



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:29 AM UTC

PDB ID : 4ASU / pdb_00004asu
Title : F1-ATPase in which all three catalytic sites contain bound nucleotide, with magnesium ion released in the Empty site
Authors : Rees, D.M.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2012-05-03
Resolution : 2.60 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

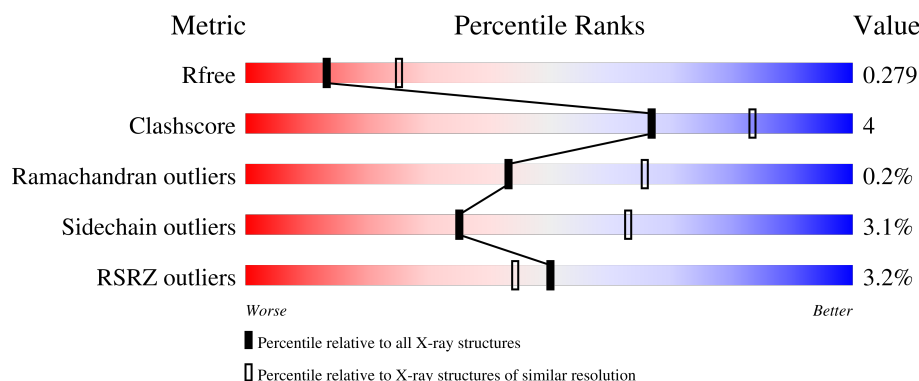
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

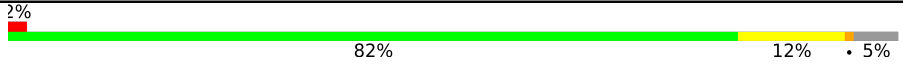
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	510	
1	B	510	
1	C	510	
2	D	480	
2	E	480	

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Mol	Chain	Length	Quality of chain
2	F	480	% 88% 8%
3	G	273	10% 58% 8% 34%
4	H	146	7% 43% 12% 43%
5	I	50	14% 42% 54%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24283 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	485	Total	C	N	O	S	0	0	0
			3695	2327	653	703	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	SEE REMARK 999	UNP P19483
B	481	GLY	SER	SEE REMARK 999	UNP P19483
C	481	GLY	SER	SEE REMARK 999	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	458	Total	C	N	O	S	0	0	0
			3472	2201	592	669	10			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	181	Total	C	N	O	S	0	0	0
			1396	881	249	260	6			

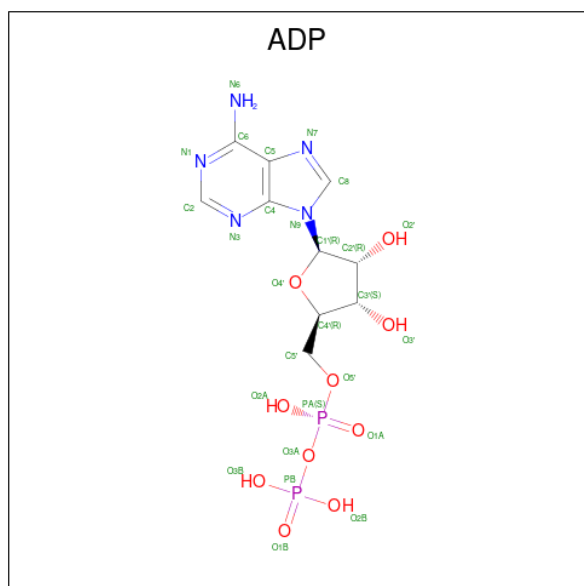
- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	83	Total	C	N	O	0	0	0
			615	392	102	121			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	23	Total	C	N	O	S	0	0	0
			183	118	33	31	1			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

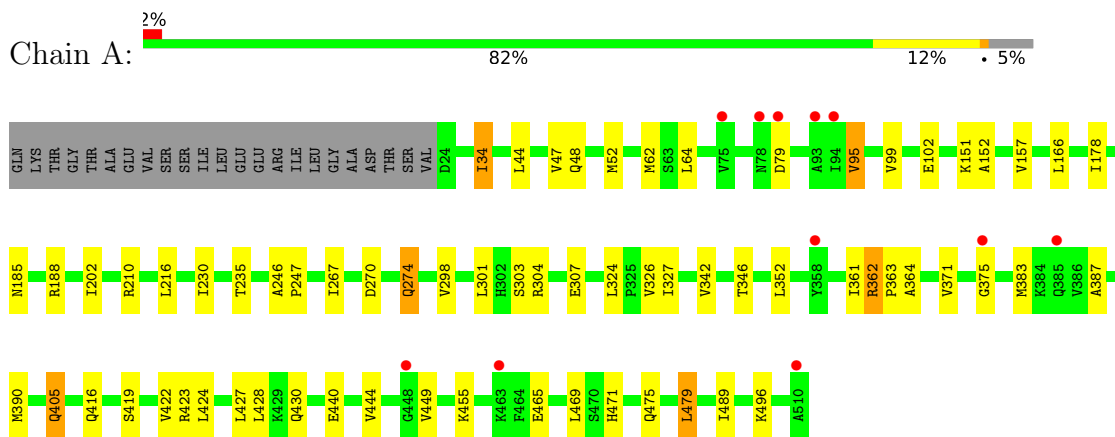
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	52	Total O 52 52	0	0
8	B	70	Total O 70 70	0	0
8	C	50	Total O 50 50	0	0
8	D	28	Total O 28 28	0	0
8	E	24	Total O 24 24	0	0
8	F	54	Total O 54 54	0	0
8	G	19	Total O 19 19	0	0
8	H	10	Total O 10 10	0	0
8	I	1	Total O 1 1	0	0

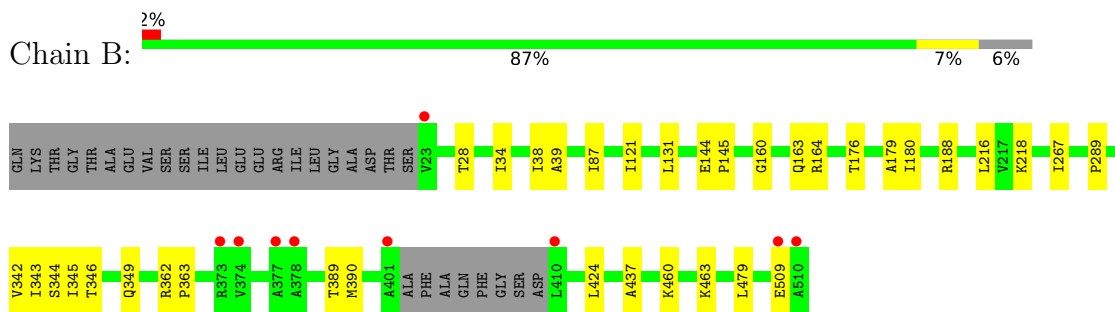
3 Residue-property plots [i](#)

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.

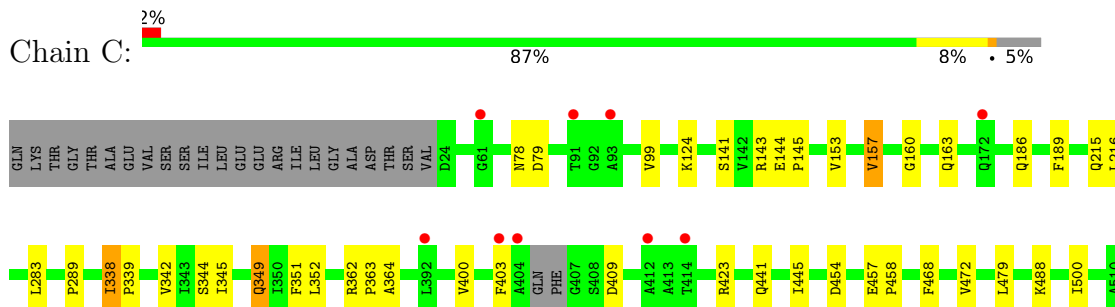
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



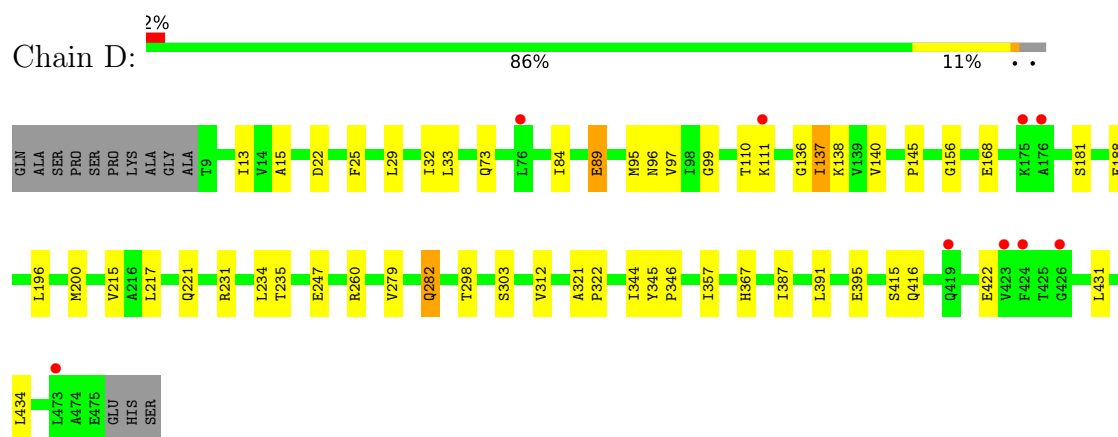
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



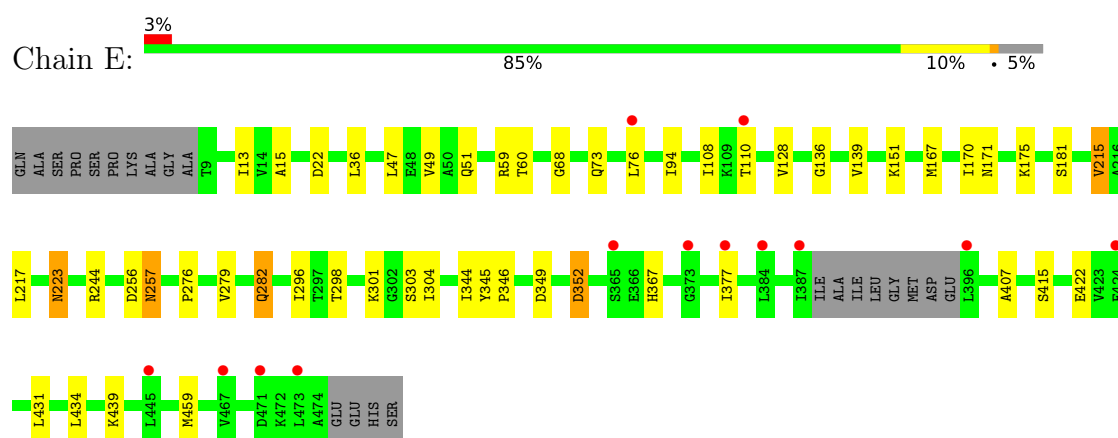
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



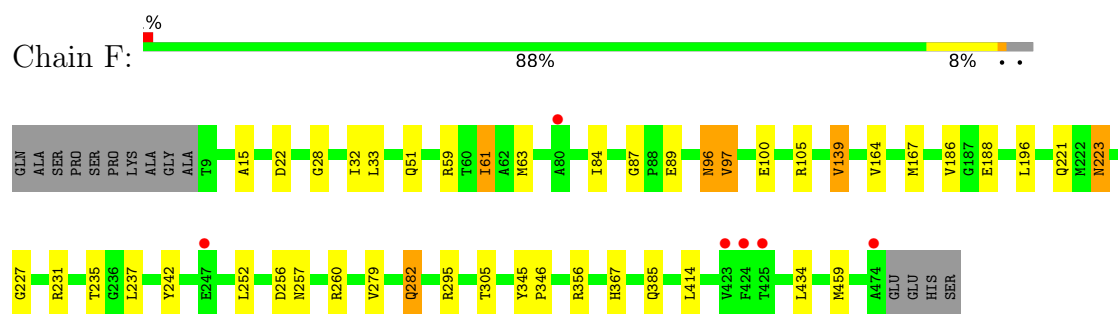
- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



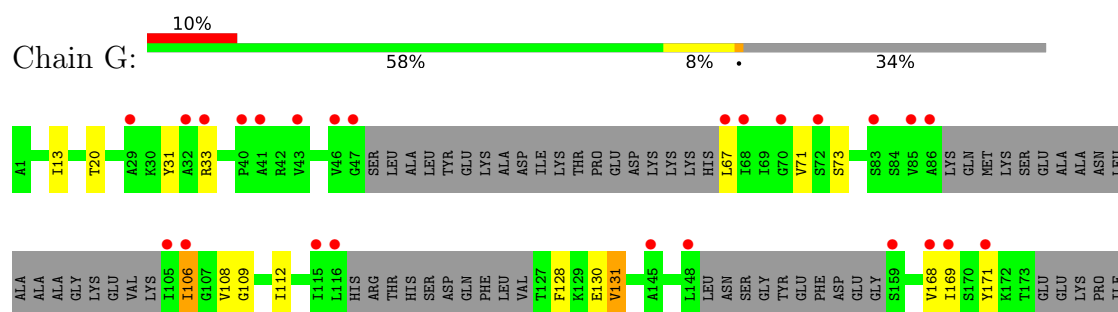
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

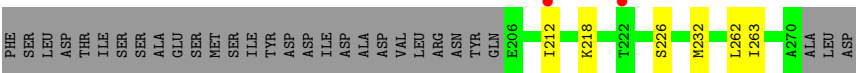


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

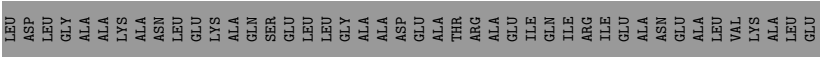


• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

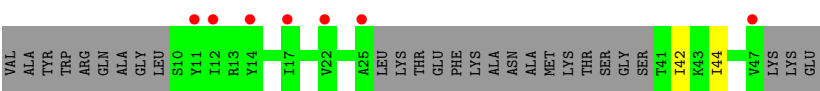




● Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



● Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.27Å 135.11Å 266.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.50 – 2.60 63.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	78.0 (63.50-2.60) 78.3 (63.50-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.245 , 0.289 0.237 , 0.279	Depositor DCC
R_{free} test set	4568 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24283	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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	0.45	0/3766	0.77	0/5080
1	B	0.45	0/3711	0.77	0/5005
1	C	0.46	0/3744	0.78	0/5049
2	D	0.50	0/3596	0.76	0/4879
2	E	0.50	0/3528	0.76	0/4786
2	F	0.50	0/3587	0.77	0/4867
3	G	0.42	0/1405	0.78	0/1878
4	H	0.57	0/627	0.72	0/860
5	I	0.43	0/183	0.78	0/243
All	All	0.48	0/24147	0.77	0/32647

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3814	35	0
1	B	3663	0	3774	17	0
1	C	3695	0	3796	22	0
2	D	3539	0	3592	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3472	0	3526	28	0
2	F	3530	0	3586	32	0
3	G	1396	0	1481	10	0
4	H	615	0	608	10	0
5	I	183	0	201	1	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	D	27	0	12	0	0
6	E	27	0	12	0	0
6	F	27	0	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	52	0	0	0	0
8	B	70	0	0	1	0
8	C	50	0	0	0	0
8	D	28	0	0	0	0
8	E	24	0	0	0	0
8	F	54	0	0	1	0
8	G	19	0	0	1	0
8	H	10	0	0	0	0
8	I	1	0	0	0	0
All	All	24283	0	24450	179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (179) 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)
2:F:282:GLN:HE21	2:F:282:GLN:H	1.05	0.93
2:D:282:GLN:H	2:D:282:GLN:HE21	1.00	0.92
2:D:282:GLN:H	2:D:282:GLN:NE2	1.73	0.86
2:E:282:GLN:HE21	2:E:282:GLN:H	1.22	0.86
2:D:282:GLN:HE21	2:D:282:GLN:N	1.82	0.77
1:C:153:VAL:HA	1:C:157:VAL:HG23	1.67	0.77
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.67	0.75
2:F:167:MET:HE1	2:F:196:LEU:HD13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:223:ASN:H	2:F:223:ASN:HD22	1.37	0.71
1:A:210:ARG:HG3	1:A:235:THR:HG21	1.78	0.66
2:E:276:PRO:HB2	3:G:262:LEU:HD21	1.78	0.65
1:A:362:ARG:HA	1:A:363:PRO:C	2.21	0.64
3:G:108:VAL:HA	3:G:128:PHE:HB2	1.79	0.64
1:C:78:ASN:HD22	1:C:79:ASP:H	1.46	0.63
2:D:196:LEU:HG	2:D:200:MET:HE2	1.81	0.63
2:F:282:GLN:H	2:F:282:GLN:NE2	1.88	0.63
3:G:171:TYR:OH	3:G:226:SER:HB2	1.98	0.62
2:F:61:ILE:HD11	2:F:227:GLY:HA2	1.82	0.62
1:A:52:MET:HG2	1:A:95:VAL:HG22	1.82	0.61
2:E:244:ARG:HD3	2:E:304:ILE:HG13	1.83	0.61
1:C:160:GLY:H	1:C:163:GLN:NE2	1.99	0.60
2:D:367:HIS:HE1	2:D:434:LEU:HD11	1.66	0.59
2:F:96:ASN:HD22	2:F:96:ASN:C	2.11	0.59
4:H:18:PHE:N	4:H:31:ALA:O	2.36	0.59
4:H:18:PHE:HB3	4:H:31:ALA:HB3	1.85	0.58
4:H:31:ALA:HA	4:H:32:ASN:CB	2.34	0.58
2:D:188:GLU:O	2:D:221:GLN:HB3	2.03	0.58
2:F:237:LEU:HD21	2:F:295:ARG:HB3	1.86	0.57
1:B:160:GLY:H	1:B:163:GLN:NE2	2.03	0.57
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.86	0.57
2:E:282:GLN:H	2:E:282:GLN:NE2	1.98	0.56
1:A:479:LEU:HG	1:A:496:LYS:HD3	1.88	0.56
1:C:215:GLN:HG2	2:F:356:ARG:HH12	1.71	0.55
2:E:13:ILE:HD12	2:E:73:GLN:HB3	1.88	0.55
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.42	0.55
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.89	0.55
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.90	0.54
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.90	0.54
4:H:54:THR:H	4:H:84:VAL:HG13	1.72	0.54
1:B:218:LYS:HD2	2:E:128:VAL:HB	1.89	0.53
2:E:51:GLN:HB2	2:E:59:ARG:HB3	1.90	0.53
2:F:188:GLU:O	2:F:221:GLN:HB3	2.08	0.53
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.91	0.53
1:C:349:GLN:HG3	1:C:351:PHE:HE2	1.74	0.52
1:C:344:SER:HB2	2:D:260:ARG:HH22	1.74	0.52
1:A:44:LEU:O	1:A:47:VAL:HG22	2.08	0.52
2:E:377:ILE:HG12	2:E:407:ALA:HB2	1.92	0.52
2:F:345:TYR:HB2	2:F:459:MET:HE1	1.91	0.52
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:223:ASN:HD22	2:E:223:ASN:H	1.58	0.52
1:A:444:VAL:HG21	1:A:465:GLU:HG3	1.91	0.51
2:F:51:GLN:HB2	2:F:59:ARG:HB3	1.93	0.51
2:F:367:HIS:CE1	2:F:434:LEU:HD11	2.46	0.51
2:D:345:TYR:HA	2:D:346:PRO:C	2.36	0.50
1:C:78:ASN:HD22	1:C:79:ASP:N	2.08	0.50
2:F:63:MET:HE3	2:F:97:VAL:HB	1.94	0.50
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.94	0.50
1:A:405:GLN:HG2	2:D:387:ILE:HD11	1.94	0.49
2:D:95:MET:HE3	2:D:99:GLY:HA2	1.95	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.94	0.49
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.95	0.49
2:D:298:THR:HG23	2:D:303:SER:HA	1.94	0.49
2:F:139:VAL:HG12	2:F:414:LEU:HD22	1.95	0.49
1:A:383:MET:HE2	1:A:387:ALA:HB2	1.95	0.48
1:C:186:GLN:HA	1:C:189:PHE:HD2	1.78	0.48
2:D:138:LYS:HE3	2:D:416:GLN:HB3	1.95	0.48
2:F:186:VAL:HG12	2:F:260:ARG:HB2	1.95	0.48
1:A:152:ALA:HA	1:A:428:LEU:HD22	1.95	0.48
1:A:151:LYS:H	1:A:430:GLN:HE22	1.60	0.48
2:E:171:ASN:O	2:E:175:LYS:HB2	2.14	0.48
1:B:160:GLY:H	1:B:163:GLN:HE21	1.60	0.48
2:D:344:ILE:HG23	2:D:415:SER:HB2	1.96	0.48
2:D:89:GLU:HG3	2:D:110:THR:HB	1.95	0.48
3:G:71:VAL:HA	3:G:108:VAL:HG13	1.95	0.48
4:H:31:ALA:HA	4:H:32:ASN:HB3	1.95	0.47
4:H:99:THR:HA	4:H:100:LEU:HA	1.59	0.47
1:A:301:LEU:HA	1:A:304:ARG:HH21	1.79	0.47
1:C:349:GLN:HG3	1:C:351:PHE:CE2	2.50	0.47
2:D:221:GLN:HE21	2:D:221:GLN:HA	1.80	0.47
2:E:49:VAL:HA	2:E:60:THR:HG22	1.97	0.47
2:E:256:ASP:HA	2:E:257:ASN:HA	1.67	0.47
3:G:73:SER:HA	3:G:131:VAL:HG23	1.97	0.47
8:G:2006:HOH:O	5:I:44:ILE:HA	2.15	0.47
2:F:252:LEU:HD23	2:F:305:THR:HB	1.96	0.46
1:B:289:PRO:HG2	3:G:263:ILE:HG12	1.97	0.46
1:A:424:LEU:HA	1:A:427:LEU:HD12	1.97	0.46
1:A:390:MET:HG3	1:A:424:LEU:HD22	1.97	0.46
2:E:223:ASN:HD22	2:E:223:ASN:N	2.13	0.46
2:E:345:TYR:HB2	2:E:459:MET:HE1	1.98	0.46
4:H:31:ALA:HB1	4:H:32:ASN:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:VAL:HA	1:C:403:PHE:HB3	1.98	0.46
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.46
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.98	0.46
2:D:391:LEU:HB3	2:D:395:GLU:HG3	1.98	0.46
1:A:151:LYS:H	1:A:430:GLN:NE2	2.14	0.46
2:D:156:GLY:H	2:D:312:VAL:HG23	1.80	0.46
2:F:63:MET:HE1	2:F:231:ARG:CB	2.40	0.46
1:A:361:ILE:O	1:A:364:ALA:HA	2.16	0.45
1:C:457:GLU:HA	1:C:458:PRO:HD3	1.87	0.45
1:A:62:MET:HE3	1:A:64:LEU:HD21	1.98	0.45
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.99	0.45
1:A:270:ASP:HB2	1:A:326:VAL:O	2.16	0.45
1:A:274:GLN:HE21	1:A:274:GLN:HB3	1.66	0.45
2:D:84:ILE:HG21	2:D:235:THR:HG23	1.98	0.45
2:F:96:ASN:HD21	2:F:100:GLU:H	1.65	0.45
4:H:65:VAL:HB	4:H:73:SER:HB2	1.97	0.45
1:C:141:SER:HB2	1:C:143:ARG:HH21	1.82	0.45
2:F:223:ASN:HD22	2:F:223:ASN:N	2.04	0.45
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.88	0.44
1:B:460:LYS:HE2	1:B:463:LYS:HD2	2.00	0.44
2:F:84:ILE:HG21	2:F:235:THR:HG23	1.97	0.44
2:F:256:ASP:HA	2:F:257:ASN:HA	1.79	0.44
1:C:160:GLY:H	1:C:163:GLN:HE21	1.64	0.44
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.99	0.44
1:B:163:GLN:HG2	1:B:164:ARG:N	2.33	0.44
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.00	0.44
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.51	0.44
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.44
1:A:352:LEU:HA	1:A:364:ALA:O	2.18	0.43
3:G:168:VAL:HG23	3:G:169:ILE:HG13	2.00	0.43
4:H:37:ASP:HB2	4:H:64:VAL:HB	2.00	0.43
2:D:231:ARG:HD3	2:D:234:LEU:HD12	1.98	0.43
1:A:34:ILE:HD11	1:A:79:ASP:HB2	1.99	0.43
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.99	0.43
1:A:298:VAL:O	1:A:301:LEU:HB3	2.18	0.43
1:B:176:THR:O	1:B:180:ILE:HG12	2.18	0.43
1:B:344:SER:HB2	8:B:2056:HOH:O	2.18	0.43
3:G:109:GLY:O	3:G:112:ILE:HG22	2.18	0.43
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.01	0.43
2:E:108:ILE:HG22	2:E:110:THR:HG23	2.01	0.43
1:C:423:ARG:HD3	1:C:454:ASP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:LEU:HB2	2:E:47:LEU:HB2	2.00	0.43
2:D:136:GLY:HA3	2:D:431:LEU:HG	2.01	0.43
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.82	0.43
2:F:345:TYR:HA	2:F:346:PRO:C	2.44	0.43
1:C:144:GLU:HA	1:C:145:PRO:HD3	1.90	0.42
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.84	0.42
1:B:390:MET:HG3	1:B:424:LEU:HD13	2.00	0.42
2:E:344:ILE:HG23	2:E:415:SER:HB3	2.00	0.42
2:F:32:ILE:HG22	2:F:33:LEU:HG	2.01	0.42
4:H:41:GLN:HA	4:H:59:ARG:HH11	1.84	0.42
2:E:349:ASP:HB3	2:E:352:ASP:HB2	2.01	0.42
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.00	0.42
2:E:298:THR:HG23	2:E:303:SER:HB3	2.02	0.42
2:F:164:VAL:HG23	6:F:600:ADP:O2A	2.19	0.42
2:E:151:LYS:HE3	2:E:296:ILE:HB	2.02	0.42
1:A:419:SER:O	1:A:423:ARG:HD3	2.20	0.42
2:D:137:ILE:HG23	2:D:140:VAL:HB	2.01	0.42
2:E:167:MET:HA	2:E:170:ILE:HD12	2.02	0.42
2:F:87:GLY:HA2	2:F:242:TYR:CE1	2.55	0.42
2:D:25:PHE:HB2	2:D:29:LEU:HD12	2.02	0.42
1:B:343:ILE:HG12	1:B:349:GLN:HG2	2.00	0.42
1:C:362:ARG:HA	1:C:363:PRO:C	2.45	0.41
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.50	0.41
1:A:166:LEU:HB2	1:A:346:THR:HG21	2.01	0.41
1:A:178:ILE:HD11	1:A:352:LEU:HD21	2.02	0.41
2:D:367:HIS:CE1	2:D:434:LEU:HD11	2.52	0.41
2:F:32:ILE:O	2:F:33:LEU:HB2	2.20	0.41
1:B:362:ARG:HA	1:B:363:PRO:C	2.44	0.41
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.03	0.41
1:B:342:VAL:HA	1:B:345:ILE:HD12	2.03	0.41
1:B:164:ARG:HB3	1:B:346:THR:HG22	2.02	0.41
2:E:136:GLY:HA3	2:E:431:LEU:HD12	2.03	0.41
1:A:440:GLU:HB3	1:A:469:LEU:HD11	2.03	0.41
1:C:352:LEU:HA	1:C:364:ALA:O	2.20	0.41
2:D:32:ILE:O	2:D:33:LEU:HB2	2.21	0.41
2:E:181:SER:HB2	2:E:215:VAL:HG13	2.03	0.41
2:E:345:TYR:HA	2:E:346:PRO:C	2.46	0.41
2:F:105:ARG:HD3	8:F:2013:HOH:O	2.21	0.41
2:F:367:HIS:HE1	2:F:434:LEU:HD11	1.86	0.41
1:A:202:ILE:HG23	1:A:230:ILE:HG13	2.01	0.41
1:C:468:PHE:O	1:C:472:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:367:HIS:HE1	2:E:434:LEU:HD11	1.85	0.40
2:F:96:ASN:ND2	2:F:100:GLU:H	2.19	0.40
1:A:422:VAL:HG23	1:A:423:ARG:HD2	2.03	0.40
2:D:15:ALA:HB3	2:D:22:ASP:HB2	2.03	0.40
3:G:171:TYR:HH	3:G:226:SER:HB2	1.83	0.40
1:A:303:SER:O	1:A:307:GLU:HB2	2.22	0.40
3:G:20:THR:HA	3:G:232:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	470 (97%)	14 (3%)	1 (0%)	43	66
1	B	476/510 (93%)	465 (98%)	11 (2%)	0	100	100
1	C	481/510 (94%)	472 (98%)	8 (2%)	1 (0%)	43	66
2	D	465/480 (97%)	439 (94%)	26 (6%)	0	100	100
2	E	454/480 (95%)	436 (96%)	17 (4%)	1 (0%)	43	66
2	F	464/480 (97%)	440 (95%)	22 (5%)	2 (0%)	30	51
3	G	169/273 (62%)	162 (96%)	5 (3%)	2 (1%)	10	23
4	H	81/146 (56%)	74 (91%)	7 (9%)	0	100	100
5	I	19/50 (38%)	19 (100%)	0	0	100	100
All	All	3094/3439 (90%)	2977 (96%)	110 (4%)	7 (0%)	43	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	GLY

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Mol	Chain	Res	Type
3	G	130	GLU
1	C	409	ASP
2	F	279	VAL
3	G	106	ILE
2	E	279	VAL
2	F	28	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	378 (96%)	15 (4%)	29	56
1	B	389/412 (94%)	380 (98%)	9 (2%)	44	71
1	C	391/412 (95%)	382 (98%)	9 (2%)	44	71
2	D	377/386 (98%)	367 (97%)	10 (3%)	39	67
2	E	370/386 (96%)	360 (97%)	10 (3%)	39	67
2	F	376/386 (97%)	368 (98%)	8 (2%)	47	73
3	G	152/231 (66%)	144 (95%)	8 (5%)	20	43
4	H	69/109 (63%)	60 (87%)	9 (13%)	4	8
5	I	20/41 (49%)	19 (95%)	1 (5%)	22	46
All	All	2537/2775 (91%)	2458 (97%)	79 (3%)	35	63

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	95	VAL
1	A	99	VAL
1	A	102	GLU
1	A	157	VAL
1	A	216	LEU
1	A	274	GLN
1	A	362	ARG

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Mol	Chain	Res	Type
1	A	371	VAL
1	A	405	GLN
1	A	416	GLN
1	A	449	VAL
1	A	455	LYS
1	A	479	LEU
1	A	489	ILE
1	B	28	THR
1	B	38	ILE
1	B	87	ILE
1	B	121	ILE
1	B	131	LEU
1	B	216	LEU
1	B	389	THR
1	B	479	LEU
1	B	509	GLU
1	C	99	VAL
1	C	124	LYS
1	C	157	VAL
1	C	216	LEU
1	C	338	ILE
1	C	349	GLN
1	C	479	LEU
1	C	488	LYS
1	C	500	ILE
2	D	89	GLU
2	D	96	ASN
2	D	97	VAL
2	D	111	LYS
2	D	137	ILE
2	D	168	GLU
2	D	247	GLU
2	D	279	VAL
2	D	282	GLN
2	D	422	GLU
2	E	76	LEU
2	E	139	VAL
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	282	GLN
2	E	301	LYS

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Mol	Chain	Res	Type
2	E	352	ASP
2	E	422	GLU
2	E	439	LYS
2	F	61	ILE
2	F	89	GLU
2	F	96	ASN
2	F	97	VAL
2	F	139	VAL
2	F	223	ASN
2	F	282	GLN
2	F	385	GLN
3	G	13	ILE
3	G	31	TYR
3	G	33	ARG
3	G	67	LEU
3	G	106	ILE
3	G	131	VAL
3	G	212	ILE
3	G	218	LYS
4	H	29	ASN
4	H	33	VAL
4	H	54	THR
4	H	57	VAL
4	H	63	VAL
4	H	72	THR
4	H	93	LEU
4	H	98	VAL
4	H	100	LEU
5	I	42	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	A	274	GLN
1	A	366	ASN
1	A	396	GLN
1	A	405	GLN
1	A	430	GLN
1	A	471	HIS
1	B	147	GLN
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	208	GLN
1	B	302	HIS
1	B	466	ASN
1	B	471	HIS
1	B	476	HIS
1	B	503	ASN
1	C	78	ASN
1	C	163	GLN
1	C	186	GLN
1	C	215	GLN
1	C	263	HIS
1	C	341	ASN
1	C	349	GLN
1	C	416	GLN
2	D	73	GLN
2	D	172	ASN
2	D	194	ASN
2	D	221	GLN
2	D	246	GLN
2	D	249	GLN
2	D	282	GLN
2	D	367	HIS
2	D	419	GLN
2	D	442	GLN
2	D	455	GLN
2	E	39	GLN
2	E	194	ASN
2	E	223	ASN
2	E	282	GLN
2	E	308	GLN
2	E	328	HIS
2	E	367	HIS
2	E	375	GLN
2	E	427	HIS
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN
2	F	112	GLN
2	F	130	GLN
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN

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Mol	Chain	Res	Type
2	F	282	GLN
2	F	367	HIS
3	G	163	ASN
3	G	211	ASN
4	H	29	ASN
4	H	35	GLN
4	H	41	GLN

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
6	ADP	A	600	7	28,29,29	1.46	4 (14%)	43,45,45	1.83	8 (18%)
6	ADP	E	600	-	28,29,29	1.45	4 (14%)	43,45,45	1.84	9 (20%)
6	ADP	F	600	7	28,29,29	1.47	5 (17%)	43,45,45	1.82	9 (20%)
6	ADP	B	600	7	28,29,29	1.49	5 (17%)	43,45,45	1.82	8 (18%)
6	ADP	C	600	7	28,29,29	1.46	5 (17%)	43,45,45	1.82	8 (18%)
6	ADP	D	600	7	28,29,29	1.47	5 (17%)	43,45,45	1.79	8 (18%)

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
6	ADP	A	600	7	-	0/16/32/32	0/3/3/3
6	ADP	E	600	-	-	0/16/32/32	0/3/3/3
6	ADP	F	600	7	-	3/16/32/32	0/3/3/3
6	ADP	B	600	7	-	0/16/32/32	0/3/3/3
6	ADP	C	600	7	-	0/16/32/32	0/3/3/3
6	ADP	D	600	7	-	1/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	ADP	C5-C4	4.96	1.47	1.39
6	A	600	ADP	C5-C4	4.92	1.47	1.39
6	E	600	ADP	C5-C4	4.90	1.47	1.39
6	F	600	ADP	C5-C4	4.89	1.47	1.39
6	D	600	ADP	C5-C4	4.88	1.47	1.39
6	C	600	ADP	C5-C4	4.85	1.47	1.39
6	B	600	ADP	C5-C6	2.91	1.49	1.41
6	A	600	ADP	C5-C6	2.89	1.49	1.41
6	D	600	ADP	C5-C6	2.86	1.49	1.41
6	F	600	ADP	C5-C6	2.84	1.48	1.41
6	E	600	ADP	C5-C6	2.83	1.48	1.41
6	C	600	ADP	C5-C6	2.80	1.48	1.41
6	B	600	ADP	C8-N7	2.44	1.36	1.31
6	A	600	ADP	C8-N7	2.40	1.36	1.31
6	C	600	ADP	C8-N7	2.38	1.36	1.31
6	D	600	ADP	C8-N7	2.36	1.36	1.31
6	C	600	ADP	C5-N7	-2.33	1.34	1.39
6	F	600	ADP	C8-N7	2.31	1.36	1.31
6	E	600	ADP	C5-N7	-2.30	1.34	1.39
6	E	600	ADP	C8-N7	2.28	1.36	1.31
6	F	600	ADP	PA-O3A	2.26	1.61	1.59
6	B	600	ADP	C5-N7	-2.26	1.35	1.39
6	F	600	ADP	C5-N7	-2.24	1.35	1.39
6	A	600	ADP	C5-N7	-2.21	1.35	1.39
6	D	600	ADP	C5-N7	-2.21	1.35	1.39
6	D	600	ADP	PA-O3A	2.18	1.61	1.59
6	B	600	ADP	PA-O3A	2.16	1.61	1.59
6	C	600	ADP	PA-O3A	2.08	1.61	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	600	ADP	C5-C4-N3	-5.91	118.58	126.72
6	F	600	ADP	C5-C4-N3	-5.89	118.61	126.72
6	C	600	ADP	C5-C4-N3	-5.77	118.77	126.72
6	A	600	ADP	C5-C4-N3	-5.77	118.78	126.72
6	B	600	ADP	C5-C4-N3	-5.76	118.79	126.72
6	D	600	ADP	C5-C4-N3	-5.75	118.79	126.72
6	E	600	ADP	N3-C4-N9	4.74	135.22	127.17
6	F	600	ADP	N3-C4-N9	4.70	135.16	127.17
6	C	600	ADP	N3-C4-N9	4.62	135.02	127.17
6	D	600	ADP	N3-C4-N9	4.60	134.99	127.17
6	A	600	ADP	N3-C4-N9	4.55	134.91	127.17
6	B	600	ADP	N3-C4-N9	4.51	134.83	127.17
6	B	600	ADP	C2-N3-C4	3.81	121.14	111.83
6	C	600	ADP	C2-N3-C4	3.81	121.14	111.83
6	E	600	ADP	C2-N3-C4	3.80	121.12	111.83
6	A	600	ADP	C2-N3-C4	3.79	121.08	111.83
6	F	600	ADP	C2-N3-C4	3.79	121.08	111.83
6	D	600	ADP	C2-N3-C4	3.76	121.02	111.83
6	C	600	ADP	N3-C2-N1	-3.55	123.20	128.58
6	B	600	ADP	N3-C2-N1	-3.52	123.25	128.58
6	A	600	ADP	C4-C5-N7	-3.50	106.58	110.58
6	B	600	ADP	C4-C5-N7	-3.50	106.58	110.58
6	A	600	ADP	N3-C2-N1	-3.46	123.34	128.58
6	D	600	ADP	N3-C2-N1	-3.43	123.39	128.58
6	D	600	ADP	C4-C5-N7	-3.41	106.69	110.58
6	E	600	ADP	N3-C2-N1	-3.40	123.44	128.58
6	E	600	ADP	C4-C5-N7	-3.39	106.70	110.58
6	F	600	ADP	N3-C2-N1	-3.38	123.46	128.58
6	F	600	ADP	C4-C5-N7	-3.37	106.72	110.58
6	C	600	ADP	C4-C5-N7	-3.30	106.80	110.58
6	A	600	ADP	C5-N7-C8	2.56	107.48	103.45
6	D	600	ADP	C4-N9-C8	2.55	108.42	105.74
6	D	600	ADP	C5-N7-C8	2.53	107.42	103.45
6	A	600	ADP	C4-N9-C8	2.52	108.39	105.74
6	B	600	ADP	C5-N7-C8	2.52	107.41	103.45
6	E	600	ADP	C3'-C2'-C1'	2.52	106.23	101.46
6	F	600	ADP	C5-N7-C8	2.48	107.34	103.45
6	C	600	ADP	C5-N7-C8	2.47	107.33	103.45
6	E	600	ADP	C5-N7-C8	2.47	107.33	103.45
6	C	600	ADP	C4-N9-C8	2.46	108.32	105.74
6	B	600	ADP	C4-N9-C8	2.45	108.31	105.74
6	E	600	ADP	C4-N9-C8	2.42	108.28	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	600	ADP	C4-N9-C8	2.37	108.23	105.74
6	B	600	ADP	C6-C5-N7	2.28	136.49	132.09
6	A	600	ADP	C6-C5-N7	2.26	136.45	132.09
6	D	600	ADP	C6-C5-N7	2.18	136.29	132.09
6	F	600	ADP	C2'-C1'-N9	-2.17	107.92	113.30
6	F	600	ADP	C6-C5-N7	2.11	136.16	132.09
6	C	600	ADP	C6-C5-N7	2.11	136.16	132.09
6	E	600	ADP	C6-C5-N7	2.11	136.15	132.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

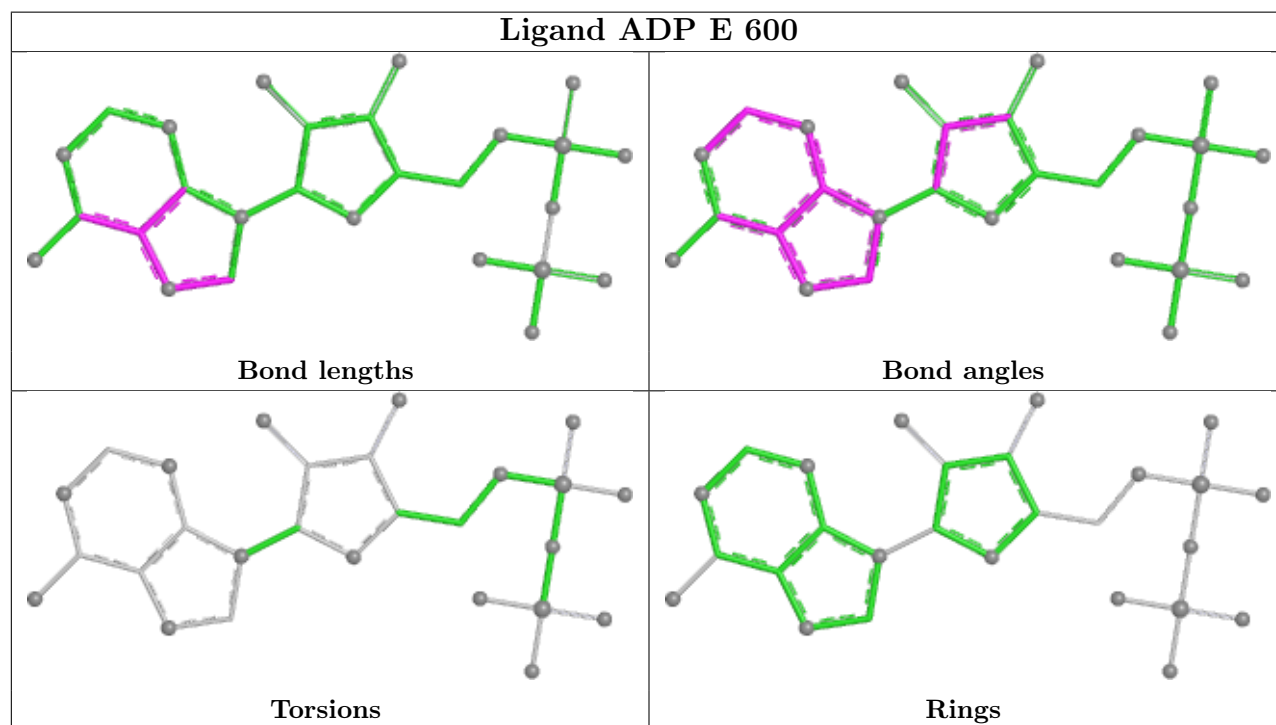
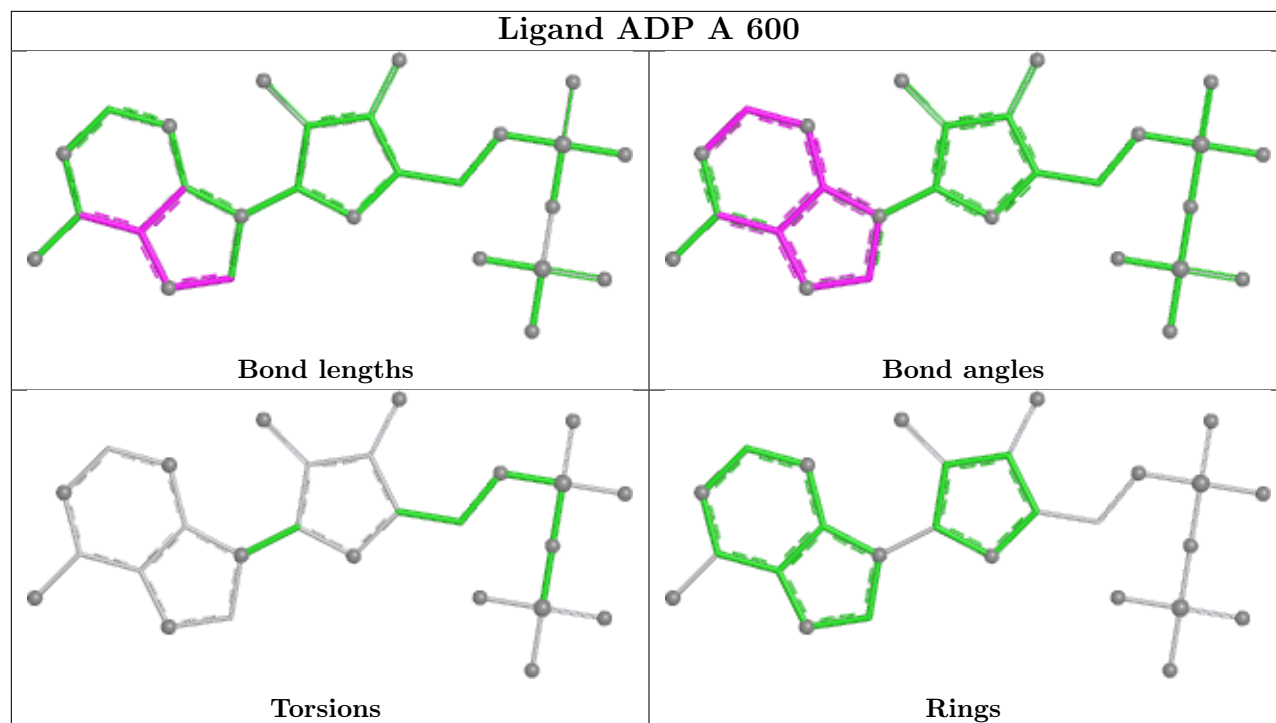
Mol	Chain	Res	Type	Atoms
6	F	600	ADP	PA-O3A-PB-O2B
6	F	600	ADP	PA-O3A-PB-O3B
6	F	600	ADP	PA-O3A-PB-O1B
6	D	600	ADP	PA-O3A-PB-O3B

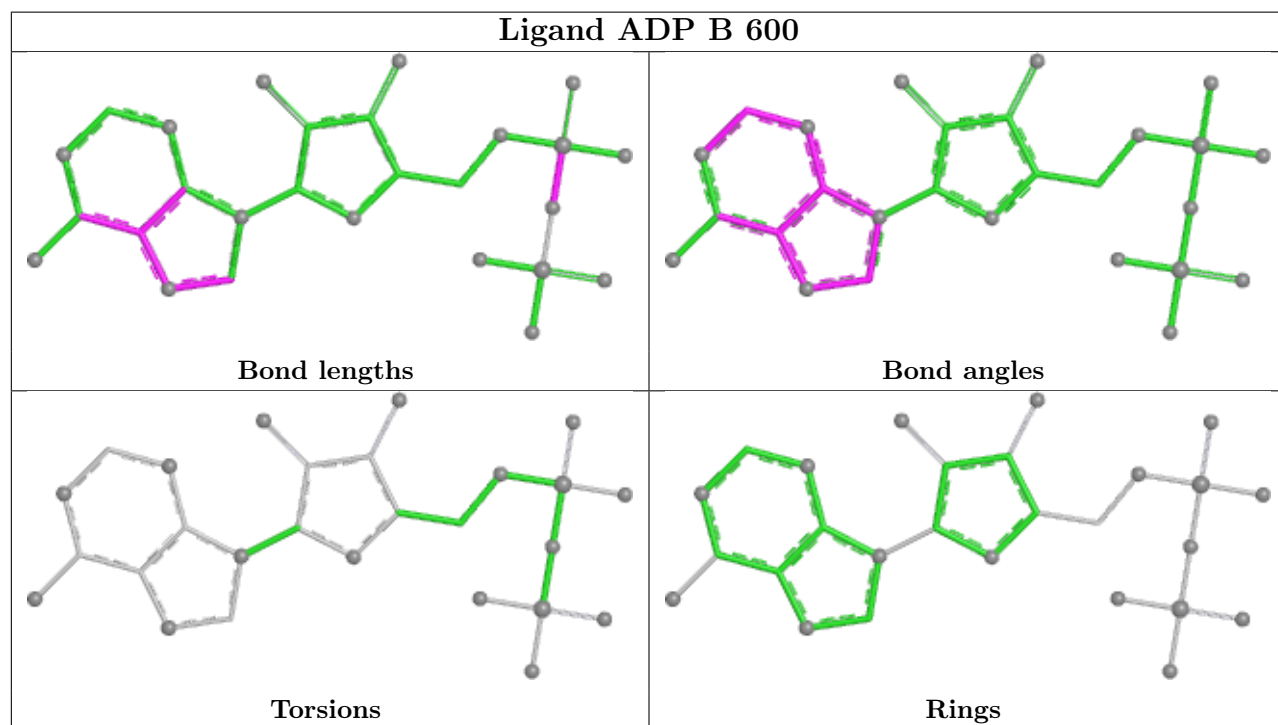
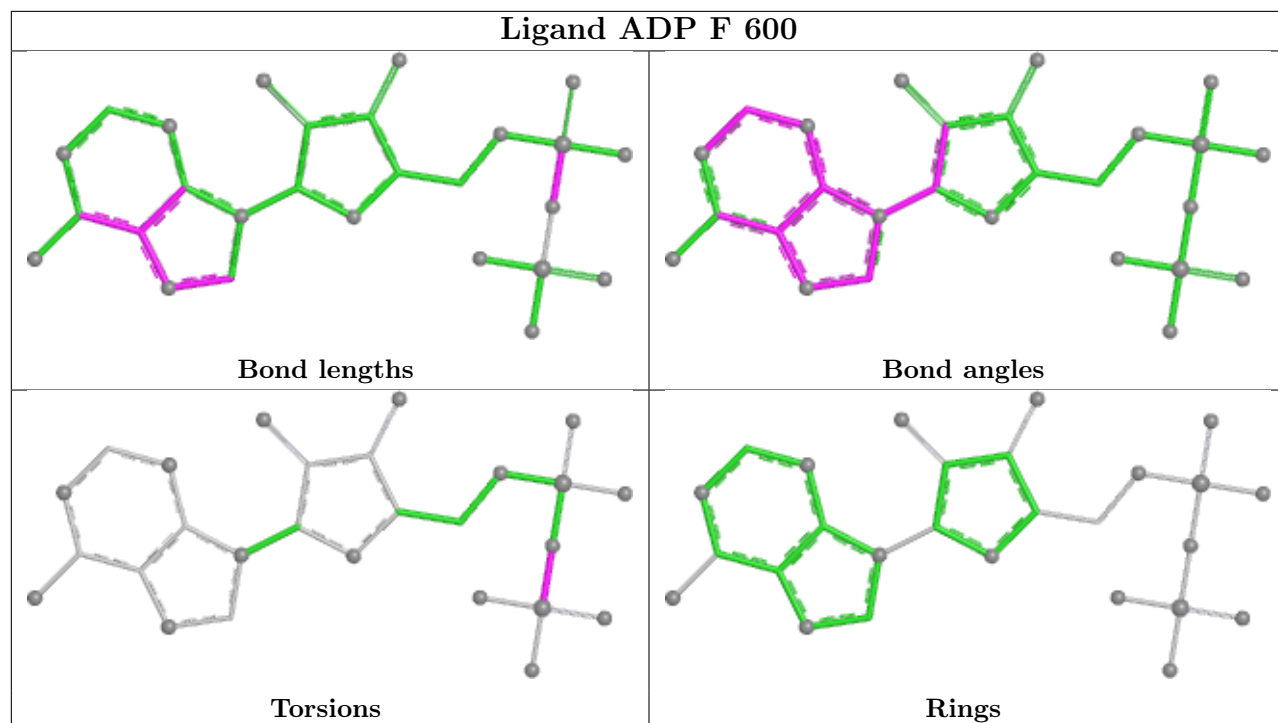
There are no ring outliers.

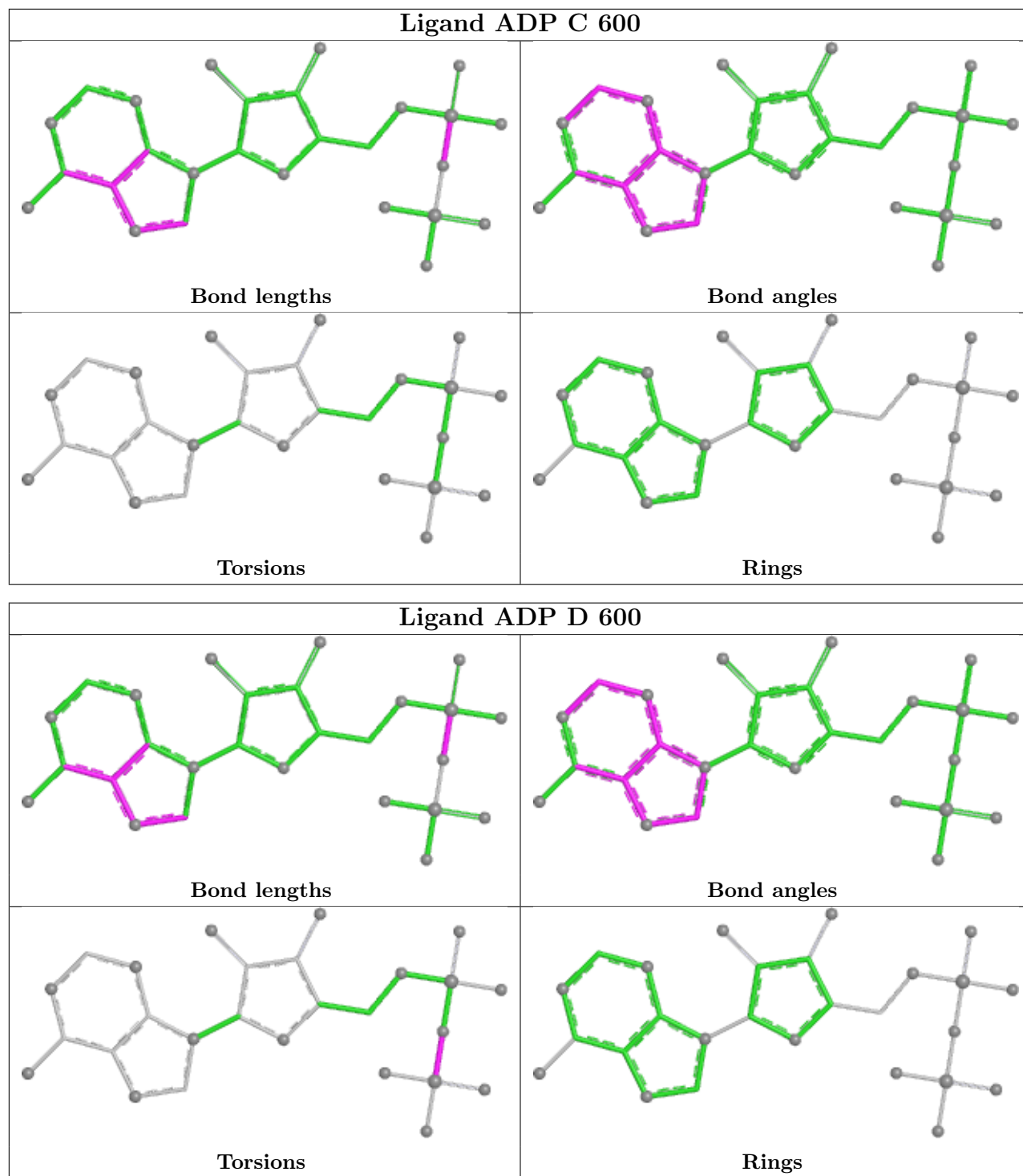
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	600	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

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	487/510 (95%)	0.32	11 (2%) 61 55	29, 49, 69, 97	0
1	B	480/510 (94%)	0.18	9 (1%) 66 61	26, 43, 74, 111	0
1	C	485/510 (95%)	0.12	9 (1%) 66 61	26, 39, 64, 97	0
2	D	467/480 (97%)	0.28	9 (1%) 66 61	29, 48, 80, 127	0
2	E	458/480 (95%)	0.42	13 (2%) 55 49	29, 53, 93, 114	0
2	F	466/480 (97%)	0.17	6 (1%) 75 71	25, 42, 74, 103	0
3	G	181/273 (66%)	1.10	27 (14%) 5 4	33, 70, 102, 138	0
4	H	83/146 (56%)	1.16	10 (12%) 9 7	55, 75, 97, 113	0
5	I	23/50 (46%)	1.58	7 (30%) 1 1	86, 113, 121, 124	0
All	All	3130/3439 (91%)	0.33	101 (3%) 50 44	25, 47, 86, 138	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	86	ALA	8.0
1	A	385	GLN	5.5
2	E	396	LEU	4.7
4	H	100	LEU	4.7
3	G	105	ILE	4.6
3	G	106	ILE	4.2
3	G	67	LEU	3.9
5	I	14	TYR	3.7
3	G	116	LEU	3.7
3	G	212	ILE	3.7
5	I	25	ALA	3.6
1	B	23	VAL	3.4
2	F	425	THR	3.4
4	H	98	VAL	3.4
5	I	47	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	H	99	THR	3.3
1	C	93	ALA	3.3
3	G	47	GLY	3.3
1	A	94	ILE	3.3
2	F	424	PHE	3.2
3	G	159	SER	3.2
2	E	387	ILE	3.1
3	G	148	LEU	3.0
1	C	61	GLY	3.0
3	G	72	SER	3.0
2	D	423	VAL	3.0
2	D	424	PHE	3.0
1	A	93	ALA	2.9
2	E	445	LEU	2.9
2	D	176	ALA	2.9
3	G	43	VAL	2.8
3	G	46	VAL	2.8
1	B	510	ALA	2.8
3	G	115	ILE	2.8
3	G	83	SER	2.8
2	E	384	LEU	2.8
1	B	377	ALA	2.7
1	B	373	ARG	2.7
1	A	78	ASN	2.7
4	H	46	GLY	2.7
1	B	410	LEU	2.7
4	H	62	LEU	2.7
2	E	110	THR	2.7
2	F	80	ALA	2.6
1	A	448	GLY	2.6
1	B	374	VAL	2.6
5	I	17	ILE	2.6
2	F	474	ALA	2.6
3	G	29	ALA	2.6
4	H	77	VAL	2.5
2	D	426	GLY	2.5
1	A	358	TYR	2.5
3	G	40	PRO	2.5
1	C	91	THR	2.4
1	A	79	ASP	2.4
1	A	463	LYS	2.4
2	E	467	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	423	VAL	2.4
1	B	401	ALA	2.4
5	I	12	ILE	2.3
1	B	509	GLU	2.3
1	C	392	LEU	2.3
1	C	403	PHE	2.3
1	B	378	ALA	2.3
2	E	365	SER	2.3
2	D	473	LEU	2.3
2	E	424	PHE	2.3
4	H	45	PHE	2.3
1	C	172	GLN	2.2
1	A	75	VAL	2.2
3	G	41	ALA	2.2
3	G	145	ALA	2.2
2	D	419	GLN	2.2
2	E	373	GLY	2.2
2	E	471	ASP	2.2
2	E	473	LEU	2.2
2	D	111	LYS	2.2
1	A	510	ALA	2.2
1	C	414	THR	2.2
2	E	377	ILE	2.2
3	G	68	ILE	2.2
4	H	57	VAL	2.2
5	I	22	VAL	2.2
3	G	32	ALA	2.1
3	G	169	ILE	2.1
1	C	412	ALA	2.1
3	G	222	THR	2.1
1	A	375	GLY	2.1
3	G	85	VAL	2.1
2	F	247	GLU	2.1
3	G	168	VAL	2.1
1	C	404	ALA	2.1
3	G	33	ARG	2.1
2	D	175	LYS	2.0
2	E	76	LEU	2.0
4	H	48	LEU	2.0
3	G	70	GLY	2.0
4	H	42	THR	2.0
2	D	76	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	G	171	TYR	2.0
5	I	11	TYR	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](#)

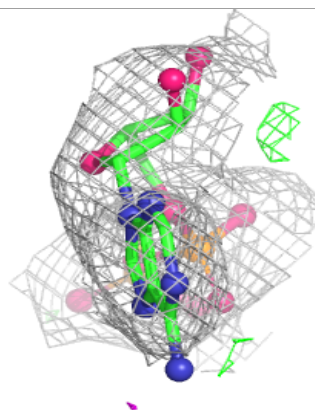
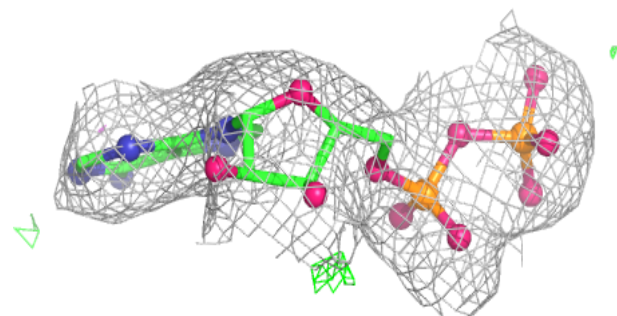
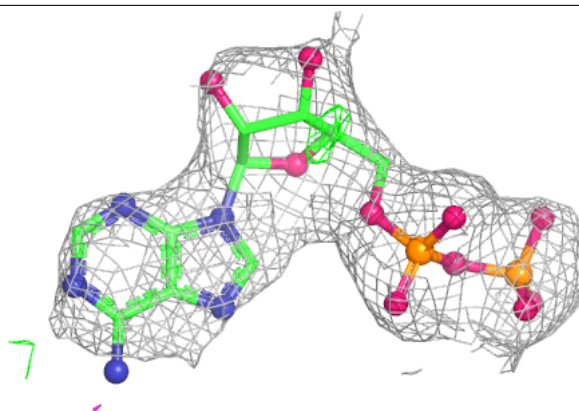
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	ADP	E	600	27/27	0.88	0.10	64,69,72,73	0
6	ADP	C	600	27/27	0.94	0.09	28,34,37,38	0
6	ADP	A	600	27/27	0.94	0.07	33,41,47,48	0
6	ADP	D	600	27/27	0.95	0.09	32,42,47,49	0
6	ADP	B	600	27/27	0.95	0.08	37,41,45,46	0
7	MG	B	601	1/1	0.95	0.06	45,45,45,45	0
6	ADP	F	600	27/27	0.96	0.07	34,40,43,44	0
7	MG	A	601	1/1	0.97	0.05	35,35,35,35	0
7	MG	C	601	1/1	0.98	0.03	34,34,34,34	0
7	MG	D	601	1/1	0.98	0.09	48,48,48,48	0
7	MG	F	601	1/1	0.98	0.05	32,32,32,32	0

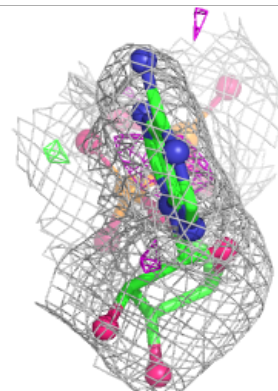
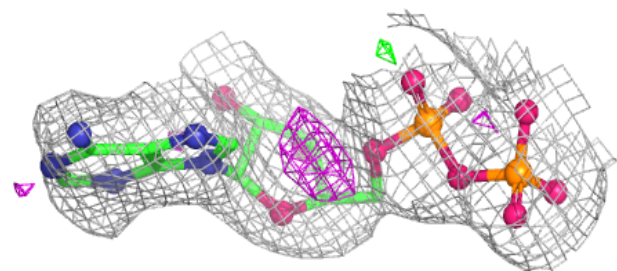
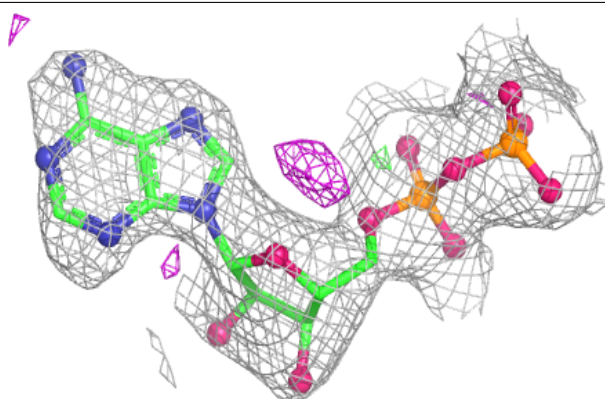
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP E 600:

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

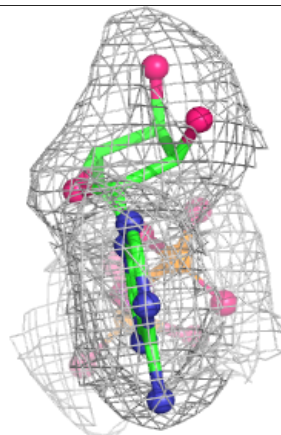
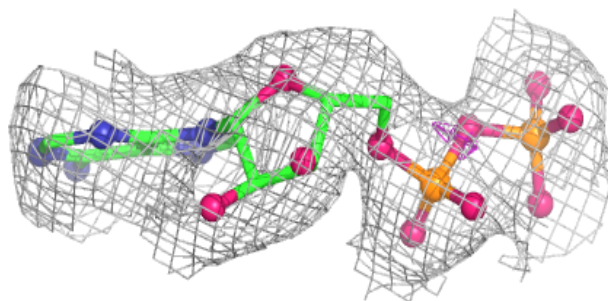
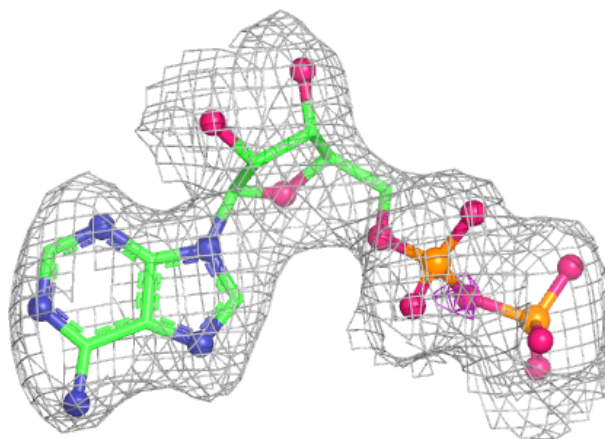
**Electron density around ADP C 600:**

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



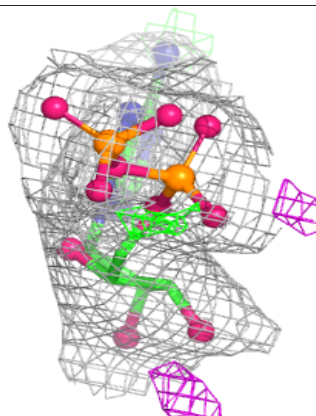
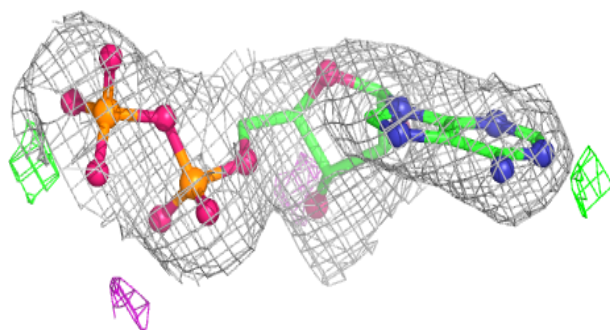
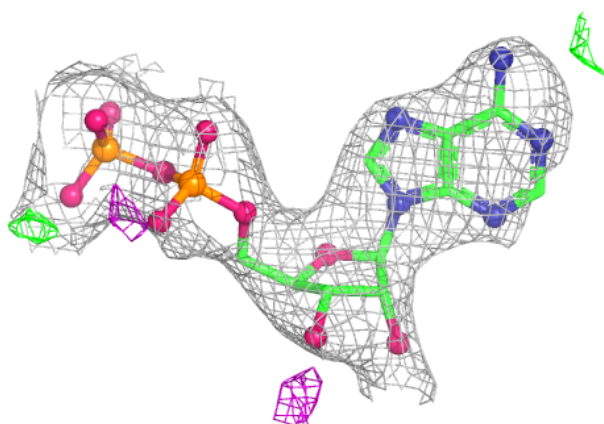
Electron density around ADP A 600:

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

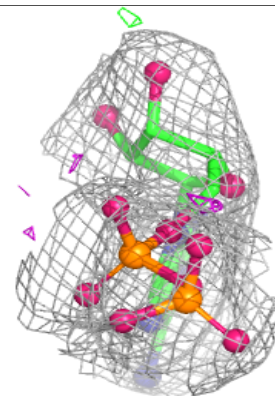
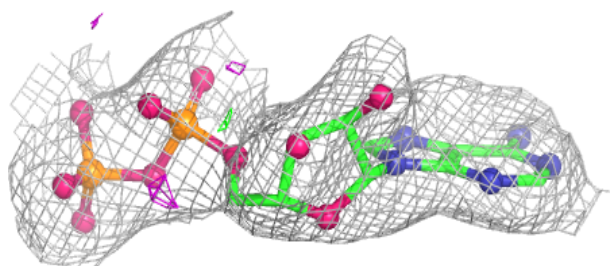
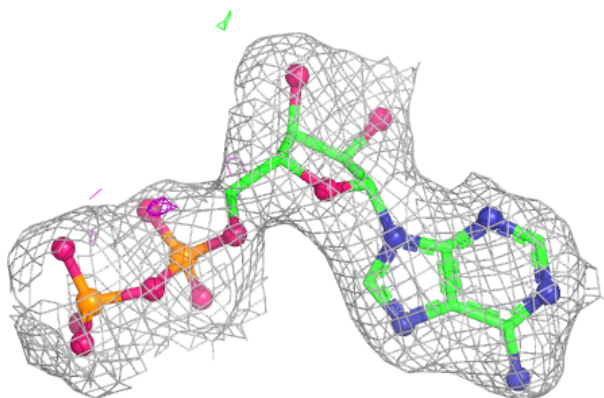


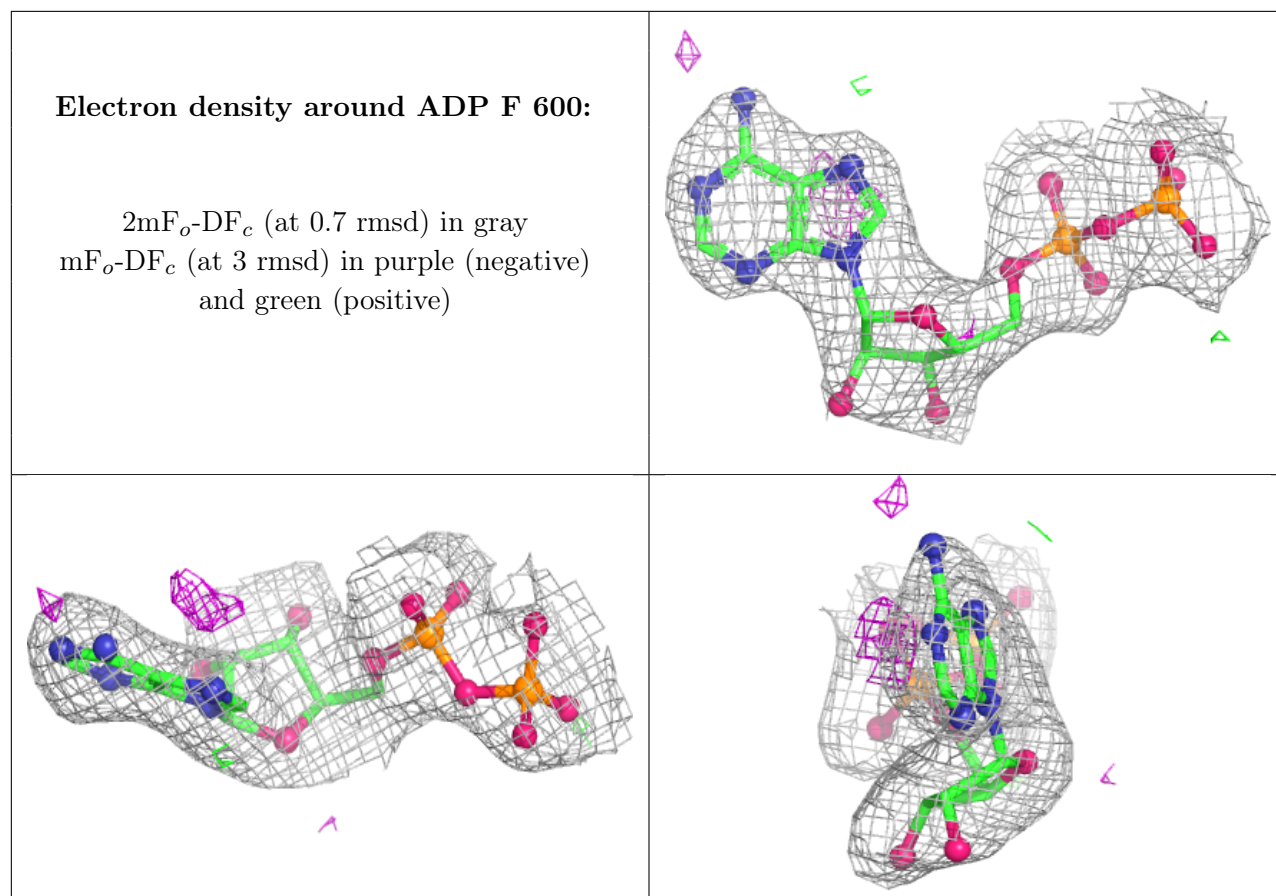
Electron density around ADP D 600:

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

**Electron density around ADP B 600:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.