



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:28 PM BST

PDB ID : 5UYZ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

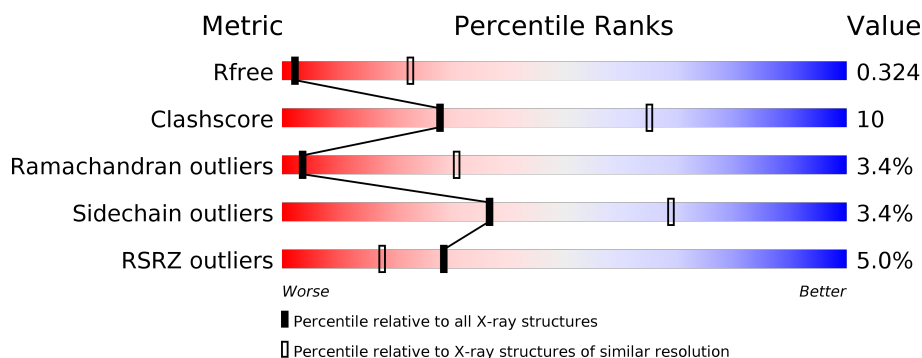
1 Overall quality at a glance

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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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 on 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	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	541	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>24%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	541	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	541	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>17%</div> <div>•</div> <div>15%</div> </div> </div>

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 (three-letter code: 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

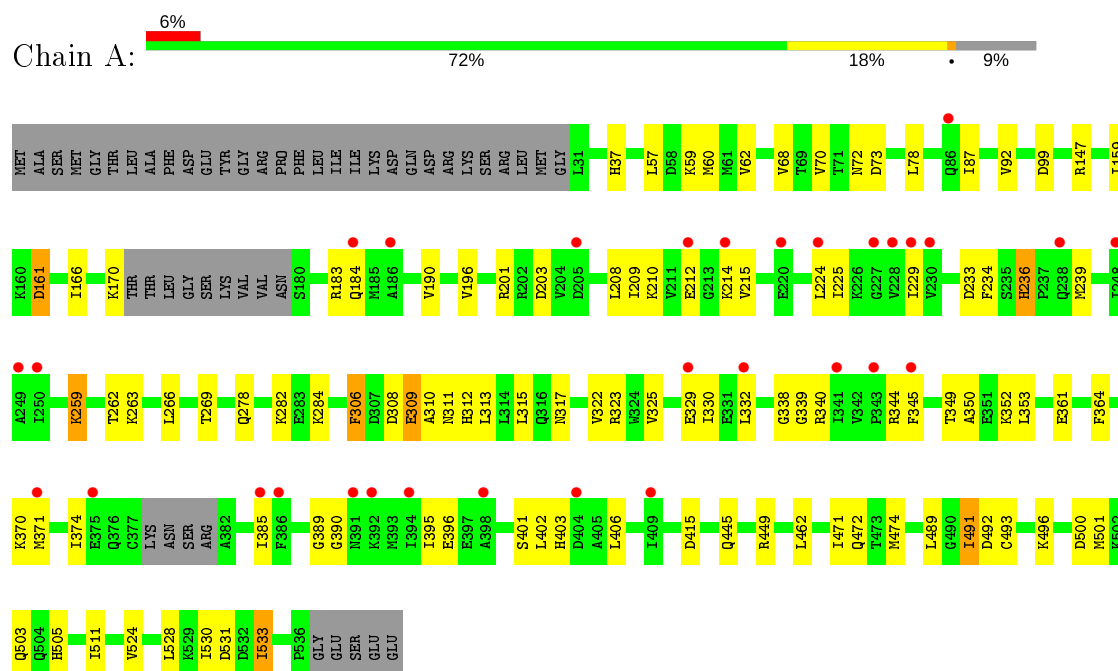
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

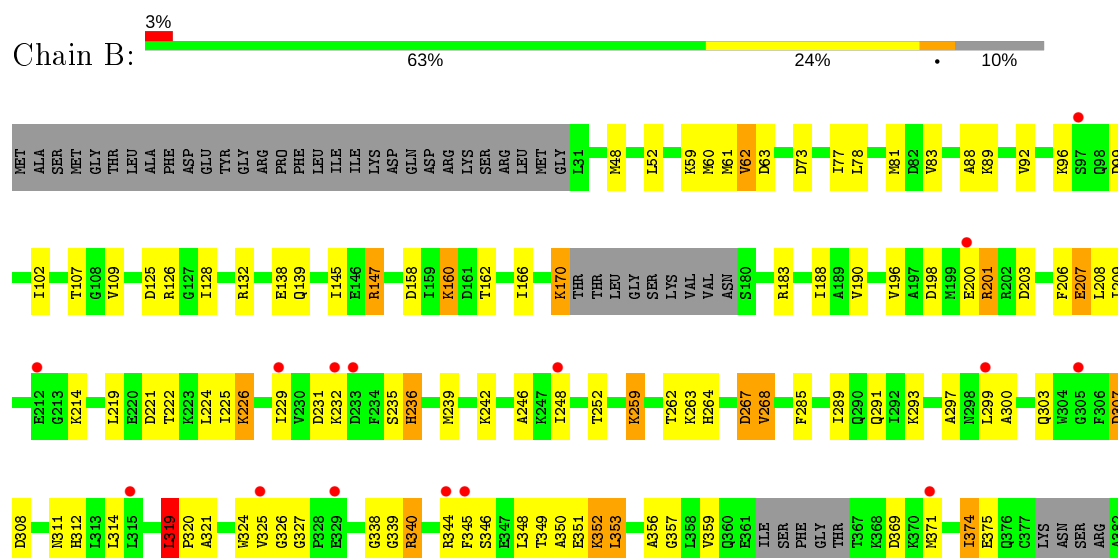
3 Residue-property plots [i](#)

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.

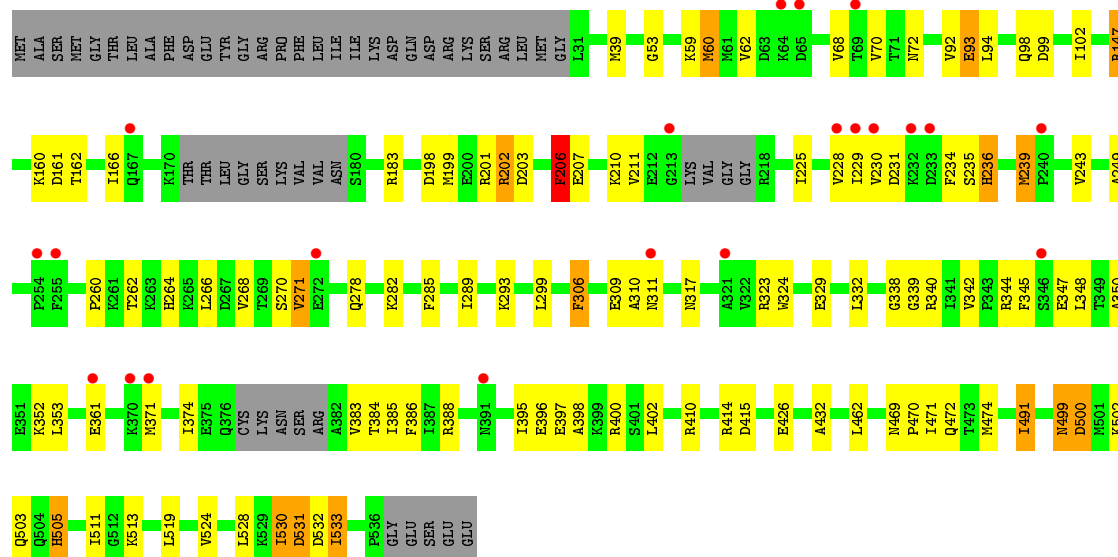
- Molecule 1: T-complex protein 1 subunit epsilon



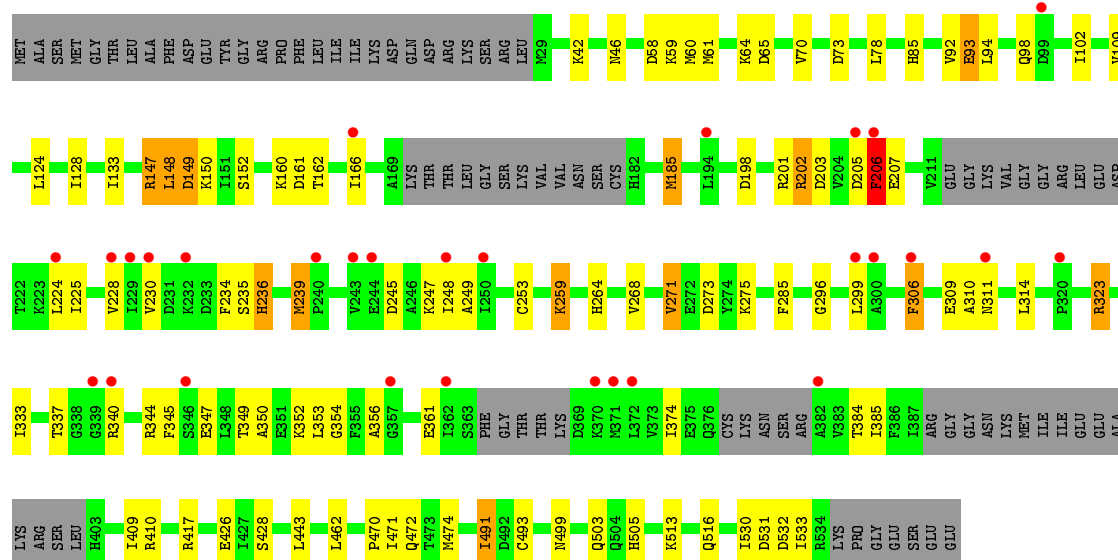
- Molecule 1: T-complex protein 1 subunit epsilon



- 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 0.275 , 0.324	Depositor DCC
R_{free} test set	2067 reflections (5.03%)	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)	0.31 , 100.8	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	0.89	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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/3837	0.49	1/5169 (0.0%)
1	B	0.26	0/3799	0.53	1/5116 (0.0%)
1	C	0.26	0/3806	0.50	0/5127
1	D	0.26	0/3573	0.50	0/4816
All	All	0.26	0/15015	0.51	2/20228 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	353	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	208	LEU	CA-CB-CG	5.37	127.66	115.30

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	70	0
1	B	3758	0	3865	100	0
1	C	3764	0	3867	69	0
1	D	3535	0	3624	70	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	301	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 10.

All (301) 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: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:B:426:GLU:OE2	1:B:513:LYS:NZ	2.16	0.72
1:A:389:GLY:CA	1:A:395:ILE:HD11	2.21	0.71
1:C:426:GLU:OE2	1:C:513:LYS:NZ	2.21	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:ARG:O	1:D:148:LEU:C	2.32	0.66
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:B:226:LYS:HZ3	1:B:375:GLU:H	1.47	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: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: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:N	1:A:395:ILE:HD12	2.19	0.58
1:D:185:MET:SD	1:D:185:MET:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:147:ARG:C	1:D:149:ASP:N	2.57	0.55
1:A:259:LYS:HD2	1:A:259:LYS:H	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: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: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:A:395:ILE:H	1:A:395:ILE:HD12	1.75	0.52
1:D:228:VAL:HA	1:D:384:THR:HB	1.92	0.52
1:B:201:ARG:O	1:B:203:ASP:N	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:THR:O	1:B:351:GLU:HB3	2.12	0.49
1:C:236:HIS:C	1:C:239:MET:HE1	2.33	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:A:322:VAL:HB	1:A:370:LYS:HZ3	1.76	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
1:C:499:ASN:ND2	1:C:499:ASN:O	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: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: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:D:205:ASP:O	1:D:206:PHE:HB2	2.14	0.47
1:B:252:THR:HA	1:B:303:GLN:HB2	1.97	0.47
1:B:503:GLN:C	1:B:505:HIS:H	2.18	0.47
1:B:83:VAL:HG13	1:B:89:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD23	1:A:225:ILE:N	2.29	0.47
1:D:236:HIS:C	1:D:239:MET:HE1	2.35	0.47
1:D:147:ARG:HH21	1:D:428:SER:HB3	1.78	0.47
1:A:389:GLY:CA	1:A:395:ILE:CD1	2.92	0.47
1:A:78:LEU:HD12	1:A:92:VAL:HG22	1.97	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:B:308:ASP:OD1	1:B:308:ASP:N	2.48	0.47
1:A:471:ILE:HD12	1:A:472:GLN:N	2.30	0.47
1:D:350:ALA:HB1	1:D:353:LEU:HG	1.96	0.47
1:A:229:ILE:HG22	1:A:371:MET:HB3	1.97	0.46
1:B:221:ASP:HB3	1:B:388:ARG:HG3	1.97	0.46
1:D:344:ARG:HB3	1:D:347:GLU:H	1.78	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:B:62:VAL:HB	1:B:63:ASP:HB2	1.97	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:344:ARG:HA	1:A:345:PHE:CB	2.45	0.45
1:A:37:HIS:HB3	1:A:87:ILE:HG12	1.98	0.45
1:D:224:LEU:HD23	1:D:225:ILE:N	2.29	0.45
1:B:352:LYS:O	1:B:353:LEU:HG	2.15	0.45
1:B:259:LYS:HE2	1:B:264:HIS:CE1	2.51	0.45
1:B:62:VAL:HB	1:B:63:ASP:CB	2.46	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:O	1:B:226:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HG11	1:B:208:LEU:CD1	2.47	0.45
1:D:271:VAL:HG13	1:D:275:LYS:HD2	1.99	0.45
1:D:64:LYS:HB3	1:D:65:ASP:H	1.54	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
1:A:60:MET:HA	1:A:70:VAL:HG12	1.99	0.44
1:B:138:GLU:HB2	1:B:525:ARG:HH22	1.81	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:253:CYS:SG	1:D:345:PHE:N	2.90	0.44
1:D:78:LEU:HB3	1:D:92:VAL:HG13	1.98	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:C:98:GLN:HG2	1:C:519:LEU:HD11	1.99	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:A:503:GLN:C	1:A:505:HIS:H	2.21	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:124:LEU:HD12	1:D:133:ILE:HD12	2.00	0.43
1:B:307:ASP:OD1	1:B:307:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ASP:C	1:C:502:LYS:H	2.21	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:D:503:GLN:C	1:D:505:HIS:H	2.22	0.43
1:B:109:VAL:HG22	1:B:516:GLN:HG2	2.01	0.43
1:B:62:VAL:HG12	1:B:63:ASP:HA	2.00	0.43
1:C:293:LYS:NZ	1:C:317:ASN:O	2.43	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: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:D:426:GLU:N	1:D:426:GLU:OE1	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:A:210:LYS:NZ	1:A:212:GLU:OE2	2.26	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:C:503:GLN:C	1:C:505:HIS:H	2.23	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: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:160:LYS:C	1:B:162:THR:H	2.21	0.42
1:B:348:LEU:O	1:B:348:LEU:HD12	2.19	0.42
1:B:226:LYS:HZ1	1:B:375:GLU:N	2.18	0.42
1:B:236:HIS:HB2	1:B:311:ASN:OD1	2.20	0.42
1:B:236:HIS:HB3	1:B:239:MET:CE	2.50	0.42
1:C:234:PHE:HE1	1:C:361:GLU:HB2	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ARG:HA	1:D:345:PHE:CB	2.48	0.41
1:D:58:ASP:HB3	1:D:70:VAL:HB	2.03	0.41
1:A:471:ILE:HG13	1:A:471:ILE:H	1.62	0.41
1:B:196:VAL:HG11	1:B:208:LEU:HD12	2.02	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:160:LYS:C	1:C:162:THR:H	2.21	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: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: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:C:386:PHE:HE2	1:C:388:ARG:HE	1.69	0.41
1:C:395:ILE:O	1:C:396:GLU:HB3	2.21	0.41
1:A:325:VAL:HG21	1:A:329:GLU:HB2	2.03	0.41
1:B:226:LYS:HD2	1:B:226:LYS:C	2.41	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:HG3	1:A:370:LYS:O	2.21	0.40
1:A:492:ASP:N	1:A:493:CYS:HA	2.36	0.40
1:B:229:ILE:HD13	1:B:371:MET:HE1	2.02	0.40
1:B:385:ILE:HG22	1:B:386:PHE:H	1.86	0.40
1:B:147:ARG:HG3	1:B:432:ALA:CB	2.51	0.40
1:D:349:THR:O	1:D:352:LYS:HG2	2.19	0.40
1:B:471:ILE:HG13	1:B:471:ILE:H	1.64	0.40
1:C:344:ARG:CB	1:C:347:GLU:HB3	2.50	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	487/541 (90%)	414 (85%)	60 (12%)	13 (3%)	5	35
1	B	480/541 (89%)	392 (82%)	68 (14%)	20 (4%)	3	25
1	C	480/541 (89%)	394 (82%)	70 (15%)	16 (3%)	4	31
1	D	447/541 (83%)	368 (82%)	63 (14%)	16 (4%)	3	29
All	All	1894/2164 (88%)	1568 (83%)	261 (14%)	65 (3%)	3	31

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

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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

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Mol	Chain	Res	Type
1	B	470	PRO

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	415/456 (91%)	407 (98%)	8 (2%)	57	80
1	B	411/456 (90%)	389 (95%)	22 (5%)	22	57
1	C	412/456 (90%)	399 (97%)	13 (3%)	39	70
1	D	387/456 (85%)	374 (97%)	13 (3%)	37	69
All	All	1625/1824 (89%)	1569 (97%)	56 (3%)	37	69

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	A	147	ARG
1	A	161	ASP
1	A	259	LYS
1	A	284	LYS
1	A	306	PHE
1	A	474	MET
1	A	500	ASP
1	B	59	LYS
1	B	96	LYS
1	B	99	ASP
1	B	125	ASP
1	B	126	ARG
1	B	139	GLN
1	B	147	ARG
1	B	170	LYS
1	B	183	ARG
1	B	201	ARG
1	B	206	PHE
1	B	219	LEU

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Mol	Chain	Res	Type
1	B	226	LYS
1	B	259	LYS
1	B	267	ASP
1	B	285	PHE
1	B	307	ASP
1	B	319	LEU
1	B	352	LYS
1	B	474	MET
1	B	500	ASP
1	B	502	LYS
1	C	39	MET
1	C	99	ASP
1	C	147	ARG
1	C	183	ARG
1	C	206	PHE
1	C	239	MET
1	C	266	LEU
1	C	306	PHE
1	C	470	PRO
1	C	474	MET
1	C	499	ASN
1	C	500	ASP
1	C	505	HIS
1	D	85	HIS
1	D	147	ARG
1	D	149	ASP
1	D	185	MET
1	D	206	PHE
1	D	239	MET
1	D	245	ASP
1	D	259	LYS
1	D	306	PHE
1	D	323	ARG
1	D	340	ARG
1	D	474	MET
1	D	499	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	601	3	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
2	ADP	A	601	3	24,29,29	0.96	1 (4%)	29,45,45	1.39	4 (13%)
2	ADP	D	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.39	4 (13%)
2	ADP	C	601	3	24,29,29	0.96	1 (4%)	29,45,45	1.39	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	601	3	-	3/12/32/32	0/3/3/3
2	ADP	A	601	3	-	4/12/32/32	0/3/3/3
2	ADP	D	601	-	-	3/12/32/32	0/3/3/3
2	ADP	C	601	3	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	C5-C4	2.46	1.47	1.40
2	C	601	ADP	C5-C4	2.43	1.47	1.40
2	D	601	ADP	C5-C4	2.42	1.47	1.40
2	B	601	ADP	C5-C4	2.41	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ADP	N3-C2-N1	-3.26	123.59	128.68
2	C	601	ADP	N3-C2-N1	-3.24	123.61	128.68
2	A	601	ADP	N3-C2-N1	-3.22	123.64	128.68
2	B	601	ADP	N3-C2-N1	-3.15	123.75	128.68
2	D	601	ADP	C4-C5-N7	-2.99	106.28	109.40
2	C	601	ADP	C4-C5-N7	-2.99	106.28	109.40
2	B	601	ADP	C4-C5-N7	-2.99	106.29	109.40
2	A	601	ADP	C4-C5-N7	-2.94	106.33	109.40
2	B	601	ADP	PA-O3A-PB	-2.83	123.10	132.83
2	A	601	ADP	C3'-C2'-C1'	2.76	105.13	100.98
2	C	601	ADP	C3'-C2'-C1'	2.74	105.11	100.98
2	D	601	ADP	C3'-C2'-C1'	2.72	105.07	100.98
2	A	601	ADP	PA-O3A-PB	-2.69	123.58	132.83
2	B	601	ADP	C3'-C2'-C1'	2.60	104.89	100.98
2	C	601	ADP	PA-O3A-PB	-2.55	124.08	132.83
2	D	601	ADP	PA-O3A-PB	-2.47	124.33	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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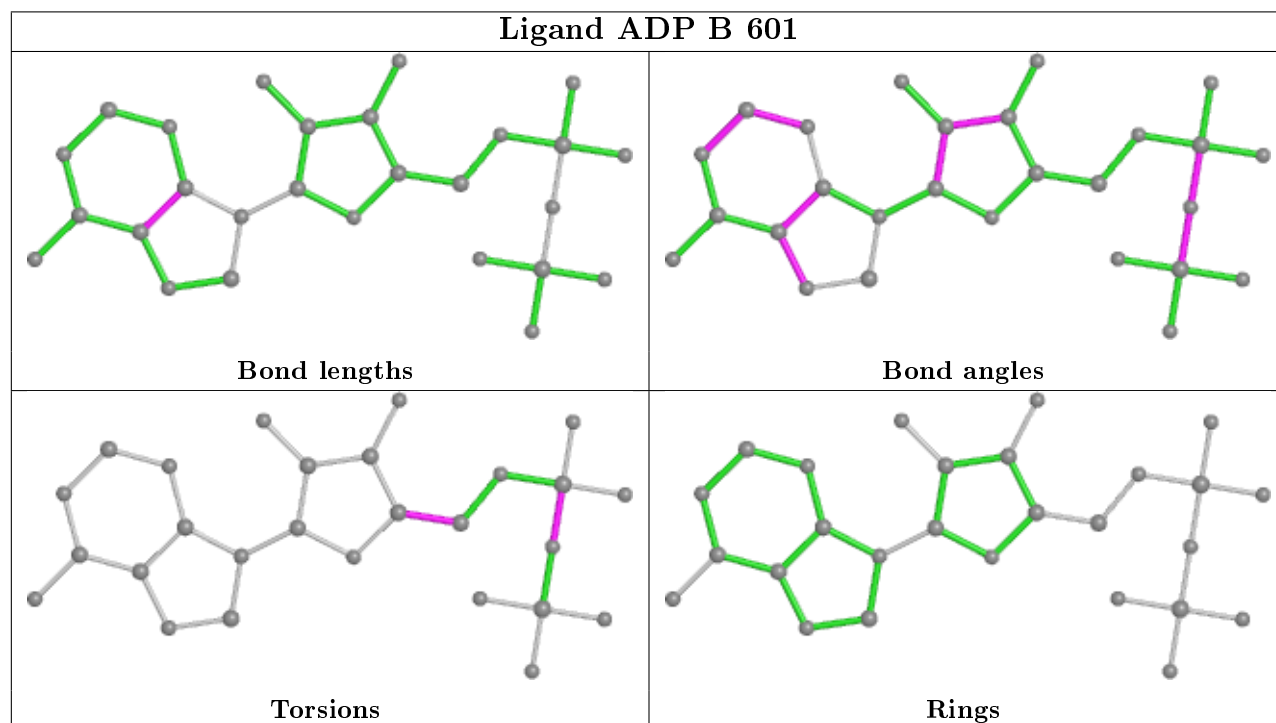
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	PB-O3A-PA-O1A
2	C	601	ADP	PB-O3A-PA-O2A

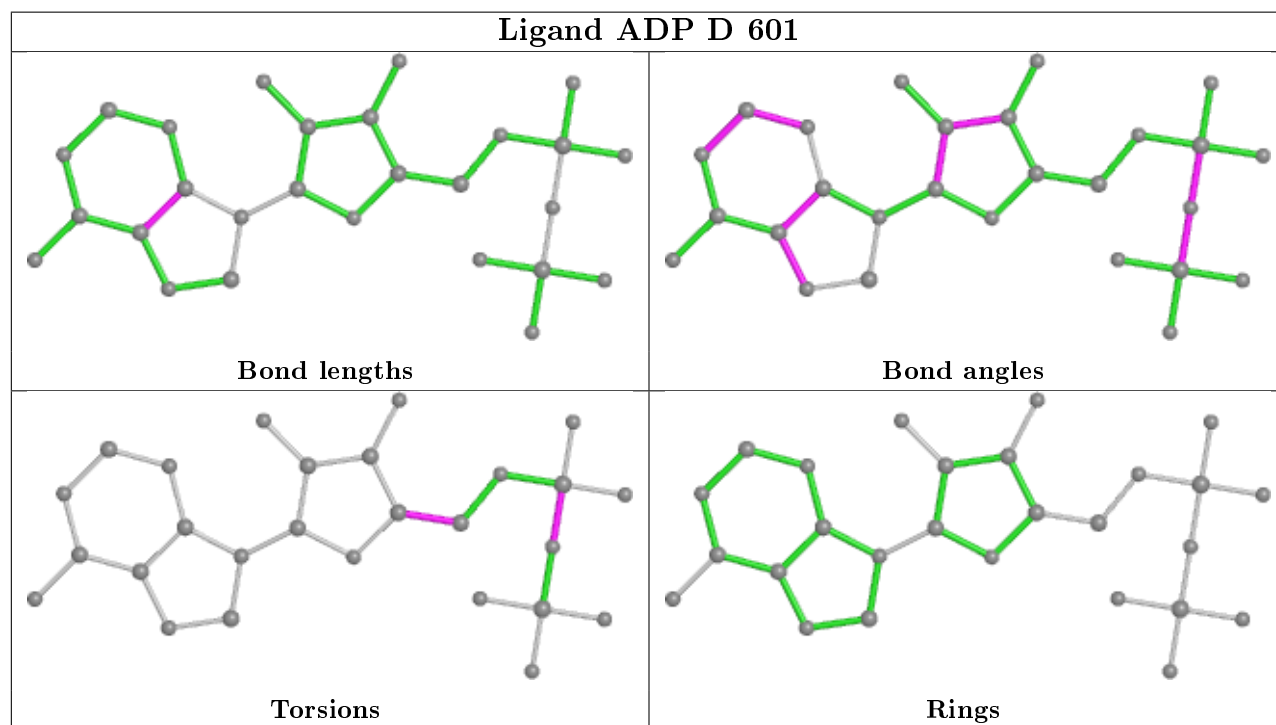
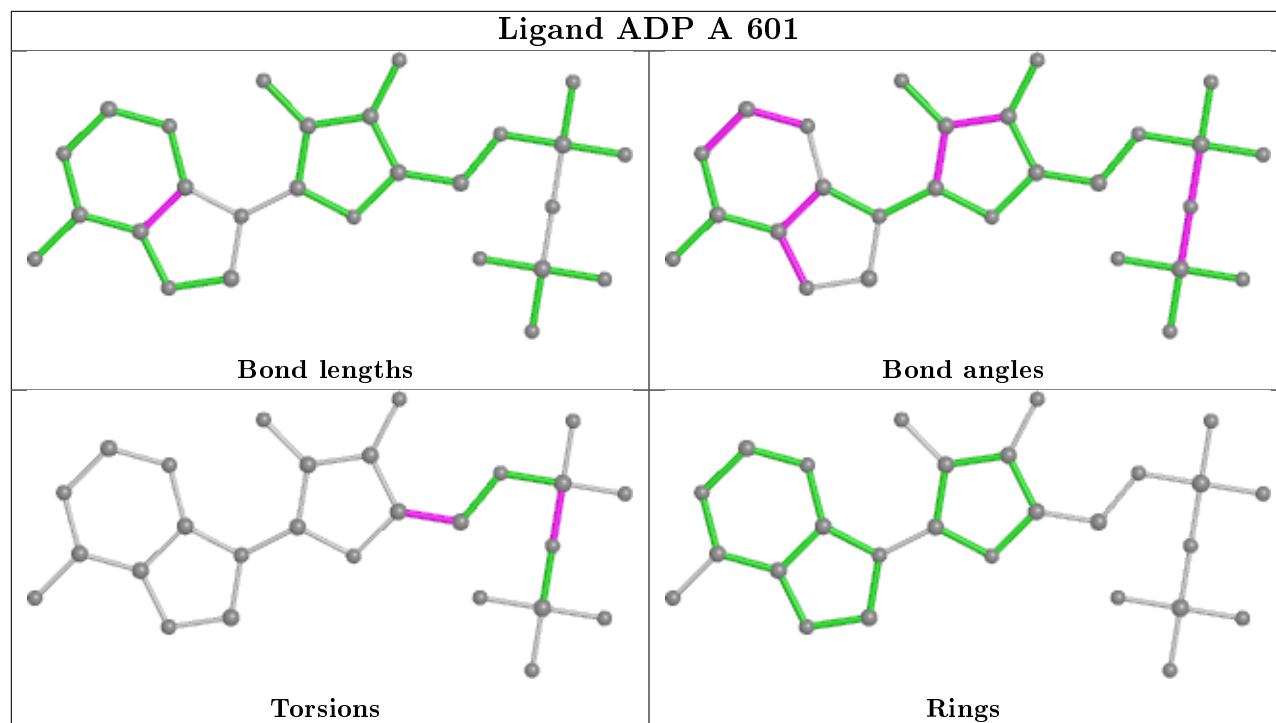
There are no ring outliers.

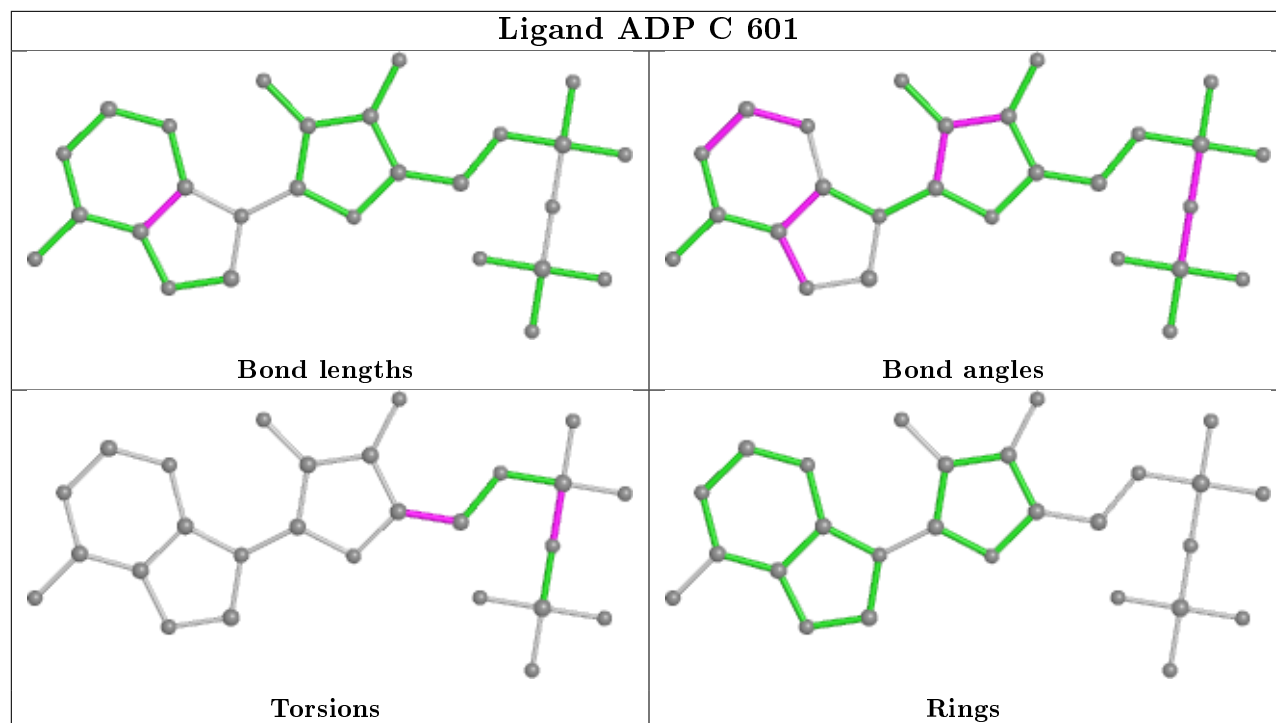
1 monomer is involved in 1 short contact:

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 [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	493/541 (91%)	0.31	31 (6%) 20 11	43, 124, 216, 273	0
1	B	488/541 (90%)	0.12	15 (3%) 49 33	34, 100, 183, 249	0
1	C	488/541 (90%)	0.25	21 (4%) 35 22	50, 127, 225, 302	0
1	D	459/541 (84%)	0.36	29 (6%) 20 11	44, 127, 204, 286	0
All	All	1928/2164 (89%)	0.26	96 (4%) 28 18	34, 119, 213, 302	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	VAL	7.0
1	D	229	ILE	5.9
1	D	370	LYS	5.3
1	C	229	ILE	5.2
1	C	233	ASP	5.0
1	A	391	ASN	4.8
1	A	343	PRO	4.8
1	C	232	LYS	4.6
1	C	228	VAL	4.5
1	B	233	ASP	4.4
1	B	345	PHE	4.2
1	C	69	THR	4.1
1	A	229	ILE	4.1
1	A	345	PHE	4.1
1	A	385	ILE	4.0
1	C	370	LYS	4.0
1	D	205	ASP	3.9
1	B	200	GLU	3.9
1	A	228	VAL	3.8
1	A	394	ILE	3.8
1	C	346	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	65	ASP	3.7
1	B	299	LEU	3.6
1	A	86	GLN	3.5
1	A	248	ILE	3.5
1	A	341	ILE	3.4
1	B	305	GLY	3.3
1	C	230	VAL	3.3
1	D	382	ALA	3.2
1	A	227	GLY	3.1
1	D	230	VAL	3.0
1	D	346	SER	3.0
1	D	340	ARG	3.0
1	D	232	LYS	3.0
1	D	299	LEU	2.9
1	D	240	PRO	2.9
1	A	404	ASP	2.9
1	D	371	MET	2.9
1	B	329	GLU	2.9
1	A	224	LEU	2.9
1	A	212	GLU	2.9
1	C	311	ASN	2.9
1	C	64	LYS	2.9
1	D	99	ASP	2.8
1	D	243	VAL	2.8
1	B	212	GLU	2.8
1	A	332	LEU	2.8
1	A	238	GLN	2.7
1	A	371	MET	2.7
1	C	371	MET	2.7
1	D	320	PRO	2.6
1	C	213	GLY	2.6
1	A	375	GLU	2.6
1	A	392	LYS	2.6
1	A	398	ALA	2.6
1	D	206	PHE	2.6
1	A	329	GLU	2.6
1	D	166	ILE	2.6
1	D	224	LEU	2.6
1	A	214	LYS	2.5
1	B	97	SER	2.5
1	D	311	ASN	2.5
1	A	205	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	2.5
1	B	344	ARG	2.5
1	A	249	ALA	2.5
1	B	229	ILE	2.5
1	C	240	PRO	2.4
1	D	372	LEU	2.4
1	C	255	PHE	2.4
1	D	300	ALA	2.3
1	B	325	VAL	2.3
1	D	250	ILE	2.3
1	D	244	GLU	2.3
1	A	409	ILE	2.3
1	B	371	MET	2.3
1	D	339	GLY	2.3
1	A	386	PHE	2.3
1	A	186	ALA	2.2
1	A	184	GLN	2.2
1	A	220	GLU	2.2
1	A	230	VAL	2.2
1	D	306	PHE	2.2
1	B	232	LYS	2.2
1	C	167	GLN	2.2
1	D	357	GLY	2.1
1	C	272	GLU	2.1
1	B	248	ILE	2.1
1	C	361	GLU	2.1
1	D	248	ILE	2.1
1	D	194	LEU	2.1
1	C	254	PRO	2.1
1	C	391	ASN	2.1
1	B	315	LEU	2.1
1	D	362	ILE	2.1
1	C	321	ALA	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 ⓘ

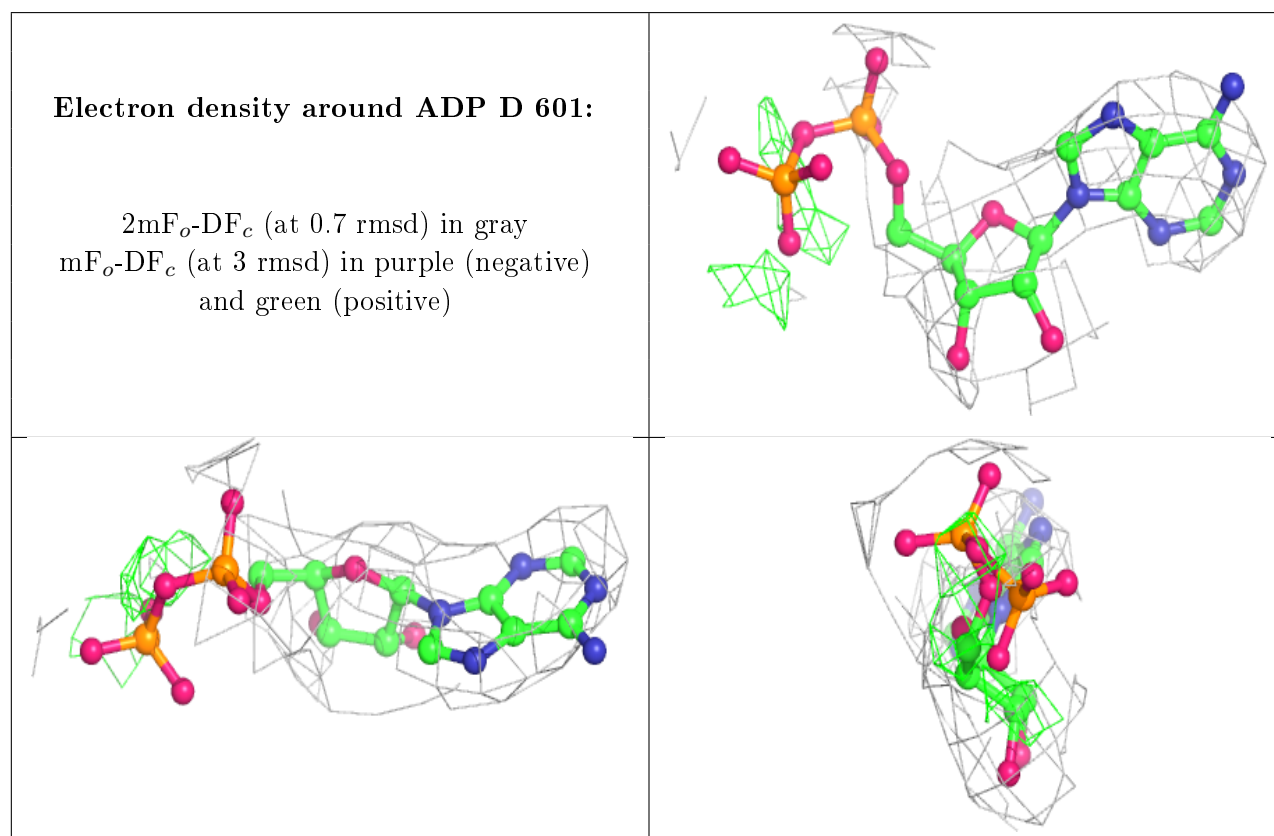
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

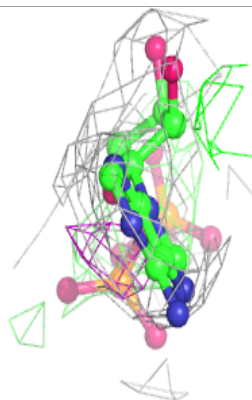
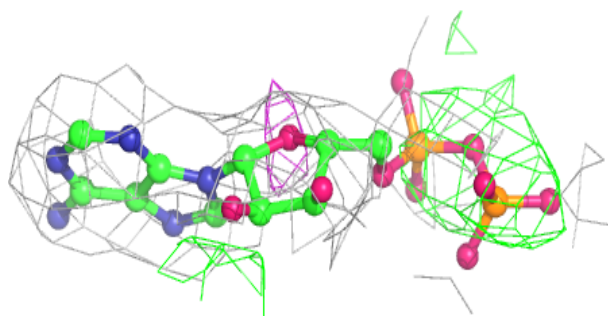
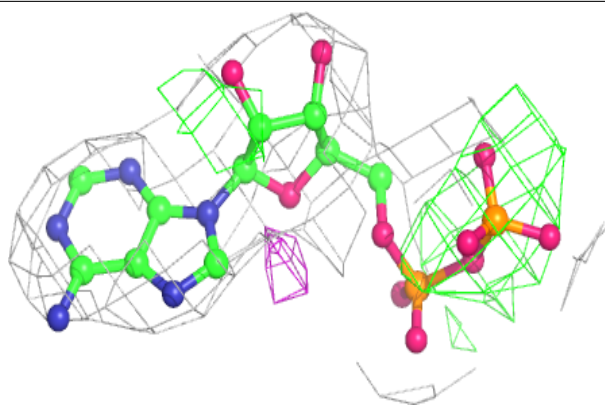
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	D	601	27/27	0.92	0.23	83,104,128,133	0
2	ADP	B	601	27/27	0.92	0.25	43,69,131,140	0
3	MG	C	602	1/1	0.93	0.52	107,107,107,107	0
2	ADP	A	601	27/27	0.94	0.21	62,71,121,130	0
2	ADP	C	601	27/27	0.94	0.23	61,92,109,122	0
3	MG	A	602	1/1	0.97	0.20	134,134,134,134	0
3	MG	B	602	1/1	0.97	0.30	132,132,132,132	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.

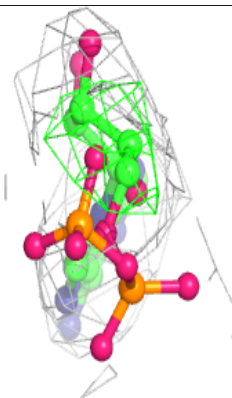
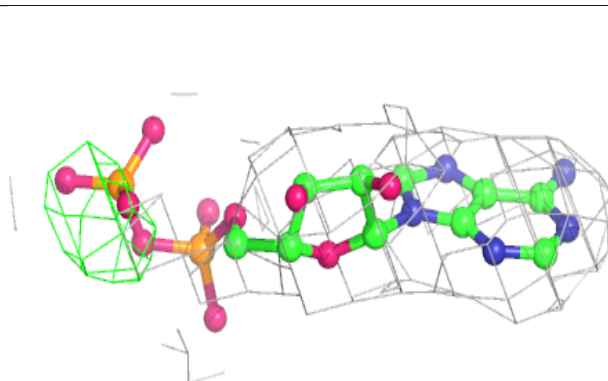
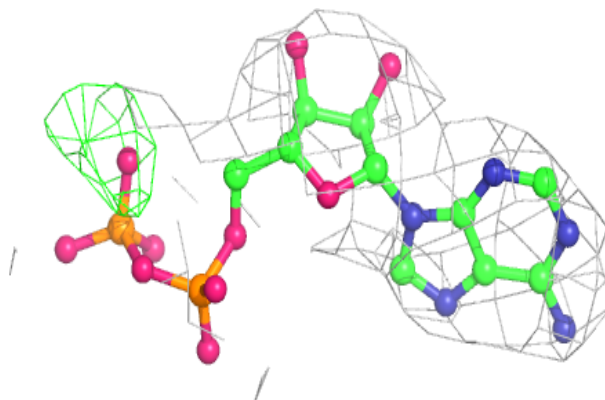


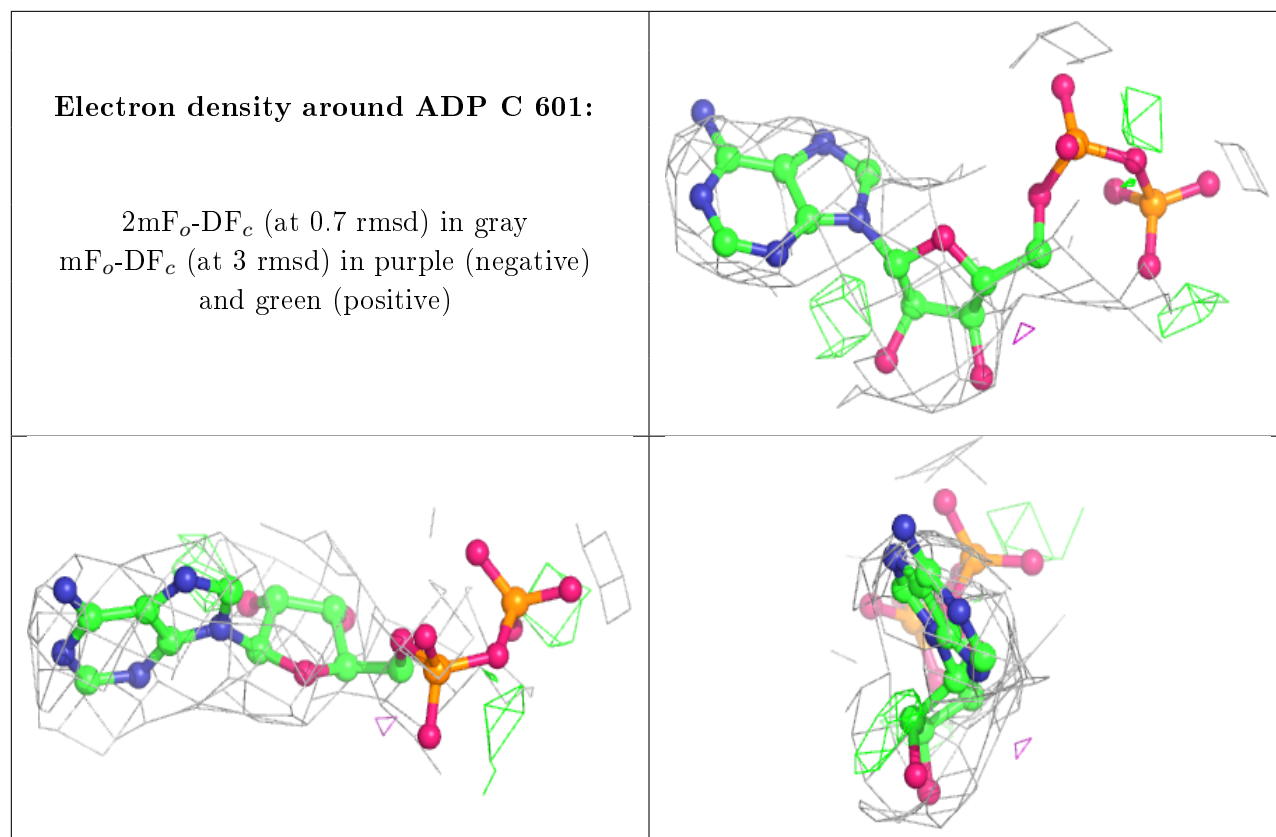
Electron density around ADP B 601:

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

**Electron density around ADP 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.