	0.50
1:A:350:ALA:CB	1:A:353:LEU:HG	2.41	0.50
1:B:188:ILE:HG23	1:B:224:LEU:HG	1.94	0.50
1:B:369:ASP:OD2	1:B:371:MET:HE3	2.11	0.50
1:B:349:THR:O	1:B:351:GLU:HB3	2.12	0.49
1:C:344:ARG:HA	1:C:345:PHE:HB3	1.94	0.49
1:B:235:SER:O	1:B:236:HIS:HB2	2.12	0.49
1:B:160:LYS:O	1:B:162:THR:N	2.42	0.49
1:B:246:ALA:N	1:B:356:ALA:O	2.45	0.49
1:C:414:ARG:HH12	1:C:511:ILE:HG21	1.76	0.49
1:C:329:GLU:HA	1:C:332:LEU:HB3	1.95	0.49
1:C:524:VAL:O	1:C:528:LEU:HB2	2.13	0.49
1:D:309:GLU:O	1:D:311:ASN:N	2.46	0.49
1:A:415:ASP:HB3	1:A:511:ILE:HD11	1.94	0.49
1:C:249:ALA:HA	1:C:353:LEU:HD22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:ASN:O	1:C:499:ASN:ND2	2.34	0.49
1:B:198:ASP:O	1:B:200:GLU:N	2.39	0.48
1:D:166:ILE:HG12	1:D:409:ILE:HD11	1.95	0.48
1:B:88:ALA:O	1:B:92:VAL:HG23	2.13	0.48
1:D:206:PHE:HD1	1:D:207:GLU:CA	2.18	0.48
1:A:236:HIS:NE2	1:A:315:LEU:HD22	2.28	0.48
1:C:60:MET:HA	1:C:70:VAL:HG12	1.94	0.48
1:D:337:THR:HG21	1:D:356:ALA:HB2	1.95	0.48
1:A:503:GLN:C	1:A:505:HIS:H	2.21	0.48
1:B:314:LEU:HD23	1:B:320:PRO:HA	1.96	0.48
1:C:228:VAL:HA	1:C:384:THR:HB	1.96	0.48
1:C:395:ILE:HG22	1:C:396:GLU:H	1.78	0.48
1:B:338:GLY:HA3	1:B:339:GLY:HA2	1.51	0.48
1:B:340:ARG:HB2	1:B:352:LYS:HB2	1.96	0.48
1:C:500:ASP:C	1:C:502:LYS:H	2.21	0.48
1:A:361:GLU:HA	1:A:370:LYS:HA	1.95	0.48
1:B:214:LYS:HB3	1:B:388:ARG:HH21	1.79	0.48
1:B:415:ASP:HB3	1:B:511:ILE:HD11	1.96	0.48
1:C:92:VAL:HG12	1:C:93:GLU:H	1.77	0.48
1:C:160:LYS:C	1:C:162:THR:H	2.21	0.48
1:D:503:GLN:C	1:D:505:HIS:H	2.22	0.48
1:D:205:ASP:O	1:D:206:PHE:HB2	2.14	0.47
1:B:83:VAL:HG13	1:B:89:LYS:HG3	1.96	0.47
1:B:252:THR:HA	1:B:303:GLN:HB2	1.97	0.47
1:A:224:LEU:HD23	1:A:225:ILE:N	2.29	0.47
1:D:147:ARG:HH21	1:D:428:SER:HB3	1.78	0.47
1:A:78:LEU:HD12	1:A:92:VAL:HG22	1.97	0.47
1:A:389:GLY:CA	1:A:395:ILE:CD1	2.92	0.47
1:B:226:LYS:NZ	1:B:375:GLU:HB2	2.30	0.47
1:C:206:PHE:HD1	1:C:207:GLU:CA	2.26	0.47
1:D:296:GLY:HA3	1:D:353:LEU:HD12	1.97	0.47
1:A:471:ILE:HD12	1:A:472:GLN:N	2.30	0.47
1:C:503:GLN:C	1:C:505:HIS:H	2.23	0.47
1:D:350:ALA:HB1	1:D:353:LEU:HG	1.96	0.47
1:A:61:MET:HE1	1:A:80:MET:HB2	1.97	0.46
1:A:229:ILE:HG22	1:A:371:MET:HB3	1.97	0.46
1:B:160:LYS:C	1:B:162:THR:H	2.21	0.46
1:B:221:ASP:HB3	1:B:388:ARG:HG3	1.97	0.46
1:B:371:MET:HE1	1:B:386:PHE:CE1	2.51	0.46
1:C:236:HIS:C	1:C:239:MET:HE2	2.40	0.46
1:D:344:ARG:HB3	1:D:347:GLU:H	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:HB	1:B:63:ASP:HB2	1.97	0.46
1:B:291:GLN:NE2	1:B:346:SER:O	2.48	0.46
1:B:387:ILE:O	1:B:388:ARG:NH2	2.49	0.46
1:C:350:ALA:HA	1:C:352:LYS:N	2.30	0.46
1:C:397:GLU:OE1	1:C:400:ARG:NH1	2.49	0.46
1:A:309:GLU:O	1:A:311:ASN:N	2.48	0.46
1:A:313:LEU:O	1:A:317:ASN:ND2	2.40	0.46
1:B:293:LYS:HA	1:B:297:ALA:HB2	1.97	0.46
1:C:340:ARG:HB2	1:C:352:LYS:HD2	1.98	0.46
1:A:225:ILE:HD13	1:A:385:ILE:HA	1.97	0.46
1:A:524:VAL:O	1:A:528:LEU:HB2	2.16	0.46
1:B:207:GLU:HA	1:B:209:ILE:N	2.31	0.46
1:C:533:ILE:HG12	1:D:60:MET:HB2	1.98	0.46
1:A:37:HIS:HB3	1:A:87:ILE:HG12	1.98	0.45
1:A:344:ARG:HA	1:A:345:PHE:CB	2.45	0.45
1:B:308:ASP:OD1	1:B:308:ASP:N	2.48	0.45
1:D:224:LEU:HD23	1:D:225:ILE:N	2.29	0.45
1:B:226:LYS:HD2	1:B:226:LYS:C	2.41	0.45
1:B:352:LYS:O	1:B:353:LEU:HG	2.15	0.45
1:D:237:PRO:HA	1:D:239:MET:HE2	1.98	0.45
1:C:201:ARG:C	1:C:203:ASP:H	2.22	0.45
1:B:62:VAL:HB	1:B:63:ASP:CB	2.46	0.45
1:B:259:LYS:HE2	1:B:264:HIS:CE1	2.51	0.45
1:A:403:HIS:HA	1:A:406:LEU:HD23	1.98	0.45
1:C:471:ILE:H	1:C:471:ILE:HG13	1.56	0.45
1:A:234:PHE:HB2	1:A:239:MET:SD	2.56	0.45
1:C:285:PHE:O	1:C:289:ILE:HG13	2.16	0.45
1:B:226:LYS:HD2	1:B:226:LYS:O	2.16	0.45
1:A:489:LEU:HD23	1:A:489:LEU:H	1.81	0.45
1:C:147:ARG:HG3	1:C:432:ALA:HB2	1.99	0.45
1:D:230:VAL:HG21	1:D:333:ILE:HD11	1.99	0.45
1:B:196:VAL:HG11	1:B:208:LEU:CD1	2.47	0.45
1:D:64:LYS:HB3	1:D:65:ASP:H	1.54	0.45
1:D:271:VAL:HG13	1:D:275:LYS:HD2	1.99	0.45
1:D:247:LYS:HA	1:D:354:GLY:O	2.17	0.44
1:C:162:THR:O	1:C:166:ILE:HG13	2.18	0.44
1:C:211:VAL:HG22	1:C:385:ILE:HB	1.99	0.44
1:A:325:VAL:HG13	1:A:330:ILE:HG12	1.98	0.44
1:A:390:GLY:H	1:A:395:ILE:HD11	1.81	0.44
1:B:147:ARG:HG3	1:B:432:ALA:HB2	2.00	0.44
1:C:230:VAL:HG12	1:C:231:ASP:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MET:HA	1:A:70:VAL:HG12	1.99	0.44
1:A:389:GLY:C	1:A:395:ILE:HD11	2.43	0.44
1:B:138:GLU:HB2	1:B:525:ARG:HH22	1.81	0.44
1:C:344:ARG:HB3	1:C:345:PHE:C	2.43	0.44
1:D:92:VAL:HG12	1:D:93:GLU:H	1.83	0.44
1:A:309:GLU:O	1:A:312:HIS:N	2.44	0.44
1:C:415:ASP:HB3	1:C:511:ILE:HD11	1.98	0.44
1:A:389:GLY:HA3	1:A:395:ILE:CD1	2.48	0.44
1:B:471:ILE:HD12	1:B:472:GLN:N	2.32	0.44
1:C:338:GLY:HA3	1:C:339:GLY:HA2	1.78	0.44
1:B:62:VAL:HB	1:B:63:ASP:HA	2.00	0.44
1:B:89:LYS:HD3	1:B:89:LYS:HA	1.82	0.44
1:D:78:LEU:HB3	1:D:92:VAL:HG13	1.98	0.44
1:D:253:CYS:SG	1:D:345:PHE:N	2.90	0.44
1:B:145:ILE:HG23	1:B:514:LYS:HG2	1.99	0.44
1:D:42:LYS:O	1:D:46:ASN:ND2	2.43	0.44
1:A:233:ASP:O	1:A:322:VAL:HG23	2.18	0.44
1:B:248:ILE:O	1:B:353:LEU:HB2	2.18	0.44
1:C:210:LYS:HG3	1:C:384:THR:CG2	2.47	0.44
1:D:500:ASP:C	1:D:502:LYS:H	2.26	0.44
1:C:98:GLN:HG2	1:C:519:LEU:HD11	1.99	0.43
1:A:500:ASP:C	1:A:502:LYS:H	2.26	0.43
1:B:128:ILE:HG23	1:B:443:LEU:HD23	1.99	0.43
1:C:199:MET:O	1:C:201:ARG:NE	2.49	0.43
1:D:109:VAL:HG22	1:D:516:GLN:HG2	2.00	0.43
1:A:159:ILE:O	1:A:161:ASP:N	2.52	0.43
1:A:349:THR:O	1:A:352:LYS:HG2	2.18	0.43
1:B:198:ASP:C	1:B:200:GLU:H	2.26	0.43
1:B:207:GLU:HA	1:B:209:ILE:H	1.84	0.43
1:B:350:ALA:HA	1:B:351:GLU:HB3	2.00	0.43
1:A:489:LEU:HA	1:A:501:MET:HB2	1.99	0.43
1:B:48:MET:HG3	1:B:107:THR:HG23	2.01	0.43
1:C:398:ALA:O	1:C:402:LEU:HB2	2.18	0.43
1:D:48:MET:HE1	1:D:78:LEU:HD11	2.01	0.43
1:D:124:LEU:HD12	1:D:133:ILE:HD12	2.00	0.43
1:B:307:ASP:N	1:B:307:ASP:OD1	2.51	0.43
1:C:53:GLY:N	2:C:601:ADP:O2A	2.51	0.43
1:C:160:LYS:O	1:C:162:THR:N	2.43	0.43
1:C:306:PHE:CB	1:C:323:ARG:HD3	2.49	0.43
1:B:62:VAL:HG12	1:B:63:ASP:HA	2.00	0.43
1:B:109:VAL:HG22	1:B:516:GLN:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:C	1:D:149:ASP:H	2.25	0.43
1:C:342:VAL:HG11	1:C:348:LEU:HB3	2.00	0.43
1:D:234:PHE:HE1	1:D:361:GLU:HB2	1.84	0.43
1:D:259:LYS:HD2	1:D:264:HIS:NE2	2.34	0.43
1:B:44:VAL:HG13	1:B:81:MET:HE1	2.01	0.43
1:C:62:VAL:HG12	1:C:68:VAL:HG12	2.01	0.43
1:D:530:ILE:HG23	1:D:533:ILE:HG21	2.00	0.43
1:A:338:GLY:HA3	1:A:339:GLY:HA2	1.51	0.42
1:B:422:GLY:HA3	1:B:501:MET:HE2	2.01	0.42
1:D:426:GLU:OE1	1:D:426:GLU:N	2.50	0.42
1:B:262:THR:HG22	1:B:263:LYS:H	1.84	0.42
1:B:489:LEU:HA	1:B:501:MET:HB2	2.01	0.42
1:C:262:THR:HG23	1:D:259:LYS:NZ	2.34	0.42
1:B:78:LEU:HD12	1:B:92:VAL:HG22	2.02	0.42
1:A:262:THR:HG22	1:A:263:LYS:H	1.84	0.42
1:B:318:ASN:C	1:B:320:PRO:HD3	2.44	0.42
1:D:344:ARG:HB3	1:D:345:PHE:C	2.44	0.42
1:A:214:LYS:HG2	1:A:364:PHE:CG	2.55	0.42
1:B:352:LYS:NZ	1:B:353:LEU:HD23	2.35	0.42
1:C:206:PHE:HD2	1:C:410:ARG:NE	2.17	0.42
1:B:236:HIS:HB3	1:B:239:MET:SD	2.60	0.42
1:B:300:ALA:HB3	1:B:321:ALA:HB2	2.01	0.42
1:C:201:ARG:C	1:C:203:ASP:N	2.78	0.42
1:B:436:GLU:HG2	1:B:448:MET:HE1	2.00	0.42
1:D:152:SER:HB2	1:D:417:ARG:HB3	2.00	0.42
1:D:491:ILE:HG22	1:D:493:CYS:HB2	2.02	0.42
1:B:348:LEU:HD12	1:B:348:LEU:O	2.19	0.42
1:B:236:HIS:HB3	1:B:239:MET:CE	2.50	0.42
1:B:236:HIS:HB2	1:B:311:ASN:OD1	2.20	0.42
1:C:234:PHE:HE1	1:C:361:GLU:HB2	1.85	0.42
1:D:236:HIS:C	1:D:239:MET:HE2	2.45	0.42
1:A:278:GLN:O	1:A:282:LYS:HD3	2.20	0.41
1:C:198:ASP:OD2	1:C:202:ARG:NE	2.53	0.41
1:A:445:GLN:OE1	1:A:449:ARG:NH2	2.53	0.41
1:B:402:LEU:O	1:B:406:LEU:HD22	2.19	0.41
1:B:201:ARG:C	1:B:203:ASP:H	2.26	0.41
1:B:418:VAL:HG12	1:B:509:THR:HA	2.03	0.41
1:C:230:VAL:HG12	1:C:231:ASP:N	2.34	0.41
1:D:58:ASP:HB3	1:D:70:VAL:HB	2.03	0.41
1:D:344:ARG:HA	1:D:345:PHE:CB	2.48	0.41
1:A:471:ILE:H	1:A:471:ILE:HG13	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HG11	1:B:208:LEU:HD12	2.02	0.41
1:C:237:PRO:CA	1:C:239:MET:HE2	2.50	0.41
1:A:329:GLU:HA	1:A:332:LEU:HD12	2.02	0.41
1:A:531:ASP:OD1	1:A:531:ASP:N	2.52	0.41
1:C:243:VAL:HG11	1:C:299:LEU:HB3	2.01	0.41
1:D:206:PHE:HA	1:D:207:GLU:HA	1.94	0.41
1:A:426:GLU:OE2	1:A:513:LYS:NZ	2.23	0.41
1:B:132:ARG:HD3	1:B:443:LEU:HD22	2.02	0.41
1:C:230:VAL:HG13	1:C:329:GLU:HG2	2.01	0.41
1:D:350:ALA:HA	1:D:352:LYS:N	2.35	0.41
1:A:350:ALA:HA	1:A:351:GLU:C	2.45	0.41
1:B:229:ILE:HG22	1:B:371:MET:HB3	2.03	0.41
1:C:323:ARG:HA	1:C:324:TRP:HA	1.79	0.41
1:D:206:PHE:CD1	1:D:207:GLU:HG2	2.56	0.41
1:D:285:PHE:HE1	1:D:314:LEU:HD11	1.86	0.41
1:D:344:ARG:HG2	1:D:347:GLU:CB	2.51	0.41
1:C:530:ILE:HG12	1:D:58:ASP:HB2	2.02	0.41
1:D:248:ILE:HG13	1:D:299:LEU:HD11	2.03	0.41
1:A:325:VAL:HG21	1:A:329:GLU:HB2	2.03	0.41
1:C:386:PHE:HE2	1:C:388:ARG:HE	1.69	0.41
1:C:390:GLY:C	1:C:392:LYS:H	2.29	0.41
1:C:395:ILE:O	1:C:396:GLU:HB3	2.21	0.41
1:D:128:ILE:HG23	1:D:443:LEU:HD23	2.02	0.41
1:A:196:VAL:HB	1:A:209:ILE:HD11	2.02	0.41
1:B:500:ASP:HB3	1:B:502:LYS:HG3	2.03	0.41
1:A:370:LYS:O	1:A:370:LYS:HG3	2.21	0.40
1:A:492:ASP:N	1:A:493:CYS:HA	2.36	0.40
1:B:147:ARG:HG3	1:B:432:ALA:CB	2.51	0.40
1:B:385:ILE:HG22	1:B:386:PHE:H	1.86	0.40
1:D:349:THR:O	1:D:352:LYS:HG2	2.19	0.40
1:B:471:ILE:H	1:B:471:ILE:HG13	1.64	0.40
1:C:344:ARG:CB	1:C:347:GLU:HB3	2.50	0.40
1:D:92:VAL:C	1:D:94:LEU:H	2.28	0.40
1:A:183:ARG:HG3	1:A:184:GLN:N	2.36	0.40
1:B:61:MET:CE	1:B:77:ILE:HG23	2.52	0.40
1:B:162:THR:O	1:B:166:ILE:HG13	2.22	0.40
1:C:160:LYS:HB3	1:C:161:ASP:H	1.71	0.40
1:C:469:ASN:HB3	1:C:472:GLN:HB3	2.03	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	466/541 (86%)	396 (85%)	57 (12%)	13 (3%)	4	26
1	B	480/541 (89%)	392 (82%)	68 (14%)	20 (4%)	2	19
1	C	480/541 (89%)	394 (82%)	70 (15%)	16 (3%)	3	24
1	D	447/541 (83%)	368 (82%)	63 (14%)	16 (4%)	2	22
All	All	1873/2164 (87%)	1550 (83%)	258 (14%)	65 (4%)	3	23

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	ALA
1	B	236	HIS
1	B	325	VAL
1	B	534	ARG
1	C	206	PHE
1	C	310	ALA
1	C	530	ILE
1	C	531	ASP
1	D	148	LEU
1	D	161	ASP
1	D	202	ARG
1	D	206	PHE
1	D	310	ALA
1	B	62	VAL
1	B	81	MET
1	C	72	ASN
1	C	93	GLU
1	C	202	ARG
1	D	271	VAL
1	A	59	LYS
1	A	308	ASP
1	A	309	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	533	ILE
1	B	326	GLY
1	B	533	ILE
1	C	59	LYS
1	C	60	MET
1	C	271	VAL
1	D	59	LYS
1	D	93	GLU
1	A	269	THR
1	A	491	ILE
1	B	158	ASP
1	B	160	LYS
1	B	232	LYS
1	B	268	VAL
1	B	491	ILE
1	C	491	ILE
1	C	532	ASP
1	D	491	ILE
1	D	532	ASP
1	A	73	ASP
1	A	215	VAL
1	A	340	ARG
1	A	530	ILE
1	B	73	ASP
1	B	207	GLU
1	B	242	LYS
1	B	327	GLY
1	B	340	ARG
1	B	374	ILE
1	C	236	HIS
1	D	235	SER
1	D	236	HIS
1	C	235	SER
1	C	533	ILE
1	D	61	MET
1	D	73	ASP
1	A	236	HIS
1	A	374	ILE
1	C	374	ILE
1	D	470	PRO
1	D	374	ILE
1	B	535	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	470	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 7 ligands modelled in this entry, 3 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	$\# Z > 2$
2	ADP	A	601	3	28,29,29	1.44	5 (17%)	43,45,45	1.88	10 (23%)
2	ADP	B	601	3	28,29,29	1.43	5 (17%)	43,45,45	1.90	10 (23%)
2	ADP	D	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.89	10 (23%)
2	ADP	C	601	3	28,29,29	1.44	5 (17%)	43,45,45	1.89	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	A	601	3	-	4/16/32/32	0/3/3/3
2	ADP	B	601	3	-	3/16/32/32	0/3/3/3
2	ADP	D	601	-	-	4/16/32/32	0/3/3/3
2	ADP	C	601	3	-	4/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	C5-C4	4.67	1.47	1.39
2	C	601	ADP	C5-C4	4.63	1.47	1.39
2	D	601	ADP	C5-C4	4.63	1.47	1.39
2	B	601	ADP	C5-C4	4.60	1.47	1.39
2	D	601	ADP	C5-C6	2.76	1.48	1.41
2	C	601	ADP	C5-C6	2.75	1.48	1.41
2	B	601	ADP	C5-C6	2.74	1.48	1.41
2	A	601	ADP	C5-C6	2.73	1.48	1.41
2	C	601	ADP	C8-N7	2.45	1.36	1.31
2	B	601	ADP	C8-N7	2.43	1.36	1.31
2	D	601	ADP	C8-N7	2.43	1.36	1.31
2	A	601	ADP	C8-N7	2.39	1.36	1.31
2	A	601	ADP	C5-N7	-2.31	1.34	1.39
2	D	601	ADP	PA-O3A	2.30	1.62	1.59
2	B	601	ADP	C5-N7	-2.29	1.34	1.39
2	C	601	ADP	PA-O3A	2.28	1.62	1.59
2	A	601	ADP	PA-O3A	2.27	1.62	1.59
2	C	601	ADP	C5-N7	-2.25	1.35	1.39
2	D	601	ADP	C5-N7	-2.25	1.35	1.39
2	B	601	ADP	PA-O3A	2.20	1.61	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-6.01	118.45	126.72
2	A	601	ADP	C5-C4-N3	-5.94	118.54	126.72
2	C	601	ADP	C5-C4-N3	-5.87	118.64	126.72
2	D	601	ADP	C5-C4-N3	-5.85	118.67	126.72
2	A	601	ADP	N3-C4-N9	4.54	134.89	127.17
2	B	601	ADP	N3-C4-N9	4.53	134.88	127.17
2	C	601	ADP	N3-C4-N9	4.42	134.69	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ADP	N3-C4-N9	4.41	134.67	127.17
2	D	601	ADP	C4-C5-N7	-3.76	106.28	110.58
2	C	601	ADP	C4-C5-N7	-3.76	106.28	110.58
2	B	601	ADP	C4-C5-N7	-3.76	106.29	110.58
2	B	601	ADP	C2-N3-C4	3.74	120.97	111.83
2	C	601	ADP	C2-N3-C4	3.73	120.95	111.83
2	A	601	ADP	C2-N3-C4	3.73	120.95	111.83
2	D	601	ADP	C2-N3-C4	3.73	120.94	111.83
2	A	601	ADP	C4-C5-N7	-3.71	106.33	110.58
2	D	601	ADP	N3-C2-N1	-3.30	123.59	128.58
2	C	601	ADP	N3-C2-N1	-3.28	123.61	128.58
2	A	601	ADP	N3-C2-N1	-3.26	123.64	128.58
2	B	601	ADP	N3-C2-N1	-3.19	123.75	128.58
2	B	601	ADP	O4'-C1'-N9	2.88	113.63	108.09
2	C	601	ADP	O4'-C1'-N9	2.86	113.57	108.09
2	D	601	ADP	O4'-C1'-N9	2.85	113.56	108.09
2	B	601	ADP	C5-N7-C8	2.75	107.78	103.45
2	A	601	ADP	C5-N7-C8	2.75	107.77	103.45
2	C	601	ADP	C5-N7-C8	2.75	107.77	103.45
2	D	601	ADP	C5-N7-C8	2.73	107.74	103.45
2	A	601	ADP	O4'-C1'-N9	2.68	113.23	108.09
2	C	601	ADP	C4-N9-C8	2.56	108.42	105.74
2	A	601	ADP	C4-N9-C8	2.51	108.38	105.74
2	D	601	ADP	C4-N9-C8	2.51	108.37	105.74
2	B	601	ADP	C4-N9-C8	2.47	108.33	105.74
2	D	601	ADP	C6-C5-N7	2.20	136.34	132.09
2	C	601	ADP	C6-C5-N7	2.19	136.31	132.09
2	C	601	ADP	N9-C8-N7	-2.17	110.85	113.94
2	A	601	ADP	C6-C5-N7	2.13	136.19	132.09
2	B	601	ADP	N9-C8-N7	-2.12	110.93	113.94
2	D	601	ADP	N9-C8-N7	-2.11	110.94	113.94
2	A	601	ADP	N9-C8-N7	-2.11	110.95	113.94
2	B	601	ADP	C6-C5-N7	2.06	136.06	132.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	O4'-C4'-C5'-O5'
2	D	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

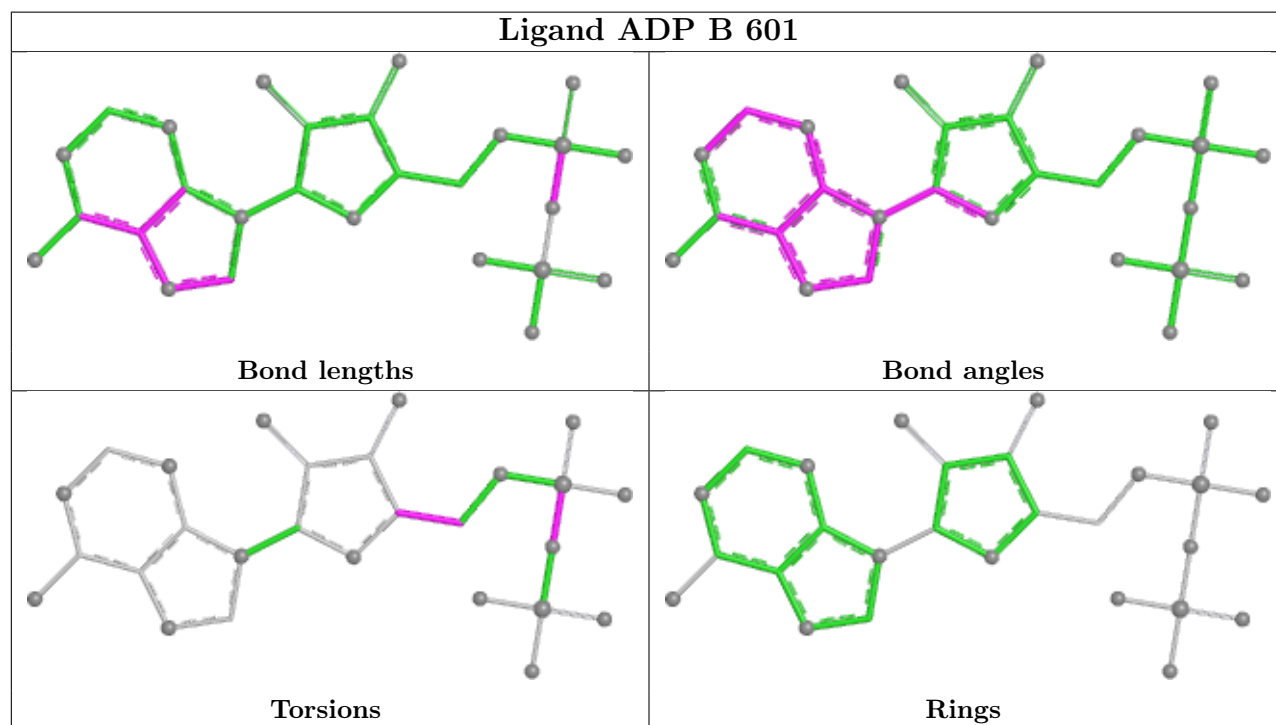
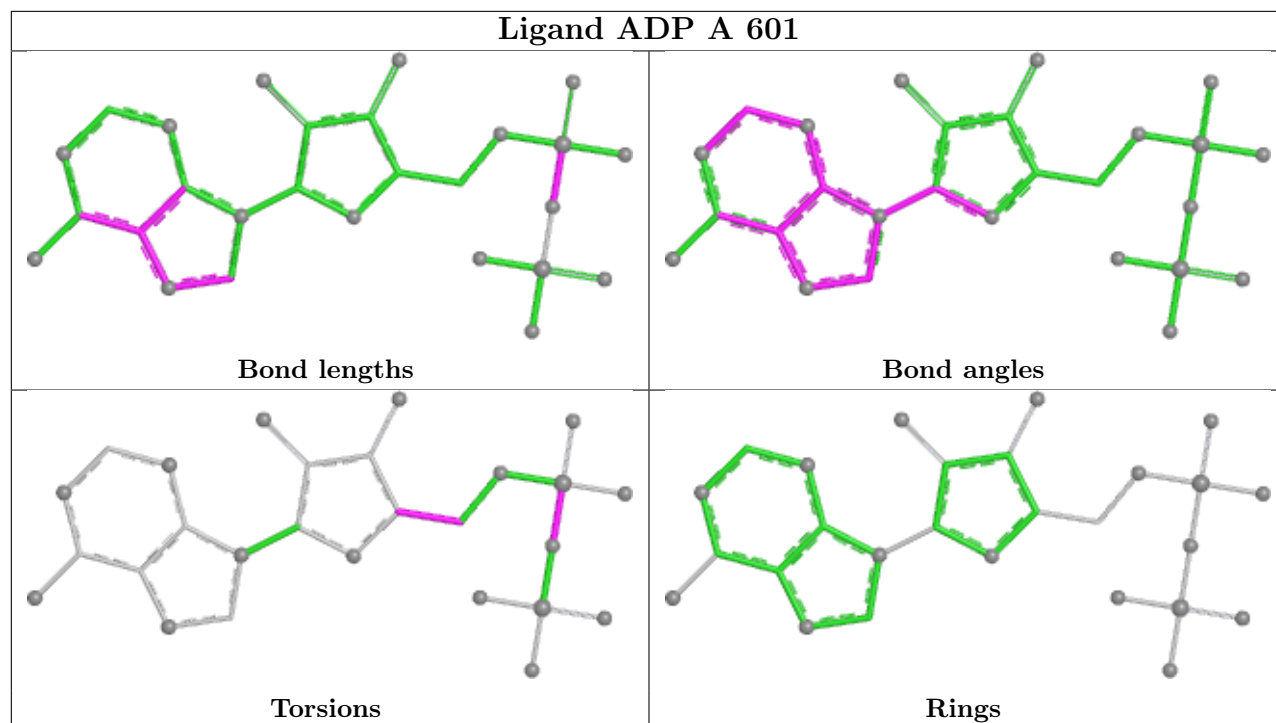
Mol	Chain	Res	Type	Atoms
2	D	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	PB-O3A-PA-O5'
2	B	601	ADP	PB-O3A-PA-O5'
2	C	601	ADP	PB-O3A-PA-O5'
2	D	601	ADP	PB-O3A-PA-O5'
2	A	601	ADP	PB-O3A-PA-O1A
2	C	601	ADP	PB-O3A-PA-O2A
2	D	601	ADP	PB-O3A-PA-O2A

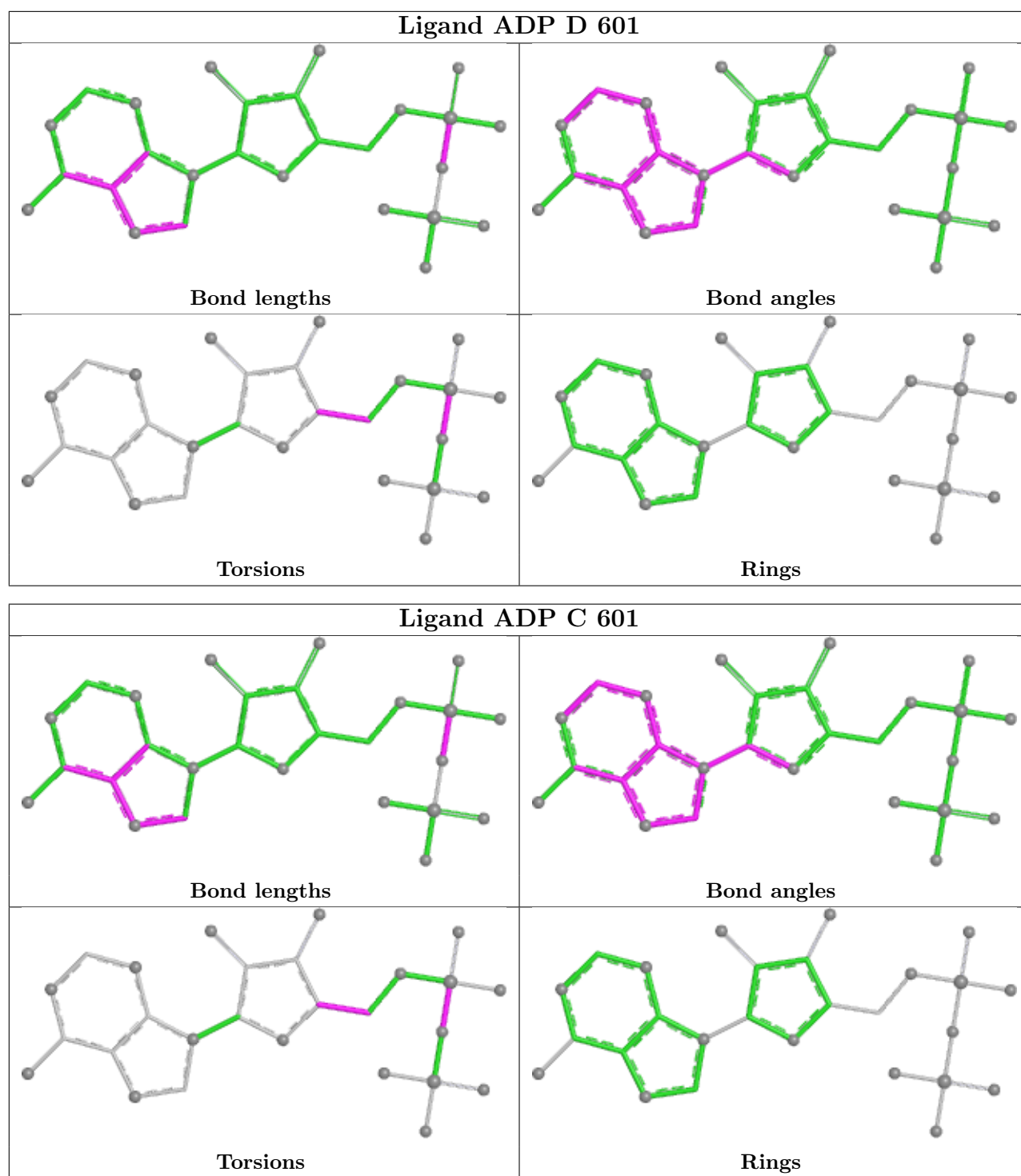
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	493/541 (91%)	0.42	25 (5%)	33 19	43, 124, 216, 273	0
1	B	488/541 (90%)	0.35	14 (2%)	53 30	34, 100, 183, 249	0
1	C	488/541 (90%)	0.44	26 (5%)	32 19	50, 127, 225, 302	0
1	D	459/541 (84%)	0.39	19 (4%)	41 23	44, 127, 204, 286	0
All	All	1928/2164 (89%)	0.40	84 (4%)	39 22	34, 119, 213, 302	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	VAL	5.8
1	D	370	LYS	5.6
1	C	370	LYS	5.3
1	C	60	MET	4.1
1	A	341	ILE	4.0
1	A	103	GLY	3.9
1	B	371	MET	3.6
1	C	228	VAL	3.5
1	C	271	VAL	3.4
1	B	500	ASP	3.4
1	D	311	ASN	3.4
1	C	311	ASN	3.3
1	A	343	PRO	3.2
1	A	394	ILE	3.1
1	A	238	GLN	3.0
1	A	311	ASN	3.0
1	A	332	LEU	3.0
1	D	271	VAL	2.9
1	A	166	ILE	2.9
1	C	308	ASP	2.9
1	D	185	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	196	VAL	2.9
1	C	285	PHE	2.9
1	A	186	ALA	2.8
1	C	270	SER	2.8
1	C	321	ALA	2.8
1	A	371	MET	2.8
1	C	194	LEU	2.8
1	C	281	GLU	2.8
1	A	165	LEU	2.7
1	D	229	ILE	2.7
1	B	259	LYS	2.7
1	A	344	ARG	2.7
1	D	493	CYS	2.7
1	D	205	ASP	2.6
1	D	345	PHE	2.6
1	A	169	ALA	2.5
1	C	254	PRO	2.5
1	B	345	PHE	2.4
1	A	345	PHE	2.4
1	A	335	ILE	2.4
1	A	397	GLU	2.4
1	C	382	ALA	2.4
1	B	160	LYS	2.4
1	A	250	ILE	2.4
1	B	86	GLN	2.3
1	C	230	VAL	2.3
1	D	339	GLY	2.3
1	B	163	GLU	2.3
1	C	166	ILE	2.3
1	C	346	SER	2.3
1	B	103	GLY	2.3
1	C	464	GLU	2.2
1	B	339	GLY	2.2
1	B	299	LEU	2.2
1	A	248	ILE	2.2
1	C	505	HIS	2.2
1	A	170	LYS	2.2
1	A	274	TYR	2.2
1	C	277	LEU	2.2
1	A	325	VAL	2.2
1	B	159	ILE	2.2
1	D	308	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	443	LEU	2.2
1	D	99	ASP	2.1
1	D	182	HIS	2.1
1	C	69	THR	2.1
1	B	369	ASP	2.1
1	C	264	HIS	2.1
1	A	355	PHE	2.1
1	D	382	ALA	2.1
1	C	234	PHE	2.1
1	B	158	ASP	2.1
1	C	347	GLU	2.1
1	A	373	VAL	2.1
1	C	343	PRO	2.1
1	C	493	CYS	2.1
1	D	263	LYS	2.1
1	A	156	LEU	2.1
1	B	320	PRO	2.0
1	A	285	PHE	2.0
1	D	257	PRO	2.0
1	D	163	GLU	2.0
1	D	500	ASP	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.

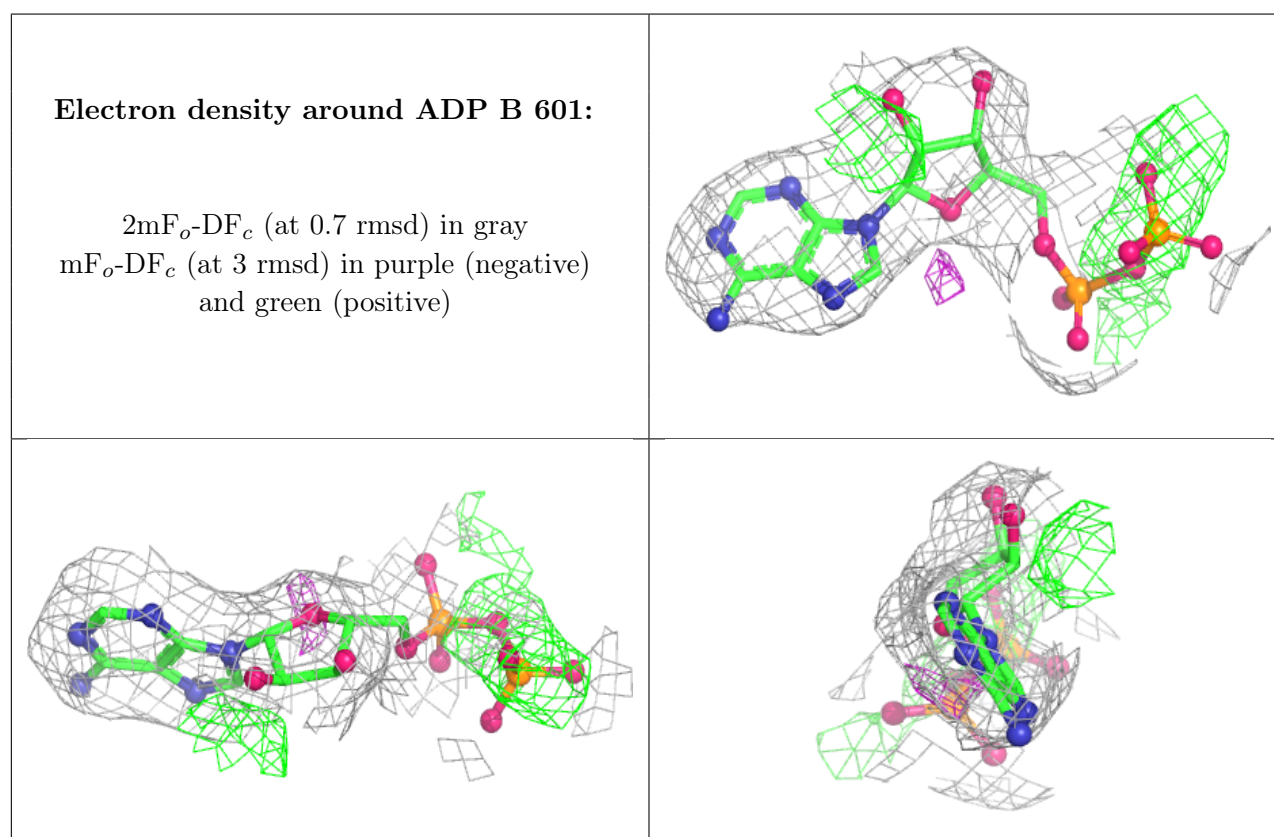
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	602	1/1	0.76	0.18	107,107,107,107	0
3	MG	A	602	1/1	0.87	0.13	134,134,134,134	0

Continued on next page...

Continued from previous page...

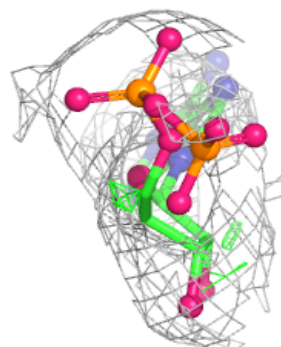
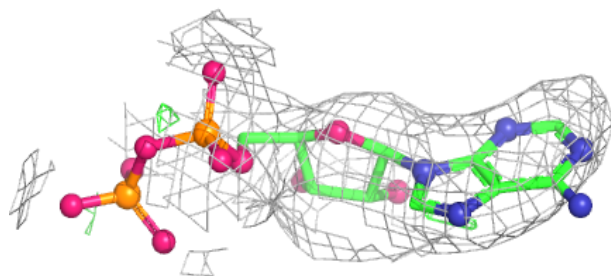
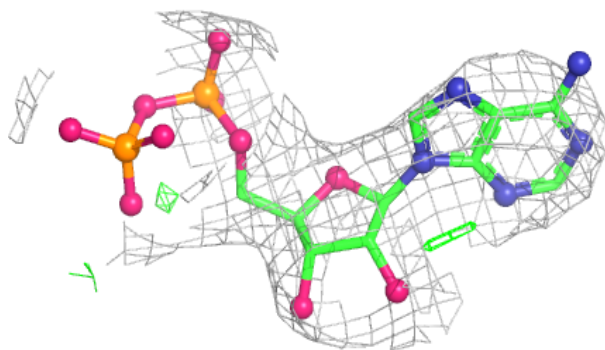
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	B	601	27/27	0.87	0.14	43,69,131,140	0
2	ADP	D	601	27/27	0.90	0.12	83,104,128,133	0
3	MG	B	602	1/1	0.92	0.12	132,132,132,132	0
2	ADP	A	601	27/27	0.93	0.08	62,71,121,130	0
2	ADP	C	601	27/27	0.94	0.10	61,92,109,122	0

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.

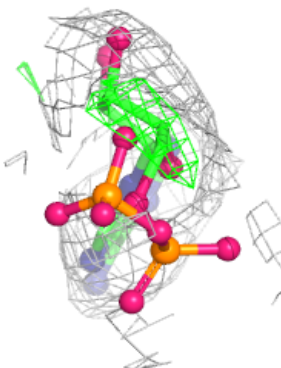
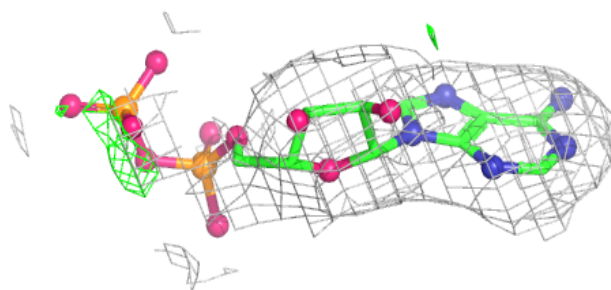
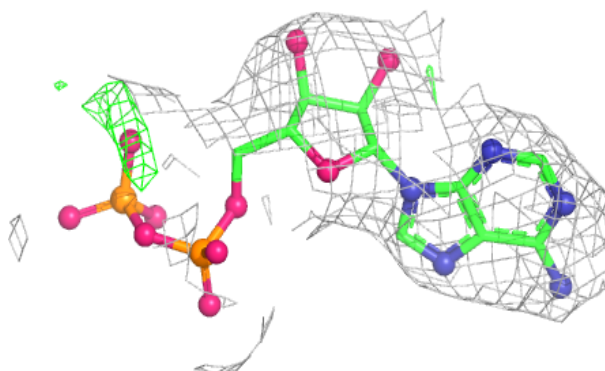


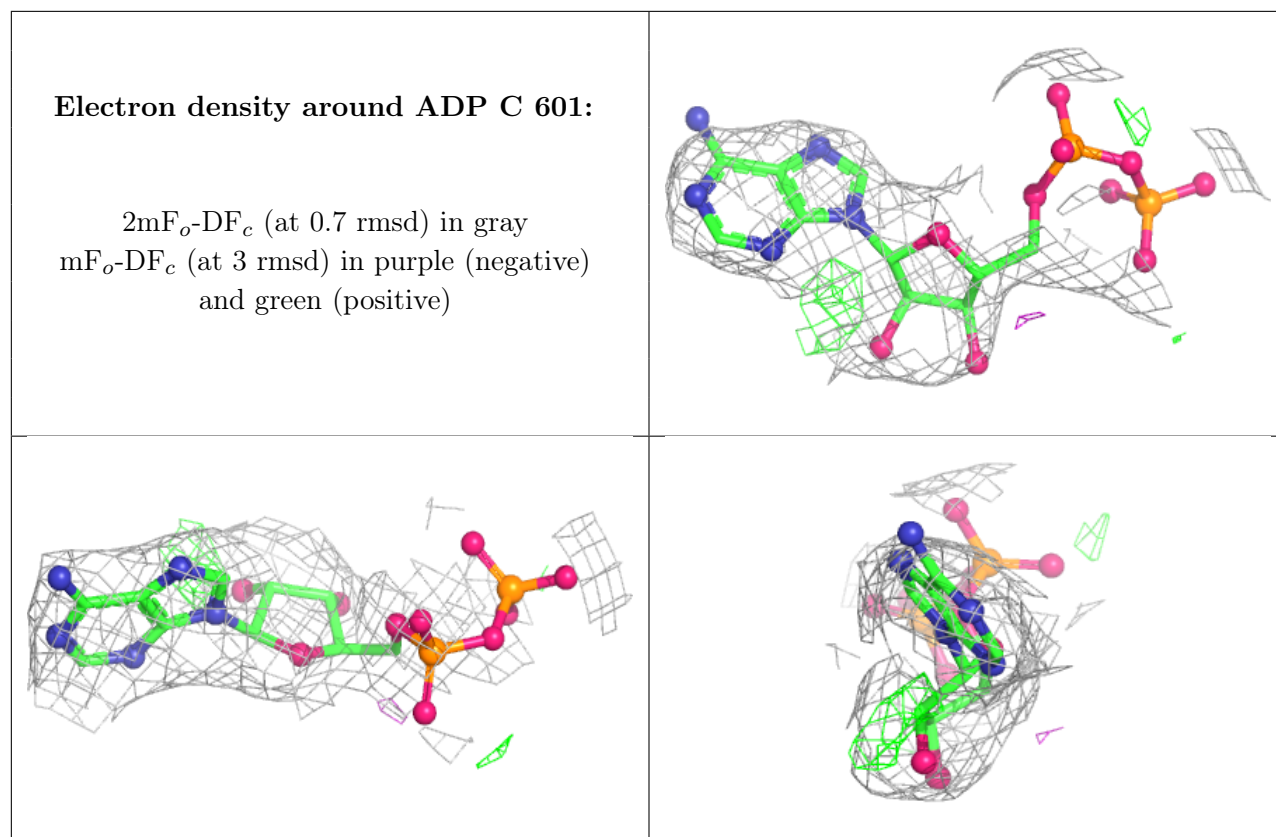
Electron density around ADP D 601:

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

**Electron density around 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.