Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:33 AM EDT

PDB ID	:	3DLS
Title	:	Crystal structure of human PAS kinase bound to ADP
Authors	:	Antonysamy, S.; Bonanno, J.B.; Romero, R.; Russell, M.; Iizuka, M.; Gheyi, T.; Wasserman, S.R.; Rutter, J.; Sauder, J.M.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-06-29
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

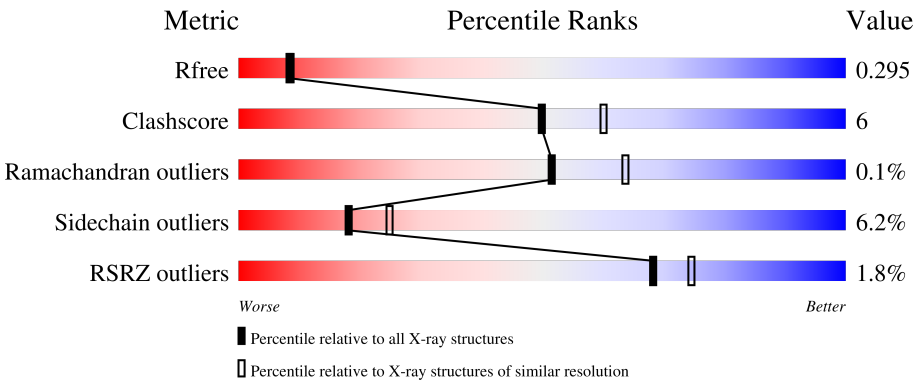
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	335	73% 11% • 15%
1	B	335	2% 68% 14% • 16%
1	C	335	2% 69% 13% • 16%
1	D	335	% 67% 16% • 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	335	% 68% 15% • 16%
1	F	335	3% 71% 12% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13724 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 PAS domain-containing serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2236	1465	350	411	10	0	0	0
1	B	280	2200	1435	353	403	9	0	0	0
1	C	281	2217	1447	355	407	8	0	0	0
1	D	284	2220	1453	351	406	10	0	0	0
1	E	282	2216	1449	353	405	9	0	0	0
1	F	281	2174	1420	345	400	9	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	974	MET	-	expression tag	UNP Q96RG2
A	975	ALA	-	expression tag	UNP Q96RG2
A	976	LEU	-	expression tag	UNP Q96RG2
A	1301	GLU	-	expression tag	UNP Q96RG2
A	1302	GLY	-	expression tag	UNP Q96RG2
A	1303	HIS	-	expression tag	UNP Q96RG2
A	1304	HIS	-	expression tag	UNP Q96RG2
A	1305	HIS	-	expression tag	UNP Q96RG2
A	1306	HIS	-	expression tag	UNP Q96RG2
A	1307	HIS	-	expression tag	UNP Q96RG2
A	1308	HIS	-	expression tag	UNP Q96RG2
B	974	MET	-	expression tag	UNP Q96RG2
B	975	ALA	-	expression tag	UNP Q96RG2
B	976	LEU	-	expression tag	UNP Q96RG2
B	1301	GLU	-	expression tag	UNP Q96RG2
B	1302	GLY	-	expression tag	UNP Q96RG2
B	1303	HIS	-	expression tag	UNP Q96RG2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1304	HIS	-	expression tag	UNP Q96RG2
B	1305	HIS	-	expression tag	UNP Q96RG2
B	1306	HIS	-	expression tag	UNP Q96RG2
B	1307	HIS	-	expression tag	UNP Q96RG2
B	1308	HIS	-	expression tag	UNP Q96RG2
C	974	MET	-	expression tag	UNP Q96RG2
C	975	ALA	-	expression tag	UNP Q96RG2
C	976	LEU	-	expression tag	UNP Q96RG2
C	1301	GLU	-	expression tag	UNP Q96RG2
C	1302	GLY	-	expression tag	UNP Q96RG2
C	1303	HIS	-	expression tag	UNP Q96RG2
C	1304	HIS	-	expression tag	UNP Q96RG2
C	1305	HIS	-	expression tag	UNP Q96RG2
C	1306	HIS	-	expression tag	UNP Q96RG2
C	1307	HIS	-	expression tag	UNP Q96RG2
C	1308	HIS	-	expression tag	UNP Q96RG2
D	974	MET	-	expression tag	UNP Q96RG2
D	975	ALA	-	expression tag	UNP Q96RG2
D	976	LEU	-	expression tag	UNP Q96RG2
D	1301	GLU	-	expression tag	UNP Q96RG2
D	1302	GLY	-	expression tag	UNP Q96RG2
D	1303	HIS	-	expression tag	UNP Q96RG2
D	1304	HIS	-	expression tag	UNP Q96RG2
D	1305	HIS	-	expression tag	UNP Q96RG2
D	1306	HIS	-	expression tag	UNP Q96RG2
D	1307	HIS	-	expression tag	UNP Q96RG2
D	1308	HIS	-	expression tag	UNP Q96RG2
E	974	MET	-	expression tag	UNP Q96RG2
E	975	ALA	-	expression tag	UNP Q96RG2
E	976	LEU	-	expression tag	UNP Q96RG2
E	1301	GLU	-	expression tag	UNP Q96RG2
E	1302	GLY	-	expression tag	UNP Q96RG2
E	1303	HIS	-	expression tag	UNP Q96RG2
E	1304	HIS	-	expression tag	UNP Q96RG2
E	1305	HIS	-	expression tag	UNP Q96RG2
E	1306	HIS	-	expression tag	UNP Q96RG2
E	1307	HIS	-	expression tag	UNP Q96RG2
E	1308	HIS	-	expression tag	UNP Q96RG2
F	974	MET	-	expression tag	UNP Q96RG2
F	975	ALA	-	expression tag	UNP Q96RG2
F	976	LEU	-	expression tag	UNP Q96RG2
F	1301	GLU	-	expression tag	UNP Q96RG2

Continued on next page...

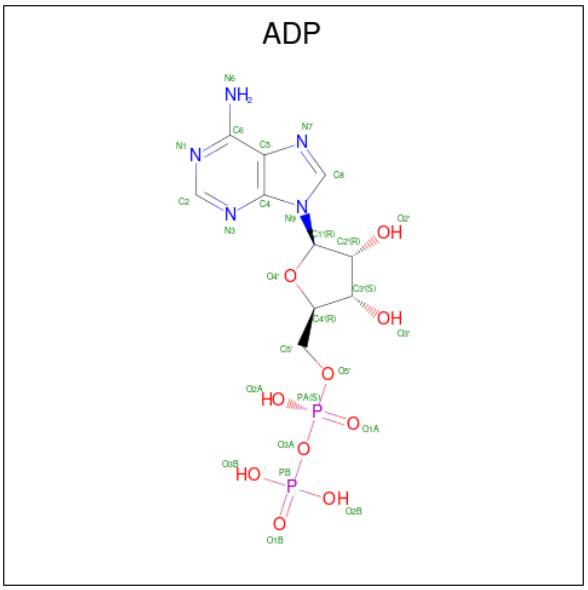
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	1302	GLY	-	expression tag	UNP Q96RG2
F	1303	HIS	-	expression tag	UNP Q96RG2
F	1304	HIS	-	expression tag	UNP Q96RG2
F	1305	HIS	-	expression tag	UNP Q96RG2
F	1306	HIS	-	expression tag	UNP Q96RG2
F	1307	HIS	-	expression tag	UNP Q96RG2
F	1308	HIS	-	expression tag	UNP Q96RG2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	4	4	4	0	0
2	B	4	4	4	0	0
2	C	4	4	4	0	0
2	D	3	3	3	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is water.

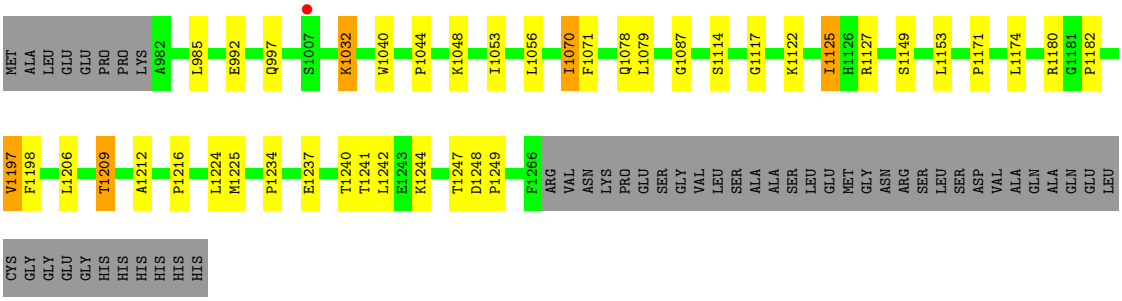
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	55	55	55	0	0
4	B	57	57	57	0	0
4	C	47	47	47	0	0
4	D	48	48	48	0	0
4	E	39	39	39	0	0
4	F	34	34	34	0	0

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.

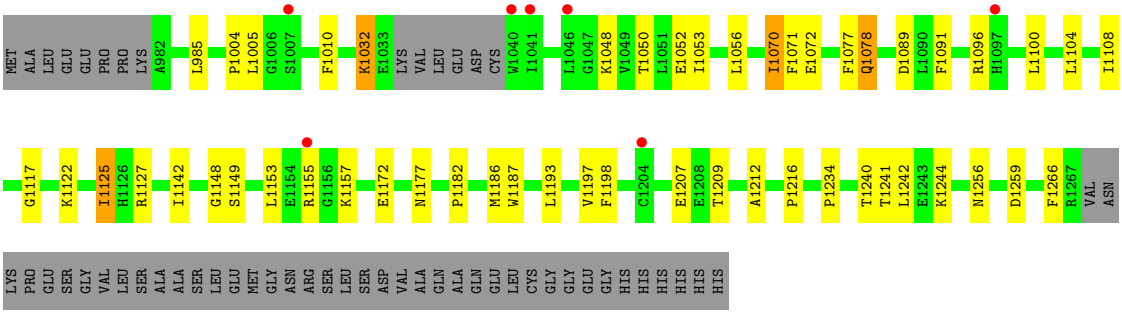
• Molecule 1: PAS domain-containing serine/threonine-protein kinase

Chain A:



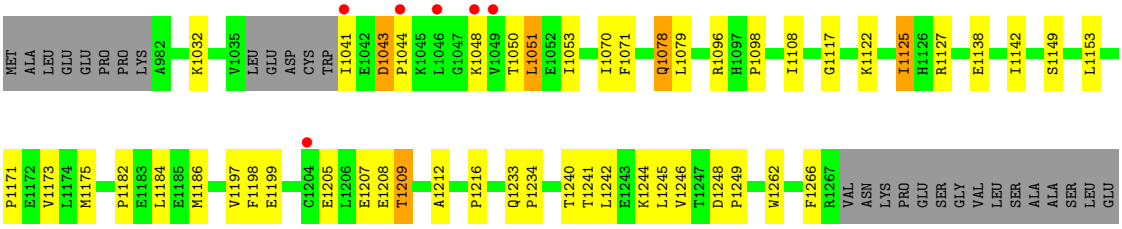
• Molecule 1: PAS domain-containing serine/threonine-protein kinase

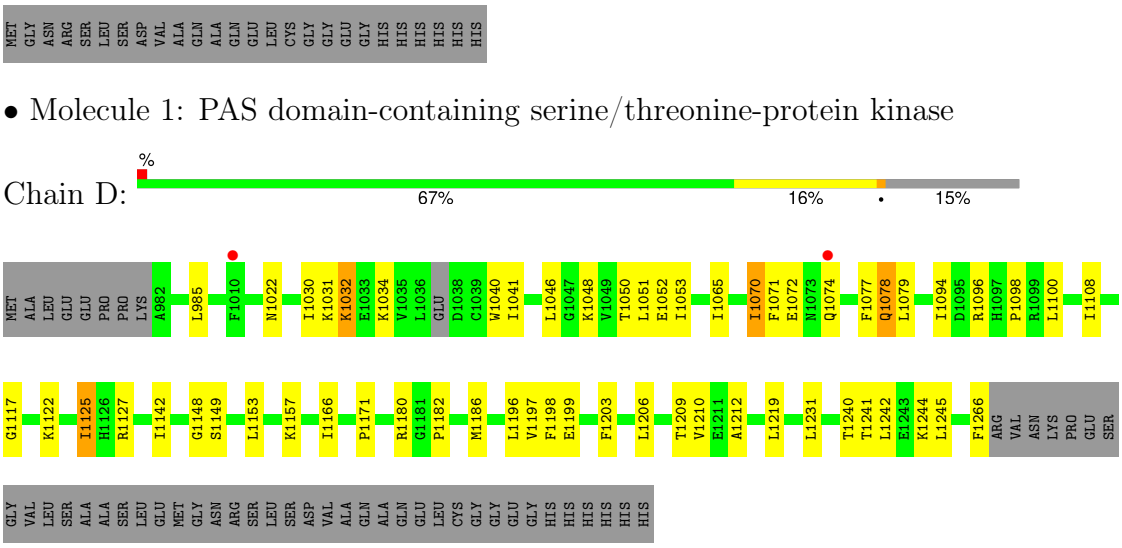
Chain B:



• Molecule 1: PAS domain-containing serine/threonine-protein kinase

Chain C:




MET GLY ASN ARG SER LEU SER ASP VAL ALA GLN ALA GLN GLU LEU CYS GLY GLY GLU GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: PAS domain-containing serine/threonine-protein kinase
Chain D:
%
67%
16%
15%
MET ALA LEU GLU GLU PRO PRO LYS A982 L985 F1010 N1022 I1030 K1031 K1032 E1033 K1034 V1035 L1036 GLU D1038 C1039 W1040 I1041 L1046 G1047 K1048 V1049 T1050 L1051 E1052 I1053 I1065 I1070 F1071 E1072 N1073 Q1074 F1077 Q1078 L1079 I1094 D1095 R1096 H1097 P1098 R1099 L1100 I1108
G1117 K1122 I1125 H1126 R1127 I1142 G1148 S1149 L1153 K1157 I1166 P1171 R1180 G1181 P1182 M1186 L1196 V1197 F1198 E1199 F1203 L1206 T1209 V1210 E1211 A1212 L1219 L1231 T1240 T1241 L1242 E1243 K1244 L1245 F1266 ARG VAL ASN LYS PRO GLU SER
GLY VAL LEU SER ALA ALA SER LEU GLU MET GLY ASN ARG SER LEU SER ASP VAL ALA ALA GLN ALA GLN GLU LEU CYS GLY GLY GLU GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: PAS domain-containing serine/threonine-protein kinase
Chain E:
%
68%
15%
16%
MET ALA LEU GLU GLU PRO PRO LYS A982 L985 G1006 S1007 G1008 A1009 D1018 N1022 I1030 K1031 K1032 V1035 LEU GLU ASP CYS W1040 I1041 E1042 K1048 I1053 A1054 I1055 I1070 F1071 F1077 Q1078 L1079 I1094 D1095 R1096 L1100 I1108 L1112 V1116 G1117
K1122 D1123 I1124 I1125 H1126 R1127 I1142 K1143 L1144 S1149 L1153 E1154 R1155 G1156 K1157 I1166 L1174 P1182 M1186 L1196 V1197 F1198 E1199 E1200 T1209 I1214 H1215 P1216 P1217 Y1218 L1219 E1237 T1241 L1242 E1243 K1244 L1245 V1246 T1247 D1248 P1249 F1266 R1267 VAL ASN LYS PRO
GLU SER GLY VAL LEU SER ALA ALA SER LEU GLU MET GLY ASN ARG SER LEU SER ASP VAL ALA ALA GLN ALA GLN GLU LEU CYS GLY GLY GLU GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: PAS domain-containing serine/threonine-protein kinase
Chain F:
3%
71%
12%
16%
MET ALA LEU GLU GLU PRO PRO LYS A982 L985 A990 C991 Y995 A1009 V1017 I1030 K1031 K1032 V1035 LEU GLU ASP CYS W1040 I1041 E1042 K1048 L1051 I1055 D1069 I1070 F1071 E1072 F1077 Q1078 L1079 I1094 L1100 L1121 K1122 D1123 I1124 I1125 H1126 R1127
S1149 L1153 I1166 P1171 M1175 P1182 M1186 L1196 F1203 C1204 E1205 L1206 E1207 E1208 T1209 V1210 E1211 A1212 L1219 V1235 T1241 K1244 L1245 L1257 Y1260 F1266 ARG VAL ASN LYS PRO GLU SER GLY VAL LEU SER ALA ALA SER LEU GLU MET GLY
ASN ARG SER LEU SER ASP VAL ALA GLN ALA GLN GLU LEU CYS GLY GLY GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.78Å 85.84Å 94.15Å 77.28° 77.50° 60.09°	Depositor
Resolution (Å)	(Not available) – 2.30 31.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 95.9 (31.20-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.297 0.240 , 0.295	Depositor DCC
R_{free} test set	4846 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 23.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.216 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13724	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/2291	0.61	0/3118
1	B	0.46	0/2252	0.61	2/3062 (0.1%)
1	C	0.46	0/2269	0.58	0/3083
1	D	0.43	0/2274	0.59	0/3094
1	E	0.42	0/2270	0.57	0/3088
1	F	0.42	0/2226	0.55	0/3033
All	All	0.44	0/13582	0.59	2/18478 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1005	LEU	O-C-N	6.14	133.64	123.20
1	B	1005	LEU	CA-C-N	-5.30	105.60	116.20

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	2236	0	2198	21	0
1	B	2200	0	2168	27	0
1	C	2217	0	2190	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2220	0	2178	31	0
1	E	2216	0	2178	28	0
1	F	2174	0	2109	18	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	2	0
3	F	27	0	12	0	0
4	A	55	0	0	1	0
4	B	57	0	0	0	0
4	C	47	0	0	2	0
4	D	48	0	0	0	0
4	E	39	0	0	2	0
4	F	34	0	0	0	0
All	All	13724	0	13093	153	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 6.

All (153) 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:C:1125:ILE:HG23	1:C:1127:ARG:HG3	1.67	0.74
1:D:1032:LYS:HZ1	1:D:1074:GLN:HA	1.51	0.74
1:A:1240:THR:HG23	1:A:1244:LYS:HD2	1.70	0.73
1:A:1125:ILE:HG23	1:A:1127:ARG:HG3	1.72	0.71
1:E:1094:ILE:HD11	1:E:1196:LEU:HA	1.71	0.71
1:C:1117:GLY:HA2	1:C:1242:LEU:HD21	1.72	0.71
1:E:1053:ILE:CG2	1:E:1070:ILE:HD12	2.23	0.68
1:F:1127:ARG:HD3	1:F:1149:SER:O	1.92	0.67
1:C:1071:PHE:HB2	1:C:1078:GLN:HE21	1.60	0.67
1:F:1041:ILE:HG13	1:F:1051:LEU:HD13	1.75	0.66
1:D:1125:ILE:HG23	1:D:1127:ARG:HG3	1.78	0.66
1:E:1174:LEU:HD12	1:E:1209:THR:HG21	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1182:PRO:O	1:B:1186:MET:HG2	1.96	0.66
1:B:1240:THR:HG23	1:B:1244:LYS:HD2	1.79	0.65
1:E:1053:ILE:HG21	1:E:1070:ILE:HD12	1.79	0.65
1:E:1241:THR:HG22	1:E:1244:LYS:HE2	1.79	0.65
1:D:1032:LYS:NZ	1:D:1074:GLN:HA	2.13	0.62
1:A:1117:GLY:HA2	1:A:1242:LEU:HD21	1.82	0.62
1:A:1053:ILE:HG21	1:A:1070:ILE:HD12	1.82	0.61
1:A:1127:ARG:HD3	1:A:1149:SER:O	2.00	0.61
1:C:1241:THR:HG23	1:C:1244:LYS:H	1.65	0.61
1:D:1166:ILE:HG22	1:D:1206:LEU:HD11	1.83	0.60
1:F:1094:ILE:HD11	1:F:1196:LEU:HA	1.83	0.60
1:D:1053:ILE:CG2	1:D:1070:ILE:HD12	2.32	0.60
1:E:1242:LEU:O	1:E:1246:VAL:HG23	2.03	0.59
1:D:1053:ILE:HG21	1:D:1070:ILE:HD12	1.85	0.59
1:B:1125:ILE:HG23	1:B:1127:ARG:HG3	1.85	0.59
1:C:1127:ARG:HD3	1:C:1149:SER:O	2.02	0.58
1:D:1041:ILE:HG13	1:D:1051:LEU:HD13	1.86	0.58
1:F:1030:ILE:HB	1:F:1077:PHE:HB2	1.84	0.58
1:F:1166:ILE:HG23	1:F:1206:LEU:HD21	1.86	0.57
1:D:1108:ILE:HG23	1:D:1142:ILE:HG21	1.87	0.56
1:A:1212:ALA:HB3	1:A:1234:PRO:HG3	1.88	0.56
1:E:1096:ARG:HG3	1:E:1266:PHE:CZ	2.42	0.55
1:E:1125:ILE:HG23	1:E:1127:ARG:HG3	1.89	0.55
1:E:1108:ILE:HG23	1:E:1142:ILE:HG21	1.88	0.54
1:B:1052:GLU:O	1:B:1056:LEU:HB2	2.08	0.54
1:D:1096:ARG:HG3	1:D:1266:PHE:CZ	2.43	0.54
1:A:1171:PRO:HB3	1:A:1209:THR:HG23	1.90	0.54
1:A:1174:LEU:HD12	1:A:1209:THR:HG21	1.90	0.53
1:E:1030:ILE:HB	1:E:1077:PHE:HB2	1.90	0.53
1:B:1117:GLY:HA2	1:B:1242:LEU:HD21	1.90	0.53
1:A:1125:ILE:HG23	1:A:1127:ARG:CG	2.37	0.53
1:A:1053:ILE:CG2	1:A:1070:ILE:HD12	2.39	0.52
1:C:1078:GLN:NE2	4:C:113:HOH:O	2.42	0.52
1:B:1052:GLU:HB2	1:B:1148:GLY:HA2	1.91	0.52
1:D:1032:LYS:HE3	1:D:1072:GLU:HG3	1.91	0.52
1:F:1205:GLU:O	1:F:1208:GLU:HG2	2.09	0.52
1:D:1030:ILE:HB	1:D:1077:PHE:HB2	1.91	0.52
1:F:1166:ILE:CG2	1:F:1206:LEU:HD21	2.40	0.52
1:D:1127:ARG:HD3	1:D:1149:SER:O	2.09	0.52
1:B:1050:THR:HG23	1:B:1053:ILE:H	1.75	0.52
1:C:1096:ARG:HB2	1:C:1266:PHE:HE1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1144:LEU:HB2	4:E:270:HOH:O	2.11	0.51
1:C:1050:THR:HG22	1:C:1053:ILE:HD12	1.92	0.51
1:D:1046:LEU:HD22	1:D:1070:ILE:HD13	1.92	0.51
1:A:1197:VAL:HG21	1:A:1224:LEU:HD21	1.93	0.51
1:D:1050:THR:HG22	1:D:1053:ILE:HD12	1.93	0.51
1:E:1078:GLN:NE2	4:E:244:HOH:O	2.43	0.50
1:C:1182:PRO:O	1:C:1186:MET:HG2	2.12	0.50
1:A:1044:PRO:HB2	1:D:1072:GLU:HB3	1.94	0.50
1:E:1127:ARG:HD3	1:E:1149:SER:O	2.12	0.50
1:F:1055:ILE:HG23	1:F:1124:ILE:HD13	1.94	0.50
1:B:1071:PHE:HB2	1:B:1078:GLN:HE21	1.77	0.49
1:D:1182:PRO:O	1:D:1186:MET:HG2	2.12	0.49
1:A:1180:ARG:NH2	1:A:1182:PRO:HG2	2.28	0.49
1:C:1125:ILE:HG23	1:C:1127:ARG:CG	2.39	0.48
1:D:1197:VAL:HG23	1:D:1198:PHE:CD2	2.47	0.48
1:E:1117:GLY:HA2	1:E:1242:LEU:HD21	1.95	0.48
1:A:1071:PHE:HB2	1:A:1078:GLN:HE21	1.78	0.48
1:B:1212:ALA:HB3	1:B:1234:PRO:HG3	1.96	0.48
1:E:1071:PHE:HB2	1:E:1078:GLN:HE21	1.79	0.48
1:D:1065:ILE:HG12	3:D:4:ADP:N6	2.29	0.48
1:E:1200:GLU:CD	1:E:1217:PRO:HG3	2.34	0.48
1:A:1078:GLN:NE2	4:A:74:HOH:O	2.46	0.47
1:E:1155:ARG:HD3	1:E:1155:ARG:H	1.79	0.47
1:C:1041:ILE:HG13	1:C:1051:LEU:HD13	1.96	0.47
1:A:1087:GLY:HA2	3:A:1:ADP:N3	2.30	0.47
1:C:1240:THR:HG23	1:C:1244:LYS:HD2	1.97	0.47
1:D:1117:GLY:HA2	1:D:1242:LEU:HD21	1.96	0.47
1:D:1244:LYS:HB2	1:D:1244:LYS:HE3	1.77	0.46
1:E:1182:PRO:O	1:E:1186:MET:HG2	2.15	0.46
1:C:1053:ILE:HG23	1:C:1070:ILE:HD13	1.97	0.46
1:B:1187:TRP:CZ2	1:B:1209:THR:HG23	2.50	0.46
1:A:1241:THR:HG23	1:A:1244:LYS:H	1.81	0.46
1:E:1094:ILE:CD1	1:E:1196:LEU:HA	2.45	0.46
1:D:1203:PHE:CE1	1:D:1212:ALA:HA	2.50	0.46
1:F:1171:PRO:HB3	1:F:1210:VAL:HG12	1.98	0.46
1:F:1203:PHE:HB3	1:F:1208:GLU:HG3	1.98	0.45
1:A:1032:LYS:HG3	1:A:1040:TRP:HH2	1.82	0.45
1:B:1096:ARG:HB2	1:B:1266:PHE:CE1	2.51	0.45
1:C:1205:GLU:O	1:C:1208:GLU:HG2	2.16	0.45
1:B:1207:GLU:C	1:B:1209:THR:H	2.20	0.45
1:B:1108:ILE:HG23	1:B:1142:ILE:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1207:GLU:C	1:C:1209:THR:H	2.20	0.44
1:A:1248:ASP:HA	1:A:1249:PRO:HD3	1.90	0.44
1:D:1071:PHE:HB2	1:D:1078:GLN:HE21	1.82	0.44
1:A:1174:LEU:CD1	1:A:1209:THR:HG21	2.48	0.44
1:B:1100:LEU:HD23	1:B:1104:LEU:HD23	1.99	0.44
1:F:995:TYR:HB2	1:F:1078:GLN:HE21	1.82	0.44
1:D:1094:ILE:HD11	1:D:1196:LEU:HA	2.00	0.44
1:F:1182:PRO:O	1:F:1186:MET:HG2	2.18	0.44
1:B:1053:ILE:CG2	1:B:1070:ILE:HD12	2.48	0.43
1:B:1256:ASN:O	1:B:1259:ASP:HB2	2.18	0.43
1:B:1172:GLU:O	1:B:1177:ASN:HB2	2.19	0.43
1:D:1052:GLU:HB2	1:D:1148:GLY:HA2	1.99	0.43
1:F:1257:LEU:HA	1:F:1260:TYR:HD2	1.82	0.43
1:D:1098:PRO:HD2	1:D:1199:GLU:OE2	2.19	0.43
1:C:1212:ALA:HB3	1:C:1234:PRO:HG3	2.01	0.43
1:C:1043:ASP:HA	1:C:1044:PRO:HD3	1.91	0.43
1:C:1096:ARG:HB2	1:C:1266:PHE:CE1	2.52	0.43
1:F:1125:ILE:HG23	1:F:1127:ARG:HG3	2.00	0.42
1:E:1155:ARG:HD3	1:E:1155:ARG:N	2.33	0.42
1:E:1006:GLY:HA2	3:E:5:ADP:H4'	2.02	0.42
1:D:1031:LYS:HD3	1:D:1034:LYS:HD3	2.02	0.42
1:B:1241:THR:HG22	1:B:1244:LYS:HE3	2.01	0.42
1:B:1241:THR:HG22	1:B:1244:LYS:HB2	2.02	0.42
1:D:1171:PRO:HB3	1:D:1210:VAL:HG12	2.01	0.42
1:E:1006:GLY:CA	3:E:5:ADP:H4'	2.50	0.42
1:A:1198:PHE:CZ	1:A:1216:PRO:HB3	2.55	0.41
1:F:1203:PHE:CD2	1:F:1209:THR:HG22	2.55	0.41
1:D:1032:LYS:HG3	1:D:1040:TRP:HH2	1.85	0.41
1:E:1018:ASP:O	1:E:1022:ASN:HA	2.21	0.41
1:B:1004:PRO:HG3	1:B:1010:PHE:CD1	2.55	0.41
1:B:1193:LEU:O	1:B:1197:VAL:HG22	2.21	0.41
1:D:1180:ARG:NH2	1:D:1182:PRO:HG2	2.36	0.41
1:E:1198:PHE:CD1	1:E:1217:PRO:HD2	2.56	0.41
1:F:1166:ILE:HD13	1:F:1166:ILE:HA	1.96	0.41
1:F:1241:THR:H	1:F:1244:LYS:HZ2	1.69	0.41
1:B:1032:LYS:HD2	1:B:1032:LYS:H	1.85	0.41
1:C:1198:PHE:CE1	1:C:1216:PRO:HB3	2.55	0.41
1:E:1216:PRO:HA	1:E:1217:PRO:HD3	1.92	0.41
1:E:1248:ASP:HA	1:E:1249:PRO:HD3	1.90	0.41
1:B:1072:GLU:HG3	1:B:1077:PHE:CE2	2.56	0.41
1:B:1089:ASP:OD1	1:B:1091:PHE:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1171:PRO:O	1:C:1175:MET:HG3	2.21	0.41
1:E:1055:ILE:HG23	1:E:1124:ILE:HD13	2.03	0.41
1:C:1173:VAL:HG21	1:C:1184:LEU:HD13	2.03	0.41
1:D:1240:THR:HG23	1:D:1244:LYS:HD2	2.02	0.41
1:B:1198:PHE:CZ	1:B:1216:PRO:HB3	2.57	0.40
1:C:1098:PRO:HD2	1:C:1199:GLU:OE2	2.21	0.40
1:C:1242:LEU:O	1:C:1246:VAL:HG23	2.20	0.40
1:C:1108:ILE:HG23	1:C:1142:ILE:HG21	2.04	0.40
1:C:1248:ASP:HA	1:C:1249:PRO:HD3	1.91	0.40
1:B:1197:VAL:HG23	1:B:1198:PHE:CD2	2.56	0.40
1:C:1233:GLN:HA	1:C:1234:PRO:HD3	1.87	0.40
1:D:1231:LEU:HD23	1:D:1240:THR:HB	2.03	0.40
1:B:1127:ARG:HD3	1:B:1149:SER:O	2.21	0.40
1:C:1197:VAL:HG23	1:C:1198:PHE:CD2	2.57	0.40
1:F:1203:PHE:CE1	1:F:1212:ALA:HA	2.57	0.40
1:C:1044:PRO:HD3	4:C:193:HOH:O	2.21	0.40
1:C:1138:GLU:HG2	1:C:1262:TRP:CE2	2.56	0.40
1:E:1112:LEU:O	1:E:1116:VAL:HG23	2.21	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	283/335 (84%)	272 (96%)	11 (4%)	0	100	100
1	B	276/335 (82%)	264 (96%)	12 (4%)	0	100	100
1	C	277/335 (83%)	260 (94%)	17 (6%)	0	100	100
1	D	280/335 (84%)	271 (97%)	9 (3%)	0	100	100
1	E	278/335 (83%)	268 (96%)	9 (3%)	1 (0%)	34	42
1	F	277/335 (83%)	260 (94%)	17 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1671/2010 (83%)	1595 (96%)	75 (4%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1009	ALA

5.3.2 Protein sidechains (i)

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	236/291 (81%)	218 (92%)	18 (8%)	13 16
1	B	233/291 (80%)	223 (96%)	10 (4%)	29 40
1	C	235/291 (81%)	224 (95%)	11 (5%)	26 37
1	D	234/291 (80%)	218 (93%)	16 (7%)	16 21
1	E	234/291 (80%)	217 (93%)	17 (7%)	14 18
1	F	226/291 (78%)	211 (93%)	15 (7%)	16 22
All	All	1398/1746 (80%)	1311 (94%)	87 (6%)	18 25

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	985	LEU
1	A	992	GLU
1	A	997	GLN
1	A	1032	LYS
1	A	1048	LYS
1	A	1056	LEU
1	A	1070	ILE
1	A	1079	LEU
1	A	1114	SER
1	A	1122	LYS
1	A	1125	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1153	LEU
1	A	1197	VAL
1	A	1206	LEU
1	A	1209	THR
1	A	1225	MET
1	A	1237	GLU
1	A	1247	THR
1	B	985	LEU
1	B	1032	LYS
1	B	1048	LYS
1	B	1070	ILE
1	B	1078	GLN
1	B	1122	LYS
1	B	1125	ILE
1	B	1153	LEU
1	B	1155	ARG
1	B	1157	LYS
1	C	1032	LYS
1	C	1043	ASP
1	C	1048	LYS
1	C	1051	LEU
1	C	1078	GLN
1	C	1079	LEU
1	C	1122	LYS
1	C	1125	ILE
1	C	1153	LEU
1	C	1209	THR
1	C	1245	LEU
1	D	985	LEU
1	D	1022	ASN
1	D	1032	LYS
1	D	1048	LYS
1	D	1070	ILE
1	D	1078	GLN
1	D	1079	LEU
1	D	1100	LEU
1	D	1122	LYS
1	D	1125	ILE
1	D	1153	LEU
1	D	1157	LYS
1	D	1209	THR
1	D	1219	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1241	THR
1	D	1245	LEU
1	E	985	LEU
1	E	1032	LYS
1	E	1042	GLU
1	E	1048	LYS
1	E	1070	ILE
1	E	1079	LEU
1	E	1100	LEU
1	E	1122	LYS
1	E	1125	ILE
1	E	1153	LEU
1	E	1155	ARG
1	E	1157	LYS
1	E	1166	ILE
1	E	1214	ILE
1	E	1219	LEU
1	E	1237	GLU
1	E	1245	LEU
1	F	985	LEU
1	F	1032	LYS
1	F	1042	GLU
1	F	1048	LYS
1	F	1069	ASP
1	F	1070	ILE
1	F	1072	GLU
1	F	1079	LEU
1	F	1100	LEU
1	F	1123	ASP
1	F	1153	LEU
1	F	1166	ILE
1	F	1175	MET
1	F	1219	LEU
1	F	1245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	997	GLN
1	A	1078	GLN
1	B	997	GLN
1	B	1078	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	997	GLN
1	C	1078	GLN
1	D	1078	GLN
1	E	1078	GLN
1	F	1253	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 19 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	$\#\|Z\| > 2$
3	ADP	B	2	2	24,29,29	1.21	3 (12%)	29,45,45	1.23	2 (6%)
3	ADP	E	5	2	24,29,29	1.21	3 (12%)	29,45,45	1.11	1 (3%)
3	ADP	A	1	2	24,29,29	1.14	2 (8%)	29,45,45	1.20	2 (6%)
3	ADP	C	3	2	24,29,29	1.15	2 (8%)	29,45,45	1.16	1 (3%)
3	ADP	F	6	2	24,29,29	1.18	3 (12%)	29,45,45	1.08	2 (6%)
3	ADP	D	4	2	24,29,29	1.12	3 (12%)	29,45,45	1.05	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	2	2	-	1/12/32/32	0/3/3/3
3	ADP	E	5	2	-	0/12/32/32	0/3/3/3
3	ADP	A	1	2	-	1/12/32/32	0/3/3/3
3	ADP	C	3	2	-	4/12/32/32	0/3/3/3
3	ADP	F	6	2	-	0/12/32/32	0/3/3/3
3	ADP	D	4	2	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	ADP	PA-O3A	3.65	1.63	1.59
3	C	3	ADP	PA-O3A	3.64	1.63	1.59
3	F	6	ADP	PA-O3A	3.54	1.63	1.59
3	A	1	ADP	PA-O3A	3.41	1.63	1.59
3	B	2	ADP	PA-O3A	3.38	1.63	1.59
3	D	4	ADP	PA-O3A	2.91	1.62	1.59
3	C	3	ADP	O4'-C1'	2.66	1.44	1.40
3	B	2	ADP	O4'-C1'	2.66	1.44	1.40
3	A	1	ADP	O4'-C1'	2.55	1.44	1.40
3	D	4	ADP	O4'-C1'	2.55	1.44	1.40
3	E	5	ADP	C2-N3	2.30	1.35	1.32
3	E	5	ADP	O4'-C1'	2.29	1.43	1.40
3	F	6	ADP	O4'-C1'	2.24	1.43	1.40
3	F	6	ADP	C2-N3	2.19	1.35	1.32
3	D	4	ADP	C2-N3	2.18	1.35	1.32
3	B	2	ADP	C2-N3	2.08	1.35	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	ADP	N3-C2-N1	-4.24	122.92	128.67
3	A	1	ADP	N3-C2-N1	-4.15	123.03	128.67
3	B	2	ADP	N3-C2-N1	-4.09	123.12	128.67
3	E	5	ADP	N3-C2-N1	-3.88	123.41	128.67
3	D	4	ADP	N3-C2-N1	-3.62	123.76	128.67
3	F	6	ADP	N3-C2-N1	-3.53	123.88	128.67
3	A	1	ADP	C4-C5-N7	-2.65	106.53	109.34
3	B	2	ADP	C4-C5-N7	-2.56	106.63	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	6	ADP	C4-C5-N7	-2.33	106.87	109.34
3	D	4	ADP	C4-C5-N7	-2.33	106.88	109.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	ADP	PA-O3A-PB-O2B
3	B	2	ADP	PB-O3A-PA-O1A
3	A	1	ADP	PA-O3A-PB-O3B
3	C	3	ADP	PA-O3A-PB-O3B
3	C	3	ADP	PA-O3A-PB-O1B
3	C	3	ADP	PB-O3A-PA-O2A

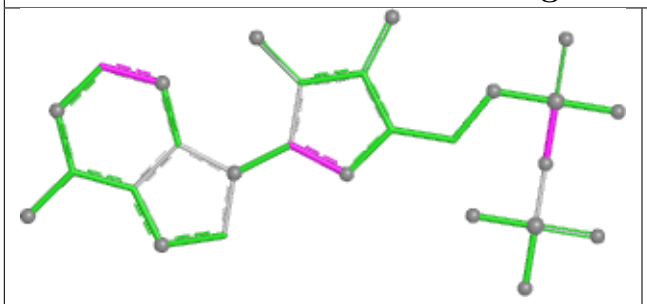
There are no ring outliers.

3 monomers are involved in 4 short contacts:

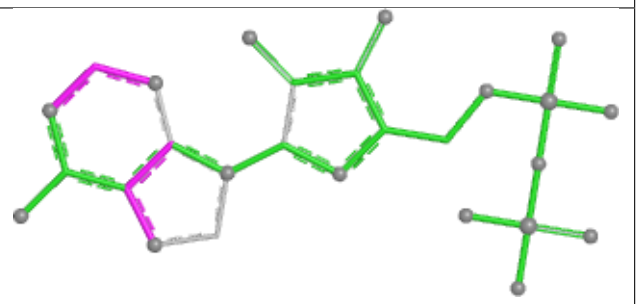
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	ADP	2	0
3	A	1	ADP	1	0
3	D	4	ADP	1	0

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 then 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.

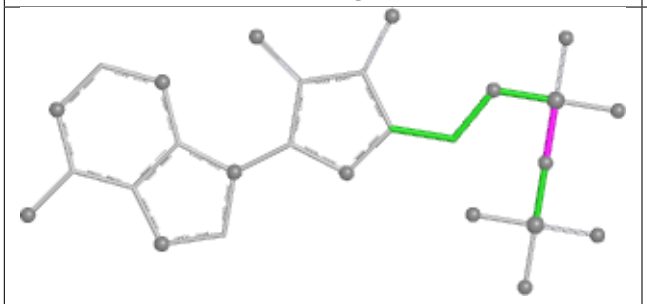
Ligand ADP B 2



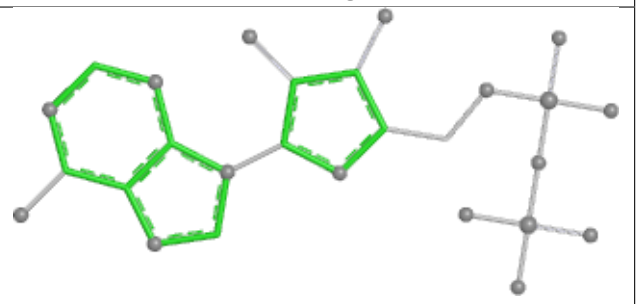
Bond lengths



Bond angles

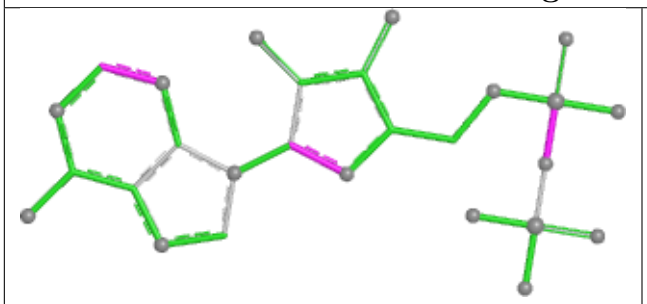


Torsions

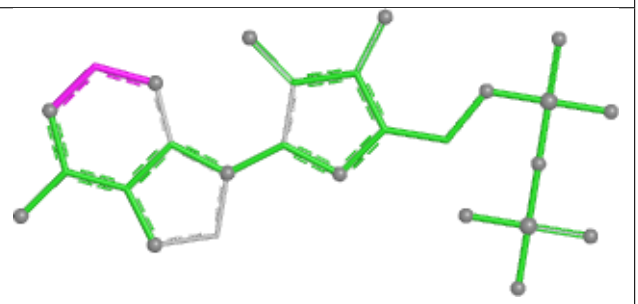


Rings

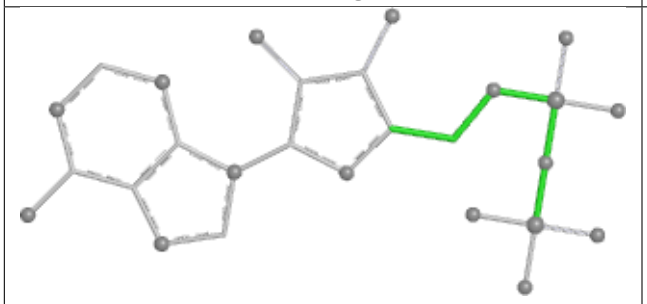
Ligand ADP E 5



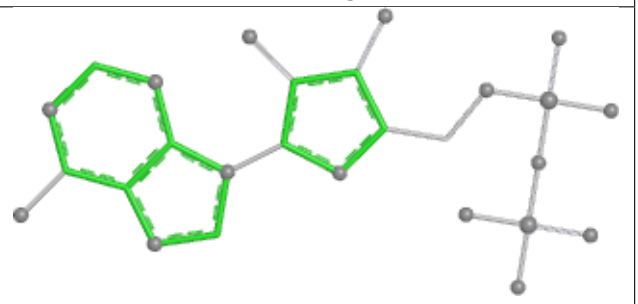
Bond lengths



Bond angles

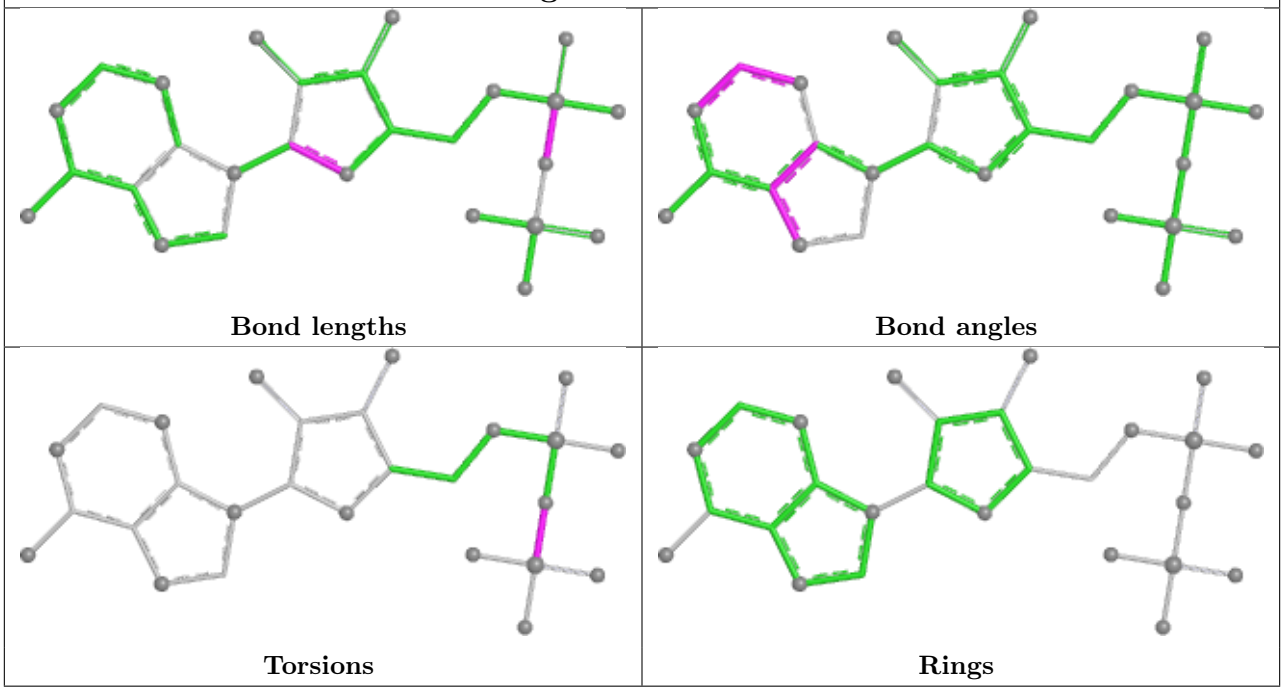


Torsions

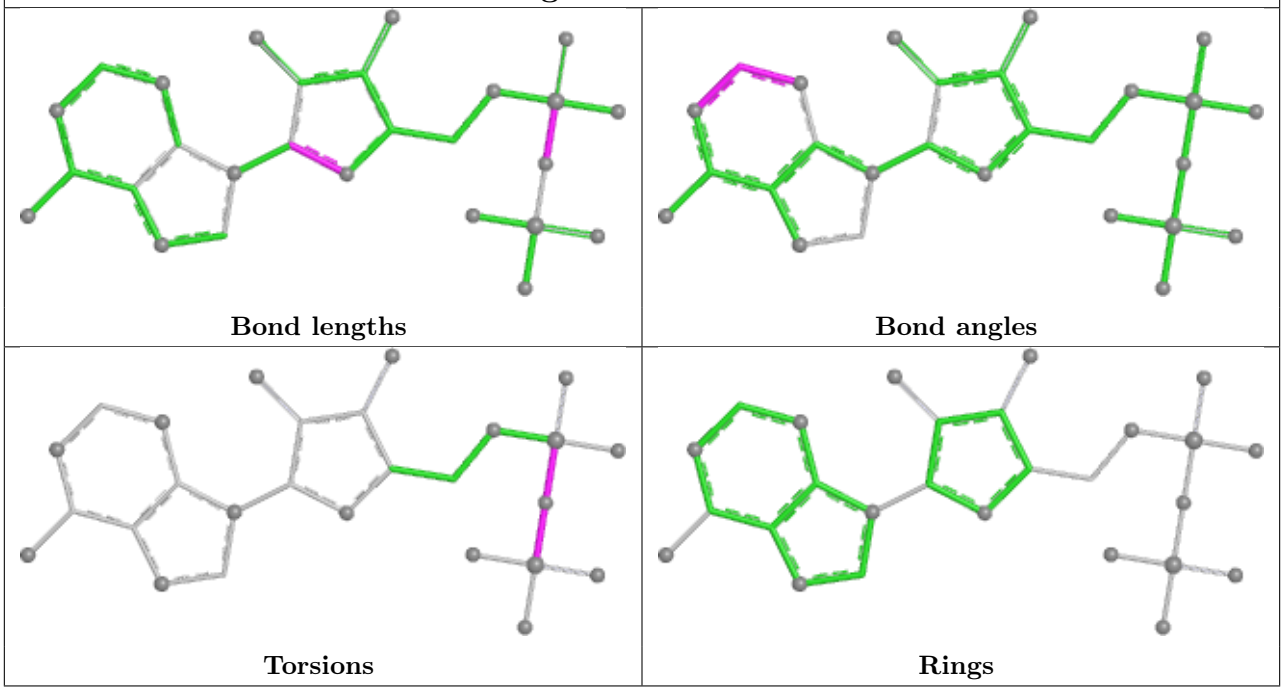


Rings

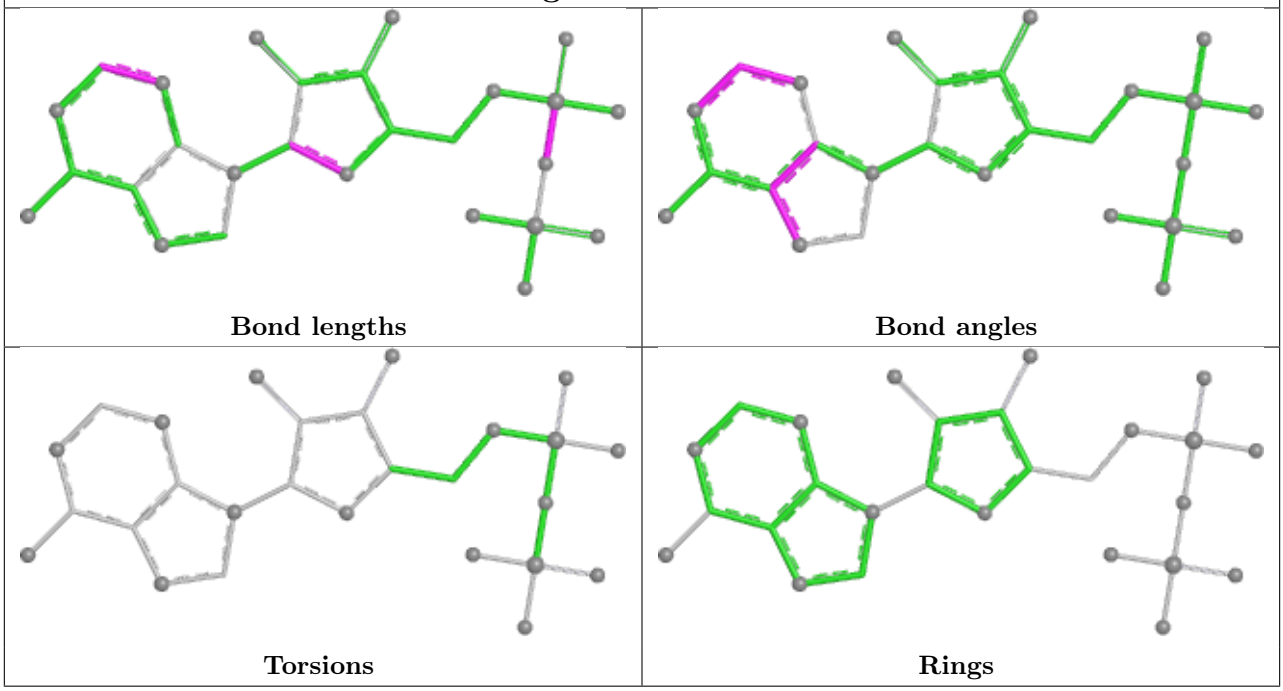
Ligand ADP A 1



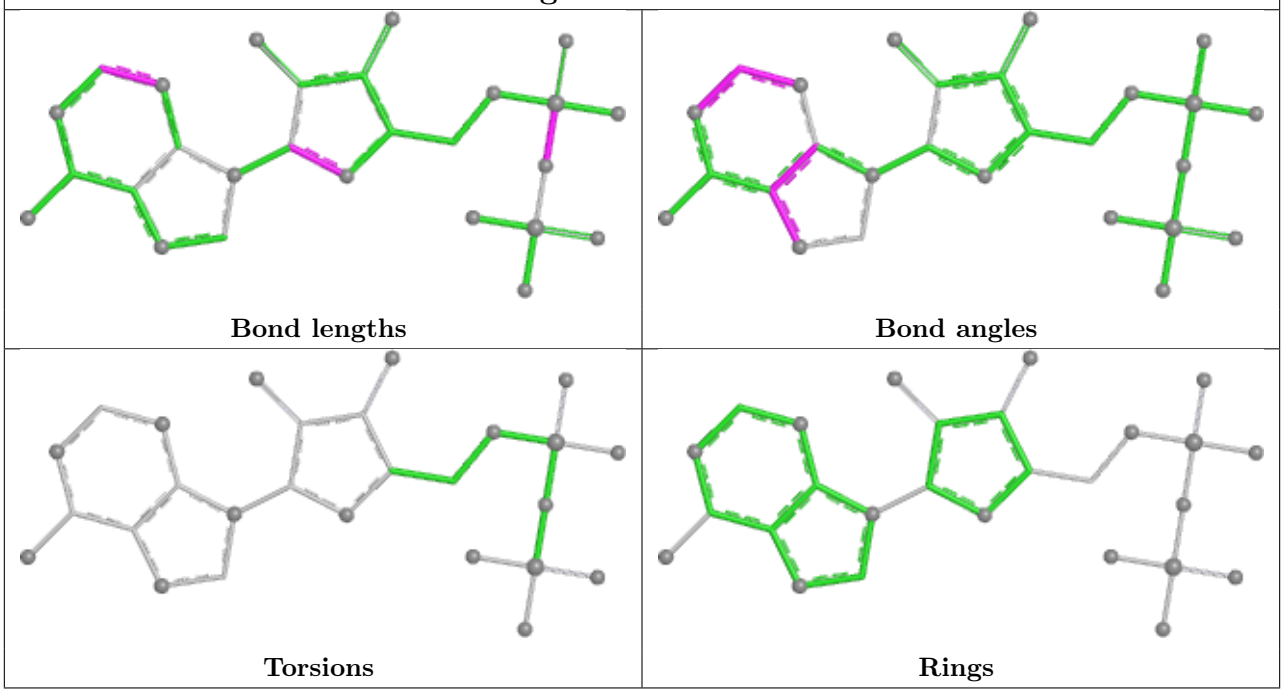
Ligand ADP C 3



Ligand ADP F 6



Ligand ADP D 4



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	285/335 (85%)	-0.14	1 (0%)	92	95	14, 29, 46, 59	0
1	B	280/335 (83%)	0.01	7 (2%)	57	64	17, 33, 53, 72	0
1	C	281/335 (83%)	-0.05	6 (2%)	63	70	17, 32, 54, 72	0
1	D	284/335 (84%)	-0.01	2 (0%)	87	91	22, 38, 56, 70	0
1	E	282/335 (84%)	0.12	4 (1%)	75	80	22, 42, 58, 73	0
1	F	281/335 (83%)	0.22	10 (3%)	42	49	26, 46, 67, 76	0
All	All	1693/2010 (84%)	0.02	30 (1%)	68	74	14, 37, 59, 76	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1204	CYS	4.8
1	C	1046	LEU	4.6
1	F	1121	LEU	4.0
1	F	1041	ILE	3.6
1	C	1048	LYS	3.5
1	B	1155	ARG	3.5
1	B	1040	TRP	3.4
1	B	1007	SER	3.3
1	F	1257	LEU	3.1
1	B	1041	ILE	2.9
1	F	1017	VAL	2.8
1	F	1235	VAL	2.8
1	C	1041	ILE	2.7
1	A	1007	SER	2.7
1	F	990	ALA	2.7
1	E	1096	ARG	2.7
1	E	1022	ASN	2.5
1	F	1070	ILE	2.5
1	C	1044	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1097	HIS	2.4
1	E	1007	SER	2.3
1	B	1046	LEU	2.3
1	C	1049	VAL	2.3
1	B	1204	CYS	2.2
1	F	1209	THR	2.2
1	D	1074	GLN	2.2
1	D	1010	PHE	2.2
1	F	1009	ALA	2.1
1	F	991	CYS	2.1
1	E	1035	VAL	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 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	MG	A	20	1/1	0.89	0.18	24,24,24,24	0
2	MG	B	19	1/1	0.90	0.20	33,33,33,33	0
2	MG	A	8	1/1	0.93	0.27	28,28,28,28	0
2	MG	C	12	1/1	0.93	0.30	35,35,35,35	0
2	MG	C	22	1/1	0.94	0.09	35,35,35,35	0
2	MG	E	16	1/1	0.94	0.25	36,36,36,36	0
2	MG	F	18	1/1	0.94	0.24	31,31,31,31	0
3	ADP	E	5	27/27	0.94	0.14	27,36,52,53	0
2	MG	B	10	1/1	0.95	0.18	23,23,23,23	0
2	MG	D	14	1/1	0.95	0.29	33,33,33,33	0
2	MG	E	15	1/1	0.95	0.21	24,24,24,24	0
2	MG	A	7	1/1	0.96	0.14	10,10,10,10	0

Continued on next page...

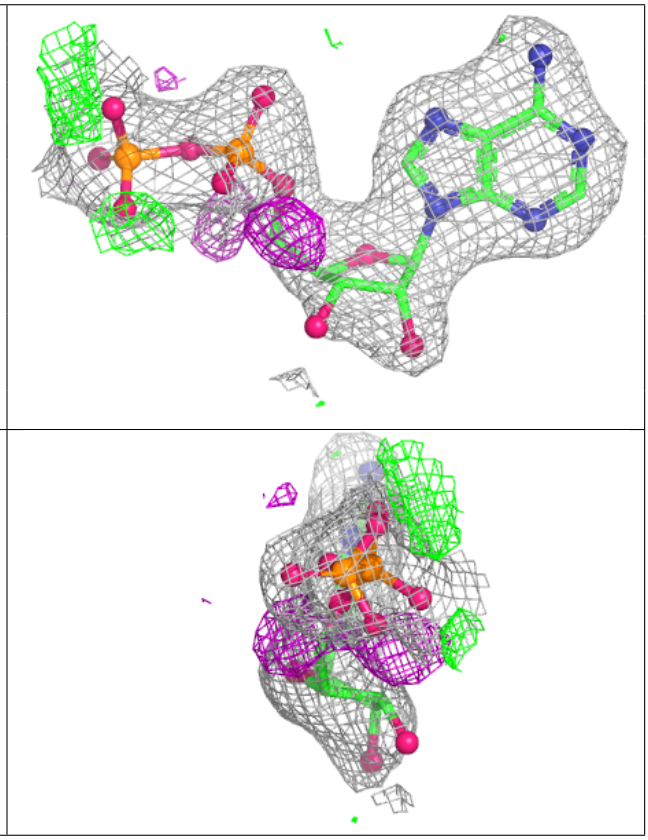
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	F	17	1/1	0.96	0.24	25,25,25,25	0
2	MG	D	23	1/1	0.96	0.12	31,31,31,31	0
3	ADP	D	4	27/27	0.96	0.13	22,32,37,43	0
2	MG	A	25	1/1	0.96	0.23	22,22,22,22	0
3	ADP	F	6	27/27	0.96	0.10	34,40,45,46	0
3	ADP	B	2	27/27	0.97	0.13	12,23,34,41	0
3	ADP	A	1	27/27	0.98	0.11	13,20,33,36	0
2	MG	B	24	1/1	0.98	0.21	26,26,26,26	0
3	ADP	C	3	27/27	0.98	0.12	17,21,30,36	0
2	MG	D	13	1/1	0.98	0.20	14,14,14,14	0
2	MG	B	9	1/1	0.98	0.16	15,15,15,15	0
2	MG	C	21	1/1	0.98	0.27	30,30,30,30	0
2	MG	C	11	1/1	0.99	0.20	13,13,13,13	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.

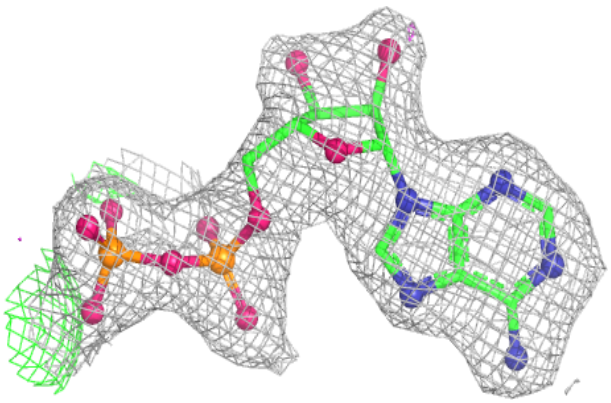
Electron density around ADP E 5:

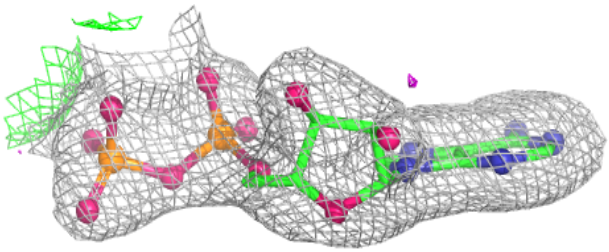
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

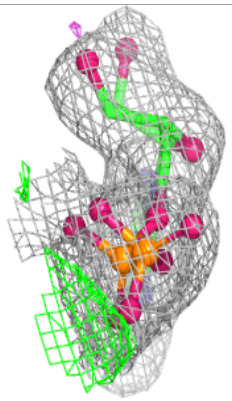


Electron density around ADP D 4:

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

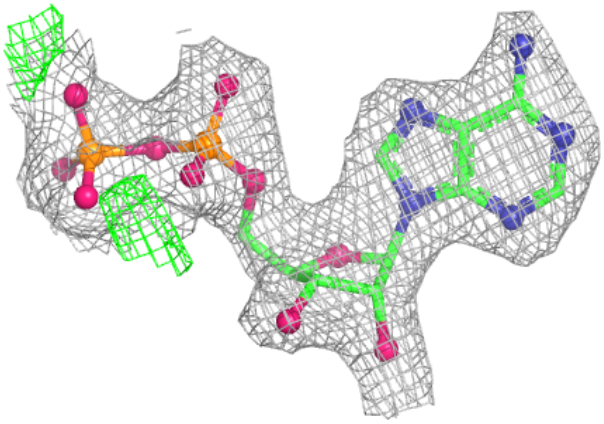


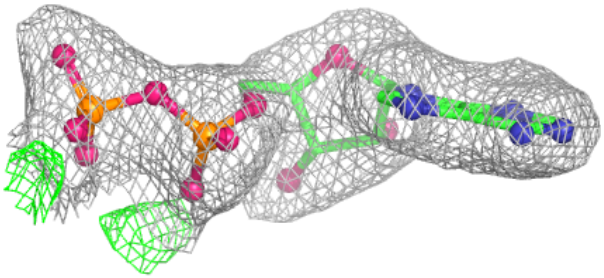


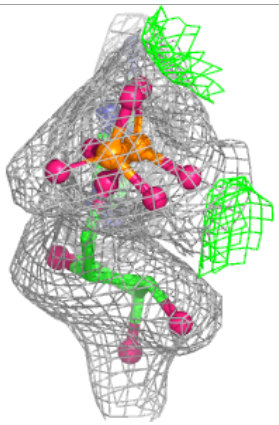


Electron density around ADP F 6:

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

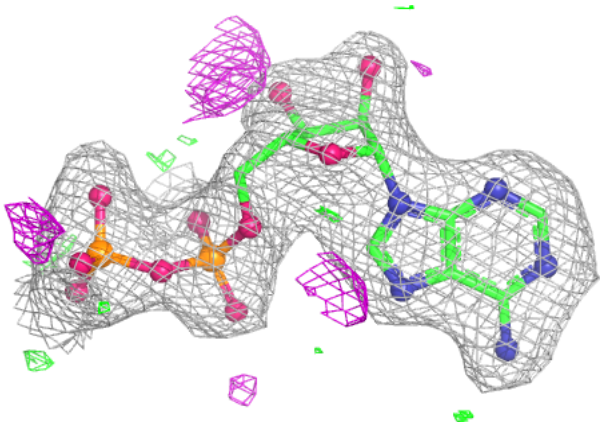


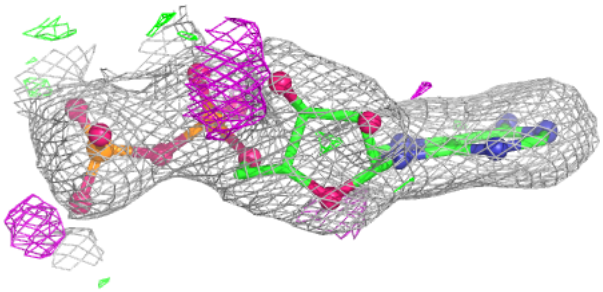


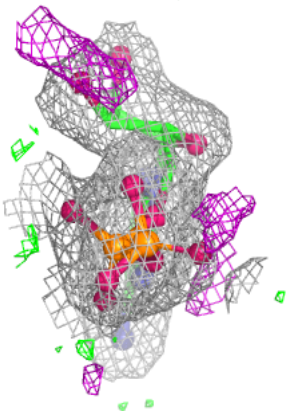


Electron density around ADP B 2:

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

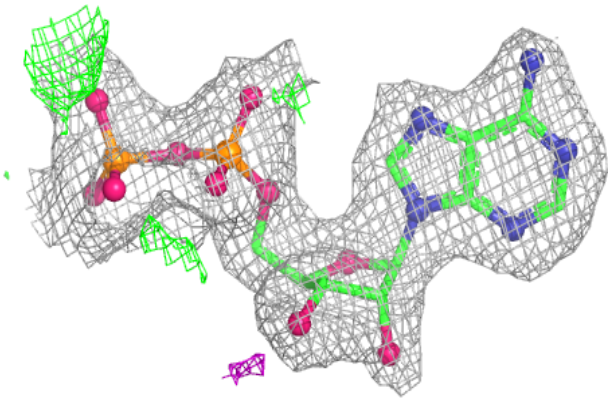


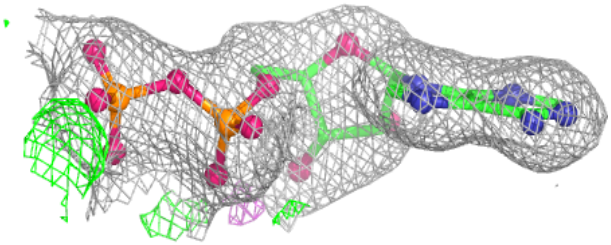


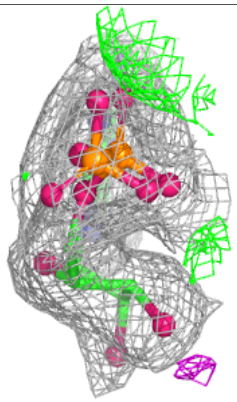


Electron density around ADP A 1:

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

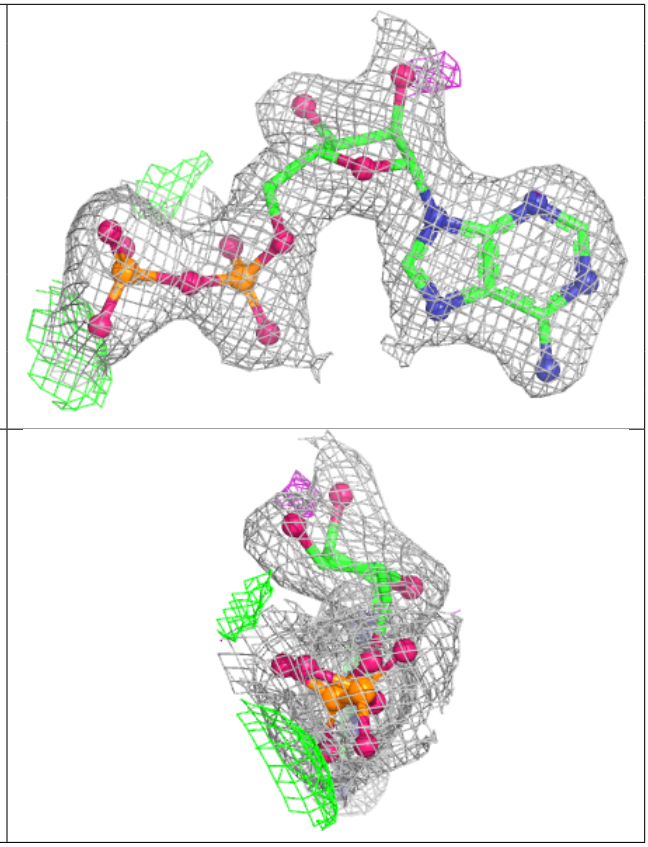






Electron density around ADP C 3:

$2mF_o$-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.