



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:41 PM UTC

PDB ID : 6UKO / pdb_00006uko
Title : Structure analysis of full-length mouse bcs1 complex
Authors : Xia, D.; Esser, L.
Deposited on : 2019-10-05
Resolution : 4.40 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

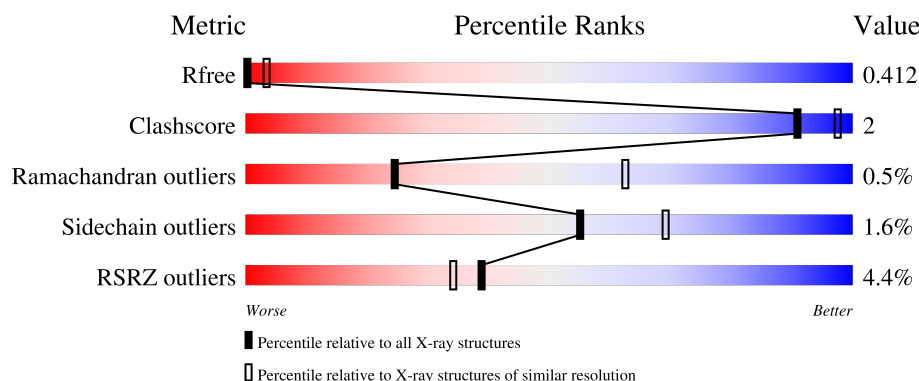
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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.



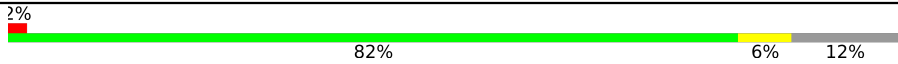
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	424	5% 82% 5% 12%
1	B	424	6% 83% • 12%
1	C	424	4% 80% 7% 12%
1	D	424	3% 81% 6% 12%
1	E	424	3% 82% 5% 12%

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Mol	Chain	Length	Quality of chain
1	F	424	 2% 82% 6% 12%
1	G	424	 3% 81% 6% 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41825 atoms, of which 20699 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 Mitochondrial chaperone BCS1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	B	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	C	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	D	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	E	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	F	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	G	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			

There are 42 discrepancies between the modelled and reference sequences:

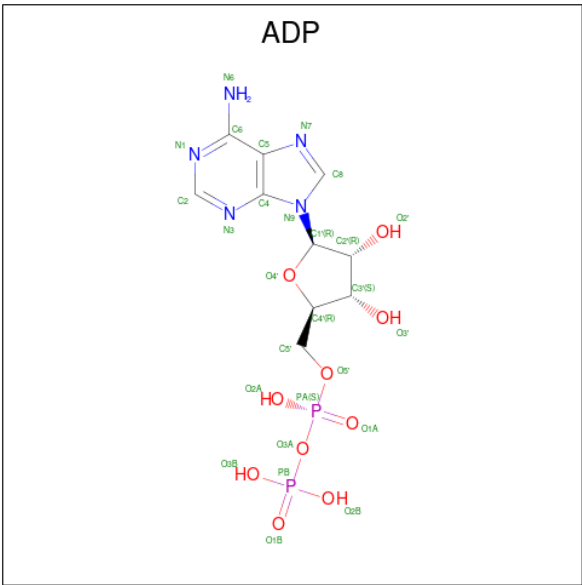
Chain	Residue	Modelled	Actual	Comment	Reference
A	1419	HIS	-	expression tag	UNP Q9CZP5
A	1420	HIS	-	expression tag	UNP Q9CZP5
A	1421	HIS	-	expression tag	UNP Q9CZP5
A	1422	HIS	-	expression tag	UNP Q9CZP5
A	1423	HIS	-	expression tag	UNP Q9CZP5
A	1424	HIS	-	expression tag	UNP Q9CZP5
B	1419	HIS	-	expression tag	UNP Q9CZP5
B	1420	HIS	-	expression tag	UNP Q9CZP5
B	1421	HIS	-	expression tag	UNP Q9CZP5
B	1422	HIS	-	expression tag	UNP Q9CZP5
B	1423	HIS	-	expression tag	UNP Q9CZP5
B	1424	HIS	-	expression tag	UNP Q9CZP5
C	1419	HIS	-	expression tag	UNP Q9CZP5
C	1420	HIS	-	expression tag	UNP Q9CZP5
C	1421	HIS	-	expression tag	UNP Q9CZP5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1422	HIS	-	expression tag	UNP Q9CZP5
C	1423	HIS	-	expression tag	UNP Q9CZP5
C	1424	HIS	-	expression tag	UNP Q9CZP5
D	1419	HIS	-	expression tag	UNP Q9CZP5
D	1420	HIS	-	expression tag	UNP Q9CZP5
D	1421	HIS	-	expression tag	UNP Q9CZP5
D	1422	HIS	-	expression tag	UNP Q9CZP5
D	1423	HIS	-	expression tag	UNP Q9CZP5
D	1424	HIS	-	expression tag	UNP Q9CZP5
E	1419	HIS	-	expression tag	UNP Q9CZP5
E	1420	HIS	-	expression tag	UNP Q9CZP5
E	1421	HIS	-	expression tag	UNP Q9CZP5
E	1422	HIS	-	expression tag	UNP Q9CZP5
E	1423	HIS	-	expression tag	UNP Q9CZP5
E	1424	HIS	-	expression tag	UNP Q9CZP5
F	1419	HIS	-	expression tag	UNP Q9CZP5
F	1420	HIS	-	expression tag	UNP Q9CZP5
F	1421	HIS	-	expression tag	UNP Q9CZP5
F	1422	HIS	-	expression tag	UNP Q9CZP5
F	1423	HIS	-	expression tag	UNP Q9CZP5
F	1424	HIS	-	expression tag	UNP Q9CZP5
G	1419	HIS	-	expression tag	UNP Q9CZP5
G	1420	HIS	-	expression tag	UNP Q9CZP5
G	1421	HIS	-	expression tag	UNP Q9CZP5
G	1422	HIS	-	expression tag	UNP Q9CZP5
G	1423	HIS	-	expression tag	UNP Q9CZP5
G	1424	HIS	-	expression tag	UNP Q9CZP5

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	E	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	F	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	G	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

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

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

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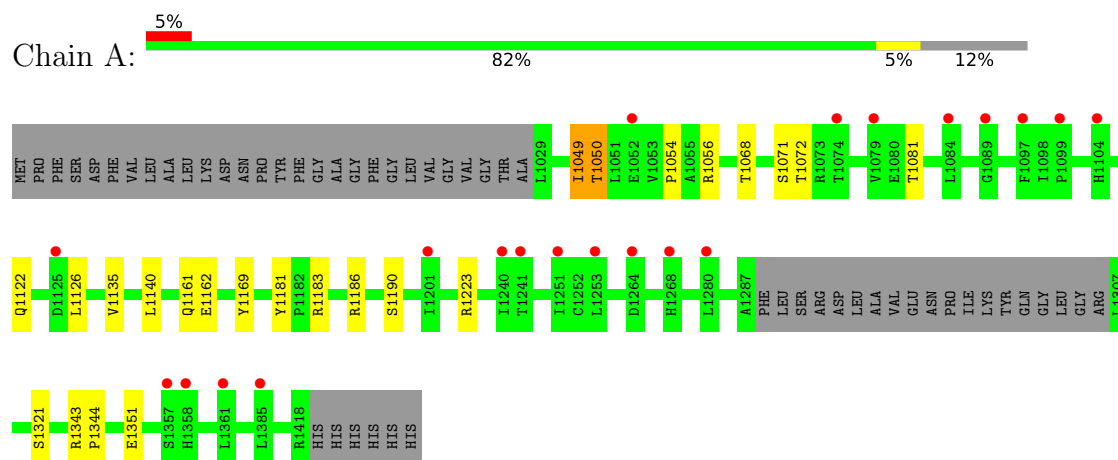
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0

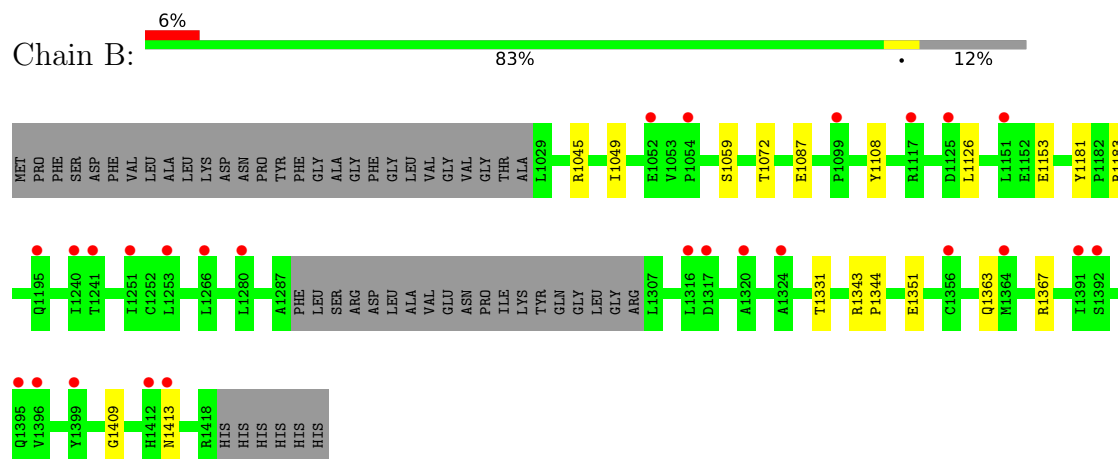
3 Residue-property plots

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.

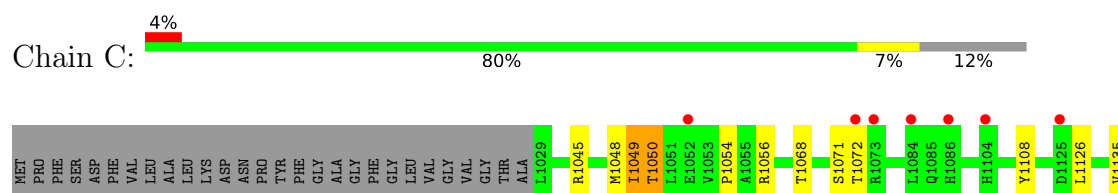
• Molecule 1: Mitochondrial chaperone BCS1

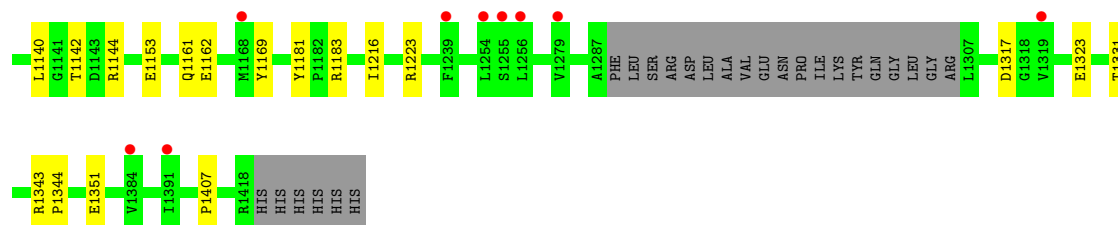


• Molecule 1: Mitochondrial chaperone BCS1

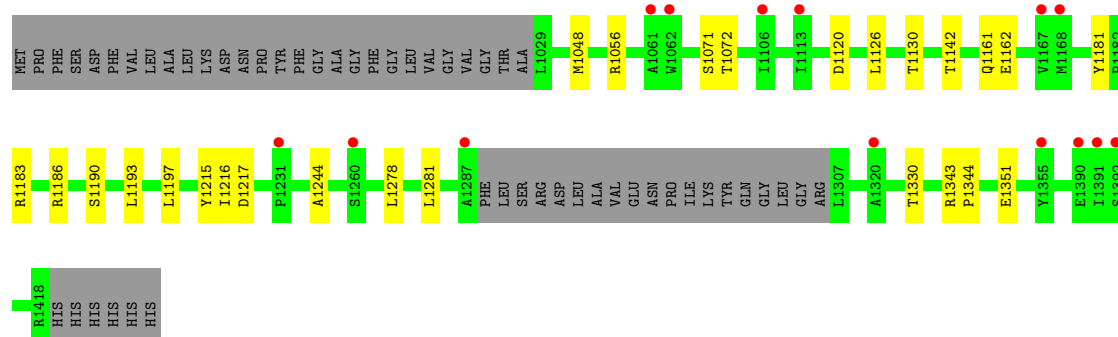
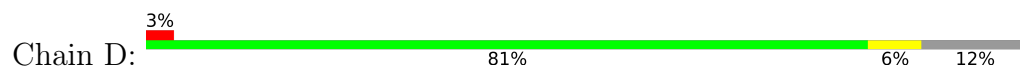


• Molecule 1: Mitochondrial chaperone BCS1

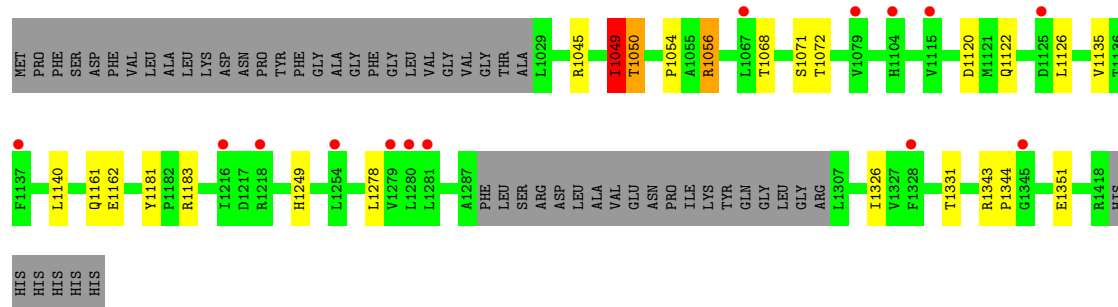
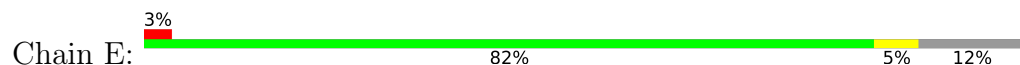




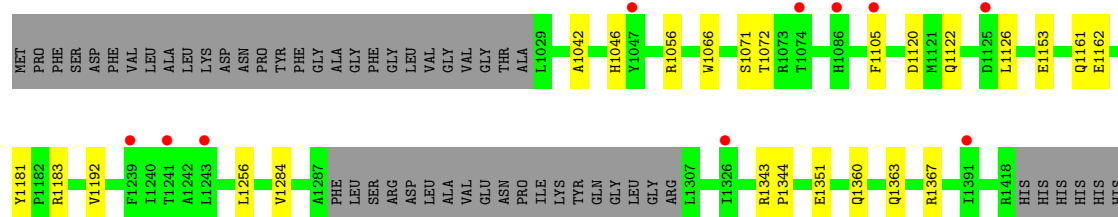
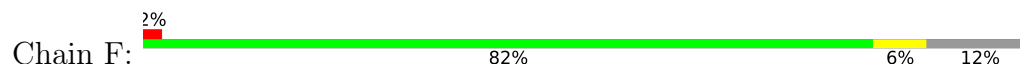
• Molecule 1: Mitochondrial chaperone BCS1



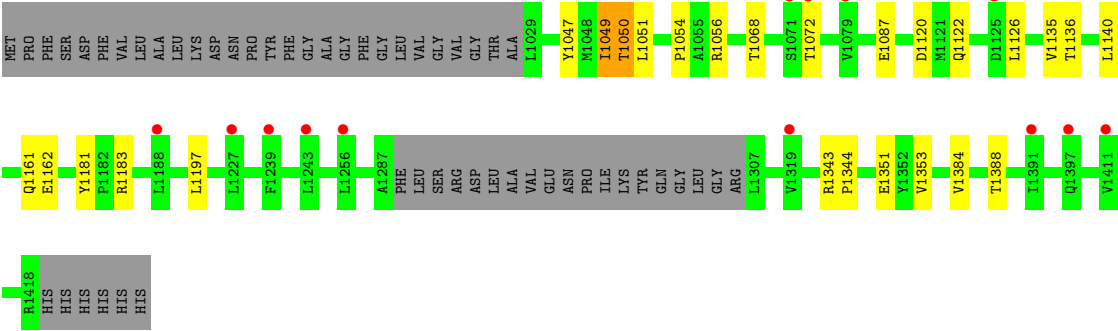
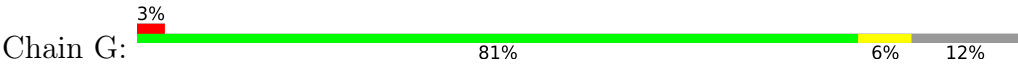
• Molecule 1: Mitochondrial chaperone BCS1



• Molecule 1: Mitochondrial chaperone BCS1



• Molecule 1: Mitochondrial chaperone BCS1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.06Å 161.13Å 132.59Å 90.00° 107.27° 90.00°	Depositor
Resolution (Å)	24.91 – 4.40 24.91 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.91-4.40) 89.6 (24.91-4.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.357 , 0.407 0.375 , 0.412	Depositor DCC
R_{free} test set	1066 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	171.0	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	41825	wwPDB-VP
Average B, all atoms (Å ²)	284.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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

5.1 Standard geometry

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	0.18	0/3063	0.48	0/4154
1	B	0.16	0/3063	0.35	0/4154
1	C	0.18	0/3063	0.48	0/4154
1	D	0.16	0/3063	0.38	0/4154
1	E	0.17	0/3063	0.47	1/4154 (0.0%)
1	F	0.15	0/3063	0.34	0/4154
1	G	0.18	0/3063	0.46	0/4154
All	All	0.17	0/21441	0.43	1/29078 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1049	ILE	CB-CA-C	5.14	119.72	111.29

There are no chirality outliers.

There are no planarity outliers.

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	2990	2945	2955	11	0
1	B	2990	2945	2955	9	1
1	C	2990	2945	2955	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2990	2945	2955	12	0
1	E	2990	2945	2955	12	0
1	F	2990	2945	2955	12	0
1	G	2990	2945	2955	13	1
2	A	27	12	12	0	0
2	B	27	12	12	0	0
2	C	27	12	12	0	0
2	D	27	12	12	0	0
2	E	27	12	12	0	0
2	F	27	12	12	0	0
2	G	27	12	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
All	All	21126	20699	20769	72	1

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 2.

All (72) 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:E:1049:ILE:HG22	1:E:1050:THR:H	1.46	0.78
1:A:1049:ILE:HG22	1:A:1050:THR:H	1.49	0.78
1:C:1049:ILE:HG22	1:C:1050:THR:H	1.48	0.78
1:G:1049:ILE:HG22	1:G:1050:THR:H	1.48	0.78
1:A:1181:TYR:O	1:A:1183:ARG:NH1	2.30	0.64
1:F:1120:ASP:O	1:G:1122:GLN:NE2	2.34	0.61
1:C:1108:TYR:OH	1:C:1153:GLU:OE2	2.19	0.60
1:C:1181:TYR:O	1:C:1183:ARG:NH1	2.35	0.59
1:B:1363:GLN:OE1	1:B:1367:ARG:NH1	2.35	0.59
1:B:1072:THR:O	1:C:1144:ARG:NH2	2.36	0.58
1:A:1122:GLN:NE2	1:G:1120:ASP:O	2.37	0.58
1:B:1087:GLU:O	1:C:1169:TYR:OH	2.21	0.58
1:B:1409:GLY:O	1:B:1413:ASN:ND2	2.36	0.56
1:D:1215:TYR:O	1:D:1217:ASP:N	2.38	0.56
1:C:1343:ARG:NH1	1:C:1344:PRO:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1071:SER:O	1:C:1072:THR:OG1	2.23	0.55
1:D:1181:TYR:O	1:D:1183:ARG:NH1	2.37	0.55
1:E:1045:ARG:HB3	1:E:1049:ILE:HD12	1.88	0.55
1:F:1071:SER:O	1:F:1072:THR:OG1	2.23	0.54
1:G:1181:TYR:O	1:G:1183:ARG:NH1	2.41	0.54
1:F:1181:TYR:O	1:F:1183:ARG:NH1	2.42	0.53
1:A:1223:ARG:NH1	1:A:1321:SER:OG	2.43	0.52
1:E:1181:TYR:O	1:E:1183:ARG:NH1	2.42	0.51
1:C:1223:ARG:NH2	1:C:1317:ASP:OD1	2.45	0.50
1:E:1071:SER:O	1:E:1072:THR:OG1	2.24	0.50
1:D:1071:SER:O	1:D:1072:THR:OG1	2.24	0.50
1:F:1363:GLN:OE1	1:F:1367:ARG:NH1	2.43	0.50
1:F:1192:VAL:O	1:F:1360:GLN:NE2	2.44	0.50
1:B:1181:TYR:O	1:B:1183:ARG:NH1	2.44	0.49
1:A:1071:SER:O	1:A:1072:THR:OG1	2.24	0.49
1:B:1343:ARG:NH1	1:B:1344:PRO:O	2.46	0.49
1:F:1343:ARG:NH1	1:F:1344:PRO:O	2.46	0.48
1:E:1343:ARG:NH1	1:E:1344:PRO:O	2.46	0.48
1:D:1048:MET:HA	1:D:1142:THR:HG22	1.95	0.48
1:D:1281:LEU:O	1:D:1330:THR:OG1	2.32	0.47
1:C:1049:ILE:HG22	1:C:1050:THR:N	2.25	0.46
1:D:1343:ARG:NH1	1:D:1344:PRO:O	2.48	0.46
1:F:1042:ALA:O	1:F:1046:HIS:N	2.46	0.46
1:F:1256:LEU:HD12	1:F:1284:VAL:HG22	1.97	0.46
1:G:1049:ILE:HG22	1:G:1050:THR:N	2.25	0.46
1:F:1161:GLN:OE1	1:F:1162:GLU:N	2.50	0.45
1:G:1161:GLN:OE1	1:G:1162:GLU:N	2.49	0.45
1:A:1161:GLN:OE1	1:A:1162:GLU:N	2.50	0.45
1:D:1161:GLN:OE1	1:D:1162:GLU:N	2.49	0.45
1:E:1161:GLN:OE1	1:E:1162:GLU:N	2.49	0.45
1:C:1161:GLN:OE1	1:C:1162:GLU:N	2.50	0.44
1:D:1244:ALA:HB2	1:D:1278:LEU:HD12	1.98	0.44
1:B:1045:ARG:HB3	1:B:1049:ILE:HD12	2.00	0.44
1:A:1169:TYR:OH	1:G:1087:GLU:O	2.27	0.44
1:G:1197:LEU:HD21	1:G:1353:VAL:HG22	1.99	0.44
1:D:1130:THR:HG22	1:E:1056:ARG:HH12	1.82	0.44
1:A:1081:THR:HG21	1:B:1059:SER:HB3	2.00	0.44
1:E:1249:HIS:HD2	1:E:1278:LEU:HD21	1.83	0.43
1:A:1049:ILE:HG22	1:A:1050:THR:N	2.25	0.43
1:E:1278:LEU:HD22	1:E:1326:ILE:HB	2.01	0.43
1:C:1045:ARG:HB3	1:C:1049:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1049:ILE:O	1:G:1050:THR:HG23	2.19	0.43
1:A:1343:ARG:NH1	1:A:1344:PRO:O	2.52	0.43
1:E:1120:ASP:O	1:F:1122:GLN:NE2	2.51	0.43
1:C:1216:ILE:HD11	1:C:1323:GLU:OE1	2.18	0.42
1:D:1193:LEU:HB3	1:D:1197:LEU:HD23	2.01	0.42
1:A:1186:ARG:HE	1:A:1190:SER:HG	1.68	0.41
1:C:1048:MET:HA	1:C:1142:THR:HG22	2.02	0.41
1:G:1384:VAL:O	1:G:1388:THR:OG1	2.35	0.41
1:B:1108:TYR:OH	1:B:1153:GLU:OE2	2.35	0.41
1:D:1120:ASP:O	1:E:1122:GLN:NE2	2.54	0.41
1:D:1186:ARG:HE	1:D:1190:SER:HG	1.67	0.41
1:F:1105:PHE:O	1:G:1047:TYR:OH	2.39	0.41
1:G:1343:ARG:NH1	1:G:1344:PRO:O	2.54	0.41
1:F:1066:TRP:NE1	1:F:1153:GLU:OE1	2.51	0.41
1:G:1051:LEU:HD11	1:G:1136:THR:OG1	2.22	0.40
1:E:1049:ILE:O	1:E:1050:THR:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1413:ASN:OD1	1:G:1072:THR:OG1[4_445]	2.14	0.06

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	367/424 (87%)	348 (95%)	16 (4%)	3 (1%)	16	52
1	B	367/424 (87%)	348 (95%)	19 (5%)	0	100	100
1	C	367/424 (87%)	347 (95%)	16 (4%)	4 (1%)	11	45
1	D	367/424 (87%)	348 (95%)	18 (5%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	367/424 (87%)	345 (94%)	19 (5%)	3 (1%)	16	52
1	F	367/424 (87%)	349 (95%)	18 (5%)	0	100	100
1	G	367/424 (87%)	344 (94%)	20 (5%)	3 (1%)	16	52
All	All	2569/2968 (87%)	2429 (95%)	126 (5%)	14 (0%)	24	62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1216	ILE
1	E	1050	THR
1	G	1050	THR
1	A	1050	THR
1	C	1050	THR
1	A	1049	ILE
1	A	1054	PRO
1	C	1049	ILE
1	C	1054	PRO
1	E	1049	ILE
1	G	1049	ILE
1	C	1407	PRO
1	E	1054	PRO
1	G	1054	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	320/362 (88%)	314 (98%)	6 (2%)	50	66
1	B	320/362 (88%)	317 (99%)	3 (1%)	70	76
1	C	320/362 (88%)	313 (98%)	7 (2%)	45	64
1	D	320/362 (88%)	317 (99%)	3 (1%)	70	76
1	E	320/362 (88%)	313 (98%)	7 (2%)	45	64
1	F	320/362 (88%)	317 (99%)	3 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	320/362 (88%)	314 (98%)	6 (2%)	50 66
All	All	2240/2534 (88%)	2205 (98%)	35 (2%)	55 69

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1056	ARG
1	A	1068	THR
1	A	1126	LEU
1	A	1135	VAL
1	A	1140	LEU
1	A	1351	GLU
1	B	1126	LEU
1	B	1331	THR
1	B	1351	GLU
1	C	1056	ARG
1	C	1068	THR
1	C	1126	LEU
1	C	1135	VAL
1	C	1140	LEU
1	C	1331	THR
1	C	1351	GLU
1	D	1056	ARG
1	D	1126	LEU
1	D	1351	GLU
1	E	1056	ARG
1	E	1068	THR
1	E	1126	LEU
1	E	1135	VAL
1	E	1140	LEU
1	E	1331	THR
1	E	1351	GLU
1	F	1056	ARG
1	F	1126	LEU
1	F	1351	GLU
1	G	1056	ARG
1	G	1068	THR
1	G	1126	LEU
1	G	1135	VAL
1	G	1140	LEU
1	G	1351	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1267	ASN
1	A	1397	GLN
1	C	1149	ASN
1	C	1267	ASN
1	C	1360	GLN
1	C	1372	GLN
1	E	1267	ASN
1	E	1397	GLN
1	F	1358	HIS
1	F	1379	ASN
1	F	1397	GLN
1	G	1267	ASN
1	G	1397	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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	C	1800	3	28,29,29	1.41	5 (17%)	43,45,45	2.02	9 (20%)
2	ADP	F	1800	3	28,29,29	1.41	5 (17%)	43,45,45	1.95	8 (18%)
2	ADP	A	1800	3	28,29,29	1.38	4 (14%)	43,45,45	1.99	9 (20%)
2	ADP	B	1800	3	28,29,29	1.41	4 (14%)	43,45,45	2.04	8 (18%)
2	ADP	D	1800	3	28,29,29	1.37	5 (17%)	43,45,45	1.96	9 (20%)
2	ADP	G	1800	3	28,29,29	1.38	4 (14%)	43,45,45	2.00	9 (20%)
2	ADP	E	1800	3	28,29,29	1.44	5 (17%)	43,45,45	2.00	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
2	ADP	C	1800	3	-	5/16/32/32	0/3/3/3
2	ADP	F	1800	3	-	5/16/32/32	0/3/3/3
2	ADP	A	1800	3	-	5/16/32/32	0/3/3/3
2	ADP	B	1800	3	-	5/16/32/32	0/3/3/3
2	ADP	D	1800	3	-	4/16/32/32	0/3/3/3
2	ADP	G	1800	3	-	5/16/32/32	0/3/3/3
2	ADP	E	1800	3	-	5/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1800	ADP	C5-C4	4.55	1.47	1.39
2	E	1800	ADP	C5-C4	4.52	1.47	1.39
2	A	1800	ADP	C5-C4	4.51	1.47	1.39
2	F	1800	ADP	C5-C4	4.48	1.47	1.39
2	B	1800	ADP	C5-C4	4.48	1.47	1.39
2	G	1800	ADP	C5-C4	4.47	1.47	1.39
2	D	1800	ADP	C5-C4	4.32	1.46	1.39
2	B	1800	ADP	C5-N7	-2.81	1.34	1.39
2	C	1800	ADP	C5-C6	2.65	1.48	1.41
2	E	1800	ADP	C5-N7	-2.63	1.34	1.39
2	G	1800	ADP	C5-N7	-2.63	1.34	1.39
2	E	1800	ADP	C5-C6	2.61	1.48	1.41
2	A	1800	ADP	C5-N7	-2.58	1.34	1.39
2	F	1800	ADP	C5-N7	-2.58	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1800	ADP	C5-C6	2.55	1.48	1.41
2	D	1800	ADP	C5-N7	-2.55	1.34	1.39
2	F	1800	ADP	C5-C6	2.54	1.48	1.41
2	A	1800	ADP	C5-C6	2.54	1.48	1.41
2	C	1800	ADP	C5-N7	-2.53	1.34	1.39
2	G	1800	ADP	C5-C6	2.48	1.47	1.41
2	D	1800	ADP	C5-C6	2.44	1.47	1.41
2	E	1800	ADP	PA-O3A	2.35	1.62	1.59
2	D	1800	ADP	PA-O3A	2.18	1.61	1.59
2	B	1800	ADP	PA-O3A	2.14	1.61	1.59
2	C	1800	ADP	C8-N7	2.14	1.35	1.31
2	F	1800	ADP	PA-O3A	2.13	1.61	1.59
2	A	1800	ADP	C8-N7	2.08	1.35	1.31
2	D	1800	ADP	C8-N7	2.07	1.35	1.31
2	F	1800	ADP	C8-N7	2.07	1.35	1.31
2	E	1800	ADP	C8-N7	2.06	1.35	1.31
2	G	1800	ADP	C8-N7	2.03	1.35	1.31
2	C	1800	ADP	PA-O3A	2.01	1.61	1.59

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1800	ADP	C5-C4-N3	-6.82	117.33	126.72
2	C	1800	ADP	C5-C4-N3	-6.76	117.41	126.72
2	G	1800	ADP	C5-C4-N3	-6.69	117.50	126.72
2	E	1800	ADP	C5-C4-N3	-6.68	117.52	126.72
2	A	1800	ADP	C5-C4-N3	-6.52	117.74	126.72
2	D	1800	ADP	C5-C4-N3	-6.37	117.94	126.72
2	F	1800	ADP	C5-C4-N3	-6.37	117.95	126.72
2	G	1800	ADP	N3-C4-N9	5.67	136.81	127.17
2	B	1800	ADP	N3-C4-N9	5.65	136.77	127.17
2	C	1800	ADP	N3-C4-N9	5.55	136.60	127.17
2	E	1800	ADP	N3-C4-N9	5.52	136.55	127.17
2	D	1800	ADP	N3-C4-N9	5.48	136.49	127.17
2	A	1800	ADP	N3-C4-N9	5.41	136.37	127.17
2	F	1800	ADP	N3-C4-N9	5.36	136.28	127.17
2	C	1800	ADP	C2-N3-C4	4.04	121.71	111.83
2	G	1800	ADP	C2-N3-C4	4.01	121.64	111.83
2	E	1800	ADP	C2-N3-C4	4.01	121.62	111.83
2	B	1800	ADP	C2-N3-C4	3.99	121.58	111.83
2	D	1800	ADP	C2-N3-C4	3.95	121.47	111.83
2	A	1800	ADP	C2-N3-C4	3.94	121.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1800	ADP	C2-N3-C4	3.94	121.45	111.83
2	B	1800	ADP	C4-C5-N7	-3.65	106.41	110.58
2	E	1800	ADP	C4-C5-N7	-3.52	106.55	110.58
2	C	1800	ADP	C4-C5-N7	-3.50	106.58	110.58
2	F	1800	ADP	N3-C2-N1	-3.38	123.47	128.58
2	A	1800	ADP	C4-C5-N7	-3.37	106.73	110.58
2	D	1800	ADP	N3-C2-N1	-3.34	123.53	128.58
2	F	1800	ADP	C4-C5-N7	-3.33	106.78	110.58
2	B	1800	ADP	C5-N7-C8	3.32	108.67	103.45
2	G	1800	ADP	N3-C2-N1	-3.28	123.62	128.58
2	E	1800	ADP	N3-C2-N1	-3.27	123.64	128.58
2	D	1800	ADP	C4-N9-C8	3.24	109.14	105.74
2	A	1800	ADP	N3-C2-N1	-3.23	123.70	128.58
2	B	1800	ADP	N3-C2-N1	-3.17	123.79	128.58
2	G	1800	ADP	C4-C5-N7	-3.15	106.98	110.58
2	C	1800	ADP	N3-C2-N1	-3.13	123.84	128.58
2	D	1800	ADP	C4-C5-N7	-3.11	107.02	110.58
2	E	1800	ADP	C5-N7-C8	3.11	108.34	103.45
2	F	1800	ADP	C4-N9-C8	3.02	108.91	105.74
2	C	1800	ADP	C5-N7-C8	3.02	108.19	103.45
2	F	1800	ADP	C5-N7-C8	2.96	108.09	103.45
2	A	1800	ADP	C5-N7-C8	2.93	108.06	103.45
2	G	1800	ADP	C5-N7-C8	2.88	107.98	103.45
2	A	1800	ADP	C4-N9-C8	2.86	108.74	105.74
2	G	1800	ADP	C4-N9-C8	2.86	108.74	105.74
2	D	1800	ADP	C5-N7-C8	2.86	107.94	103.45
2	E	1800	ADP	C4-N9-C8	2.82	108.70	105.74
2	B	1800	ADP	C4-N9-C8	2.81	108.69	105.74
2	C	1800	ADP	C4-N9-C8	2.74	108.62	105.74
2	D	1800	ADP	N9-C8-N7	-2.55	110.33	113.94
2	B	1800	ADP	N9-C8-N7	-2.54	110.33	113.94
2	F	1800	ADP	N9-C8-N7	-2.46	110.45	113.94
2	E	1800	ADP	N9-C8-N7	-2.43	110.49	113.94
2	A	1800	ADP	N9-C8-N7	-2.37	110.58	113.94
2	G	1800	ADP	N9-C8-N7	-2.34	110.61	113.94
2	C	1800	ADP	N9-C8-N7	-2.34	110.62	113.94
2	A	1800	ADP	O3B-PB-O2B	2.19	116.01	107.80
2	G	1800	ADP	N6-C6-N1	2.07	122.99	118.38
2	D	1800	ADP	N6-C6-N1	2.03	122.91	118.38
2	C	1800	ADP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (34) torsion outliers are listed below:

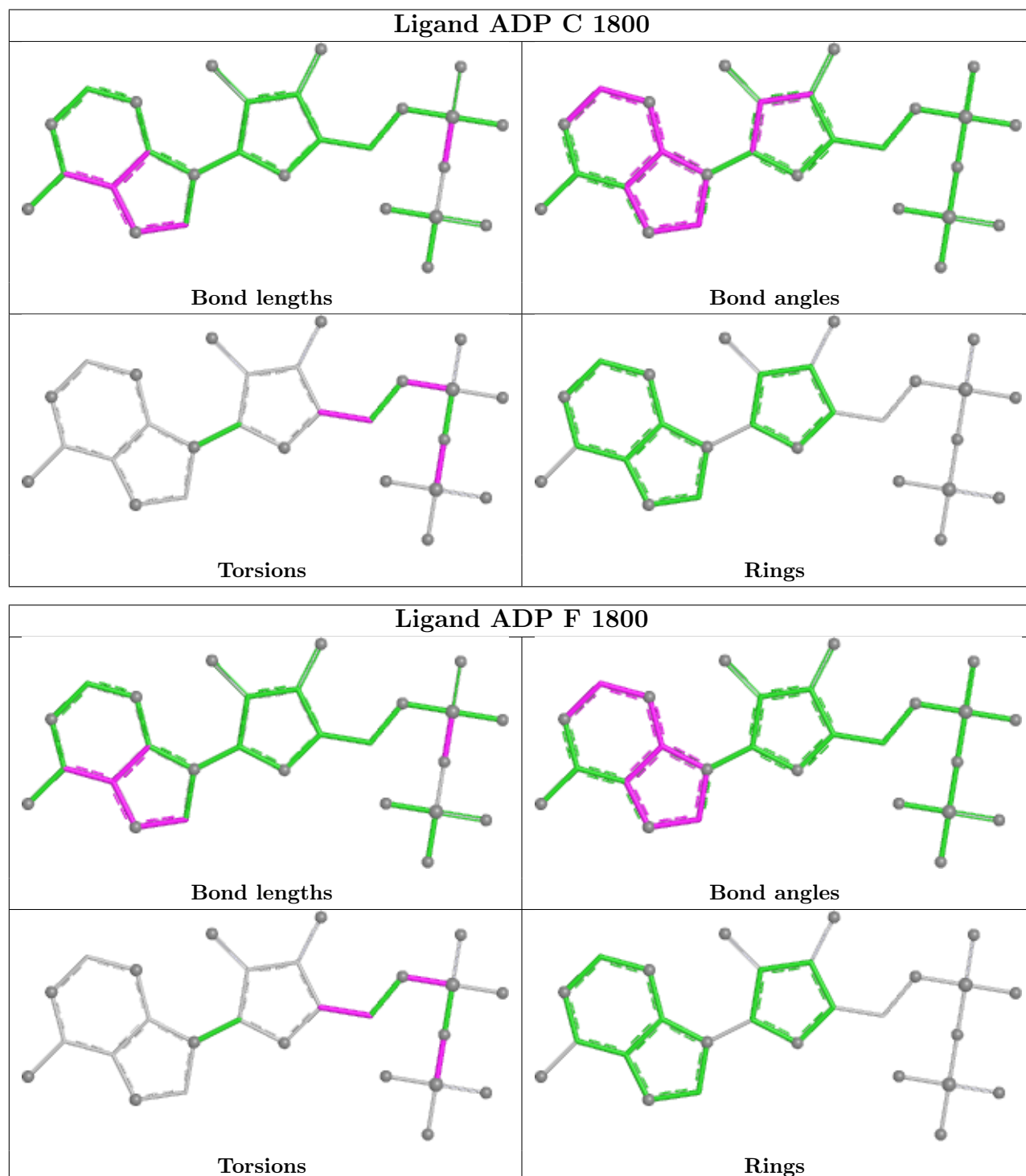
Mol	Chain	Res	Type	Atoms
2	A	1800	ADP	C5'-O5'-PA-O3A
2	B	1800	ADP	C5'-O5'-PA-O3A
2	C	1800	ADP	C5'-O5'-PA-O3A
2	D	1800	ADP	C5'-O5'-PA-O3A
2	E	1800	ADP	C5'-O5'-PA-O3A
2	F	1800	ADP	C5'-O5'-PA-O3A
2	G	1800	ADP	C5'-O5'-PA-O3A
2	A	1800	ADP	O4'-C4'-C5'-O5'
2	B	1800	ADP	O4'-C4'-C5'-O5'
2	C	1800	ADP	O4'-C4'-C5'-O5'
2	D	1800	ADP	O4'-C4'-C5'-O5'
2	E	1800	ADP	O4'-C4'-C5'-O5'
2	F	1800	ADP	O4'-C4'-C5'-O5'
2	G	1800	ADP	O4'-C4'-C5'-O5'
2	B	1800	ADP	C3'-C4'-C5'-O5'
2	C	1800	ADP	C3'-C4'-C5'-O5'
2	E	1800	ADP	C3'-C4'-C5'-O5'
2	A	1800	ADP	C3'-C4'-C5'-O5'
2	D	1800	ADP	C3'-C4'-C5'-O5'
2	F	1800	ADP	C3'-C4'-C5'-O5'
2	G	1800	ADP	C3'-C4'-C5'-O5'
2	E	1800	ADP	PA-O3A-PB-O1B
2	F	1800	ADP	PA-O3A-PB-O1B
2	C	1800	ADP	PA-O3A-PB-O2B
2	A	1800	ADP	C5'-O5'-PA-O1A
2	B	1800	ADP	C5'-O5'-PA-O1A
2	C	1800	ADP	C5'-O5'-PA-O1A
2	D	1800	ADP	C5'-O5'-PA-O1A
2	E	1800	ADP	C5'-O5'-PA-O1A
2	F	1800	ADP	C5'-O5'-PA-O1A
2	G	1800	ADP	C5'-O5'-PA-O1A
2	A	1800	ADP	PA-O3A-PB-O2B
2	B	1800	ADP	PA-O3A-PB-O2B
2	G	1800	ADP	PA-O3A-PB-O2B

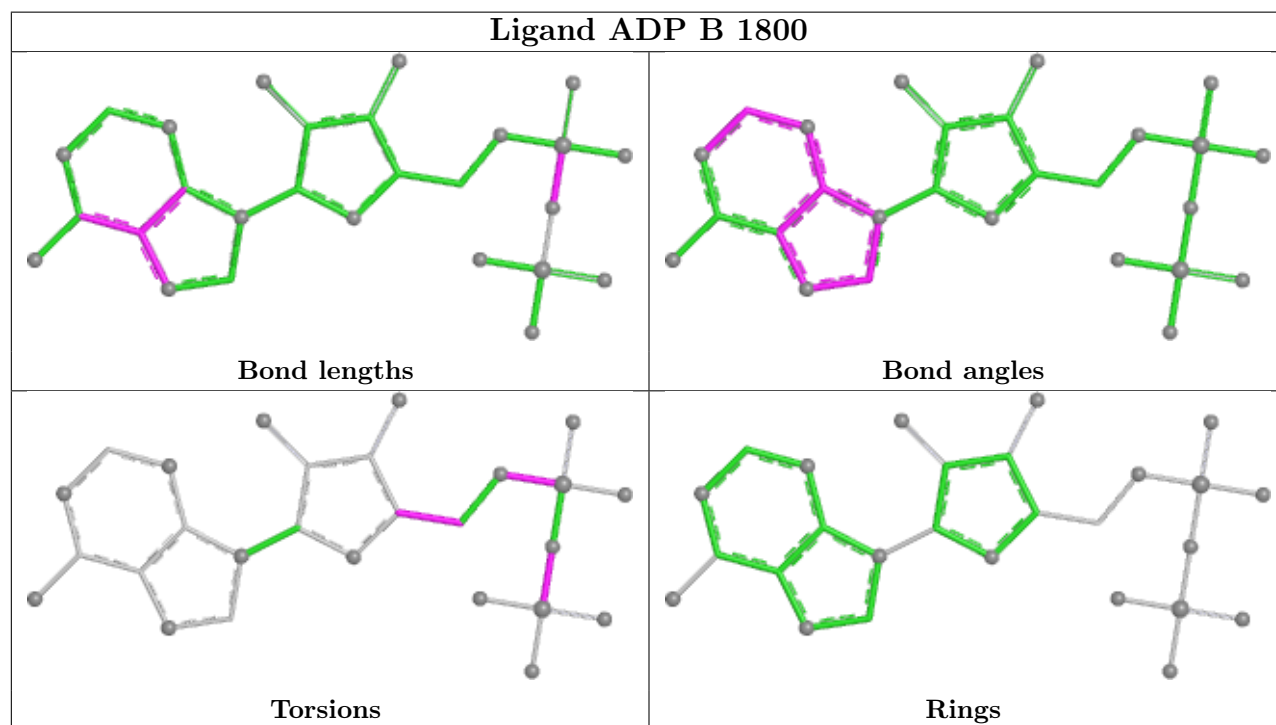
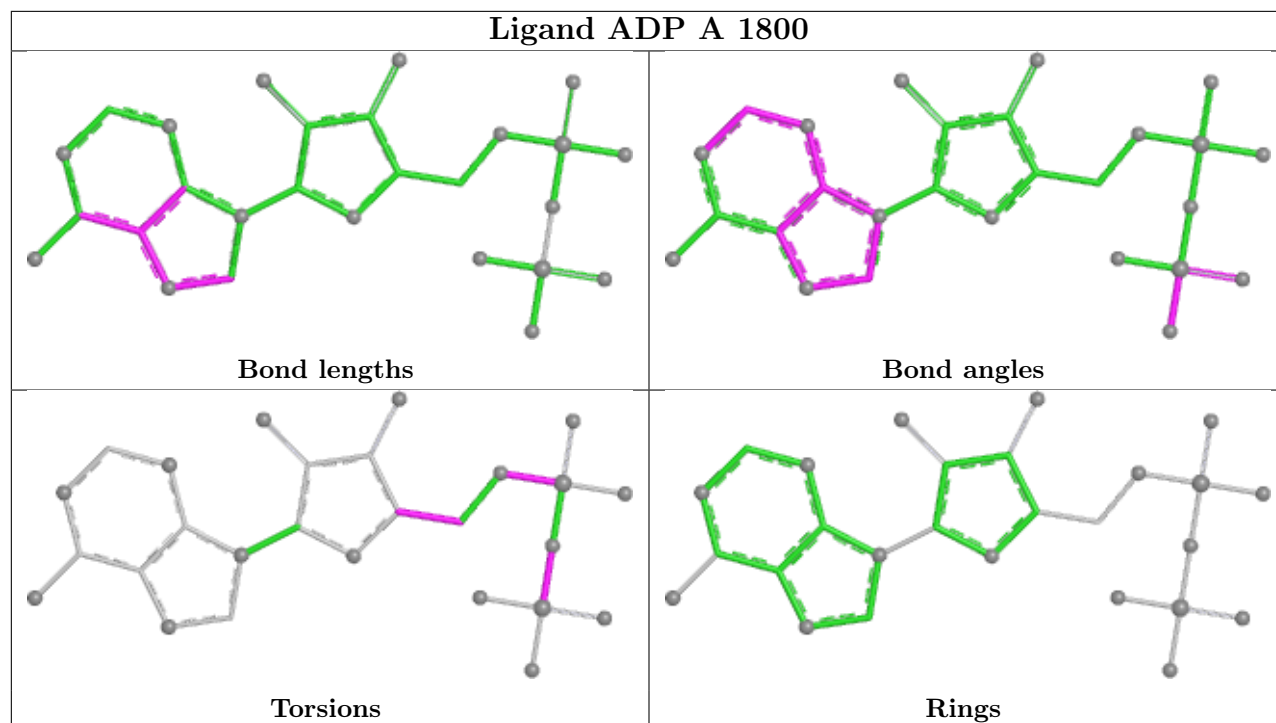
There are no ring outliers.

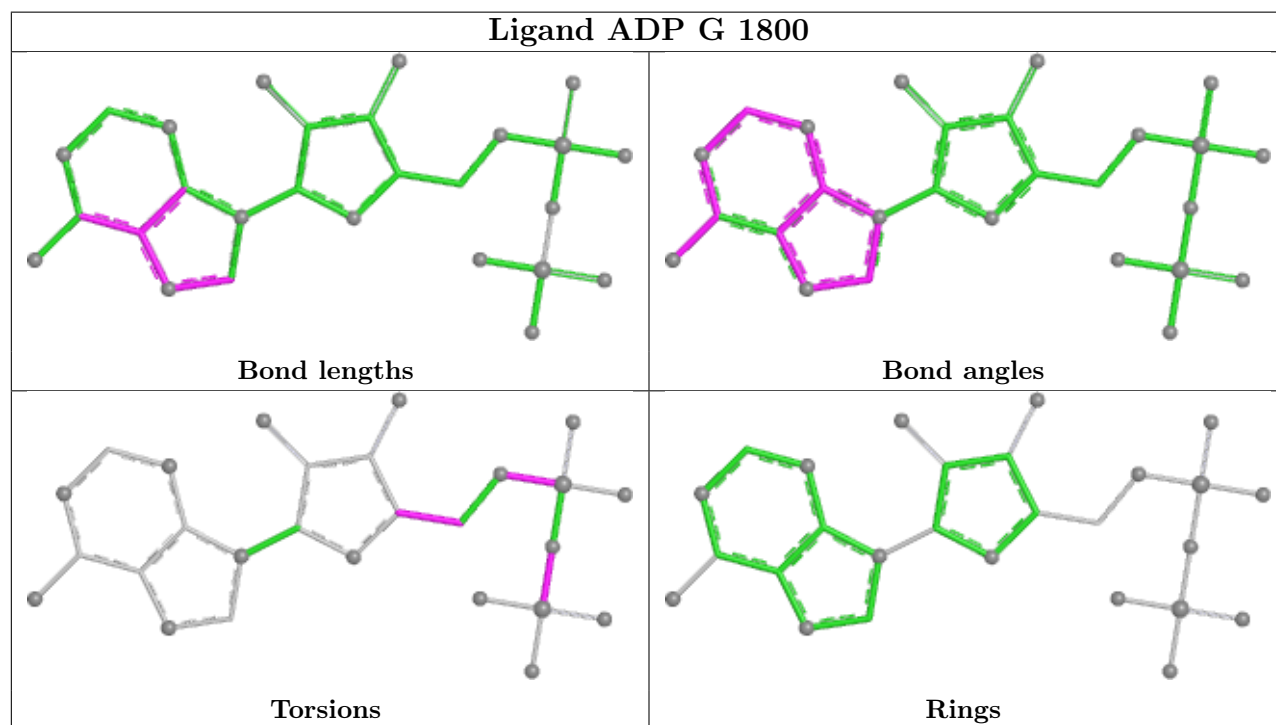
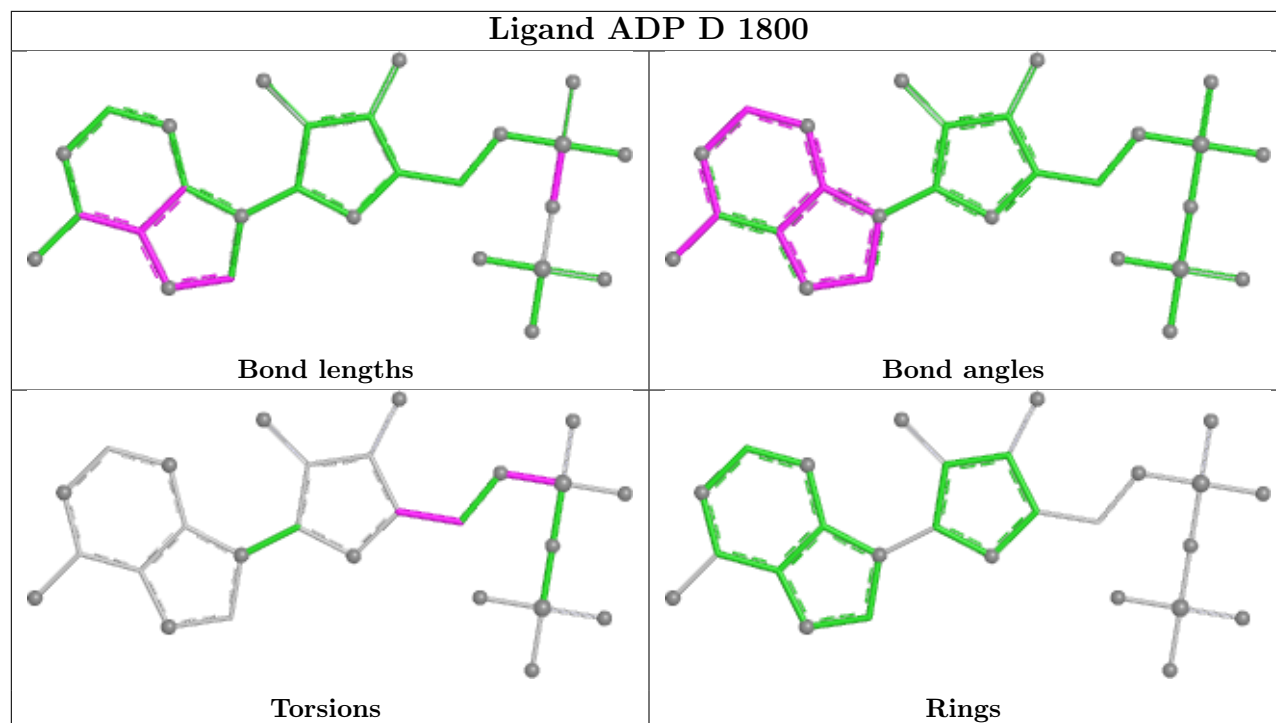
No monomer is involved in short contacts.

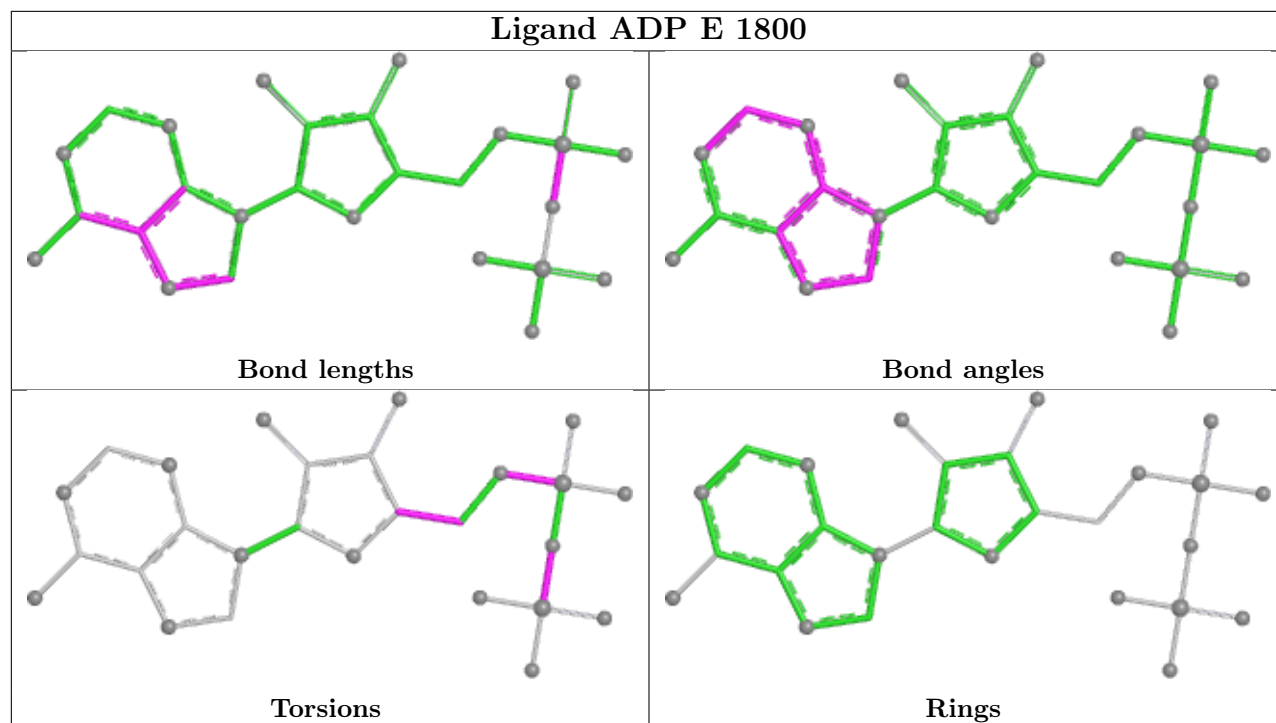
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	371/424 (87%)	0.29	21 (5%)	29	29	266, 283, 293, 299	0
1	B	371/424 (87%)	0.25	26 (7%)	22	24	265, 283, 293, 300	0
1	C	371/424 (87%)	0.19	16 (4%)	40	35	261, 283, 292, 299	0
1	D	371/424 (87%)	0.10	14 (3%)	44	37	271, 284, 295, 303	0
1	E	371/424 (87%)	0.01	14 (3%)	44	37	270, 285, 294, 305	0
1	F	371/424 (87%)	0.04	10 (2%)	56	44	270, 286, 295, 307	0
1	G	371/424 (87%)	0.06	13 (3%)	47	38	269, 284, 294, 303	0
All	All	2597/2968 (87%)	0.13	114 (4%)	39	34	261, 284, 294, 307	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1319	VAL	6.6
1	A	1125	ASP	6.2
1	C	1072	THR	5.9
1	E	1279	VAL	5.6
1	F	1125	ASP	4.9
1	A	1361	LEU	4.9
1	B	1316	LEU	4.8
1	B	1125	ASP	4.7
1	D	1391	ILE	4.4
1	G	1125	ASP	4.4
1	A	1253	LEU	4.3
1	B	1195	GLN	4.3
1	B	1391	ILE	4.2
1	A	1358	HIS	4.2
1	F	1105	PHE	4.2
1	F	1239	PHE	4.1
1	E	1125	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	1256	LEU	3.9
1	F	1391	ILE	3.7
1	G	1411	VAL	3.7
1	C	1254	LEU	3.7
1	F	1326	ILE	3.7
1	D	1168	MET	3.6
1	D	1355	TYR	3.6
1	B	1320	ALA	3.5
1	E	1104	HIS	3.5
1	A	1385	LEU	3.4
1	C	1052	GLU	3.4
1	E	1328	PHE	3.3
1	G	1391	ILE	3.3
1	C	1104	HIS	3.3
1	B	1364	MET	3.3
1	A	1099	PRO	3.2
1	D	1260	SER	3.2
1	B	1413	ASN	3.2
1	B	1395	GLN	3.2
1	E	1137	PHE	3.1
1	G	1239	PHE	3.1
1	B	1392	SER	3.0
1	C	1125	ASP	3.0
1	A	1268	HIS	3.0
1	C	1279	VAL	2.9
1	E	1216	ILE	2.9
1	D	1061	ALA	2.9
1	E	1218	ARG	2.8
1	C	1384	VAL	2.8
1	D	1231	PRO	2.8
1	E	1280	LEU	2.7
1	A	1357	SER	2.7
1	D	1113	ILE	2.7
1	D	1167	VAL	2.7
1	B	1412	HIS	2.7
1	A	1052	GLU	2.6
1	E	1345	GLY	2.6
1	D	1390	GLU	2.6
1	B	1399	TYR	2.6
1	C	1084	LEU	2.6
1	A	1089	GLY	2.6
1	B	1052	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1280	LEU	2.6
1	E	1115	VAL	2.6
1	B	1253	LEU	2.5
1	A	1084	LEU	2.5
1	D	1287	ALA	2.5
1	B	1099	PRO	2.5
1	B	1324	ALA	2.5
1	C	1319	VAL	2.5
1	B	1240	ILE	2.4
1	C	1391	ILE	2.4
1	G	1397	GLN	2.4
1	A	1097	PHE	2.4
1	B	1117	ARG	2.4
1	B	1396	VAL	2.4
1	F	1074	THR	2.3
1	C	1086	HIS	2.3
1	D	1320	ALA	2.3
1	B	1317	ASP	2.3
1	A	1240	ILE	2.3
1	E	1079	VAL	2.3
1	F	1241	THR	2.3
1	E	1281	LEU	2.3
1	C	1168	MET	2.3
1	A	1251	ILE	2.2
1	G	1188	LEU	2.2
1	B	1054	PRO	2.2
1	D	1106	ILE	2.2
1	C	1073	ARG	2.2
1	E	1067	LEU	2.2
1	E	1254	LEU	2.2
1	A	1079	VAL	2.2
1	A	1074	THR	2.2
1	G	1071	SER	2.2
1	G	1227	LEU	2.2
1	A	1201	ILE	2.1
1	B	1251	ILE	2.1
1	B	1151	LEU	2.1
1	B	1266	LEU	2.1
1	B	1356	CYS	2.1
1	A	1104	HIS	2.1
1	A	1241	THR	2.1
1	B	1241	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1062	TRP	2.1
1	F	1243	LEU	2.1
1	A	1280	LEU	2.1
1	C	1239	PHE	2.1
1	D	1392	SER	2.1
1	G	1079	VAL	2.1
1	C	1255	SER	2.0
1	G	1256	LEU	2.0
1	F	1047	TYR	2.0
1	A	1264	ASP	2.0
1	F	1086	HIS	2.0
1	G	1072	THR	2.0
1	G	1243	LEU	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	E	1801	1/1	-0.18	0.22	251,251,251,251	0
3	MG	C	1801	1/1	0.25	0.17	253,253,253,253	0
3	MG	F	1801	1/1	0.39	0.19	250,250,250,250	0
3	MG	G	1801	1/1	0.55	0.11	251,251,251,251	0
3	MG	D	1801	1/1	0.61	0.06	254,254,254,254	0
3	MG	B	1801	1/1	0.70	0.14	251,251,251,251	0
3	MG	A	1801	1/1	0.80	0.09	256,256,256,256	0
2	ADP	C	1800	27/27	0.82	0.13	243,259,312,312	0
2	ADP	E	1800	27/27	0.85	0.11	260,263,316,317	0
2	ADP	B	1800	27/27	0.88	0.08	253,258,310,311	0

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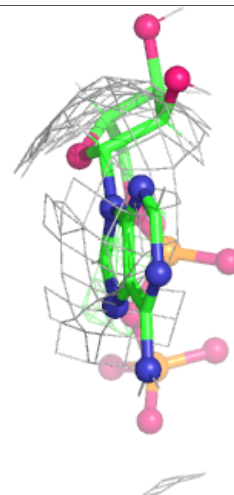
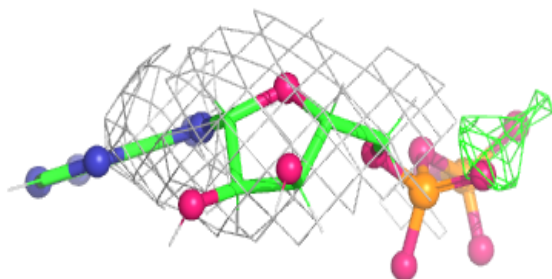
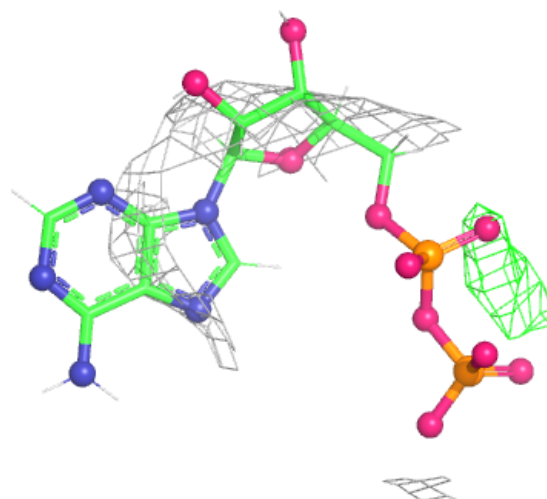
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1800	27/27	0.90	0.10	252,257,311,315	0
2	ADP	D	1800	27/27	0.92	0.08	246,254,305,306	0
2	ADP	G	1800	27/27	0.93	0.11	248,257,310,311	0
2	ADP	F	1800	27/27	0.95	0.10	256,260,314,316	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.

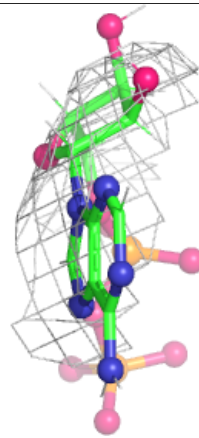
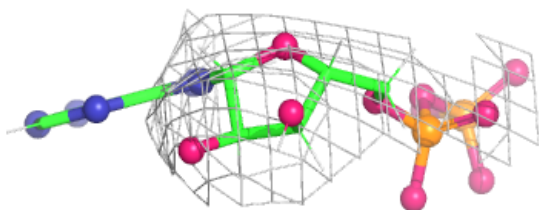
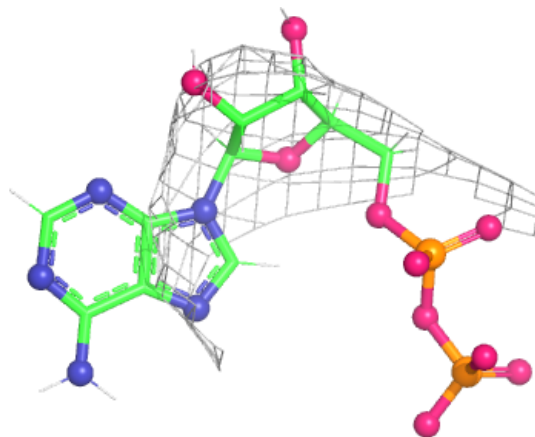
Electron density around ADP C 1800:

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



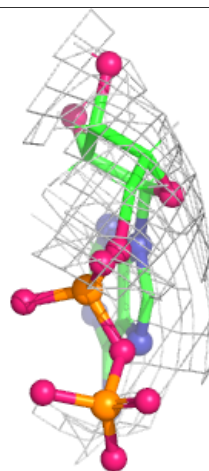
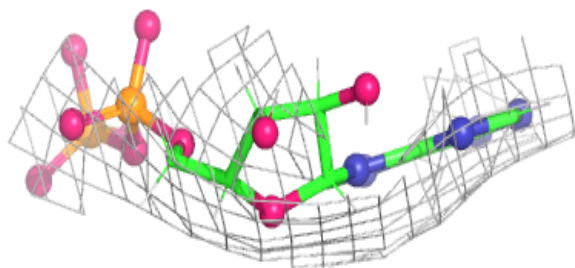
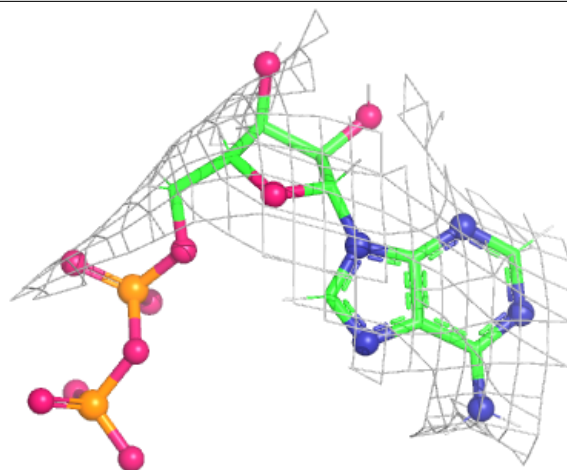
Electron density around ADP E 1800:

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



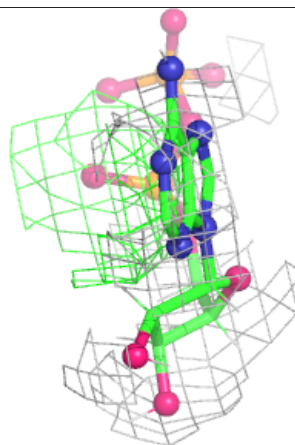
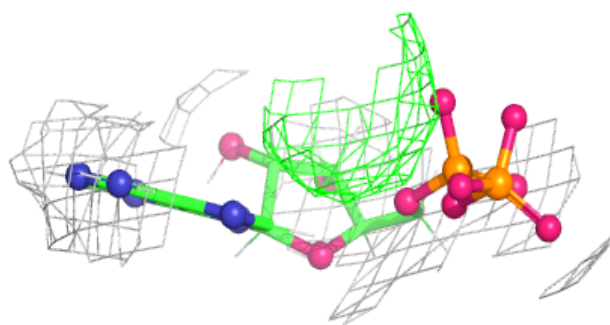
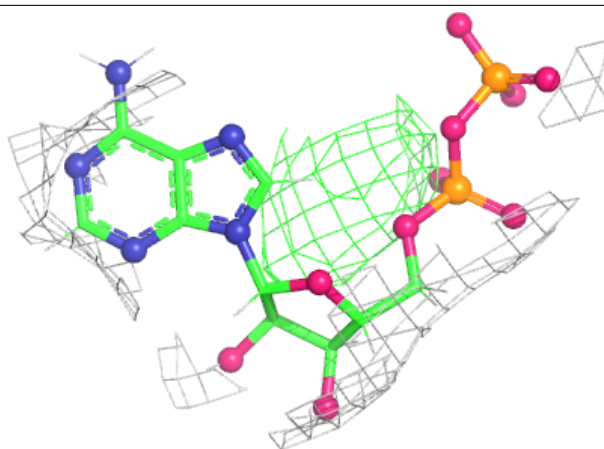
Electron density around ADP B 1800:

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



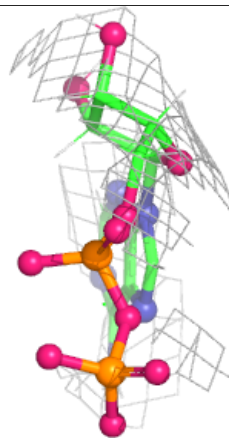
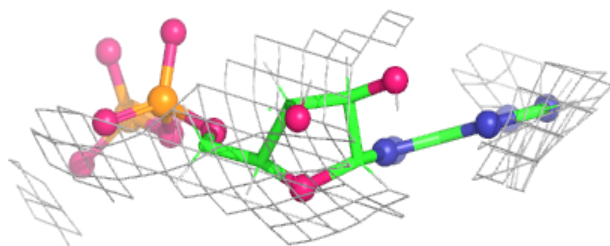
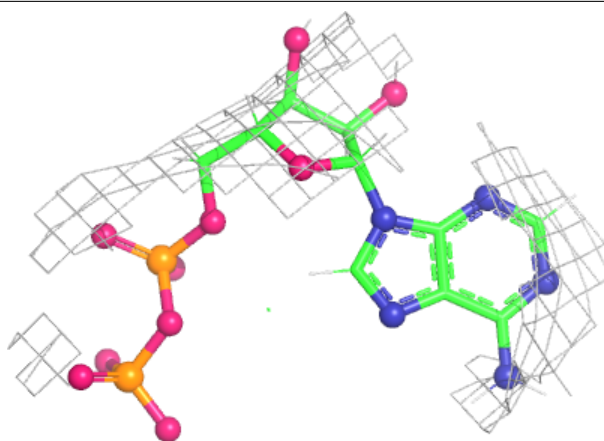
Electron density around ADP A 1800:

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



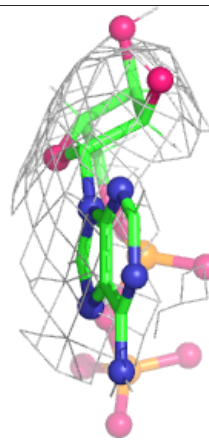
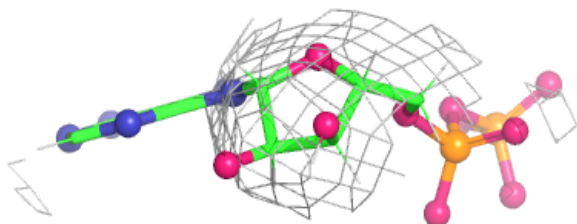
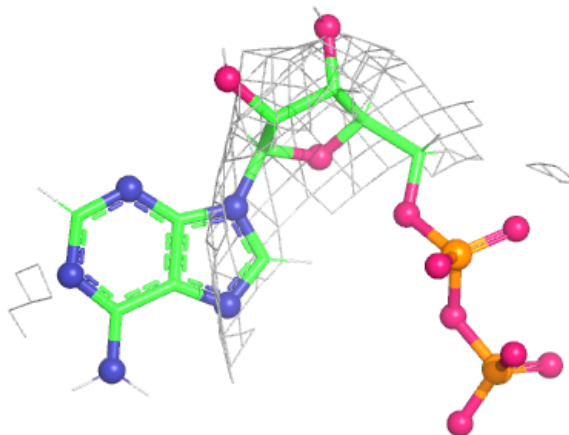
Electron density around ADP D 1800:

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



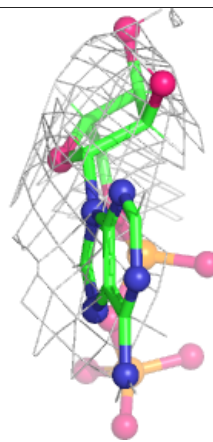
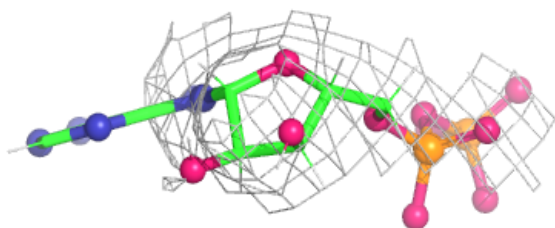
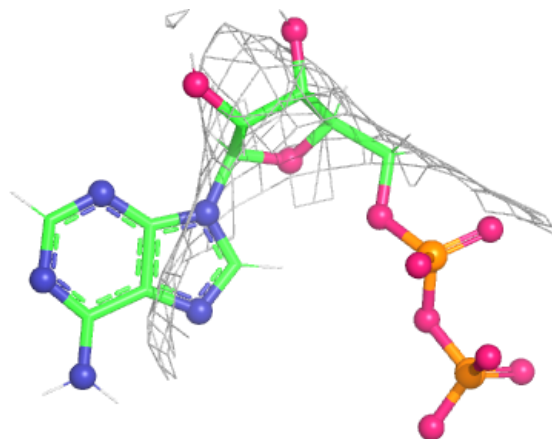
Electron density around ADP G 1800:

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



Electron density around ADP F 1800:

$2mF_o-DF_c$ (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.