Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 07:52 AM EDT

PDB ID	:	2HV7
Title	:	Crystal structure of phosphotyrosyl phosphatase activator bound to ATPgammaS
Authors	:	Chao, Y.; Jeffrey, J.D.; Shi, Y.
Deposited on	:	2006-07-27
Resolution	:	2.50 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 (1)) were used in the production of this report:

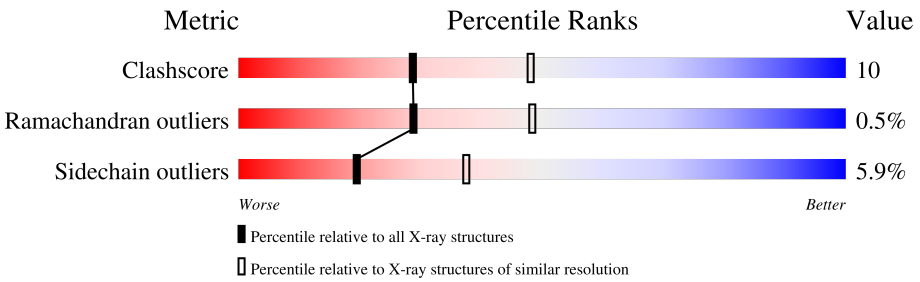
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	69% 22% • 7%
1	B	323	70% 21% • 7%
1	C	323	72% 20% • 7%
1	D	323	68% 23% • 7%
1	E	323	67% 25% • 7%
1	F	323	68% 22% • 7%
1	G	323	69% 21% • 7%
1	H	323	74% 18% • 7%

2 Entry composition (i)

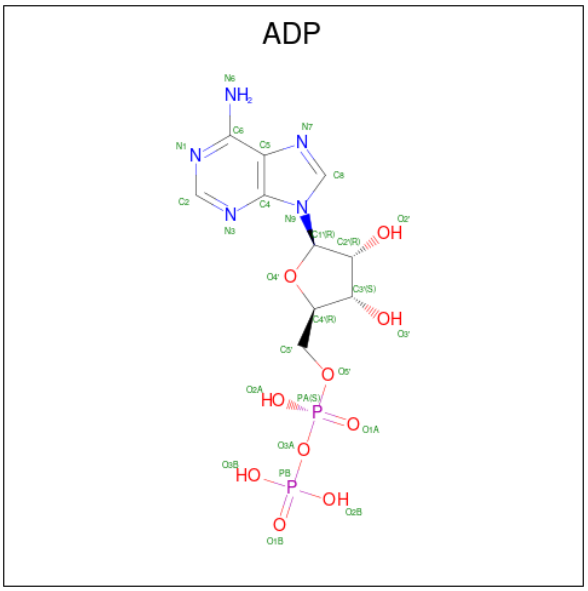
There are 2 unique types of molecules in this entry. The entry contains 19612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein phosphatase 2A, regulatory subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2438	1586	406	435	11	0	0	0
1	B	301	2438	1586	406	435	11	0	0	0
1	C	301	2438	1586	406	435	11	0	0	0
1	D	301	2438	1586	406	435	11	0	0	0
1	E	301	2438	1586	406	435	11	0	0	0
1	F	301	2438	1586	406	435	11	0	0	0
1	G	301	2438	1586	406	435	11	0	0	0
1	H	301	2438	1586	406	435	11	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

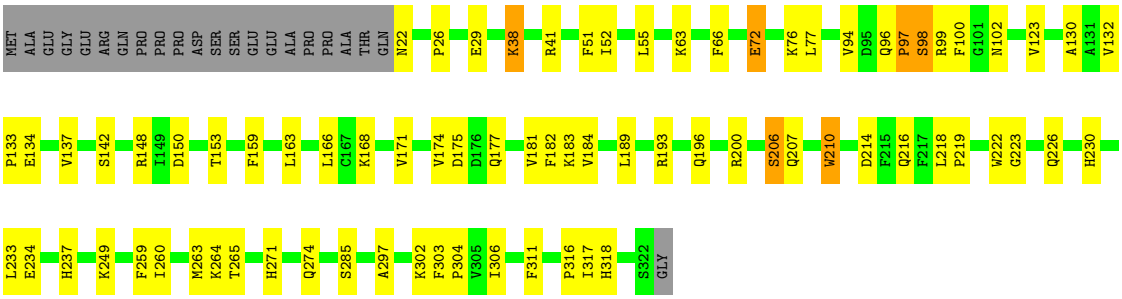
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

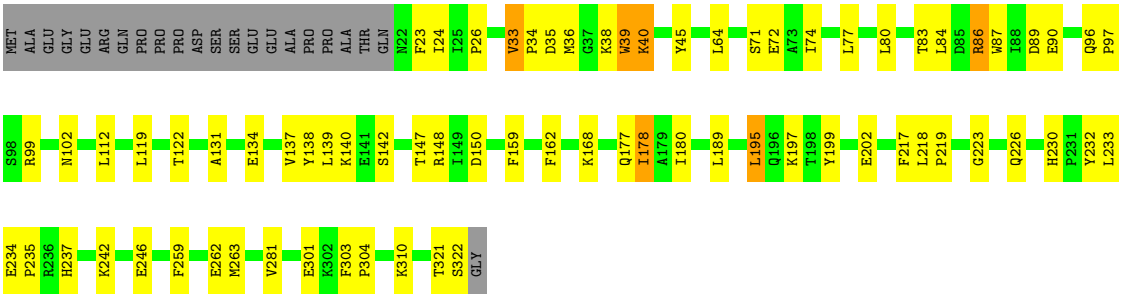
• Molecule 1: Protein phosphatase 2A, regulatory subunit B

Chain A: 69% 22% • 7%



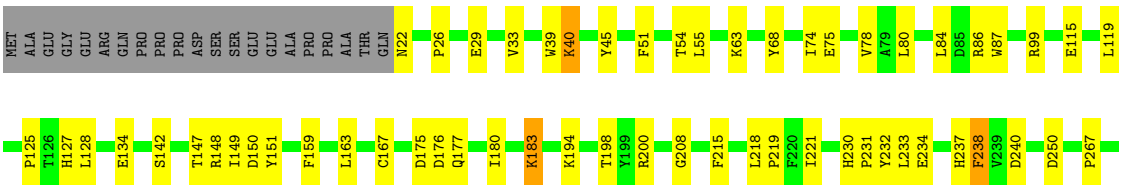
• Molecule 1: Protein phosphatase 2A, regulatory subunit B

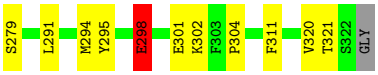
Chain B: 70% 21% • 7%



• Molecule 1: Protein phosphatase 2A, regulatory subunit B

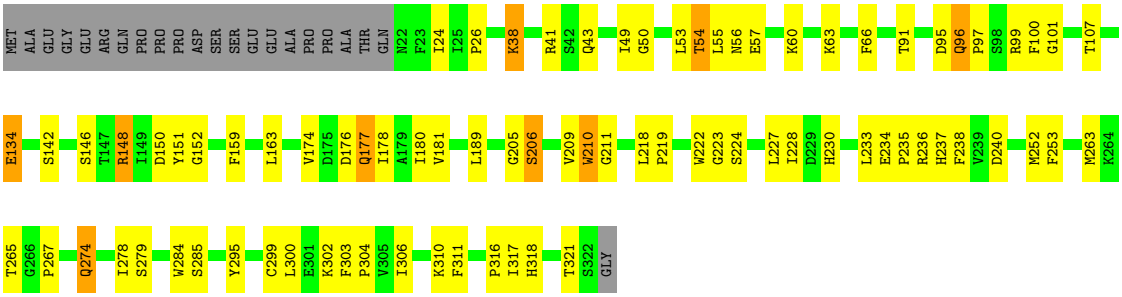
Chain C: 72% 20% • 7%





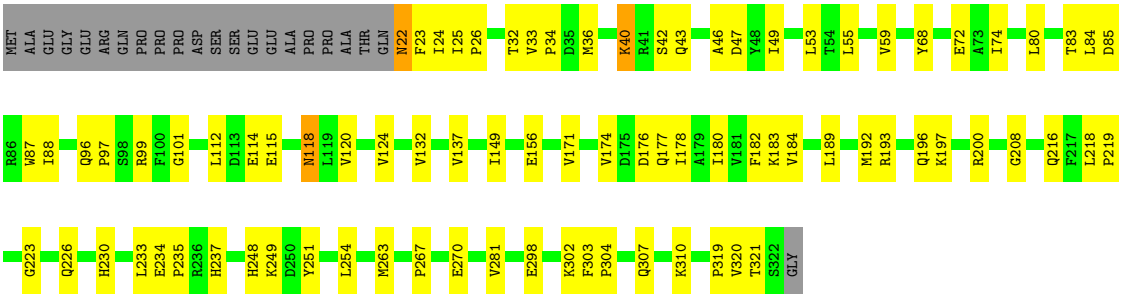
• Molecule 1: Protein phosphatase 2A, regulatory subunit B

Chain D:



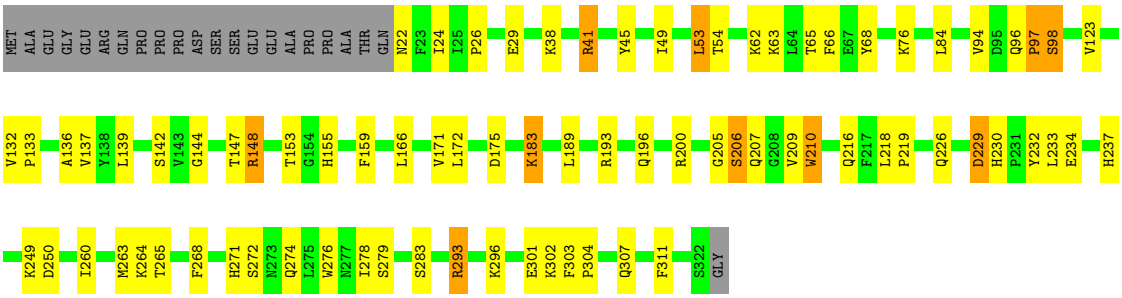
• Molecule 1: Protein phosphatase 2A, regulatory subunit B

Chain E:



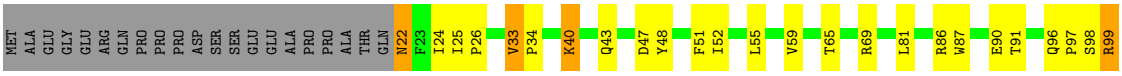
• Molecule 1: Protein phosphatase 2A, regulatory subunit B

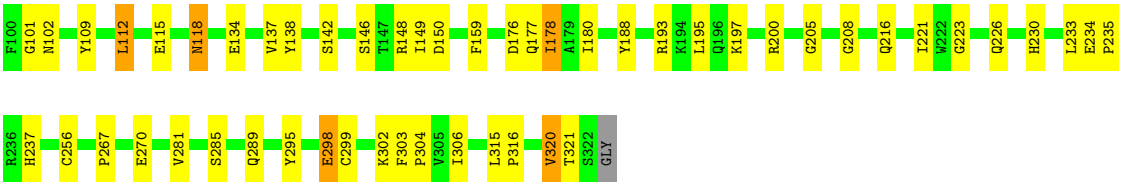
Chain F:



• Molecule 1: Protein phosphatase 2A, regulatory subunit B

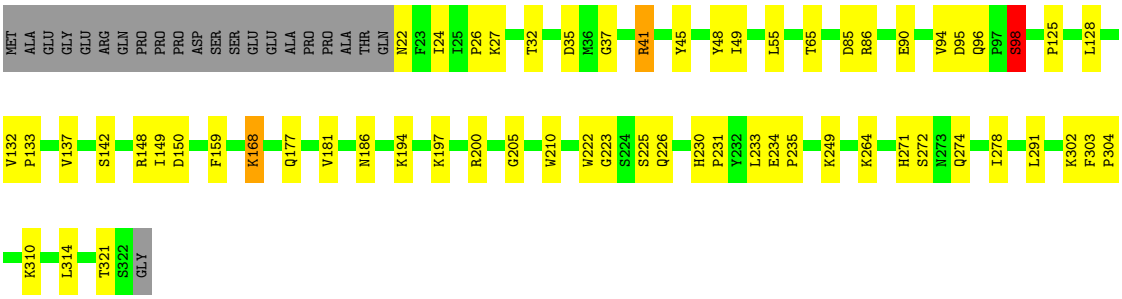
Chain G:





• Molecule 1: Protein phosphatase 2A, regulatory subunit B

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.04Å 86.10Å 95.10Å 73.91° 89.97° 73.31°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	87.7 (50.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.249 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19612	wwPDB-VP
Average B, all atoms ($Å^2$)	11.0	wwPDB-VP

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

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	0.55	0/2506	0.61	0/3401
1	B	0.55	0/2506	0.61	0/3401
1	C	0.55	1/2506 (0.0%)	0.59	0/3401
1	D	0.50	1/2506 (0.0%)	0.58	0/3401
1	E	0.51	0/2506	0.59	0/3401
1	F	0.73	4/2506 (0.2%)	0.64	2/3401 (0.1%)
1	G	0.51	0/2506	0.57	0/3401
1	H	0.53	0/2506	0.62	1/3401 (0.0%)
All	All	0.56	6/20048 (0.0%)	0.60	3/27208 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	229	ASP	CG-OD1	18.58	1.68	1.25
1	F	229	ASP	CG-OD2	14.23	1.58	1.25
1	D	176	ASP	CG-OD1	7.17	1.41	1.25
1	F	53	LEU	CG-CD2	6.77	1.76	1.51
1	F	53	LEU	CG-CD1	5.71	1.73	1.51
1	C	298	GLU	CG-CD	5.34	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	229	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	F	229	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	H	98	SER	N-CA-C	5.34	125.42	111.00

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	2438	0	2423	52	0
1	B	2438	0	2423	48	0
1	C	2438	0	2423	43	0
1	D	2438	0	2423	55	0
1	E	2438	0	2423	54	0
1	F	2438	0	2423	59	0
1	G	2438	0	2423	55	0
1	H	2438	0	2423	34	0
2	B	27	0	12	2	0
2	C	27	0	12	1	0
2	E	27	0	12	0	0
2	G	27	0	12	3	0
All	All	19612	0	19432	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (378) 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:F:53:LEU:CD2	1:F:53:LEU:CG	1.76	1.59
1:F:229:ASP:CG	1:F:229:ASP:OD1	1.68	1.30
1:F:263:MET:HE3	1:G:97:PRO:HB2	1.38	1.00
1:E:235:PRO:HG2	1:E:281:VAL:O	1.64	0.97
1:F:293:ARG:HH11	1:F:293:ARG:HG3	1.32	0.94
1:F:234:GLU:H	1:F:237:HIS:HD2	1.12	0.94
1:C:68:TYR:OH	1:C:183:LYS:HE2	1.69	0.92
1:F:263:MET:CE	1:G:97:PRO:HB2	1.99	0.91
1:D:316:PRO:HB2	1:D:318:HIS:HD2	1.36	0.91
1:F:96:GLN:HG3	1:F:98:SER:HB2	1.55	0.87
1:G:118:ASN:H	1:G:118:ASN:HD22	1.21	0.87
2:B:324:ADP:H5'2	2:B:324:ADP:O3B	1.75	0.87
1:A:96:GLN:HG3	1:A:98:SER:HB2	1.56	0.86
1:H:96:GLN:HG3	1:H:98:SER:HB3	1.55	0.86
1:G:205:GLY:HA3	2:G:324:ADP:C8	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:PRO:HG2	1:G:281:VAL:O	1.76	0.84
1:H:230:HIS:CD2	1:H:233:LEU:H	1.95	0.84
1:A:234:GLU:H	1:A:237:HIS:HD2	1.26	0.83
1:B:97:PRO:HB2	1:D:263:MET:HE2	1.60	0.83
1:B:230:HIS:HD2	1:B:232:TYR:H	1.25	0.83
1:H:230:HIS:HD2	1:H:233:LEU:H	1.23	0.82
1:F:230:HIS:CD2	1:F:233:LEU:H	1.98	0.81
1:H:148:ARG:HD3	1:H:150:ASP:OD2	1.82	0.80
1:A:206:SER:HB2	1:A:210:TRP:CH2	2.16	0.79
1:F:142:SER:HB2	1:F:159:PHE:HB2	1.63	0.78
1:A:230:HIS:HD2	1:A:233:LEU:H	1.31	0.78
1:D:230:HIS:CD2	1:D:233:LEU:H	2.04	0.76
1:E:118:ASN:H	1:E:118:ASN:HD22	1.35	0.75
1:G:230:HIS:CD2	1:G:233:LEU:H	2.04	0.74
1:G:230:HIS:HD2	1:G:233:LEU:H	1.32	0.74
1:F:53:LEU:CD2	1:F:53:LEU:CB	2.65	0.74
1:F:153:THR:HG23	1:F:207:GLN:NE2	2.02	0.74
1:E:230:HIS:CD2	1:E:233:LEU:H	2.07	0.73
1:C:99:ARG:O	1:C:200:ARG:NH1	2.21	0.73
1:H:37:GLY:O	1:H:41:ARG:HG3	1.89	0.72
1:G:205:GLY:CA	2:G:324:ADP:C8	2.73	0.72
1:D:230:HIS:HD2	1:D:233:LEU:H	1.35	0.72
1:E:118:ASN:H	1:E:118:ASN:ND2	1.88	0.72
1:B:142:SER:HB2	1:B:159:PHE:HB2	1.70	0.71
1:A:230:HIS:CD2	1:A:233:LEU:H	2.07	0.71
1:A:153:THR:HG23	1:A:207:GLN:NE2	2.04	0.71
1:F:234:GLU:H	1:F:237:HIS:CD2	2.03	0.70
1:E:80:LEU:O	1:E:84:LEU:HD13	1.91	0.70
1:A:196:GLN:HE22	1:A:216:GLN:HE22	1.37	0.70
1:F:230:HIS:HD2	1:F:233:LEU:H	1.40	0.69
1:F:293:ARG:HH11	1:F:293:ARG:CG	2.06	0.69
1:A:207:GLN:HG2	1:A:214:ASP:O	1.94	0.68
1:F:166:LEU:HB2	1:F:172:LEU:HD12	1.76	0.68
1:B:234:GLU:H	1:B:237:HIS:CD2	2.11	0.67
1:C:54:THR:HG22	1:C:177:GLN:HE22	1.58	0.67
1:B:230:HIS:CD2	1:B:233:LEU:H	2.13	0.66
1:B:195:LEU:HD23	1:B:199:TYR:HD2	1.60	0.66
1:G:118:ASN:H	1:G:118:ASN:ND2	1.92	0.65
1:G:177:GLN:HA	1:G:180:ILE:HD12	1.79	0.65
1:H:96:GLN:CG	1:H:98:SER:HB3	2.25	0.65
1:A:200:ARG:NH2	1:E:96:GLN:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LYS:HE2	1:B:301:GLU:HG2	1.79	0.64
1:C:142:SER:HB2	1:C:159:PHE:HB2	1.79	0.64
1:E:177:GLN:HA	1:E:180:ILE:HD12	1.79	0.64
1:A:316:PRO:HB2	1:A:318:HIS:CD2	2.33	0.64
1:G:118:ASN:ND2	1:G:118:ASN:N	2.46	0.64
1:C:177:GLN:HA	1:C:180:ILE:HD12	1.79	0.63
1:G:234:GLU:H	1:G:237:HIS:CD2	2.16	0.63
1:A:148:ARG:NH1	1:A:150:ASP:OD2	2.32	0.63
1:C:176:ASP:O	1:C:180:ILE:HG13	1.98	0.63
1:F:153:THR:HG23	1:F:207:GLN:HE22	1.62	0.62
1:C:302:LYS:HG3	1:C:304:PRO:HD2	1.80	0.62
1:G:118:ASN:HD22	1:G:118:ASN:N	1.93	0.62
1:B:178:ILE:H	1:B:178:ILE:HD12	1.63	0.62
1:E:248:HIS:CE1	1:E:249:LYS:HG2	2.34	0.61
1:E:230:HIS:HD2	1:E:233:LEU:H	1.48	0.61
1:G:33:VAL:HG23	1:G:34:PRO:HD3	1.82	0.60
2:C:324:ADP:O3B	2:C:324:ADP:H5'2	2.02	0.60
1:D:218:LEU:N	1:D:219:PRO:HD2	2.17	0.60
1:B:137:VAL:HA	1:B:140:LYS:HE3	1.84	0.60
1:D:234:GLU:H	1:D:237:HIS:HD2	1.49	0.59
1:G:96:GLN:OE1	1:G:102:ASN:HA	2.02	0.59
1:C:40:LYS:HE2	1:C:301:GLU:HG3	1.84	0.59
1:A:260:ILE:HG23	1:A:264:LYS:HD2	1.85	0.58
1:C:230:HIS:HD2	1:C:233:LEU:H	1.51	0.58
1:H:55:LEU:HD23	1:H:177:GLN:HB2	1.83	0.58
1:E:302:LYS:HG3	1:E:304:PRO:HD2	1.86	0.58
1:F:26:PRO:HD2	1:F:137:VAL:HG21	1.86	0.58
1:G:22:ASN:N	1:G:22:ASN:HD22	2.01	0.58
1:A:142:SER:HB2	1:A:159:PHE:HB2	1.85	0.58
1:F:196:GLN:HE22	1:F:216:GLN:HE22	1.52	0.58
1:C:230:HIS:CD2	1:C:233:LEU:H	2.22	0.58
1:A:38:LYS:HD3	1:A:317:ILE:HG13	1.85	0.58
1:E:218:LEU:N	1:E:219:PRO:HD2	2.18	0.57
1:E:32:THR:HB	1:E:34:PRO:HD2	1.84	0.57
1:E:74:ILE:HG23	1:E:184:VAL:HG23	1.87	0.57
1:B:303:PHE:HB3	1:B:304:PRO:HD3	1.84	0.57
1:B:242:LYS:O	1:B:246:GLU:HG3	2.04	0.57
1:E:99:ARG:O	1:E:200:ARG:NH1	2.36	0.57
1:F:234:GLU:N	1:F:237:HIS:HD2	1.94	0.57
1:H:32:THR:O	1:H:35:ASP:HB2	2.04	0.57
1:F:97:PRO:CB	1:G:197:LYS:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:GLY:HA3	2:G:324:ADP:N7	2.18	0.57
1:B:263:MET:SD	1:D:99:ARG:HG2	2.46	0.56
1:F:200:ARG:HG2	1:F:200:ARG:HH11	1.69	0.56
1:D:316:PRO:HB2	1:D:318:HIS:CD2	2.28	0.56
1:F:97:PRO:HB2	1:G:197:LYS:HB3	1.88	0.56
1:A:153:THR:HG23	1:A:207:GLN:HE22	1.69	0.56
1:H:149:ILE:O	1:H:149:ILE:HG22	2.06	0.56
1:A:29:GLU:HB2	1:A:311:PHE:CD2	2.41	0.56
1:B:97:PRO:HB2	1:D:263:MET:CE	2.35	0.56
1:A:26:PRO:HD2	1:A:137:VAL:HG21	1.88	0.55
1:D:235:PRO:O	1:D:238:PHE:CD2	2.58	0.55
1:B:97:PRO:CB	1:D:263:MET:HE2	2.35	0.55
1:D:181:VAL:HG12	1:D:252:MET:HE1	1.87	0.55
1:A:234:GLU:H	1:A:237:HIS:CD2	2.15	0.55
1:B:33:VAL:HG23	1:B:34:PRO:HD3	1.88	0.55
1:E:84:LEU:HG	1:E:112:LEU:CD1	2.37	0.55
1:F:45:TYR:O	1:F:49:ILE:HG22	2.07	0.54
1:F:260:ILE:HG23	1:F:264:LYS:HD2	1.88	0.54
1:D:50:GLY:O	1:D:54:THR:OG1	2.25	0.54
1:A:302:LYS:O	1:A:306:ILE:HG22	2.06	0.54
1:C:40:LYS:HE2	1:C:301:GLU:CG	2.37	0.54
1:D:177:GLN:HA	1:D:180:ILE:HD12	1.89	0.54
1:F:96:GLN:CG	1:F:98:SER:HB2	2.32	0.54
1:G:48:TYR:O	1:G:52:ILE:HG12	2.06	0.54
1:D:303:PHE:HB3	1:D:304:PRO:HD3	1.89	0.54
1:G:81:LEU:HD13	1:G:188:TYR:HA	1.90	0.54
1:A:94:VAL:HG22	1:A:102:ASN:OD1	2.08	0.54
1:C:230:HIS:CD2	1:C:232:TYR:H	2.25	0.54
1:E:235:PRO:CG	1:E:281:VAL:O	2.47	0.54
1:B:97:PRO:HB3	1:D:263:MET:HE1	1.90	0.54
1:G:142:SER:HB2	1:G:159:PHE:HB2	1.90	0.54
1:E:32:THR:CB	1:E:34:PRO:HD2	2.37	0.53
1:B:97:PRO:CB	1:D:263:MET:CE	2.87	0.53
1:B:235:PRO:HG2	1:B:281:VAL:O	2.08	0.53
1:H:230:HIS:HD2	1:H:233:LEU:N	2.00	0.53
1:G:26:PRO:HG3	1:G:134:GLU:HG3	1.90	0.53
1:E:234:GLU:H	1:E:237:HIS:CD2	2.26	0.53
1:F:189:LEU:O	1:F:193:ARG:HG3	2.07	0.53
1:E:36:MET:O	1:E:40:LYS:HD3	2.08	0.53
1:F:293:ARG:HG3	1:F:293:ARG:NH1	2.13	0.53
1:B:90:GLU:HG2	1:F:249:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:GLU:HG3	1:C:311:PHE:HB2	1.91	0.52
1:A:72:GLU:O	1:A:76:LYS:HG2	2.10	0.52
1:C:26:PRO:HD3	1:C:134:GLU:HG3	1.90	0.52
1:B:197:LYS:HE3	1:B:259:PHE:HE1	1.74	0.52
1:C:68:TYR:HH	1:C:183:LYS:HE2	1.74	0.52
1:F:132:VAL:HB	1:F:133:PRO:HD3	1.90	0.52
1:E:55:LEU:O	1:E:59:VAL:HG22	2.10	0.52
1:F:153:THR:H	1:F:207:GLN:HE22	1.58	0.52
1:F:148:ARG:HH12	1:F:205:GLY:H	1.57	0.52
1:H:223:GLY:O	1:H:226:GLN:HB2	2.10	0.52
1:C:218:LEU:N	1:C:219:PRO:HD2	2.25	0.52
1:F:53:LEU:CD2	1:F:53:LEU:CD1	2.85	0.52
1:G:223:GLY:O	1:G:226:GLN:HB2	2.10	0.52
1:A:51:PHE:CZ	1:A:55:LEU:HD11	2.45	0.51
1:F:303:PHE:CE2	1:F:307:GLN:NE2	2.78	0.51
1:D:311:PHE:CE1	1:D:317:ILE:HD13	2.45	0.51
1:C:234:GLU:H	1:C:237:HIS:CD2	2.28	0.51
1:D:235:PRO:O	1:D:238:PHE:HD2	1.94	0.51
1:E:84:LEU:HG	1:E:112:LEU:HD11	1.93	0.51
1:D:38:LYS:HD2	1:D:317:ILE:HG13	1.92	0.51
1:G:51:PHE:CZ	1:G:55:LEU:HD11	2.46	0.51
1:G:109:TYR:CD2	1:G:146:SER:HB2	2.46	0.51
1:H:85:ASP:OD2	1:H:194:LYS:NZ	2.26	0.51
1:F:63:LYS:O	1:F:66:PHE:HB2	2.10	0.51
1:A:316:PRO:HB2	1:A:318:HIS:HD2	1.75	0.51
1:B:177:GLN:HA	1:B:180:ILE:HD12	1.92	0.51
1:E:189:LEU:O	1:E:193:ARG:HG3	2.10	0.51
1:H:148:ARG:NH1	1:H:205:GLY:H	2.09	0.51
1:B:138:TYR:HB3	1:B:162:PHE:HB2	1.92	0.50
1:E:85:ASP:O	1:E:88:ILE:HB	2.12	0.50
1:A:99:ARG:HG2	1:E:263:MET:SD	2.51	0.50
1:D:26:PRO:HB2	1:D:310:LYS:HB3	1.93	0.50
1:G:33:VAL:HG23	1:G:34:PRO:CD	2.41	0.50
1:A:193:ARG:HD3	1:A:259:PHE:CD1	2.47	0.50
1:D:49:ILE:O	1:D:53:LEU:HG	2.11	0.50
1:E:178:ILE:O	1:E:182:PHE:HB2	2.12	0.50
1:G:55:LEU:O	1:G:59:VAL:HG22	2.12	0.50
1:H:303:PHE:HB3	1:H:304:PRO:HD3	1.94	0.50
1:E:303:PHE:O	1:E:307:GLN:HB3	2.11	0.50
1:F:144:GLY:HA2	1:F:155:HIS:CE1	2.46	0.50
1:G:267:PRO:O	1:G:270:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:TYR:O	1:H:49:ILE:HG22	2.12	0.50
1:A:218:LEU:N	1:A:219:PRO:HD2	2.27	0.49
1:C:87:TRP:CH2	1:C:119:LEU:HD11	2.47	0.49
1:D:211:GLY:O	1:D:274:GLN:NE2	2.45	0.49
1:A:97:PRO:HB3	1:E:197:LYS:HD3	1.94	0.49
1:C:230:HIS:CG	1:C:231:PRO:HD2	2.47	0.49
1:H:264:LYS:HD2	1:H:271:HIS:HB2	1.95	0.49
1:F:63:LYS:HB3	1:F:250:ASP:HB3	1.94	0.49
1:H:142:SER:HB2	1:H:159:PHE:HB2	1.95	0.49
1:A:38:LYS:HD3	1:A:317:ILE:CG1	2.43	0.49
1:B:230:HIS:CD2	1:B:232:TYR:H	2.17	0.49
1:C:221:ILE:HG12	1:C:291:LEU:HB3	1.94	0.49
1:B:234:GLU:H	1:B:237:HIS:HD2	1.59	0.49
1:D:142:SER:HB2	1:D:159:PHE:HB2	1.94	0.49
1:C:320:VAL:HG13	1:C:320:VAL:O	2.13	0.48
1:D:236:ARG:HA	1:D:279:SER:HB2	1.94	0.48
1:E:156:GLU:OE2	1:E:216:GLN:HB3	2.12	0.48
1:G:55:LEU:HD23	1:G:177:GLN:HB2	1.94	0.48
1:G:96:GLN:HE21	1:G:98:SER:HB3	1.78	0.48
1:E:223:GLY:O	1:E:226:GLN:HB2	2.14	0.48
1:F:218:LEU:N	1:F:219:PRO:HD2	2.28	0.48
1:H:132:VAL:HB	1:H:133:PRO:HD3	1.95	0.48
1:B:39:TRP:O	1:B:45:TYR:HB2	2.14	0.48
1:D:306:ILE:HG13	1:D:306:ILE:O	2.12	0.48
1:G:138:TYR:CZ	1:G:315:LEU:HD12	2.49	0.48
1:D:235:PRO:HA	1:D:284:TRP:CZ2	2.47	0.48
1:A:55:LEU:HD23	1:A:177:GLN:HB2	1.96	0.48
1:E:87:TRP:HH2	1:E:115:GLU:HB2	1.77	0.48
1:A:163:LEU:HA	1:A:166:LEU:HD12	1.96	0.48
1:C:148:ARG:HD3	1:C:150:ASP:OD2	2.13	0.48
1:B:148:ARG:NH1	2:B:324:ADP:O2B	2.46	0.48
1:G:26:PRO:HD3	1:G:134:GLU:HA	1.96	0.48
1:B:26:PRO:HB2	1:B:310:LYS:HB3	1.95	0.48
1:D:43:GLN:HG2	1:D:316:PRO:HD2	1.95	0.48
1:E:26:PRO:HB2	1:E:310:LYS:HB3	1.95	0.48
1:F:29:GLU:HB2	1:F:311:PHE:CD2	2.49	0.48
1:G:25:ILE:HG23	1:G:137:VAL:HG21	1.96	0.48
1:H:181:VAL:HG13	1:H:222:TRP:CE3	2.49	0.48
1:A:303:PHE:HB3	1:A:304:PRO:HD3	1.96	0.47
1:D:96:GLN:O	1:D:96:GLN:HG2	2.13	0.47
1:E:25:ILE:HG23	1:E:137:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ARG:NH2	1:G:256:CYS:SG	2.87	0.47
1:B:35:ASP:O	1:B:38:LYS:HB2	2.14	0.47
1:H:26:PRO:HD2	1:H:137:VAL:HG21	1.95	0.47
1:B:84:LEU:HG	1:B:112:LEU:HD12	1.95	0.47
1:E:22:ASN:HD22	1:E:22:ASN:N	2.13	0.47
1:E:46:ALA:HA	1:E:49:ILE:HG22	1.97	0.47
1:G:148:ARG:HD3	1:G:150:ASP:OD2	2.15	0.47
1:C:87:TRP:HH2	1:C:115:GLU:HB2	1.79	0.47
1:E:42:SER:HA	1:E:319:PRO:HA	1.96	0.47
1:E:267:PRO:O	1:E:270:GLU:HB2	2.15	0.47
1:F:263:MET:HE1	1:G:97:PRO:HB2	1.91	0.47
1:A:55:LEU:CD2	1:A:177:GLN:HB2	2.44	0.47
1:E:114:GLU:OE2	1:E:114:GLU:HA	2.13	0.47
1:F:268:PHE:HA	1:F:271:HIS:CE1	2.50	0.47
1:G:178:ILE:H	1:G:178:ILE:HG13	1.47	0.47
1:H:86:ARG:HG2	1:H:90:GLU:OE2	2.14	0.47
1:A:302:LYS:HG3	1:A:304:PRO:HD2	1.96	0.47
1:B:223:GLY:O	1:B:226:GLN:HB2	2.14	0.47
1:C:26:PRO:HA	1:C:311:PHE:O	2.14	0.47
1:D:91:THR:HG21	1:D:107:THR:HB	1.97	0.47
1:G:43:GLN:HB3	1:G:316:PRO:HD2	1.96	0.47
1:D:223:GLY:HA3	1:D:253:PHE:HB2	1.96	0.46
1:E:118:ASN:ND2	1:E:118:ASN:N	2.59	0.46
1:B:168:LYS:HB3	1:B:168:LYS:HE2	1.67	0.46
1:B:195:LEU:HD23	1:B:199:TYR:CD2	2.46	0.46
1:H:168:LYS:HB3	1:H:314:LEU:HD22	1.96	0.46
1:H:230:HIS:CG	1:H:231:PRO:HD2	2.50	0.46
1:D:56:ASN:HA	1:D:222:TRP:CD1	2.50	0.46
1:B:197:LYS:HB3	1:D:97:PRO:HB2	1.97	0.46
1:E:192:MET:O	1:E:196:GLN:HG3	2.16	0.46
1:E:124:VAL:HG22	1:E:171:VAL:HG21	1.97	0.46
1:D:174:VAL:O	1:D:177:GLN:HG2	2.15	0.46
1:E:174:VAL:O	1:E:177:GLN:HG2	2.16	0.46
1:F:38:LYS:HA	1:F:41:ARG:HG3	1.97	0.46
1:F:53:LEU:HA	1:F:53:LEU:HD23	1.97	0.46
1:F:62:LYS:O	1:F:226:GLN:HG3	2.16	0.46
1:G:112:LEU:O	1:G:112:LEU:HG	2.15	0.46
1:D:295:TYR:O	1:D:299:CYS:HB3	2.15	0.46
1:F:200:ARG:HG2	1:F:200:ARG:NH1	2.31	0.45
1:H:168:LYS:HA	1:H:168:LYS:HE2	1.97	0.45
1:B:189:LEU:HD11	1:B:219:PRO:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:LEU:HD11	1:D:219:PRO:HB3	1.98	0.45
1:A:96:GLN:CG	1:A:98:SER:HB2	2.36	0.45
1:B:321:THR:O	1:B:322:SER:HB3	2.16	0.45
1:G:99:ARG:O	1:G:200:ARG:NH2	2.45	0.45
1:D:148:ARG:HD3	1:D:150:ASP:OD2	2.17	0.45
1:E:149:ILE:O	1:E:149:ILE:HG22	2.16	0.45
1:F:206:SER:HB2	1:F:210:TRP:CZ2	2.51	0.45
1:A:153:THR:CG2	1:A:207:GLN:HE22	2.30	0.45
1:A:206:SER:HB2	1:A:210:TRP:CZ3	2.52	0.45
1:B:90:GLU:CG	1:F:249:LYS:HE3	2.47	0.45
1:H:26:PRO:HB2	1:H:310:LYS:HB3	1.97	0.45
1:A:249:LYS:NZ	1:C:86:ARG:HG3	2.30	0.45
1:H:125:PRO:HG2	1:H:128:LEU:HD12	1.99	0.45
1:B:71:SER:HB3	1:B:74:ILE:HG12	1.98	0.45
1:A:223:GLY:O	1:A:226:GLN:HB2	2.17	0.45
1:C:238:PHE:CZ	1:C:279:SER:HB3	2.52	0.45
1:C:149:ILE:O	1:C:149:ILE:HG22	2.17	0.44
1:E:251:TYR:HB2	1:E:254:LEU:HD12	1.99	0.44
1:G:230:HIS:CD2	1:G:233:LEU:HB2	2.51	0.44
1:H:48:TYR:O	1:H:49:ILE:C	2.55	0.44
1:C:151:TYR:O	1:C:215:PHE:HD1	2.01	0.44
1:A:264:LYS:HD3	1:A:271:HIS:HB2	1.99	0.44
1:B:87:TRP:CH2	1:B:119:LEU:HD11	2.52	0.44
1:F:303:PHE:HB3	1:F:304:PRO:HD3	1.99	0.44
1:G:298:GLU:HA	1:G:302:LYS:HE2	1.99	0.44
1:C:74:ILE:O	1:C:78:VAL:HG23	2.17	0.44
1:D:206:SER:HB2	1:D:210:TRP:CZ2	2.53	0.44
1:F:296:LYS:O	1:F:301:GLU:HB2	2.17	0.44
1:B:87:TRP:HH2	1:B:119:LEU:HD11	1.81	0.44
1:G:101:GLY:HA3	1:G:149:ILE:CG2	2.48	0.44
1:A:123:VAL:HG12	1:A:171:VAL:HG11	1.98	0.44
1:C:39:TRP:O	1:C:45:TYR:HB2	2.17	0.44
1:C:151:TYR:C	1:C:151:TYR:CD2	2.91	0.44
1:B:83:THR:HG23	1:B:86:ARG:NH2	2.33	0.44
1:A:100:PHE:O	1:E:200:ARG:NH2	2.51	0.43
1:G:221:ILE:HD11	1:G:295:TYR:HB2	2.01	0.43
1:G:303:PHE:HB3	1:G:304:PRO:HD3	1.99	0.43
1:A:63:LYS:O	1:A:66:PHE:HB2	2.18	0.43
1:B:218:LEU:N	1:B:219:PRO:HD2	2.33	0.43
1:F:293:ARG:CG	1:F:293:ARG:NH1	2.71	0.43
1:E:101:GLY:HA3	1:E:149:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:ALA:O	1:F:139:LEU:HB3	2.18	0.43
1:A:181:VAL:HG12	1:A:182:PHE:HD1	1.84	0.43
1:C:51:PHE:O	1:C:55:LEU:HG	2.17	0.43
1:D:300:LEU:HA	1:D:306:ILE:HD13	2.00	0.43
1:D:303:PHE:CD2	1:D:303:PHE:C	2.91	0.43
1:F:276:TRP:O	1:F:279:SER:OG	2.37	0.43
1:A:132:VAL:HB	1:A:133:PRO:HD3	2.00	0.43
1:D:148:ARG:NH1	1:D:205:GLY:H	2.17	0.43
1:F:123:VAL:HG12	1:F:171:VAL:HG11	2.01	0.43
1:F:302:LYS:HG3	1:F:304:PRO:HD2	2.01	0.43
1:A:51:PHE:O	1:A:55:LEU:HG	2.18	0.43
1:C:291:LEU:O	1:C:295:TYR:N	2.47	0.43
1:D:63:LYS:O	1:D:66:PHE:HB2	2.19	0.43
1:D:302:LYS:O	1:D:306:ILE:HG22	2.19	0.43
1:H:41:ARG:HH11	1:H:41:ARG:HB3	1.84	0.43
1:B:26:PRO:HD3	1:B:134:GLU:HA	2.00	0.43
1:D:24:ILE:O	1:D:134:GLU:HB2	2.18	0.43
1:G:87:TRP:HH2	1:G:115:GLU:HB2	1.84	0.42
1:C:127:HIS:CD2	1:C:128:LEU:HG	2.54	0.42
1:C:267:PRO:HA	1:D:240:ASP:OD1	2.19	0.42
1:E:43:GLN:NE2	1:E:47:ASP:OD1	2.53	0.42
1:B:23:PHE:CZ	1:B:131:ALA:HB2	2.53	0.42
1:B:150:ASP:HB3	1:B:202:GLU:HB2	2.01	0.42
1:H:222:TRP:O	1:H:225:SER:HB3	2.20	0.42
1:B:96:GLN:OE1	1:B:102:ASN:HA	2.20	0.42
1:D:163:LEU:HD13	1:D:180:ILE:HG23	2.00	0.42
1:F:97:PRO:HB3	1:G:197:LYS:HB3	2.02	0.42
1:E:25:ILE:HA	1:E:26:PRO:HD3	1.92	0.42
1:H:197:LYS:O	1:H:200:ARG:HD2	2.20	0.42
1:C:294:MET:O	1:C:298:GLU:HB2	2.19	0.42
1:D:206:SER:HB2	1:D:210:TRP:CH2	2.55	0.42
1:E:68:TYR:OH	1:E:183:LYS:HE2	2.20	0.42
1:C:87:TRP:HH2	1:C:119:LEU:HD11	1.84	0.41
1:C:240:ASP:OD2	1:D:267:PRO:HA	2.21	0.41
1:G:25:ILE:HA	1:G:26:PRO:HD3	1.91	0.41
1:D:227:LEU:HD13	1:D:284:TRP:CH2	2.56	0.41
1:G:40:LYS:HD3	1:G:40:LYS:HA	1.70	0.41
1:G:295:TYR:O	1:G:299:CYS:HB3	2.20	0.41
1:A:26:PRO:HD3	1:A:134:GLU:HA	2.03	0.41
1:A:263:MET:HE1	1:E:97:PRO:HB3	2.02	0.41
1:C:298:GLU:HA	1:C:302:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:PRO:CB	1:D:318:HIS:HD2	2.20	0.41
1:E:196:GLN:HE22	1:E:216:GLN:NE2	2.18	0.41
1:G:320:VAL:HG13	1:G:320:VAL:O	2.19	0.41
1:H:291:LEU:HD23	1:H:291:LEU:HA	1.91	0.41
1:A:52:ILE:HD12	1:A:222:TRP:HZ2	1.85	0.41
1:D:55:LEU:HD23	1:D:177:GLN:HB3	2.02	0.41
1:D:100:PHE:HB3	1:D:101:GLY:H	1.56	0.41
1:G:90:GLU:HG2	1:H:249:LYS:HE3	2.03	0.41
1:A:77:LEU:HD13	1:A:184:VAL:HG11	2.02	0.41
1:C:194:LYS:O	1:C:198:THR:OG1	2.31	0.41
1:F:53:LEU:CD2	1:F:53:LEU:HA	2.51	0.41
1:E:23:PHE:O	1:E:24:ILE:HG23	2.20	0.41
1:A:297:ALA:O	1:A:302:LYS:HE2	2.20	0.41
1:C:159:PHE:CE2	1:C:163:LEU:HD11	2.56	0.41
1:D:177:GLN:HG2	1:D:177:GLN:H	1.60	0.41
1:F:206:SER:HB2	1:F:210:TRP:CH2	2.56	0.41
1:B:77:LEU:O	1:B:80:LEU:HB3	2.21	0.41
1:C:63:LYS:HG2	1:C:250:ASP:HB3	2.02	0.41
1:C:125:PRO:HG2	1:C:128:LEU:HB2	2.02	0.41
1:D:151:TYR:CD2	1:D:152:GLY:N	2.89	0.41
1:G:22:ASN:N	1:G:22:ASN:ND2	2.67	0.41
1:B:33:VAL:O	1:B:36:MET:HB2	2.21	0.40
1:E:120:VAL:HG12	1:E:132:VAL:HG22	2.03	0.40
1:H:234:GLU:O	1:H:235:PRO:C	2.59	0.40
1:G:43:GLN:HG3	1:G:47:ASP:OD2	2.21	0.40
1:D:60:LYS:HG3	1:D:228:ILE:HD12	2.03	0.40
1:E:99:ARG:O	1:E:99:ARG:HG2	2.21	0.40
1:F:76:LYS:HA	1:F:76:LYS:HD3	1.88	0.40
1:A:189:LEU:HD11	1:A:219:PRO:HB3	2.04	0.40
1:F:68:TYR:OH	1:F:183:LYS:HE2	2.22	0.40
1:A:52:ILE:HD13	1:A:52:ILE:HA	1.78	0.40
1:B:217:PHE:C	1:B:219:PRO:HD2	2.42	0.40
1:E:230:HIS:HD2	1:E:233:LEU:N	2.17	0.40
1:F:230:HIS:CD2	1:F:232:TYR:H	2.40	0.40
1:H:302:LYS:HA	1:H:302:LYS:HD3	1.93	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	299/323 (93%)	280 (94%)	16 (5%)	3 (1%)	15	28
1	B	299/323 (93%)	277 (93%)	22 (7%)	0	100	100
1	C	299/323 (93%)	278 (93%)	20 (7%)	1 (0%)	41	61
1	D	299/323 (93%)	278 (93%)	20 (7%)	1 (0%)	41	61
1	E	299/323 (93%)	267 (89%)	30 (10%)	2 (1%)	22	39
1	F	299/323 (93%)	276 (92%)	21 (7%)	2 (1%)	22	39
1	G	299/323 (93%)	270 (90%)	27 (9%)	2 (1%)	22	39
1	H	299/323 (93%)	272 (91%)	26 (9%)	1 (0%)	41	61
All	All	2392/2584 (93%)	2198 (92%)	182 (8%)	12 (0%)	29	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	98	SER
1	A	97	PRO
1	A	98	SER
1	C	208	GLY
1	D	209	VAL
1	G	208	GLY
1	A	130	ALA
1	F	209	VAL
1	E	208	GLY
1	E	320	VAL
1	F	97	PRO
1	G	320	VAL

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	263/280 (94%)	250 (95%)	13 (5%)	25	47
1	B	263/280 (94%)	248 (94%)	15 (6%)	20	39
1	C	263/280 (94%)	250 (95%)	13 (5%)	25	47
1	D	263/280 (94%)	244 (93%)	19 (7%)	14	28
1	E	263/280 (94%)	253 (96%)	10 (4%)	33	58
1	F	263/280 (94%)	243 (92%)	20 (8%)	13	25
1	G	263/280 (94%)	243 (92%)	20 (8%)	13	25
1	H	263/280 (94%)	248 (94%)	15 (6%)	20	39
All	All	2104/2240 (94%)	1979 (94%)	125 (6%)	19	37

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	38	LYS
1	A	41	ARG
1	A	72	GLU
1	A	168	LYS
1	A	174	VAL
1	A	175	ASP
1	A	183	LYS
1	A	206	SER
1	A	210	TRP
1	A	265	THR
1	A	274	GLN
1	A	285	SER
1	B	24	ILE
1	B	33	VAL
1	B	39	TRP
1	B	40	LYS
1	B	64	LEU
1	B	72	GLU
1	B	86	ARG
1	B	89	ASP
1	B	99	ARG
1	B	122	THR

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Mol	Chain	Res	Type
1	B	139	LEU
1	B	147	THR
1	B	178	ILE
1	B	195	LEU
1	B	262	GLU
1	C	22	ASN
1	C	33	VAL
1	C	40	LYS
1	C	75	GLU
1	C	80	LEU
1	C	84	LEU
1	C	147	THR
1	C	167	CYS
1	C	175	ASP
1	C	183	LYS
1	C	238	PHE
1	C	298	GLU
1	C	321	THR
1	D	38	LYS
1	D	41	ARG
1	D	54	THR
1	D	57	GLU
1	D	95	ASP
1	D	96	GLN
1	D	134	GLU
1	D	146	SER
1	D	148	ARG
1	D	177	GLN
1	D	178	ILE
1	D	206	SER
1	D	210	TRP
1	D	224	SER
1	D	265	THR
1	D	274	GLN
1	D	278	ILE
1	D	285	SER
1	D	321	THR
1	E	22	ASN
1	E	33	VAL
1	E	40	LYS
1	E	53	LEU
1	E	72	GLU

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Mol	Chain	Res	Type
1	E	83	THR
1	E	118	ASN
1	E	176	ASP
1	E	298	GLU
1	E	321	THR
1	F	22	ASN
1	F	24	ILE
1	F	41	ARG
1	F	54	THR
1	F	65	THR
1	F	84	LEU
1	F	94	VAL
1	F	98	SER
1	F	147	THR
1	F	148	ARG
1	F	175	ASP
1	F	183	LYS
1	F	206	SER
1	F	210	TRP
1	F	265	THR
1	F	272	SER
1	F	274	GLN
1	F	278	ILE
1	F	283	SER
1	F	293	ARG
1	G	22	ASN
1	G	24	ILE
1	G	33	VAL
1	G	40	LYS
1	G	65	THR
1	G	69	ARG
1	G	86	ARG
1	G	91	THR
1	G	99	ARG
1	G	112	LEU
1	G	118	ASN
1	G	176	ASP
1	G	178	ILE
1	G	195	LEU
1	G	216	GLN
1	G	285	SER
1	G	289	GLN

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Mol	Chain	Res	Type
1	G	298	GLU
1	G	306	ILE
1	G	321	THR
1	H	22	ASN
1	H	24	ILE
1	H	27	LYS
1	H	41	ARG
1	H	65	THR
1	H	94	VAL
1	H	95	ASP
1	H	98	SER
1	H	168	LYS
1	H	186	ASN
1	H	210	TRP
1	H	272	SER
1	H	274	GLN
1	H	278	ILE
1	H	321	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	31	HIS
1	A	96	GLN
1	A	207	GLN
1	A	216	GLN
1	A	230	HIS
1	A	237	HIS
1	B	186	ASN
1	B	230	HIS
1	B	237	HIS
1	B	274	GLN
1	B	277	ASN
1	C	31	HIS
1	C	177	GLN
1	C	186	ASN
1	C	230	HIS
1	C	237	HIS
1	C	277	ASN
1	D	186	ASN
1	D	216	GLN

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Mol	Chain	Res	Type
1	D	230	HIS
1	D	237	HIS
1	D	274	GLN
1	D	277	ASN
1	D	318	HIS
1	E	118	ASN
1	E	177	GLN
1	E	216	GLN
1	E	230	HIS
1	E	237	HIS
1	E	248	HIS
1	E	274	GLN
1	E	277	ASN
1	F	22	ASN
1	F	96	GLN
1	F	207	GLN
1	F	216	GLN
1	F	230	HIS
1	F	237	HIS
1	F	274	GLN
1	F	288	ASN
1	G	118	ASN
1	G	230	HIS
1	G	237	HIS
1	G	274	GLN
1	G	277	ASN
1	H	22	ASN
1	H	96	GLN
1	H	186	ASN
1	H	216	GLN
1	H	230	HIS
1	H	237	HIS
1	H	274	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)

4 ligands are modelled in this entry.

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	E	324	-	24,29,29	1.11	3 (12%)	29,45,45	1.36	5 (17%)
2	ADP	B	324	-	24,29,29	1.07	3 (12%)	29,45,45	1.36	3 (10%)
2	ADP	G	324	-	24,29,29	1.15	3 (12%)	29,45,45	1.20	3 (10%)
2	ADP	C	324	-	24,29,29	1.11	3 (12%)	29,45,45	1.31	3 (10%)

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	E	324	-	-	3/12/32/32	0/3/3/3
2	ADP	B	324	-	-	5/12/32/32	0/3/3/3
2	ADP	G	324	-	-	2/12/32/32	0/3/3/3
2	ADP	C	324	-	-	8/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	324	ADP	O4'-C1'	3.05	1.45	1.41
2	E	324	ADP	C5-C4	2.71	1.48	1.40
2	C	324	ADP	C5-C4	2.70	1.48	1.40
2	G	324	ADP	C5-C4	2.69	1.48	1.40
2	E	324	ADP	O4'-C1'	2.58	1.44	1.41
2	B	324	ADP	C5-C4	2.58	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	324	ADP	O4'-C1'	2.48	1.44	1.41
2	B	324	ADP	C2-N3	2.30	1.35	1.32
2	C	324	ADP	C2-N3	2.29	1.35	1.32
2	B	324	ADP	O4'-C1'	2.22	1.44	1.41
2	E	324	ADP	C2-N3	2.18	1.35	1.32
2	G	324	ADP	C2-N3	2.12	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	324	ADP	C4-C5-N7	-3.65	105.59	109.40
2	E	324	ADP	C3'-C2'-C1'	3.46	106.19	100.98
2	E	324	ADP	N3-C2-N1	-3.38	123.40	128.68
2	C	324	ADP	N3-C2-N1	-3.22	123.64	128.68
2	G	324	ADP	N3-C2-N1	-3.19	123.69	128.68
2	B	324	ADP	N3-C2-N1	-3.13	123.78	128.68
2	C	324	ADP	C3'-C2'-C1'	3.09	105.63	100.98
2	G	324	ADP	C4-C5-N7	-2.79	106.49	109.40
2	C	324	ADP	C4-C5-N7	-2.59	106.70	109.40
2	B	324	ADP	O5'-C5'-C4'	2.44	117.40	108.99
2	E	324	ADP	C4-C5-N7	-2.42	106.87	109.40
2	G	324	ADP	PA-O3A-PB	-2.40	124.61	132.83
2	E	324	ADP	PA-O3A-PB	-2.17	125.36	132.83
2	E	324	ADP	C2'-C3'-C4'	2.12	106.76	102.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	324	ADP	C5'-O5'-PA-O1A
2	B	324	ADP	C5'-O5'-PA-O2A
2	B	324	ADP	C5'-O5'-PA-O3A
2	B	324	ADP	O4'-C4'-C5'-O5'
2	C	324	ADP	PA-O3A-PB-O3B
2	C	324	ADP	PB-O3A-PA-O5'
2	C	324	ADP	C5'-O5'-PA-O3A
2	E	324	ADP	PB-O3A-PA-O5'
2	C	324	ADP	O4'-C4'-C5'-O5'
2	G	324	ADP	O4'-C4'-C5'-O5'
2	B	324	ADP	C3'-C4'-C5'-O5'
2	C	324	ADP	C3'-C4'-C5'-O5'
2	G	324	ADP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
2	C	324	ADP	C5'-O5'-PA-O1A
2	C	324	ADP	C5'-O5'-PA-O2A
2	E	324	ADP	C4'-C5'-O5'-PA
2	C	324	ADP	PA-O3A-PB-O2B
2	E	324	ADP	O4'-C4'-C5'-O5'

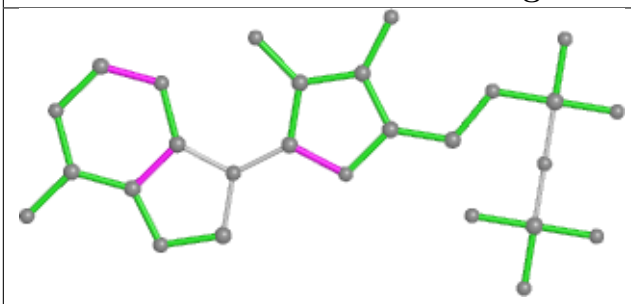
There are no ring outliers.

3 monomers are involved in 6 short contacts:

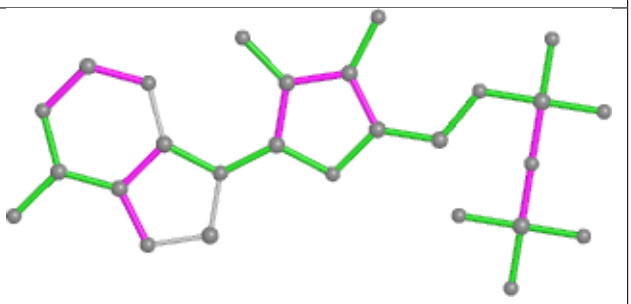
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	324	ADP	2	0
2	G	324	ADP	3	0
2	C	324	ADP	1	0

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.

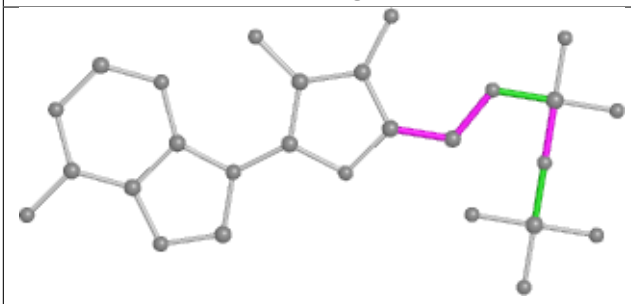
Ligand ADP E 324



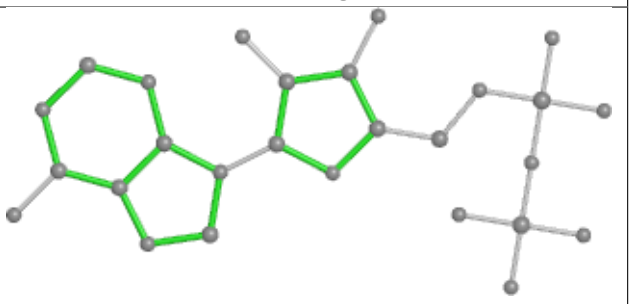
Bond lengths



Bond angles

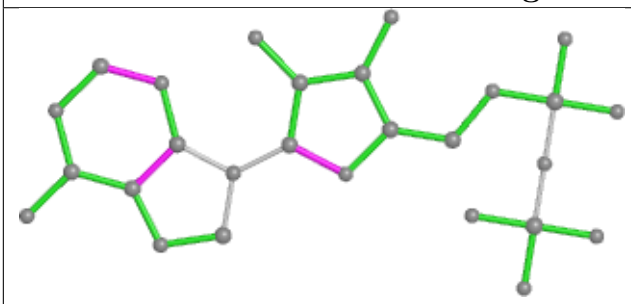


Torsions

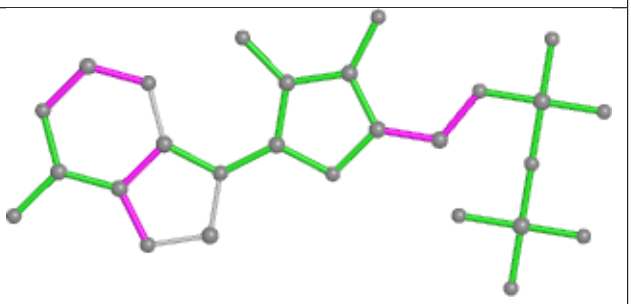


Rings

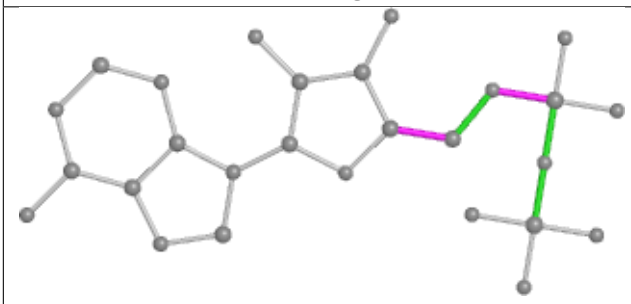
Ligand ADP B 324



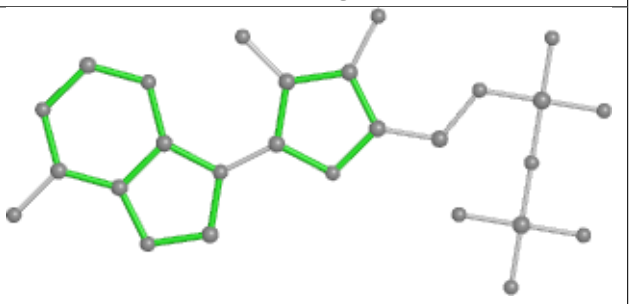
Bond lengths



Bond angles

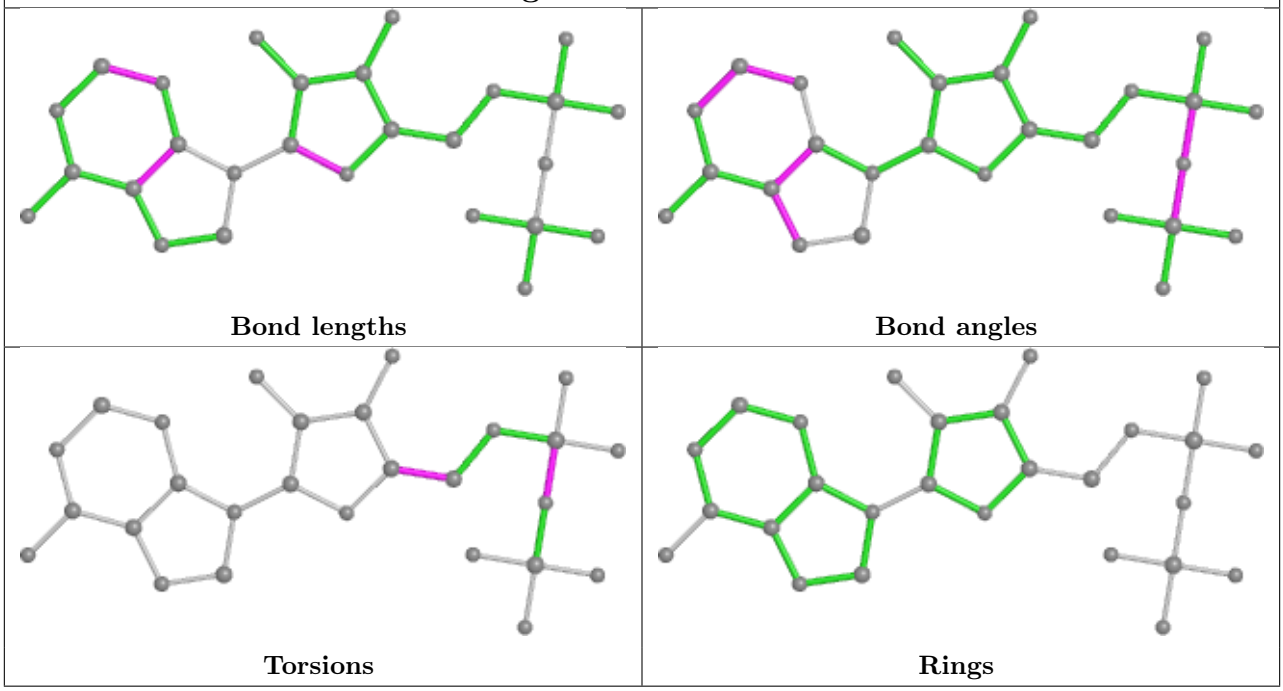


Torsions

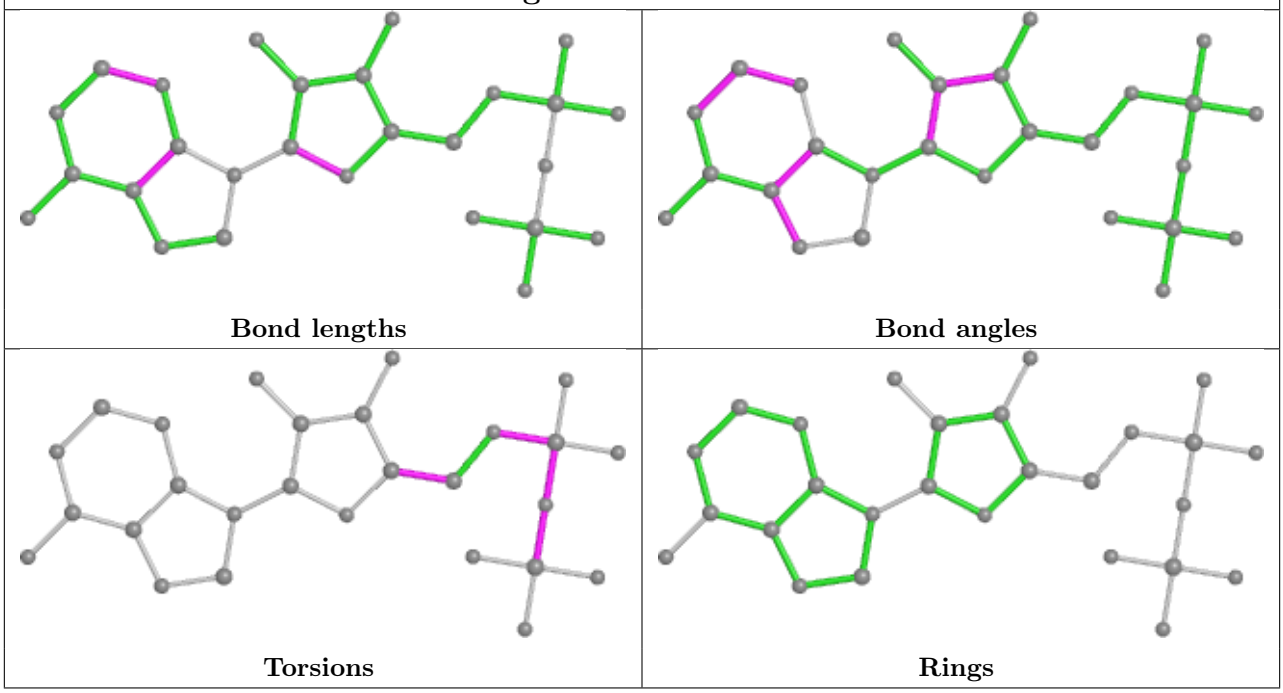


Rings

Ligand ADP G 324



Ligand ADP C 324



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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.