



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:31 AM UTC

PDB ID : 1OSN / pdb_00001osn
Title : Crystal structure of Varicella zoster virus thymidine kinase in complex with BVDU-MP and ADP
Authors : Bird, L.E.; Ren, J.; Wright, A.; Leslie, K.D.; Degreve, B.; Balzarini, J.; Stammers, D.K.
Deposited on : 2003-03-20
Resolution : 3.20 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

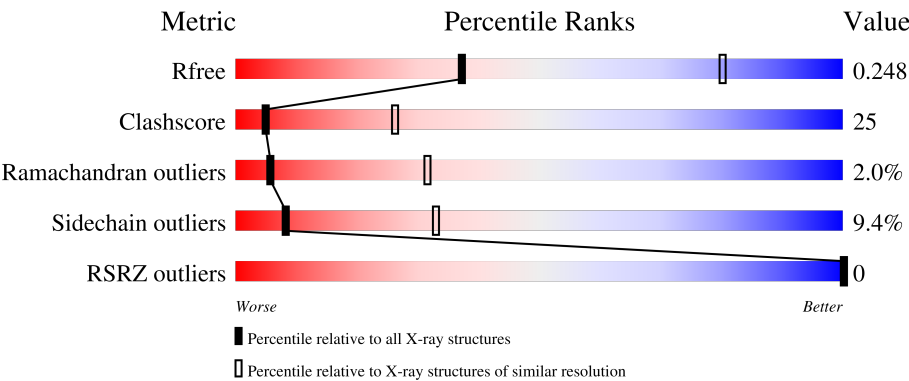
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	341	56%31%8%5%
1	B	341	52%32%8%8%
1	C	341	51%33%7%8%
1	D	341	53%32%7%8%

2 Entry composition [i](#)

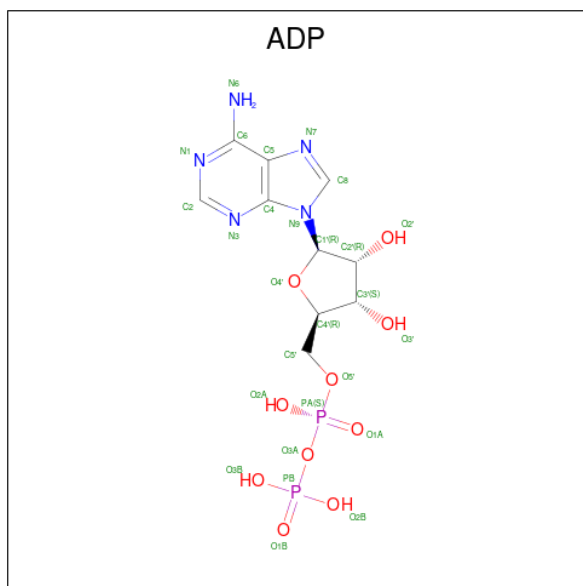
There are 4 unique types of molecules in this entry. The entry contains 10038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thymidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2524	1623	426	456	19			
1	B	315	Total	C	N	O	S	0	0	0
			2446	1574	412	441	19			
1	C	313	Total	C	N	O	S	0	0	0
			2433	1568	411	435	19			
1	D	315	Total	C	N	O	S	0	0	0
			2452	1579	413	441	19			

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



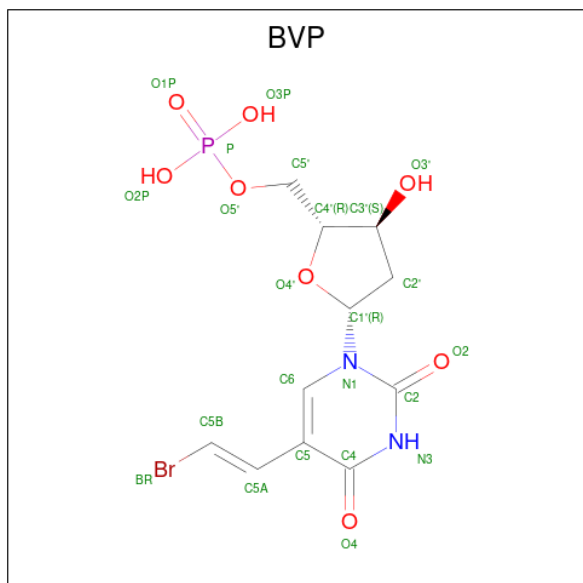
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	O	P			0	0
			8	6	2				
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 3 is (E)-5-(2-BROMOVINYL)-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: BVP) (formula: $C_{11}H_{14}BrN_2O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 23	Br 1	C 11	N 2	O 8	P 1	0	0
3	B	1	Total 23	Br 1	C 11	N 2	O 8	P 1	0	0
3	C	1	Total 23	Br 1	C 11	N 2	O 8	P 1	0	0
3	D	1	Total 23	Br 1	C 11	N 2	O 8	P 1	0	0

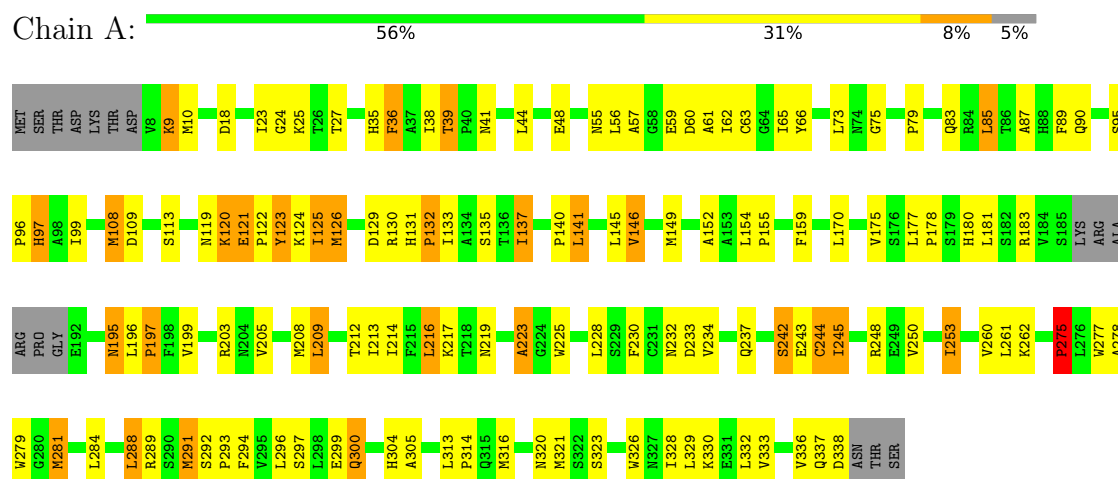
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		

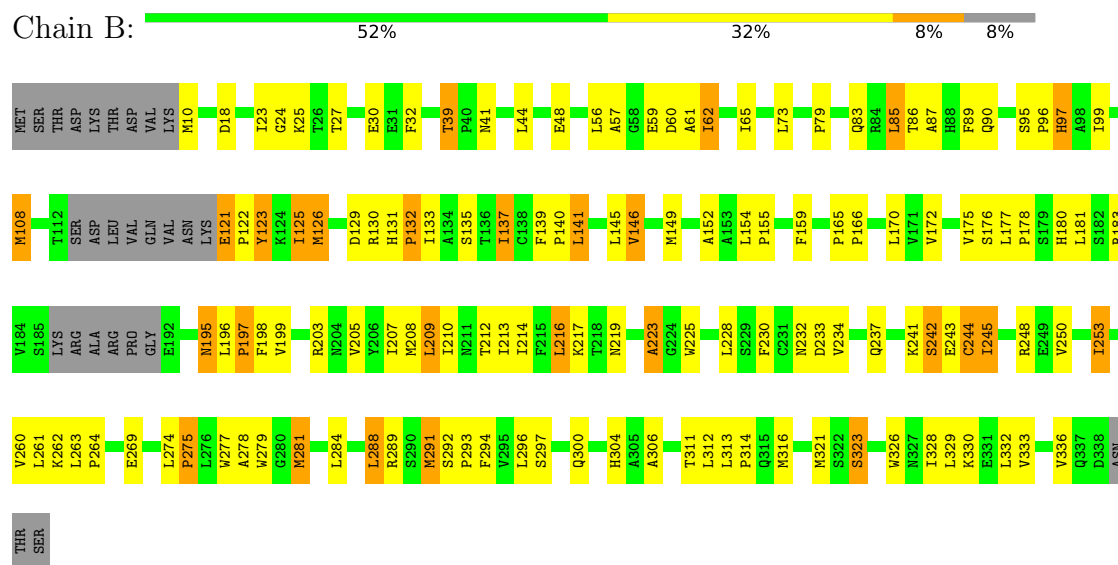
3 Residue-property plots

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: Thymidine kinase

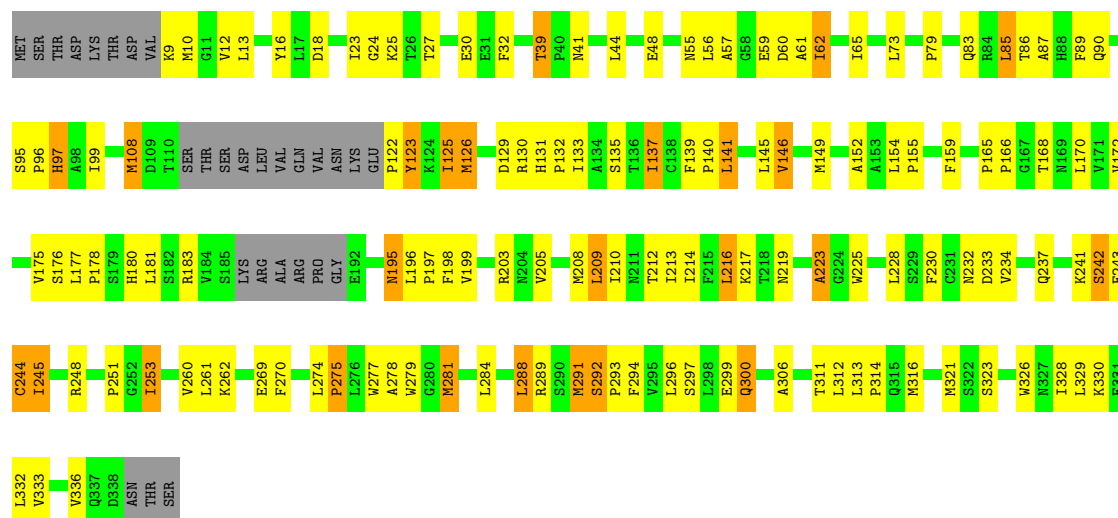


• Molecule 1: Thymidine kinase



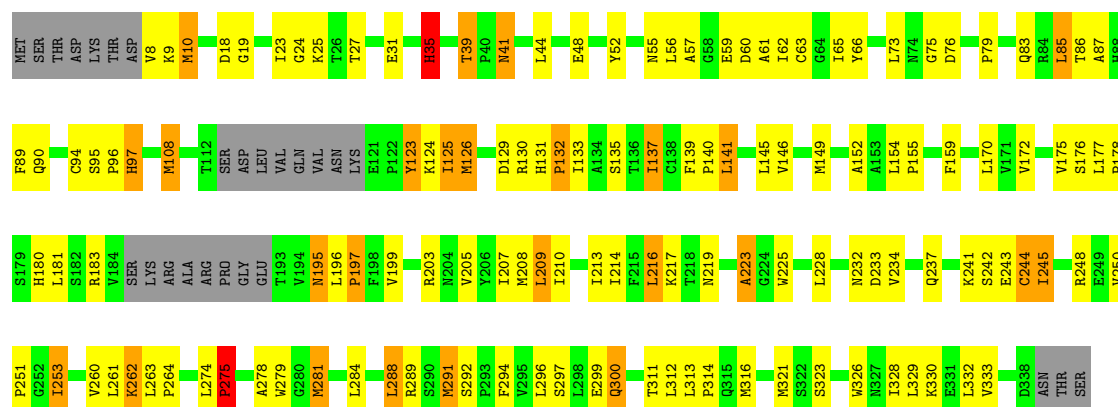
• Molecule 1: Thymidine kinase





• Molecule 1: Thymidine kinase

Chain D: 53% 32% 7% • 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 54.20Å 167.80Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	29.78 – 3.20 29.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.78-3.20) 78.2 (29.78-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.268 0.215 , 0.248	Depositor DCC
R_{free} test set	1490 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10038	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% 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: BVP, 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	0.58	0/2584	1.04	14/3519 (0.4%)
1	B	0.51	0/2505	1.02	15/3411 (0.4%)
1	C	0.51	0/2492	1.01	13/3391 (0.4%)
1	D	0.52	0/2511	1.02	15/3418 (0.4%)
All	All	0.53	0/10092	1.02	57/13739 (0.4%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	CYS	N-CA-C	8.17	119.88	110.97
1	A	291	MET	N-CA-C	8.16	121.45	110.35
1	B	291	MET	N-CA-C	8.12	121.39	110.35
1	B	242	SER	N-CA-C	8.00	123.04	113.28
1	D	291	MET	N-CA-C	7.97	121.19	110.35
1	C	291	MET	N-CA-C	7.74	121.45	110.23
1	C	242	SER	N-CA-C	7.62	122.58	113.28
1	A	242	SER	N-CA-C	7.61	122.56	113.28
1	D	242	SER	N-CA-C	7.26	122.31	113.38
1	A	337	GLN	N-CA-C	-6.83	104.93	113.20
1	C	292	SER	CA-C-N	6.28	126.50	119.90
1	C	292	SER	C-N-CA	6.28	126.50	119.90
1	A	121	GLU	N-CA-C	6.20	119.00	110.01
1	A	248	ARG	N-CA-C	6.16	119.53	109.06
1	B	248	ARG	N-CA-C	6.07	119.39	109.06
1	D	248	ARG	N-CA-C	5.92	119.12	109.06
1	A	292	SER	CA-C-N	5.91	126.11	119.90
1	A	292	SER	C-N-CA	5.91	126.11	119.90
1	C	248	ARG	N-CA-C	5.81	118.93	109.06
1	B	39	THR	CA-C-N	5.80	127.09	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	THR	C-N-CA	5.80	127.09	119.84
1	C	39	THR	CA-C-N	5.71	126.98	119.84
1	C	39	THR	C-N-CA	5.71	126.98	119.84
1	B	292	SER	CA-C-N	5.70	125.89	119.90
1	B	292	SER	C-N-CA	5.70	125.89	119.90
1	A	293	PRO	N-CA-C	5.57	119.21	110.80
1	A	121	GLU	CA-C-N	5.56	125.53	120.03
1	A	121	GLU	C-N-CA	5.56	125.53	120.03
1	C	62	ILE	N-CA-C	5.55	115.69	110.30
1	C	241	LYS	N-CA-C	5.52	119.51	112.12
1	D	39	THR	CA-C-N	5.38	126.56	119.84
1	D	39	THR	C-N-CA	5.38	126.56	119.84
1	B	62	ILE	N-CA-C	5.36	115.50	110.30
1	B	274	LEU	CA-C-N	5.33	126.50	119.84
1	B	274	LEU	C-N-CA	5.33	126.50	119.84
1	D	292	SER	CA-C-N	5.32	125.49	119.90
1	D	292	SER	C-N-CA	5.32	125.49	119.90
1	B	241	LYS	N-CA-C	5.32	119.25	112.12
1	A	250	VAL	CA-C-N	5.31	125.22	119.85
1	A	250	VAL	C-N-CA	5.31	125.22	119.85
1	C	274	LEU	CA-C-N	5.21	126.35	119.84
1	C	274	LEU	C-N-CA	5.21	126.35	119.84
1	A	39	THR	CA-C-N	5.16	126.28	119.84
1	A	39	THR	C-N-CA	5.16	126.28	119.84
1	D	241	LYS	N-CA-C	5.15	119.32	112.72
1	B	250	VAL	CA-C-N	5.10	125.00	119.85
1	B	250	VAL	C-N-CA	5.10	125.00	119.85
1	B	323	SER	N-CA-C	-5.07	105.75	111.28
1	D	35	HIS	N-CA-C	5.07	116.66	111.03
1	C	122	PRO	CA-C-N	5.06	128.66	121.42
1	C	122	PRO	C-N-CA	5.06	128.66	121.42
1	B	293	PRO	N-CA-C	5.06	118.44	110.80
1	D	250	VAL	CA-C-N	5.06	124.96	119.85
1	D	250	VAL	C-N-CA	5.06	124.96	119.85
1	D	76	ASP	N-CA-C	-5.02	106.98	113.01
1	D	274	LEU	CA-C-N	5.00	126.09	119.84
1	D	274	LEU	C-N-CA	5.00	126.09	119.84

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	2524	0	2544	139	0
1	B	2446	0	2456	131	0
1	C	2433	0	2452	138	0
1	D	2452	0	2474	131	0
2	A	8	0	0	2	0
2	B	27	0	12	2	0
2	C	27	0	12	3	0
2	D	27	0	12	2	0
3	A	23	0	10	2	0
3	B	23	0	10	2	0
3	C	23	0	10	3	0
3	D	23	0	10	2	0
4	A	2	0	0	1	0
All	All	10038	0	10002	503	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 25.

All (503) 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:B:205:VAL:HA	1:B:208:MET:HE3	1.36	1.07
1:C:205:VAL:HA	1:C:208:MET:HE3	1.42	1.01
1:D:87:ALA:HA	1:D:149:MET:HE2	1.43	1.00
1:A:87:ALA:HA	1:A:149:MET:HE2	1.42	0.99
1:C:87:ALA:HA	1:C:149:MET:HE2	1.48	0.94
1:A:205:VAL:HA	1:A:208:MET:HE3	1.47	0.94
1:B:87:ALA:HA	1:B:149:MET:HE2	1.48	0.93
1:D:205:VAL:HA	1:D:208:MET:HE3	1.52	0.92
1:D:159:PHE:HE1	1:D:281:MET:HE3	1.41	0.85
1:B:126:MET:HE2	1:B:329:LEU:HD21	1.59	0.84
1:D:126:MET:HE2	1:D:329:LEU:HD21	1.59	0.83
1:A:63:CYS:HB2	1:D:63:CYS:SG	2.20	0.81
1:A:126:MET:HE2	1:A:329:LEU:HD21	1.61	0.81
1:B:159:PHE:HE1	1:B:281:MET:HE3	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:CYS:SG	1:D:63:CYS:HB2	2.21	0.80
1:A:159:PHE:HE1	1:A:281:MET:HE3	1.45	0.80
1:C:85:LEU:HD13	1:D:85:LEU:HD13	1.63	0.79
1:C:126:MET:HE2	1:C:329:LEU:HD21	1.64	0.78
1:A:9:LYS:HE3	1:A:109:ASP:OD2	1.83	0.77
1:A:275:PRO:HB3	1:B:336:VAL:HG12	1.66	0.77
1:C:159:PHE:HE1	1:C:281:MET:HE3	1.49	0.76
1:D:159:PHE:CE1	1:D:281:MET:HE3	2.20	0.76
1:A:288:LEU:HA	1:A:291:MET:HE3	1.66	0.76
1:C:284:LEU:C	1:C:284:LEU:HD23	2.11	0.75
1:A:108:MET:HE2	1:A:321:MET:HB3	1.68	0.75
1:D:228:LEU:HD11	1:D:253:ILE:HD12	1.68	0.75
1:D:288:LEU:HA	1:D:291:MET:HE3	1.69	0.74
1:B:108:MET:HE2	1:B:321:MET:HB3	1.69	0.74
1:B:159:PHE:CE1	1:B:281:MET:HE3	2.23	0.73
1:B:288:LEU:HA	1:B:291:MET:HE3	1.69	0.73
1:C:177:LEU:HB3	1:C:178:PRO:HD3	1.70	0.72
1:A:152:ALA:HA	1:B:57:ALA:HB3	1.71	0.72
1:A:159:PHE:CE1	1:A:281:MET:HE3	2.24	0.72
1:B:284:LEU:HD23	1:B:284:LEU:C	2.14	0.72
1:B:196:LEU:HB2	1:B:197:PRO:HD3	1.72	0.72
1:D:177:LEU:HB3	1:D:178:PRO:HD3	1.71	0.71
1:D:196:LEU:HB2	1:D:197:PRO:HD3	1.72	0.71
1:A:196:LEU:HB2	1:A:197:PRO:HD3	1.71	0.71
1:C:196:LEU:HB2	1:C:197:PRO:HD3	1.71	0.71
1:A:177:LEU:HB3	1:A:178:PRO:HD3	1.72	0.71
1:D:108:MET:HE2	1:D:321:MET:HB3	1.72	0.71
1:A:279:TRP:CZ2	1:B:332:LEU:HB3	2.25	0.70
1:C:57:ALA:HB3	1:D:152:ALA:HA	1.74	0.70
1:A:281:MET:HE2	1:A:281:MET:HA	1.74	0.70
1:B:228:LEU:HD11	1:B:253:ILE:HD12	1.74	0.70
1:C:108:MET:HE2	1:C:321:MET:HB3	1.74	0.70
1:B:177:LEU:HB3	1:B:178:PRO:HD3	1.72	0.69
1:A:63:CYS:CB	1:D:63:CYS:SG	2.80	0.69
1:C:288:LEU:HA	1:C:291:MET:HE3	1.74	0.68
1:D:281:MET:HE2	1:D:281:MET:HA	1.76	0.68
1:C:228:LEU:HD11	1:C:253:ILE:HD12	1.74	0.68
1:C:195:ASN:H	1:C:195:ASN:HD22	1.42	0.68
1:C:159:PHE:CE1	1:C:281:MET:HE3	2.27	0.68
1:D:195:ASN:HD22	1:D:195:ASN:H	1.41	0.68
1:A:284:LEU:C	1:A:284:LEU:HD23	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HD23	1:D:284:LEU:C	2.18	0.67
1:B:195:ASN:HD22	1:B:195:ASN:H	1.41	0.67
1:A:199:VAL:O	1:A:203:ARG:HG3	1.94	0.67
1:A:195:ASN:HD22	1:A:195:ASN:H	1.41	0.67
1:A:10:MET:O	1:A:10:MET:HG3	1.93	0.66
1:B:24:GLY:HA2	2:B:1400:ADP:PA	2.35	0.66
1:C:281:MET:HA	1:C:281:MET:HE2	1.76	0.66
1:C:145:LEU:HD21	1:C:260:VAL:HG13	1.77	0.66
1:B:329:LEU:O	1:B:333:VAL:HG23	1.96	0.66
1:C:87:ALA:CA	1:C:149:MET:HE2	2.25	0.66
1:C:24:GLY:HA2	2:C:2400:ADP:PA	2.36	0.65
1:B:216:LEU:O	1:B:289:ARG:HD3	1.96	0.65
1:C:329:LEU:O	1:C:333:VAL:HG23	1.96	0.65
1:D:261:LEU:HD13	1:D:281:MET:HE1	1.79	0.65
1:C:44:LEU:HD21	1:C:333:VAL:HG21	1.79	0.65
1:D:145:LEU:HD21	1:D:260:VAL:HG13	1.77	0.65
1:D:213:ILE:HG23	1:D:288:LEU:O	1.97	0.65
1:B:294:PHE:CE1	1:B:316:MET:HG2	2.32	0.65
1:C:152:ALA:HA	1:D:57:ALA:HB3	1.78	0.65
1:C:261:LEU:HD13	1:C:281:MET:HE1	1.77	0.65
1:A:228:LEU:HD11	1:A:253:ILE:HD12	1.78	0.64
1:B:199:VAL:O	1:B:203:ARG:HG3	1.97	0.64
1:A:85:LEU:HD13	1:B:85:LEU:HD13	1.77	0.64
1:A:261:LEU:HD13	1:A:281:MET:HE1	1.80	0.64
1:C:133:ILE:CD1	1:C:209:LEU:HD11	2.27	0.64
1:B:44:LEU:HD21	1:B:333:VAL:HG21	1.79	0.64
1:A:57:ALA:HB3	1:B:152:ALA:HA	1.79	0.64
1:B:62:ILE:O	1:B:65:ILE:HG22	1.98	0.64
1:B:79:PRO:O	1:B:83:GLN:HG3	1.97	0.64
1:C:10:MET:HE3	1:C:323:SER:OG	1.97	0.64
1:A:208:MET:HG3	1:A:245:ILE:HG21	1.80	0.64
1:B:208:MET:HG3	1:B:245:ILE:HG21	1.78	0.64
1:C:213:ILE:HG23	1:C:288:LEU:O	1.97	0.64
1:A:63:CYS:SG	1:D:63:CYS:CB	2.85	0.63
1:B:281:MET:HE2	1:B:281:MET:HA	1.79	0.63
1:D:208:MET:HG3	1:D:245:ILE:HG21	1.80	0.63
1:D:79:PRO:O	1:D:83:GLN:HG3	1.98	0.63
1:B:133:ILE:CD1	1:B:209:LEU:HD11	2.28	0.63
1:C:216:LEU:O	1:C:289:ARG:HD3	1.99	0.63
1:A:87:ALA:CA	1:A:149:MET:HE2	2.23	0.63
1:A:213:ILE:HG23	1:A:288:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LEU:HD13	1:B:281:MET:HE1	1.80	0.63
1:A:145:LEU:HD21	1:A:260:VAL:HG13	1.80	0.62
1:A:62:ILE:O	1:A:65:ILE:HG22	1.99	0.62
1:A:24:GLY:HA2	2:A:400:ADP:PA	2.38	0.62
1:C:208:MET:HG3	1:C:245:ILE:HG21	1.81	0.62
1:A:133:ILE:CD1	1:A:209:LEU:HD11	2.30	0.62
1:D:87:ALA:CA	1:D:149:MET:HE2	2.26	0.62
1:A:296:LEU:C	1:A:296:LEU:HD23	2.25	0.62
1:D:62:ILE:O	1:D:65:ILE:HG22	2.00	0.61
1:C:199:VAL:O	1:C:203:ARG:HG3	1.99	0.61
1:C:133:ILE:HD11	1:C:170:LEU:HD11	1.82	0.61
1:D:24:GLY:HA2	2:D:3400:ADP:PA	2.40	0.61
1:A:294:PHE:CE1	1:A:316:MET:HG2	2.36	0.61
1:D:294:PHE:CE1	1:D:316:MET:HG2	2.36	0.61
1:A:10:MET:SD	1:A:124:LYS:HD2	2.40	0.61
1:C:62:ILE:O	1:C:65:ILE:HG22	2.01	0.61
1:A:225:TRP:CZ2	1:A:262:LYS:HD3	2.36	0.61
1:D:137:ILE:O	1:D:141:LEU:HB2	2.01	0.61
1:D:225:TRP:CZ2	1:D:262:LYS:HD3	2.37	0.60
1:B:95:SER:OG	1:B:96:PRO:HD3	2.02	0.60
1:B:213:ILE:HG23	1:B:288:LEU:O	2.02	0.60
1:A:96:PRO:HB2	4:A:601:HOH:O	2.00	0.60
1:D:133:ILE:HD11	1:D:170:LEU:HD11	1.83	0.59
1:D:228:LEU:HG	1:D:253:ILE:CG2	2.32	0.59
1:B:137:ILE:O	1:B:141:LEU:HB2	2.02	0.59
1:C:296:LEU:C	1:C:296:LEU:HD23	2.26	0.59
1:B:133:ILE:HD11	1:B:170:LEU:HD11	1.84	0.59
1:A:137:ILE:O	1:A:141:LEU:HB2	2.03	0.59
1:C:79:PRO:O	1:C:83:GLN:HG3	2.03	0.59
1:C:133:ILE:HD12	1:C:209:LEU:HD11	1.84	0.59
1:D:296:LEU:C	1:D:296:LEU:HD23	2.28	0.59
1:C:95:SER:OG	1:C:96:PRO:HD3	2.03	0.59
1:B:87:ALA:CA	1:B:149:MET:HE2	2.27	0.59
1:B:244:CYS:O	1:B:245:ILE:C	2.46	0.58
1:C:332:LEU:HB3	1:D:279:TRP:CZ2	2.38	0.58
1:A:159:PHE:CB	1:B:99:ILE:HD11	2.33	0.58
1:B:228:LEU:HG	1:B:253:ILE:CG2	2.33	0.58
1:C:244:CYS:O	1:C:245:ILE:C	2.46	0.58
1:C:225:TRP:CZ2	1:C:262:LYS:HD3	2.38	0.58
1:B:296:LEU:C	1:B:296:LEU:HD23	2.29	0.58
1:C:336:VAL:HG12	1:D:275:PRO:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:OG	1:A:96:PRO:HD3	2.04	0.58
1:D:95:SER:OG	1:D:96:PRO:HD3	2.03	0.58
1:A:79:PRO:O	1:A:83:GLN:HG3	2.02	0.58
1:D:133:ILE:CD1	1:D:209:LEU:HD11	2.33	0.58
1:D:56:LEU:HD23	1:D:56:LEU:C	2.28	0.58
1:A:119:ASN:HD22	1:A:120:LYS:N	2.02	0.58
1:A:133:ILE:HD12	1:A:209:LEU:HD11	1.85	0.58
1:B:145:LEU:HD21	1:B:260:VAL:HG13	1.85	0.58
1:C:137:ILE:O	1:C:141:LEU:HB2	2.04	0.57
1:D:313:LEU:N	1:D:314:PRO:HD2	2.19	0.57
1:A:243:GLU:O	1:A:243:GLU:HG2	2.04	0.57
1:B:313:LEU:N	1:B:314:PRO:HD2	2.19	0.57
1:A:133:ILE:HD11	1:A:170:LEU:HD11	1.87	0.57
1:A:216:LEU:O	1:A:289:ARG:HD3	2.04	0.57
1:B:135:SER:HB3	3:B:1500:BVP:BR	2.59	0.57
1:B:225:TRP:CZ2	1:B:262:LYS:HD3	2.39	0.57
1:B:121:GLU:OE2	1:B:122:PRO:HD2	2.04	0.57
1:A:313:LEU:N	1:A:314:PRO:HD2	2.20	0.57
1:B:129:ASP:O	1:B:130:ARG:HB2	2.05	0.56
1:C:195:ASN:O	1:C:195:ASN:ND2	2.38	0.56
1:B:133:ILE:HD12	1:B:209:LEU:HD11	1.87	0.56
1:D:199:VAL:O	1:D:203:ARG:HG3	2.04	0.56
1:C:135:SER:HB3	3:C:2500:BVP:BR	2.61	0.56
1:C:294:PHE:CE1	1:C:316:MET:HG2	2.40	0.56
1:C:313:LEU:N	1:C:314:PRO:HD2	2.20	0.56
1:A:44:LEU:HD21	1:A:333:VAL:HG21	1.87	0.56
1:A:228:LEU:HG	1:A:253:ILE:CG2	2.36	0.56
1:D:44:LEU:HD21	1:D:333:VAL:HG21	1.88	0.56
1:A:56:LEU:C	1:A:56:LEU:HD23	2.31	0.56
1:D:133:ILE:HD12	1:D:209:LEU:HD11	1.87	0.56
1:C:209:LEU:HD22	1:C:213:ILE:HD11	1.88	0.56
1:A:329:LEU:O	1:A:333:VAL:HG23	2.05	0.55
1:B:195:ASN:HD22	1:B:195:ASN:N	2.05	0.55
1:C:228:LEU:HG	1:C:253:ILE:CG2	2.36	0.55
1:D:244:CYS:O	1:D:245:ILE:C	2.49	0.55
1:A:275:PRO:CB	1:B:336:VAL:HG12	2.35	0.55
1:B:243:GLU:HG2	1:B:243:GLU:O	2.06	0.55
1:D:48:GLU:OE1	1:D:130:ARG:HD2	2.07	0.55
1:B:56:LEU:HD23	1:B:56:LEU:C	2.31	0.55
1:D:216:LEU:O	1:D:289:ARG:HD3	2.07	0.54
1:A:48:GLU:OE1	1:A:130:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HG12	1:A:125:ILE:O	2.07	0.54
1:B:208:MET:O	1:B:209:LEU:C	2.50	0.54
1:D:228:LEU:CD1	1:D:253:ILE:HD12	2.38	0.54
1:A:199:VAL:HG12	1:A:203:ARG:HD2	1.88	0.54
1:A:279:TRP:HZ2	1:B:332:LEU:HB3	1.71	0.54
1:C:56:LEU:C	1:C:56:LEU:HD23	2.32	0.54
1:B:199:VAL:HG12	1:B:203:ARG:HD2	1.89	0.54
1:A:159:PHE:HB3	1:B:99:ILE:CD1	2.37	0.53
1:A:244:CYS:O	1:A:245:ILE:C	2.50	0.53
1:D:199:VAL:HG12	1:D:203:ARG:HD2	1.90	0.53
1:C:10:MET:HE3	1:C:323:SER:CB	2.38	0.53
1:D:90:GLN:CB	1:D:149:MET:HE1	2.39	0.53
1:C:232:ASN:OD1	1:C:234:VAL:HB	2.09	0.53
1:A:119:ASN:ND2	1:A:120:LYS:N	2.57	0.52
1:D:135:SER:HB3	3:D:3500:BVP:BR	2.65	0.52
1:A:321:MET:HE2	1:A:326:TRP:N	2.25	0.52
1:A:63:CYS:SG	1:D:63:CYS:SG	3.07	0.52
1:D:329:LEU:O	1:D:333:VAL:HG23	2.10	0.52
1:A:135:SER:HB3	3:A:500:BVP:BR	2.65	0.52
1:C:48:GLU:OE1	1:C:130:ARG:HD2	2.09	0.52
1:C:133:ILE:HD11	1:C:209:LEU:HD11	1.92	0.51
1:C:228:LEU:CD1	1:C:253:ILE:HD12	2.40	0.51
1:D:243:GLU:O	1:D:243:GLU:HG2	2.10	0.51
1:C:59:GLU:HG3	1:D:152:ALA:HB2	1.92	0.51
1:C:90:GLN:NE2	1:C:140:PRO:HD3	2.26	0.51
1:A:126:MET:HE2	1:A:329:LEU:CD2	2.38	0.51
1:A:332:LEU:HB3	1:B:279:TRP:CZ2	2.46	0.51
1:D:228:LEU:HG	1:D:253:ILE:HG23	1.91	0.51
1:D:214:ILE:O	1:D:217:LYS:HB2	2.09	0.51
1:C:131:HIS:ND1	1:C:132:PRO:HD2	2.25	0.51
1:B:123:TYR:O	1:B:123:TYR:HD1	1.94	0.51
1:A:214:ILE:O	1:A:217:LYS:HB2	2.11	0.51
1:C:199:VAL:HG12	1:C:203:ARG:HD2	1.93	0.51
1:C:208:MET:O	1:C:209:LEU:C	2.52	0.51
1:C:214:ILE:O	1:C:217:LYS:HB2	2.10	0.51
1:C:243:GLU:O	1:C:243:GLU:HG2	2.10	0.51
1:B:121:GLU:CD	1:B:122:PRO:HD2	2.36	0.51
1:D:195:ASN:O	1:D:195:ASN:ND2	2.44	0.51
1:A:23:ILE:HG13	1:A:25:LYS:HG2	1.93	0.51
1:A:159:PHE:HB3	1:B:99:ILE:HD11	1.91	0.51
1:A:60:ASP:O	1:A:61:ALA:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:HD11	1:B:209:LEU:HD11	1.93	0.50
1:B:131:HIS:CG	1:B:132:PRO:HD2	2.47	0.50
1:B:321:MET:HE2	1:B:326:TRP:N	2.27	0.50
1:A:131:HIS:ND1	1:A:132:PRO:HD2	2.27	0.50
1:D:208:MET:O	1:D:209:LEU:C	2.54	0.50
1:B:232:ASN:OD1	1:B:234:VAL:HB	2.12	0.50
1:A:131:HIS:CG	1:A:132:PRO:HD2	2.47	0.50
1:D:23:ILE:HG13	1:D:25:LYS:HG2	1.93	0.50
1:A:159:PHE:HB2	1:B:99:ILE:HD11	1.93	0.50
1:B:195:ASN:ND2	1:B:195:ASN:O	2.44	0.50
1:B:90:GLN:NE2	1:B:140:PRO:HD3	2.27	0.50
1:C:60:ASP:O	1:C:61:ALA:C	2.53	0.50
1:C:321:MET:HE2	1:C:326:TRP:N	2.26	0.50
1:B:214:ILE:O	1:B:217:LYS:HB2	2.11	0.49
1:D:48:GLU:HG3	1:D:129:ASP:CG	2.37	0.49
1:D:125:ILE:O	1:D:125:ILE:HG12	2.12	0.49
1:B:131:HIS:ND1	1:B:132:PRO:HD2	2.28	0.49
1:A:180:HIS:HD2	1:A:180:HIS:O	1.95	0.49
1:C:129:ASP:O	1:C:130:ARG:HB2	2.10	0.49
1:C:230:PHE:CD2	1:C:262:LYS:HG3	2.48	0.49
1:A:75:GLY:O	1:C:269:GLU:HB2	2.13	0.49
1:A:129:ASP:O	1:A:130:ARG:HB2	2.12	0.49
1:A:228:LEU:HG	1:A:253:ILE:HG23	1.95	0.49
1:B:228:LEU:HG	1:B:253:ILE:HG23	1.95	0.49
1:A:195:ASN:HD22	1:A:195:ASN:N	2.05	0.49
1:B:278:ALA:O	1:B:279:TRP:C	2.55	0.49
1:A:89:PHE:O	1:A:90:GLN:C	2.56	0.49
1:A:146:VAL:O	1:A:146:VAL:CG1	2.61	0.49
1:B:228:LEU:CD1	1:B:253:ILE:HD12	2.43	0.49
1:C:131:HIS:CG	1:C:132:PRO:HD2	2.48	0.49
1:A:175:VAL:O	1:A:203:ARG:NH2	2.46	0.48
1:C:180:HIS:HD2	1:C:180:HIS:O	1.95	0.48
1:A:195:ASN:O	1:A:195:ASN:ND2	2.46	0.48
1:C:123:TYR:HD1	1:C:123:TYR:O	1.96	0.48
1:C:195:ASN:HD22	1:C:195:ASN:N	2.05	0.48
1:A:90:GLN:CB	1:A:149:MET:HE1	2.43	0.48
1:B:126:MET:HG3	1:B:126:MET:O	2.12	0.48
1:B:60:ASP:O	1:B:61:ALA:C	2.56	0.48
1:D:131:HIS:ND1	1:D:132:PRO:HD2	2.29	0.48
1:B:230:PHE:CD2	1:B:262:LYS:HG3	2.48	0.48
1:A:25:LYS:HG3	2:A:400:ADP:O2B	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:OE1	1:B:130:ARG:HD2	2.14	0.48
1:C:90:GLN:CB	1:C:149:MET:HE1	2.43	0.48
1:D:131:HIS:CG	1:D:132:PRO:HD2	2.48	0.48
1:B:326:TRP:O	1:B:330:LYS:HG3	2.13	0.48
1:D:126:MET:HE2	1:D:329:LEU:CD2	2.37	0.48
1:A:208:MET:O	1:A:209:LEU:C	2.56	0.48
1:B:48:GLU:HG3	1:B:129:ASP:CG	2.38	0.48
1:D:233:ASP:O	1:D:237:GLN:HG2	2.14	0.48
1:A:36:PHE:C	1:A:38:ILE:H	2.22	0.47
1:B:90:GLN:CB	1:B:149:MET:HE1	2.44	0.47
1:D:131:HIS:ND1	1:D:133:ILE:HG23	2.29	0.47
1:C:23:ILE:HG13	1:C:25:LYS:HG2	1.96	0.47
1:D:60:ASP:O	1:D:61:ALA:C	2.57	0.47
1:D:321:MET:HE2	1:D:326:TRP:N	2.29	0.47
1:B:139:PHE:O	1:B:140:PRO:C	2.57	0.47
1:B:207:ILE:HD13	1:B:207:ILE:HA	1.79	0.47
1:C:25:LYS:NZ	1:C:129:ASP:OD2	2.45	0.47
1:C:48:GLU:HG3	1:C:129:ASP:CG	2.39	0.47
1:C:133:ILE:O	1:C:137:ILE:HG23	2.15	0.47
1:C:152:ALA:HB2	1:D:59:GLU:HG3	1.96	0.47
1:A:223:ALA:C	1:A:225:TRP:H	2.23	0.47
1:A:233:ASP:O	1:A:237:GLN:HG2	2.14	0.47
1:A:131:HIS:ND1	1:A:133:ILE:HG23	2.30	0.47
1:A:232:ASN:OD1	1:A:234:VAL:HB	2.14	0.47
1:C:212:THR:HG22	1:C:216:LEU:HD22	1.97	0.47
1:A:133:ILE:HD11	1:A:209:LEU:HD11	1.97	0.47
1:A:328:ILE:O	1:A:329:LEU:C	2.57	0.47
1:C:228:LEU:HG	1:C:253:ILE:HG23	1.96	0.47
1:C:25:LYS:HG3	2:C:2400:ADP:O2B	2.14	0.47
1:D:195:ASN:HD22	1:D:195:ASN:N	2.04	0.47
1:A:230:PHE:CD2	1:A:262:LYS:HG3	2.49	0.47
1:B:23:ILE:HG13	1:B:25:LYS:HG2	1.97	0.47
1:D:180:HIS:HD2	1:D:180:HIS:O	1.97	0.47
1:A:10:MET:HE3	1:A:323:SER:HA	1.97	0.47
1:A:123:TYR:HD1	1:A:123:TYR:O	1.98	0.47
1:B:48:GLU:HG3	1:B:129:ASP:OD1	2.15	0.47
1:A:48:GLU:HG3	1:A:129:ASP:CG	2.40	0.46
1:B:328:ILE:O	1:B:329:LEU:C	2.58	0.46
1:C:284:LEU:HD23	1:C:284:LEU:O	2.16	0.46
1:B:125:ILE:O	1:B:125:ILE:HG12	2.12	0.46
1:C:12:VAL:HG11	1:C:321:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PHE:O	1:C:140:PRO:C	2.58	0.46
1:D:55:ASN:CG	1:D:55:ASN:O	2.58	0.46
1:D:126:MET:HG3	1:D:126:MET:O	2.16	0.46
1:C:278:ALA:O	1:C:279:TRP:C	2.58	0.46
1:D:129:ASP:O	1:D:130:ARG:HB2	2.16	0.46
1:B:133:ILE:O	1:B:137:ILE:HG23	2.15	0.46
1:B:180:HIS:HD2	1:B:180:HIS:O	1.98	0.46
1:C:85:LEU:HD13	1:D:85:LEU:CD1	2.41	0.46
1:C:284:LEU:C	1:C:284:LEU:CD2	2.83	0.46
1:A:90:GLN:NE2	1:A:140:PRO:HD3	2.30	0.46
1:A:326:TRP:O	1:A:330:LYS:HG3	2.15	0.46
1:C:279:TRP:CZ2	1:D:332:LEU:HB3	2.51	0.46
1:C:328:ILE:O	1:C:329:LEU:C	2.59	0.46
1:D:124:LYS:HD3	1:D:326:TRP:CE2	2.51	0.46
1:D:25:LYS:HG3	2:D:3400:ADP:O2B	2.16	0.46
1:C:260:VAL:O	1:C:260:VAL:HG12	2.16	0.45
1:D:296:LEU:HD23	1:D:297:SER:N	2.31	0.45
1:D:177:LEU:O	1:D:181:LEU:HG	2.16	0.45
1:A:196:LEU:O	1:A:197:PRO:C	2.59	0.45
1:B:85:LEU:HD12	1:B:85:LEU:HA	1.71	0.45
1:C:9:LYS:O	1:C:9:LYS:HG2	2.16	0.45
1:D:328:ILE:O	1:D:329:LEU:C	2.58	0.45
1:B:25:LYS:NZ	1:B:129:ASP:OD2	2.48	0.45
1:A:177:LEU:O	1:A:181:LEU:HG	2.17	0.45
1:B:86:THR:O	1:B:87:ALA:C	2.60	0.45
1:A:131:HIS:CE1	1:A:133:ILE:HG23	2.52	0.45
1:B:25:LYS:HG3	2:B:1400:ADP:O2B	2.17	0.45
1:B:175:VAL:O	1:B:203:ARG:NH2	2.50	0.45
1:C:86:THR:O	1:C:87:ALA:C	2.60	0.45
1:B:131:HIS:ND1	1:B:133:ILE:HG23	2.32	0.45
1:C:87:ALA:HA	1:C:149:MET:CE	2.34	0.45
1:D:8:VAL:O	1:D:9:LYS:HD3	2.17	0.45
1:B:212:THR:HG22	1:B:216:LEU:HD22	1.98	0.44
1:B:284:LEU:HD23	1:B:284:LEU:O	2.17	0.44
1:C:99:ILE:HD11	1:D:159:PHE:CB	2.47	0.44
1:C:131:HIS:CE1	1:C:132:PRO:HD2	2.51	0.44
1:A:55:ASN:CG	1:A:55:ASN:O	2.60	0.44
1:B:23:ILE:O	1:B:183:ARG:NH1	2.50	0.44
1:C:89:PHE:O	1:C:90:GLN:C	2.60	0.44
1:A:296:LEU:C	1:A:296:LEU:CD2	2.90	0.44
1:D:278:ALA:O	1:D:279:TRP:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:C	1:B:225:TRP:H	2.25	0.44
1:B:228:LEU:HG	1:B:253:ILE:HG21	1.99	0.44
1:C:48:GLU:HG3	1:C:129:ASP:OD1	2.17	0.44
1:C:326:TRP:O	1:C:330:LYS:HG3	2.17	0.44
1:A:133:ILE:O	1:A:137:ILE:HG23	2.18	0.44
1:C:32:PHE:HD1	1:C:306:ALA:HB1	1.83	0.44
1:D:10:MET:HE3	1:D:323:SER:OG	2.17	0.44
1:D:123:TYR:HD1	1:D:123:TYR:O	2.00	0.44
1:D:131:HIS:CE1	1:D:133:ILE:HG23	2.53	0.44
1:B:209:LEU:HD22	1:B:213:ILE:HD11	2.00	0.44
1:D:90:GLN:NE2	1:D:140:PRO:HD3	2.33	0.44
1:A:97:HIS:CD2	3:A:500:BVP:BR	3.26	0.43
1:A:196:LEU:HB2	1:A:197:PRO:CD	2.44	0.43
1:B:172:VAL:CG2	1:B:210:ILE:HD11	2.47	0.43
1:B:284:LEU:C	1:B:284:LEU:CD2	2.86	0.43
1:C:165:PRO:HA	1:C:166:PRO:HD3	1.92	0.43
1:C:312:LEU:C	1:C:314:PRO:HD2	2.42	0.43
1:D:19:GLY:O	1:D:130:ARG:NH2	2.51	0.43
1:A:119:ASN:HD22	1:A:120:LYS:H	1.64	0.43
1:C:209:LEU:O	1:C:213:ILE:HG13	2.17	0.43
1:C:214:ILE:HB	1:C:251:PRO:HG3	2.00	0.43
1:D:48:GLU:HG3	1:D:129:ASP:OD1	2.18	0.43
1:D:223:ALA:C	1:D:225:TRP:H	2.26	0.43
1:D:261:LEU:HA	1:D:261:LEU:HD23	1.83	0.43
1:C:23:ILE:O	1:C:183:ARG:NH1	2.50	0.43
1:C:154:LEU:N	1:C:155:PRO:CD	2.82	0.43
1:C:175:VAL:O	1:C:203:ARG:NH2	2.51	0.43
1:C:233:ASP:O	1:C:237:GLN:HG2	2.18	0.43
1:A:296:LEU:HD23	1:A:297:SER:N	2.32	0.43
1:D:196:LEU:O	1:D:197:PRO:C	2.61	0.43
1:D:214:ILE:HB	1:D:251:PRO:HG3	1.99	0.43
1:A:99:ILE:HD11	1:B:159:PHE:CB	2.48	0.43
1:C:97:HIS:CD2	3:C:2500:BVP:BR	3.27	0.43
1:C:172:VAL:CG2	1:C:210:ILE:HD11	2.49	0.43
1:C:223:ALA:C	1:C:225:TRP:H	2.27	0.43
1:D:154:LEU:N	1:D:155:PRO:CD	2.82	0.43
1:D:232:ASN:OD1	1:D:234:VAL:HB	2.19	0.43
1:A:228:LEU:CD1	1:A:253:ILE:HD12	2.45	0.43
1:C:296:LEU:C	1:C:296:LEU:CD2	2.90	0.43
1:C:296:LEU:HD23	1:C:297:SER:N	2.34	0.43
1:D:86:THR:O	1:D:87:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:LEU:HG	1:D:253:ILE:HG21	2.01	0.43
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.77	0.43
1:A:212:THR:HG22	1:A:216:LEU:HD22	2.01	0.43
1:A:242:SER:O	1:A:243:GLU:HB3	2.18	0.43
1:B:146:VAL:O	1:B:146:VAL:CG1	2.66	0.43
1:B:177:LEU:O	1:B:181:LEU:HG	2.19	0.43
1:D:133:ILE:O	1:D:137:ILE:HG23	2.19	0.43
1:A:23:ILE:O	1:A:183:ARG:NH1	2.52	0.43
1:D:175:VAL:HG12	1:D:176:SER:N	2.33	0.43
1:A:87:ALA:HA	1:A:149:MET:CE	2.31	0.43
1:B:242:SER:O	1:B:243:GLU:HB3	2.19	0.43
1:D:108:MET:HA	1:D:108:MET:HE3	2.01	0.43
1:D:326:TRP:O	1:D:330:LYS:HG3	2.19	0.43
1:B:269:GLU:HB2	1:D:75:GLY:O	2.19	0.43
1:B:296:LEU:C	1:B:296:LEU:CD2	2.92	0.43
1:C:175:VAL:HG12	1:C:176:SER:N	2.33	0.43
1:D:196:LEU:HB2	1:D:197:PRO:CD	2.45	0.43
1:A:278:ALA:O	1:A:279:TRP:C	2.62	0.42
1:C:13:LEU:HD12	1:C:13:LEU:HA	1.91	0.42
1:C:126:MET:HE2	1:C:329:LEU:CD2	2.42	0.42
1:A:9:LYS:HE2	1:A:320:ASN:HB3	2.01	0.42
1:B:175:VAL:HG12	1:B:176:SER:N	2.32	0.42
1:C:145:LEU:HD21	1:C:260:VAL:CG1	2.47	0.42
1:B:89:PHE:O	1:B:90:GLN:C	2.62	0.42
1:A:131:HIS:CE1	1:A:132:PRO:HD2	2.54	0.42
1:C:30:GLU:C	1:C:32:PHE:N	2.77	0.42
1:C:125:ILE:O	1:C:125:ILE:HG12	2.15	0.42
1:D:139:PHE:O	1:D:140:PRO:C	2.63	0.42
1:A:336:VAL:C	1:A:338:ASP:H	2.26	0.42
1:B:146:VAL:HG21	1:B:198:PHE:HA	2.02	0.42
1:A:180:HIS:O	1:A:180:HIS:CD2	2.73	0.42
1:B:126:MET:HE2	1:B:329:LEU:CD2	2.41	0.42
1:B:196:LEU:O	1:B:197:PRO:C	2.62	0.42
1:C:131:HIS:ND1	1:C:133:ILE:HG23	2.35	0.42
1:D:97:HIS:CD2	3:D:3500:BVP:BR	3.28	0.42
1:D:133:ILE:HD11	1:D:209:LEU:HD11	2.01	0.42
1:A:59:GLU:HG3	1:B:152:ALA:HB2	2.02	0.42
1:A:108:MET:HE3	1:A:108:MET:HA	2.02	0.42
1:A:284:LEU:C	1:A:284:LEU:CD2	2.91	0.42
1:C:299:GLU:O	1:C:300:GLN:HB3	2.20	0.42
1:D:25:LYS:NZ	1:D:129:ASP:OD2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ASN:O	1:D:196:LEU:C	2.62	0.42
1:A:35:HIS:C	1:A:35:HIS:CD2	2.97	0.42
1:A:48:GLU:HG3	1:A:129:ASP:OD1	2.20	0.42
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.83	0.42
1:D:23:ILE:O	1:D:183:ARG:NH1	2.53	0.42
1:D:299:GLU:O	1:D:300:GLN:HB3	2.19	0.42
1:C:242:SER:O	1:C:243:GLU:HB3	2.20	0.42
1:D:10:MET:HE3	1:D:323:SER:CB	2.49	0.42
1:A:85:LEU:HD13	1:B:85:LEU:CD1	2.49	0.41
1:A:120:LYS:NZ	1:A:120:LYS:CB	2.83	0.41
1:A:126:MET:O	1:A:126:MET:HG3	2.20	0.41
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.86	0.41
1:B:154:LEU:N	1:B:155:PRO:CD	2.82	0.41
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.90	0.41
1:B:296:LEU:HD23	1:B:297:SER:N	2.35	0.41
1:C:24:GLY:HA2	2:C:2400:ADP:O1A	2.20	0.41
1:C:55:ASN:O	1:C:55:ASN:CG	2.63	0.41
1:D:296:LEU:C	1:D:296:LEU:CD2	2.92	0.41
1:A:99:ILE:HD11	1:B:159:PHE:HB3	2.02	0.41
1:D:172:VAL:CG2	1:D:210:ILE:HD11	2.50	0.41
1:A:65:ILE:HG23	1:A:66:TYR:N	2.34	0.41
1:A:119:ASN:ND2	1:A:119:ASN:C	2.75	0.41
1:C:172:VAL:HG21	1:C:210:ILE:HD11	2.02	0.41
1:D:23:ILE:CG1	1:D:25:LYS:HG2	2.50	0.41
1:B:131:HIS:CE1	1:B:132:PRO:HD2	2.55	0.41
1:B:233:ASP:O	1:B:237:GLN:HG2	2.21	0.41
1:B:260:VAL:O	1:B:260:VAL:HG12	2.19	0.41
1:C:177:LEU:O	1:C:181:LEU:HG	2.21	0.41
1:C:196:LEU:O	1:C:197:PRO:C	2.63	0.41
1:D:312:LEU:C	1:D:314:PRO:HD2	2.45	0.41
1:A:95:SER:O	1:A:96:PRO:C	2.63	0.41
1:A:154:LEU:N	1:A:155:PRO:CD	2.83	0.41
1:A:299:GLU:O	1:A:300:GLN:HB3	2.21	0.41
1:B:32:PHE:HD1	1:B:306:ALA:HB1	1.86	0.41
1:B:172:VAL:HG21	1:B:210:ILE:HD11	2.03	0.41
1:C:12:VAL:HG13	1:C:321:MET:HG2	2.02	0.41
1:D:175:VAL:O	1:D:203:ARG:NH2	2.50	0.41
1:C:146:VAL:HG21	1:C:198:PHE:HA	2.03	0.41
1:B:123:TYR:CD1	1:B:123:TYR:N	2.89	0.41
1:C:16:TYR:CD2	1:C:168:THR:HG23	2.55	0.41
1:C:130:ARG:NH1	3:C:2500:BVP:O1P	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLN:CD	1:B:304:HIS:HB3	2.45	0.41
1:C:99:ILE:CD1	1:D:159:PHE:HB3	2.51	0.41
1:C:270:PHE:N	1:C:270:PHE:CD2	2.89	0.41
1:D:41:ASN:HD22	1:D:41:ASN:HA	1.70	0.41
1:D:89:PHE:O	1:D:90:GLN:C	2.60	0.41
1:A:121:GLU:HB3	1:A:122:PRO:HD2	2.02	0.41
1:B:30:GLU:C	1:B:32:PHE:N	2.77	0.41
1:C:60:ASP:O	1:C:60:ASP:OD1	2.38	0.41
1:C:90:GLN:HB3	1:C:149:MET:HE1	2.02	0.41
1:C:99:ILE:HD11	1:D:159:PHE:HB3	2.02	0.41
1:C:196:LEU:HB2	1:C:197:PRO:CD	2.45	0.41
1:D:207:ILE:HD13	1:D:207:ILE:HA	1.82	0.41
1:C:30:GLU:C	1:C:32:PHE:H	2.28	0.41
1:C:85:LEU:HD12	1:C:85:LEU:HA	1.73	0.41
1:D:209:LEU:HD22	1:D:213:ILE:HD11	2.03	0.40
1:D:263:LEU:HA	1:D:264:PRO:HD3	1.88	0.40
1:B:10:MET:HE3	1:B:323:SER:OG	2.21	0.40
1:B:97:HIS:CD2	3:B:1500:BVP:BR	3.29	0.40
1:B:108:MET:HE2	1:B:321:MET:CB	2.46	0.40
1:B:312:LEU:C	1:B:314:PRO:HD2	2.45	0.40
1:C:131:HIS:CE1	1:C:133:ILE:HG23	2.57	0.40
1:C:292:SER:HA	1:C:293:PRO:HD2	1.96	0.40
1:A:108:MET:HE2	1:A:321:MET:CB	2.46	0.40
1:C:180:HIS:O	1:C:180:HIS:CD2	2.73	0.40
1:D:172:VAL:HB	1:D:210:ILE:HD11	2.03	0.40
1:A:152:ALA:HB2	1:B:59:GLU:HG3	2.03	0.40
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.84	0.40
1:B:263:LEU:HA	1:B:264:PRO:HD3	1.95	0.40
1:C:126:MET:O	1:C:126:MET:HG3	2.20	0.40
1:D:65:ILE:HG23	1:D:66:TYR:N	2.36	0.40
1:D:90:GLN:HB3	1:D:149:MET:HE1	2.03	0.40
1:D:180:HIS:O	1:D:180:HIS:CD2	2.73	0.40
1:A:304:HIS:O	1:A:305:ALA:C	2.65	0.40
1:B:165:PRO:HA	1:B:166:PRO:HD3	1.90	0.40
1:C:228:LEU:HG	1:C:253:ILE:HG21	2.03	0.40
1:D:31:GLU:O	1:D:35:HIS:HB2	2.22	0.40
1:D:52:TYR:O	1:D:56:LEU:HB2	2.21	0.40
1:D:60:ASP:O	1:D:60:ASP:OD1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/341 (94%)	278 (87%)	35 (11%)	8 (2%)	4	27
1	B	309/341 (91%)	264 (85%)	40 (13%)	5 (2%)	7	36
1	C	307/341 (90%)	267 (87%)	35 (11%)	5 (2%)	7	36
1	D	309/341 (91%)	267 (86%)	35 (11%)	7 (2%)	5	29
All	All	1246/1364 (91%)	1076 (86%)	145 (12%)	25 (2%)	6	31

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ALA
1	A	245	ILE
1	B	223	ALA
1	B	245	ILE
1	C	223	ALA
1	C	245	ILE
1	D	223	ALA
1	D	245	ILE
1	A	244	CYS
1	B	244	CYS
1	C	244	CYS
1	D	244	CYS
1	A	9	LYS
1	D	10	MET
1	A	36	PHE
1	A	300	GLN
1	B	275	PRO
1	C	300	GLN
1	D	275	PRO
1	D	300	GLN
1	A	275	PRO
1	C	275	PRO

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Mol	Chain	Res	Type
1	A	197	PRO
1	D	197	PRO
1	B	197	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	280/298 (94%)	254 (91%)	26 (9%)	8	33
1	B	270/298 (91%)	244 (90%)	26 (10%)	8	32
1	C	268/298 (90%)	244 (91%)	24 (9%)	9	34
1	D	272/298 (91%)	246 (90%)	26 (10%)	8	32
All	All	1090/1192 (91%)	988 (91%)	102 (9%)	8	33

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	27	THR
1	A	39	THR
1	A	41	ASN
1	A	73	LEU
1	A	85	LEU
1	A	97	HIS
1	A	108	MET
1	A	113	SER
1	A	120	LYS
1	A	123	TYR
1	A	125	ILE
1	A	126	MET
1	A	132	PRO
1	A	137	ILE
1	A	141	LEU
1	A	146	VAL
1	A	195	ASN

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Mol	Chain	Res	Type
1	A	209	LEU
1	A	216	LEU
1	A	219	ASN
1	A	253	ILE
1	A	275	PRO
1	A	277	TRP
1	A	281	MET
1	A	288	LEU
1	B	18	ASP
1	B	27	THR
1	B	39	THR
1	B	41	ASN
1	B	73	LEU
1	B	85	LEU
1	B	97	HIS
1	B	108	MET
1	B	121	GLU
1	B	123	TYR
1	B	125	ILE
1	B	126	MET
1	B	132	PRO
1	B	137	ILE
1	B	141	LEU
1	B	146	VAL
1	B	195	ASN
1	B	209	LEU
1	B	216	LEU
1	B	219	ASN
1	B	253	ILE
1	B	275	PRO
1	B	277	TRP
1	B	281	MET
1	B	288	LEU
1	B	311	THR
1	C	18	ASP
1	C	27	THR
1	C	39	THR
1	C	41	ASN
1	C	73	LEU
1	C	85	LEU
1	C	97	HIS
1	C	108	MET

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Mol	Chain	Res	Type
1	C	123	TYR
1	C	125	ILE
1	C	126	MET
1	C	137	ILE
1	C	141	LEU
1	C	146	VAL
1	C	195	ASN
1	C	209	LEU
1	C	216	LEU
1	C	219	ASN
1	C	253	ILE
1	C	275	PRO
1	C	277	TRP
1	C	281	MET
1	C	288	LEU
1	C	311	THR
1	D	18	ASP
1	D	27	THR
1	D	35	HIS
1	D	39	THR
1	D	41	ASN
1	D	73	LEU
1	D	85	LEU
1	D	97	HIS
1	D	108	MET
1	D	123	TYR
1	D	125	ILE
1	D	126	MET
1	D	132	PRO
1	D	137	ILE
1	D	141	LEU
1	D	146	VAL
1	D	195	ASN
1	D	209	LEU
1	D	216	LEU
1	D	219	ASN
1	D	253	ILE
1	D	262	LYS
1	D	275	PRO
1	D	281	MET
1	D	288	LEU
1	D	311	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	74	ASN
1	A	97	HIS
1	A	119	ASN
1	A	180	HIS
1	A	195	ASN
1	A	204	ASN
1	A	220	ASN
1	A	300	GLN
1	A	337	GLN
1	B	41	ASN
1	B	74	ASN
1	B	97	HIS
1	B	195	ASN
1	B	204	ASN
1	B	220	ASN
1	B	240	GLN
1	B	300	GLN
1	C	41	ASN
1	C	74	ASN
1	C	97	HIS
1	C	180	HIS
1	C	195	ASN
1	C	204	ASN
1	C	220	ASN
1	C	300	GLN
1	D	35	HIS
1	D	41	ASN
1	D	55	ASN
1	D	74	ASN
1	D	97	HIS
1	D	180	HIS
1	D	195	ASN
1	D	204	ASN
1	D	220	ASN
1	D	300	GLN

5.3.3 RNA ⓘ

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](#)

8 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	B	1400	-	28,29,29	2.07	4 (14%)	43,45,45	1.07	4 (9%)
3	BVP	B	1500	-	24,24,24	3.08	4 (16%)	32,35,35	1.44	4 (12%)
2	ADP	D	3400	-	28,29,29	2.11	6 (21%)	43,45,45	1.07	4 (9%)
2	ADP	A	400	-	3,7,29	1.57	0	6,10,45	0.91	1 (16%)
3	BVP	D	3500	-	24,24,24	3.10	3 (12%)	32,35,35	1.46	4 (12%)
3	BVP	A	500	-	24,24,24	3.07	4 (16%)	32,35,35	1.44	4 (12%)
3	BVP	C	2500	-	24,24,24	3.11	4 (16%)	32,35,35	1.45	4 (12%)
2	ADP	C	2400	-	28,29,29	2.04	4 (14%)	43,45,45	1.08	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	1400	-	-	3/16/32/32	0/3/3/3
3	BVP	B	1500	-	-	6/13/25/25	0/2/2/2
2	ADP	D	3400	-	-	3/16/32/32	0/3/3/3
2	ADP	A	400	-	-	0/2/5/32	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BVP	D	3500	-	-	5/13/25/25	0/2/2/2
3	BVP	A	500	-	-	6/13/25/25	0/2/2/2
3	BVP	C	2500	-	-	6/13/25/25	0/2/2/2
2	ADP	C	2400	-	-	3/16/32/32	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3500	BVP	C5A-C5	-14.13	1.14	1.46
3	C	2500	BVP	C5A-C5	-14.08	1.14	1.46
3	B	1500	BVP	C5A-C5	-13.90	1.14	1.46
3	A	500	BVP	C5A-C5	-13.89	1.14	1.46
2	B	1400	ADP	PA-O3A	-8.20	1.50	1.59
2	D	3400	ADP	PA-O3A	-8.05	1.50	1.59
2	C	2400	ADP	PA-O3A	-7.79	1.51	1.59
2	D	3400	ADP	C4-N3	3.41	1.40	1.34
2	C	2400	ADP	C4-N3	3.13	1.40	1.34
2	C	2400	ADP	C5-C4	3.00	1.44	1.39
2	D	3400	ADP	C5-C4	2.99	1.44	1.39
2	B	1400	ADP	C5-C4	2.94	1.44	1.39
2	B	1400	ADP	C4-N3	2.87	1.39	1.34
3	B	1500	BVP	C6-C5	2.79	1.45	1.37
3	A	500	BVP	C6-C5	2.76	1.45	1.37
3	D	3500	BVP	C6-C5	2.73	1.45	1.37
2	D	3400	ADP	O4'-C1'	2.73	1.48	1.42
3	C	2500	BVP	C6-C5	2.68	1.45	1.37
2	C	2400	ADP	O4'-C1'	2.61	1.48	1.42
2	B	1400	ADP	O4'-C1'	2.56	1.47	1.42
2	D	3400	ADP	C4-N9	2.32	1.42	1.37
3	A	500	BVP	C1'-N1	2.29	1.53	1.48
3	C	2500	BVP	P-O3P	-2.25	1.46	1.54
3	B	1500	BVP	P-O3P	-2.20	1.46	1.54
3	C	2500	BVP	C1'-N1	2.18	1.53	1.48
3	B	1500	BVP	C1'-N1	2.16	1.53	1.48
3	A	500	BVP	P-O3P	-2.06	1.47	1.54
3	D	3500	BVP	C1'-N1	2.06	1.53	1.48
2	D	3400	ADP	PB-O3B	-2.00	1.47	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2500	BVP	C5A-C5-C4	-5.55	111.24	120.85
3	B	1500	BVP	C5A-C5-C4	-5.46	111.40	120.85
3	D	3500	BVP	C5A-C5-C4	-5.42	111.47	120.85
3	A	500	BVP	C5A-C5-C4	-5.37	111.55	120.85
3	A	500	BVP	N3-C2-N1	3.48	119.42	114.89
3	D	3500	BVP	N3-C2-N1	3.47	119.41	114.89
3	C	2500	BVP	N3-C2-N1	3.37	119.28	114.89
3	B	1500	BVP	N3-C2-N1	3.35	119.25	114.89
2	B	1400	ADP	C3'-C2'-C1'	2.84	106.84	101.46
2	C	2400	ADP	C3'-C2'-C1'	2.84	106.84	101.46
2	D	3400	ADP	C3'-C2'-C1'	2.83	106.81	101.46
2	C	2400	ADP	C5-N7-C8	2.59	107.52	103.45
2	D	3400	ADP	C5-N7-C8	2.58	107.50	103.45
2	B	1400	ADP	C5-N7-C8	2.55	107.45	103.45
3	B	1500	BVP	C5-C4-N3	2.53	118.08	114.43
3	C	2500	BVP	C5-C4-N3	2.50	118.04	114.43
3	A	500	BVP	C5-C4-N3	2.43	117.94	114.43
3	C	2500	BVP	C4-N3-C2	-2.39	124.21	127.34
3	D	3500	BVP	C5-C4-N3	2.35	117.83	114.43
3	B	1500	BVP	C4-N3-C2	-2.28	124.35	127.34
2	C	2400	ADP	C4-C5-N7	-2.22	108.04	110.58
3	A	500	BVP	C4-N3-C2	-2.20	124.45	127.34
3	D	3500	BVP	C4-N3-C2	-2.19	124.46	127.34
2	B	1400	ADP	C5-C4-N3	-2.19	123.71	126.72
2	B	1400	ADP	C4-C5-N7	-2.15	108.13	110.58
2	D	3400	ADP	C5-C4-N3	-2.08	123.85	126.72
2	D	3400	ADP	C4-C5-N7	-2.07	108.21	110.58
2	A	400	ADP	O2B-PB-O3A	2.06	111.52	104.64
2	C	2400	ADP	C5-C4-N3	-2.04	123.90	126.72

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1400	ADP	C5'-O5'-PA-O2A
2	B	1400	ADP	C5'-O5'-PA-O3A
2	C	2400	ADP	C5'-O5'-PA-O2A
2	C	2400	ADP	C5'-O5'-PA-O3A
2	D	3400	ADP	C5'-O5'-PA-O2A
2	D	3400	ADP	C5'-O5'-PA-O3A
3	A	500	BVP	C5'-O5'-P-O1P
3	A	500	BVP	C5'-O5'-P-O2P
3	A	500	BVP	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
3	A	500	BVP	C6-C5-C5A-C5B
3	A	500	BVP	C4-C5-C5A-C5B
3	B	1500	BVP	C5'-O5'-P-O1P
3	B	1500	BVP	C5'-O5'-P-O2P
3	B	1500	BVP	C5'-O5'-P-O3P
3	B	1500	BVP	C6-C5-C5A-C5B
3	B	1500	BVP	C4-C5-C5A-C5B
3	B	1500	BVP	C5-C5A-C5B-BR
3	C	2500	BVP	C5'-O5'-P-O1P
3	C	2500	BVP	C5'-O5'-P-O2P
3	C	2500	BVP	C5'-O5'-P-O3P
3	C	2500	BVP	C6-C5-C5A-C5B
3	C	2500	BVP	C4-C5-C5A-C5B
3	C	2500	BVP	C5-C5A-C5B-BR
3	D	3500	BVP	C5'-O5'-P-O1P
3	D	3500	BVP	C5'-O5'-P-O2P
3	D	3500	BVP	C5'-O5'-P-O3P
3	D	3500	BVP	C6-C5-C5A-C5B
3	D	3500	BVP	C4-C5-C5A-C5B
2	B	1400	ADP	C5'-O5'-PA-O1A
2	C	2400	ADP	C5'-O5'-PA-O1A
2	D	3400	ADP	C5'-O5'-PA-O1A
3	A	500	BVP	C5-C5A-C5B-BR

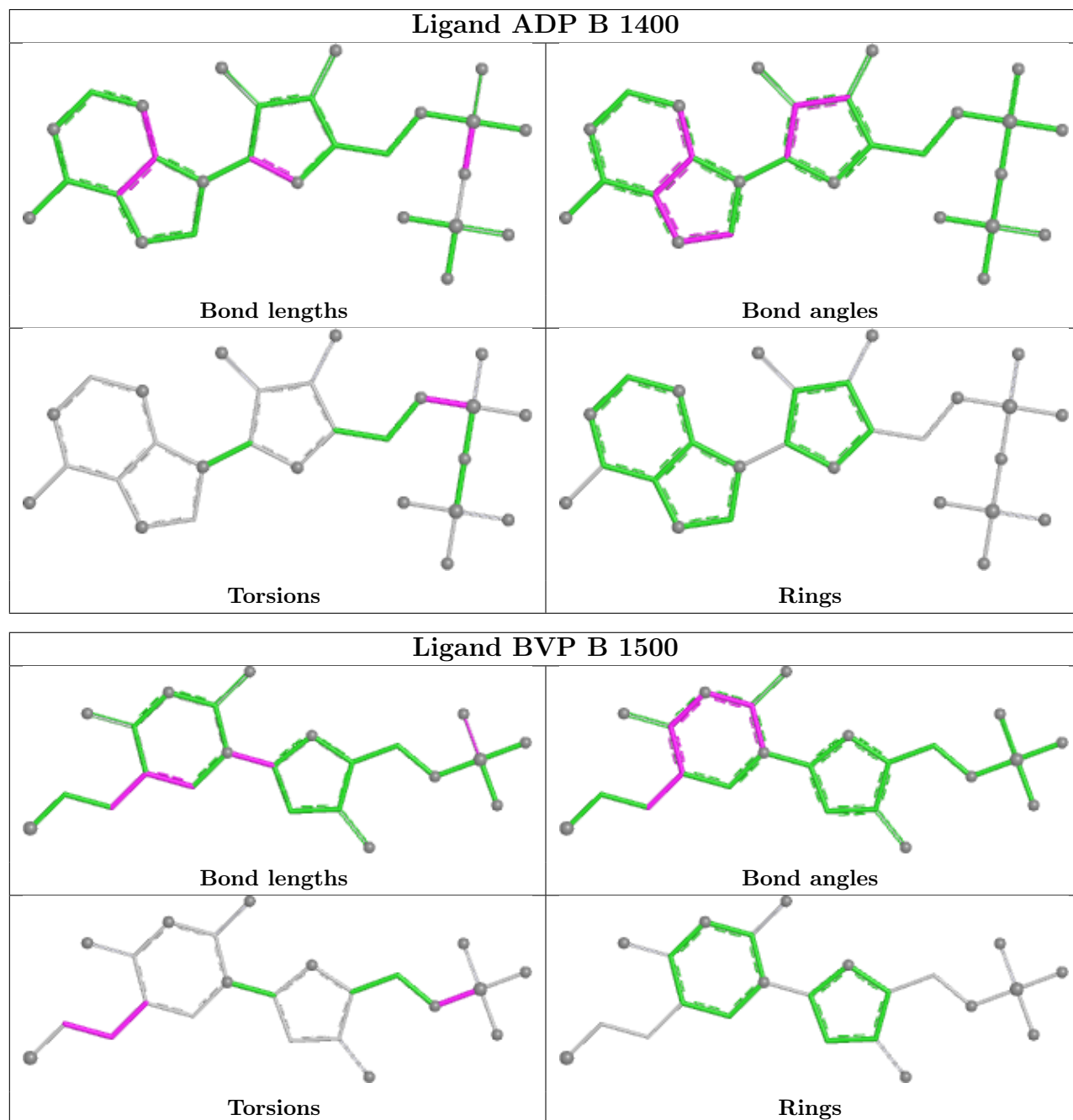
There are no ring outliers.

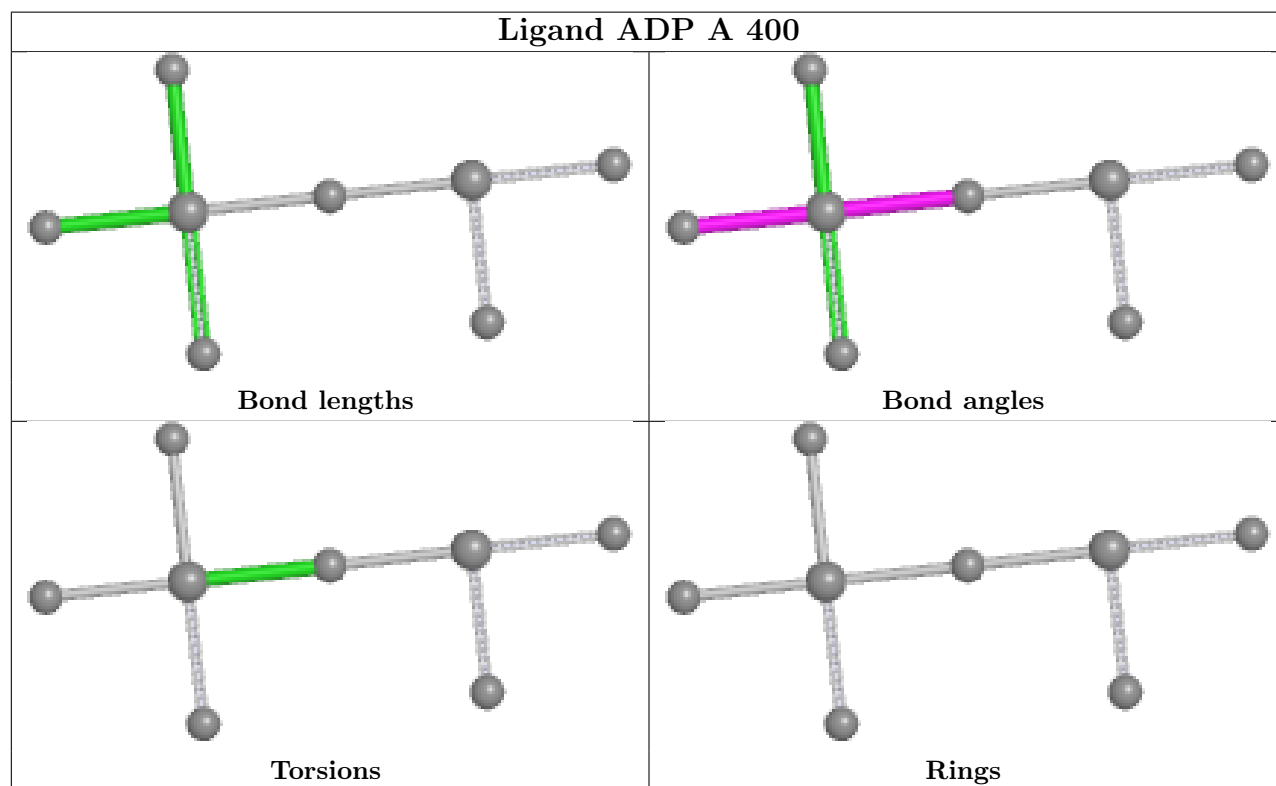
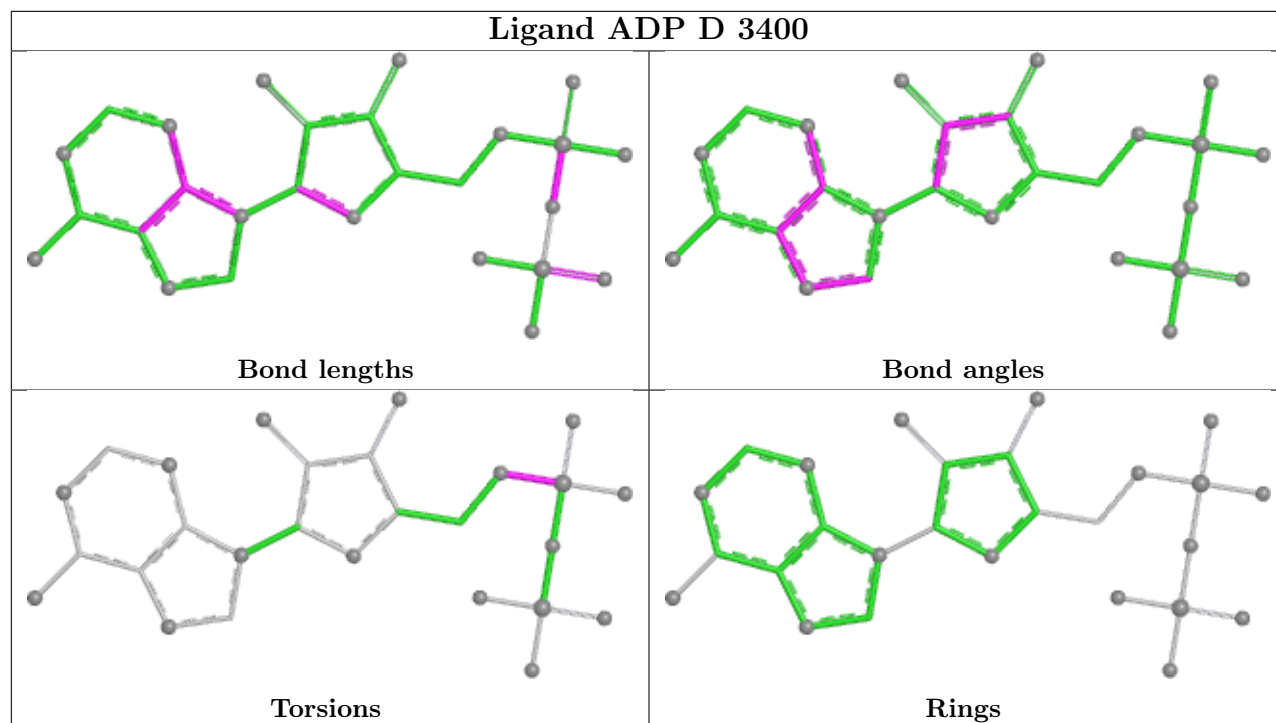
8 monomers are involved in 18 short contacts:

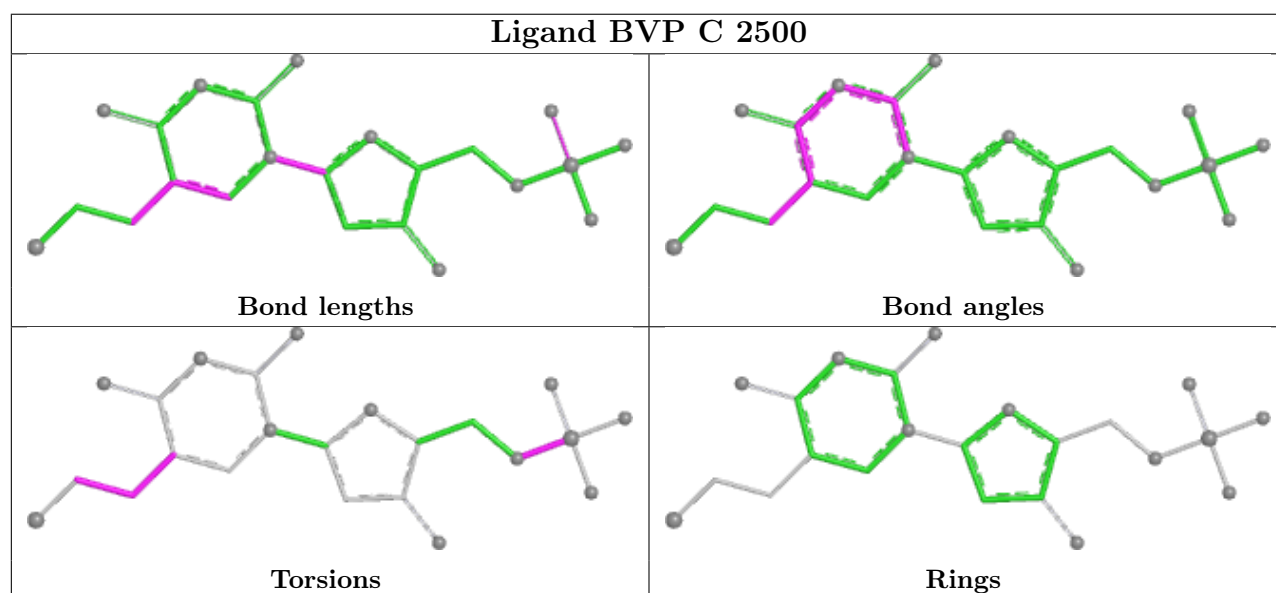
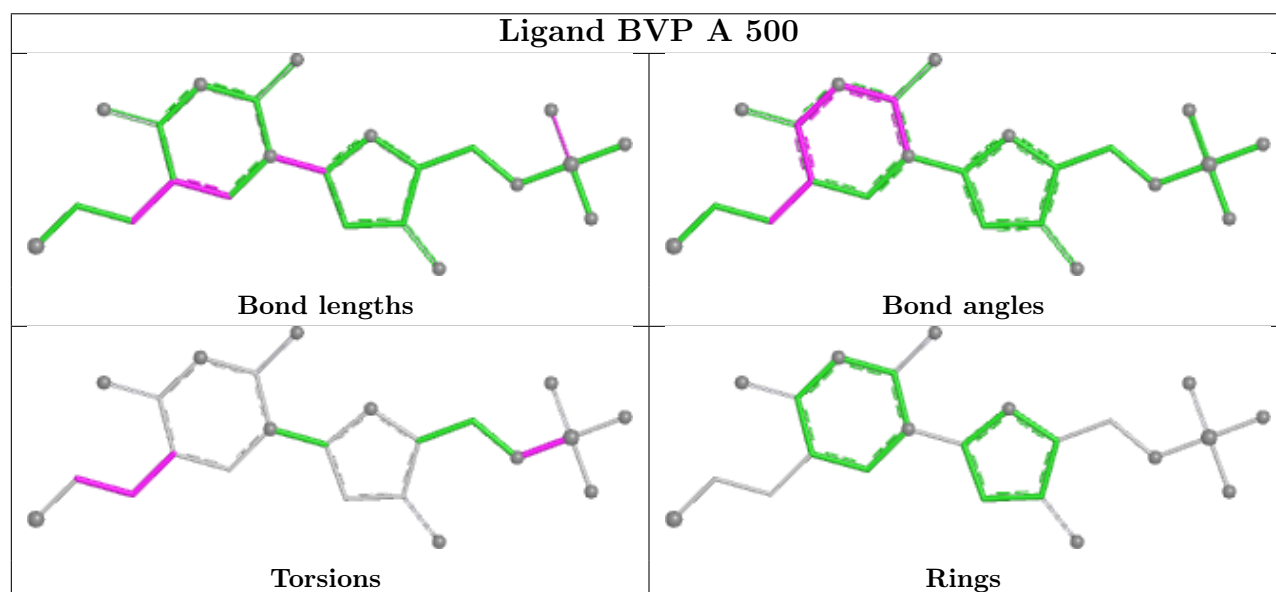
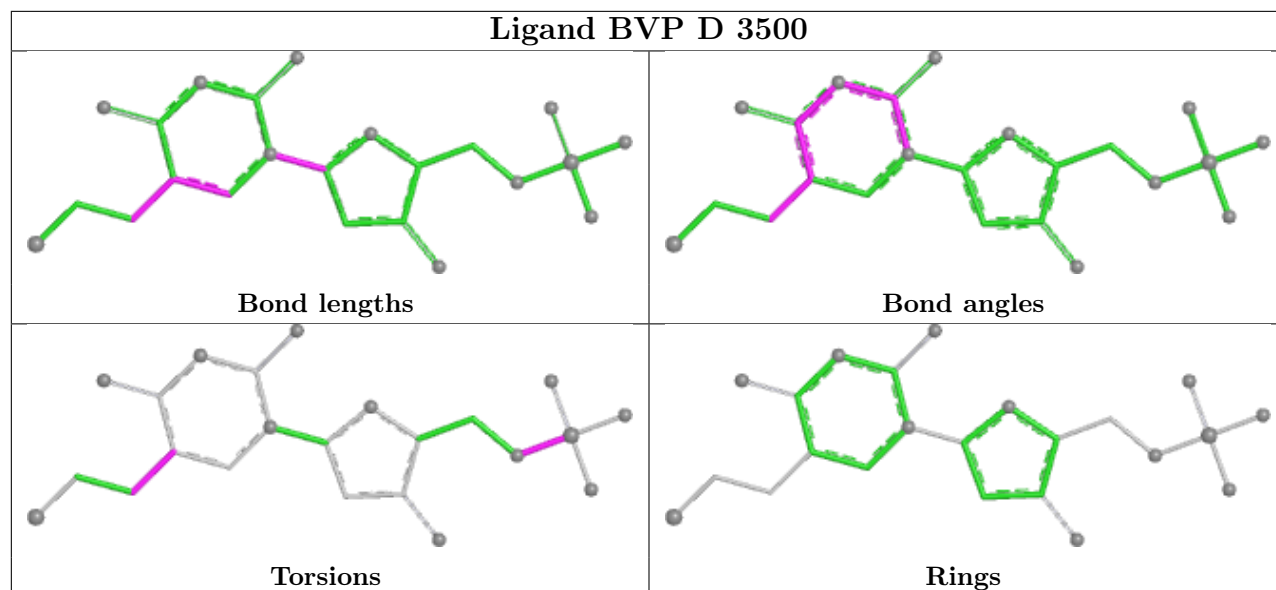
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1400	ADP	2	0
3	B	1500	BVP	2	0
2	D	3400	ADP	2	0
2	A	400	ADP	2	0
3	D	3500	BVP	2	0
3	A	500	BVP	2	0
3	C	2500	BVP	3	0
2	C	2400	ADP	3	0

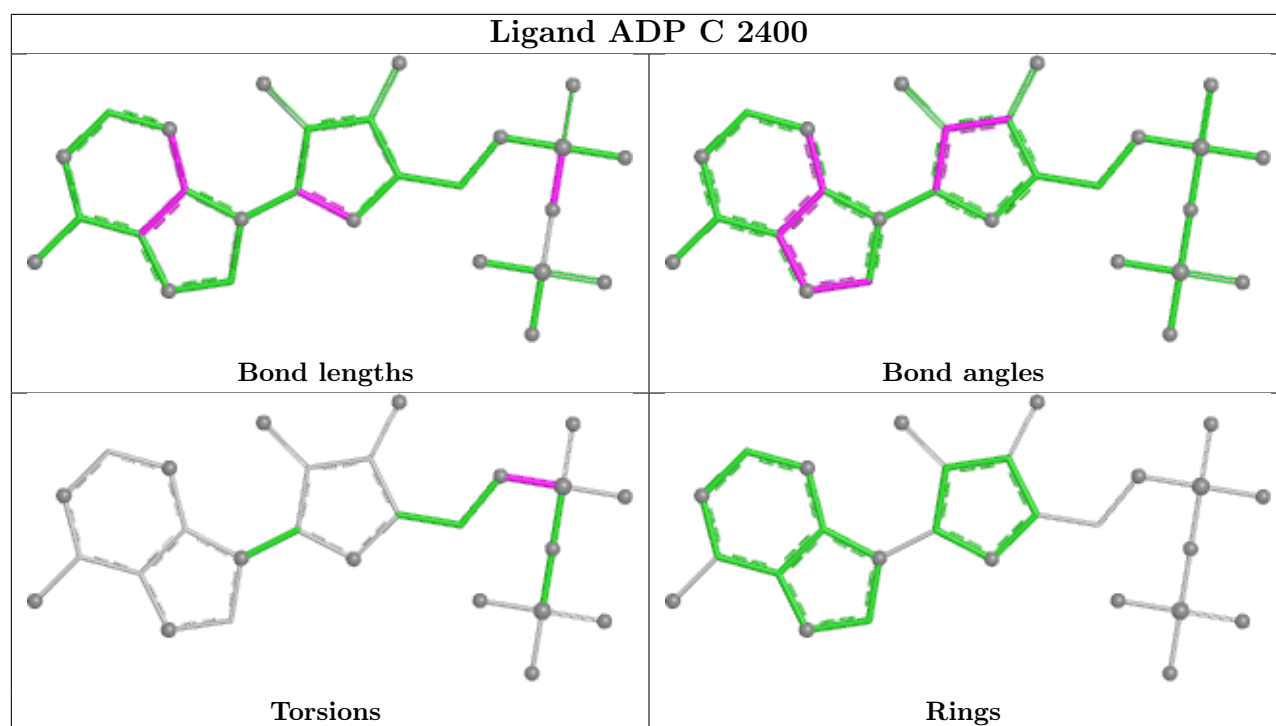
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	325/341 (95%)	-1.66	0 100 100	5, 26, 88, 105	0
1	B	315/341 (92%)	-1.64	0 100 100	5, 30, 87, 103	0
1	C	313/341 (91%)	-1.67	0 100 100	5, 30, 87, 102	0
1	D	315/341 (92%)	-1.66	0 100 100	7, 29, 89, 107	0
All	All	1268/1364 (92%)	-1.66	0 100 100	5, 29, 88, 107	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	ADP	D	3400	27/27	0.98	0.05	90,113,118,119	0
2	ADP	B	1400	27/27	0.99	0.04	85,109,116,123	0
2	ADP	C	2400	27/27	0.99	0.04	84,110,117,122	0
2	ADP	A	400	8/27	0.99	0.03	94,97,105,107	0

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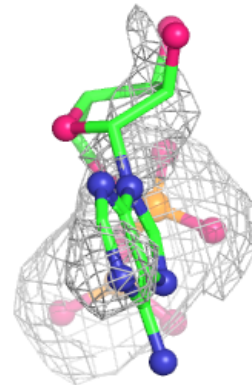
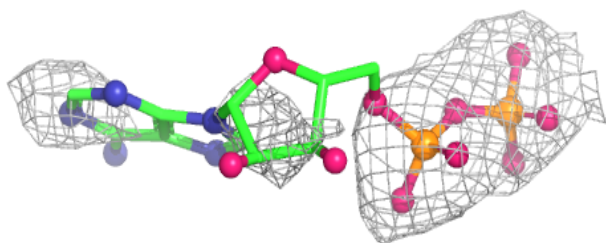
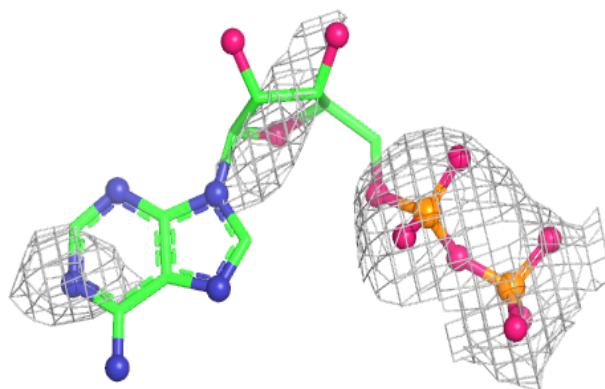
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BVP	A	500	23/23	1.00	0.02	13,28,58,77	0
3	BVP	B	1500	23/23	1.00	0.03	24,35,53,74	0
3	BVP	C	2500	23/23	1.00	0.02	23,31,50,86	0
3	BVP	D	3500	23/23	1.00	0.02	13,30,58,98	0

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.

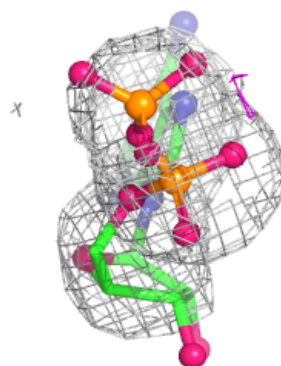
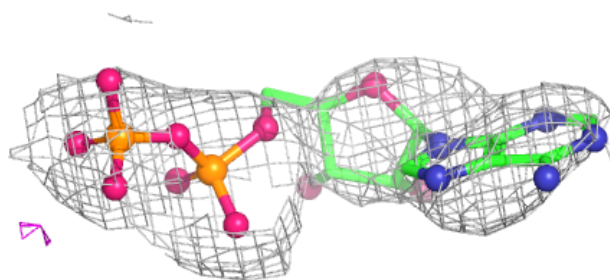
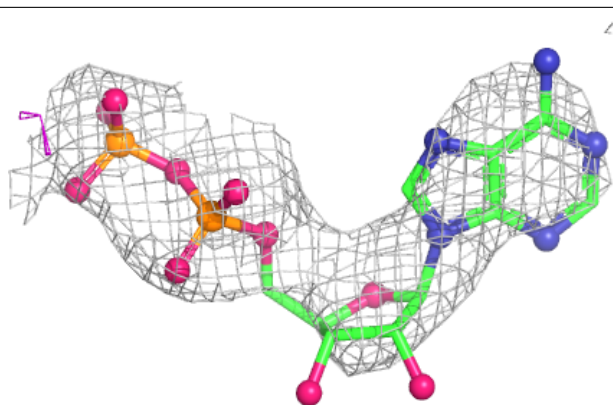
Electron density around ADP D 3400:

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

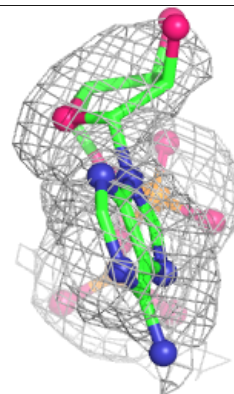
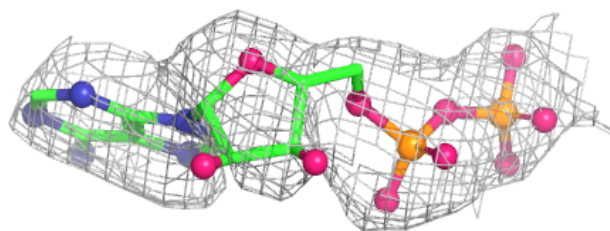
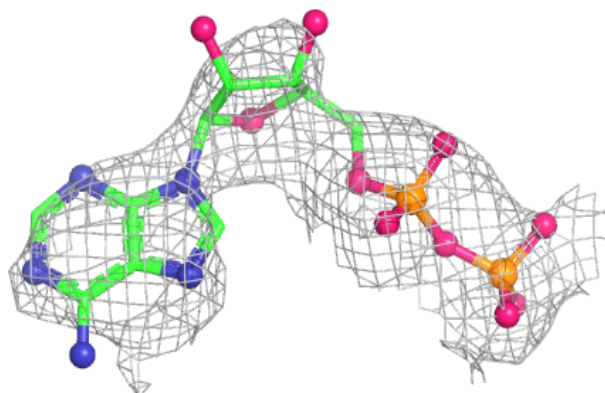


Electron density around ADP B 1400:

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

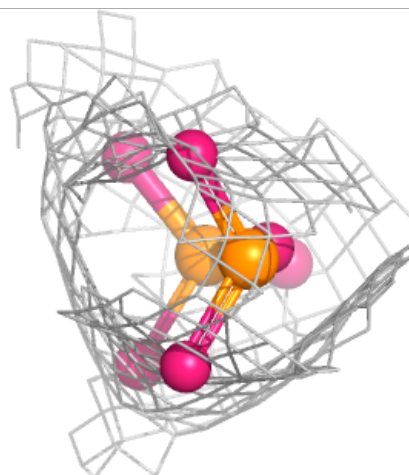
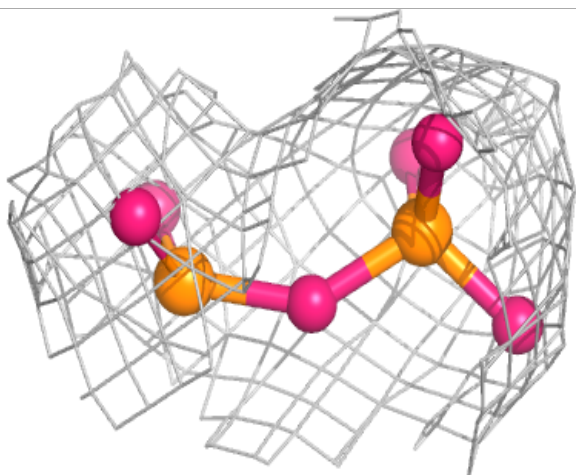
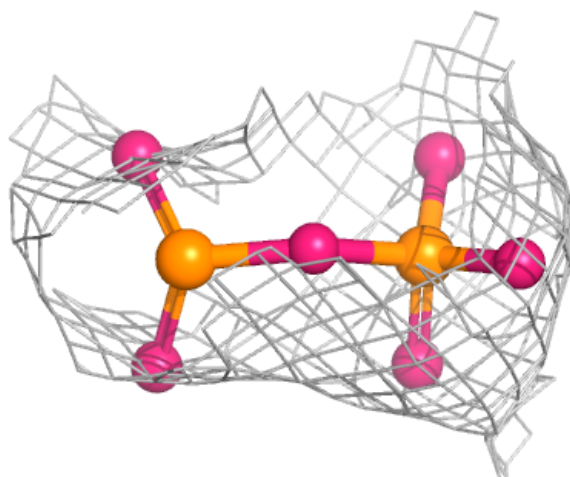
**Electron density around ADP C 2400:**

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



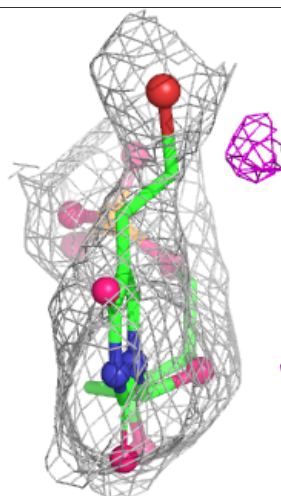
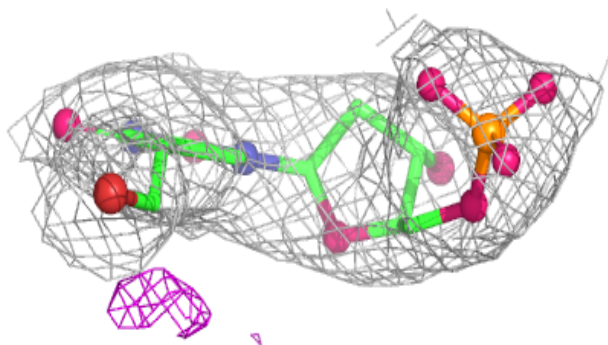
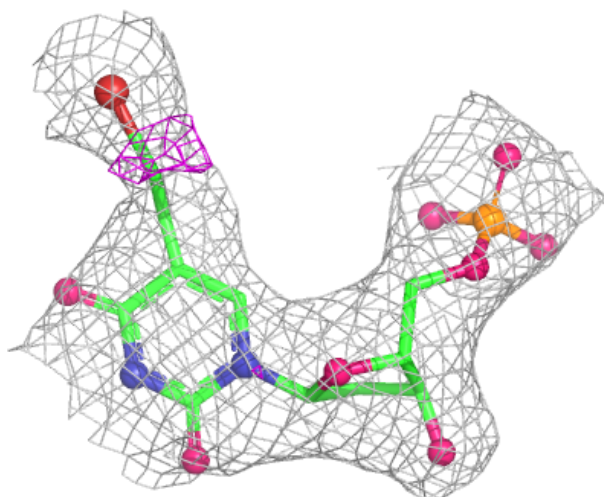
Electron density around ADP A 400:

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



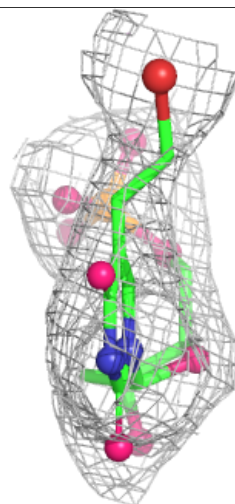
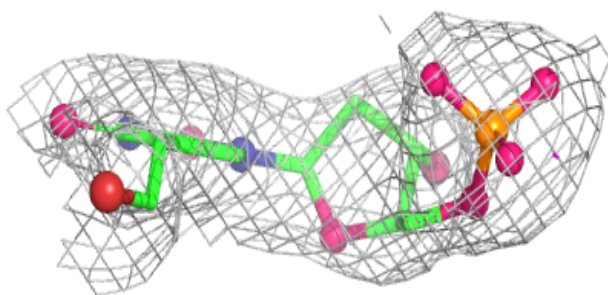
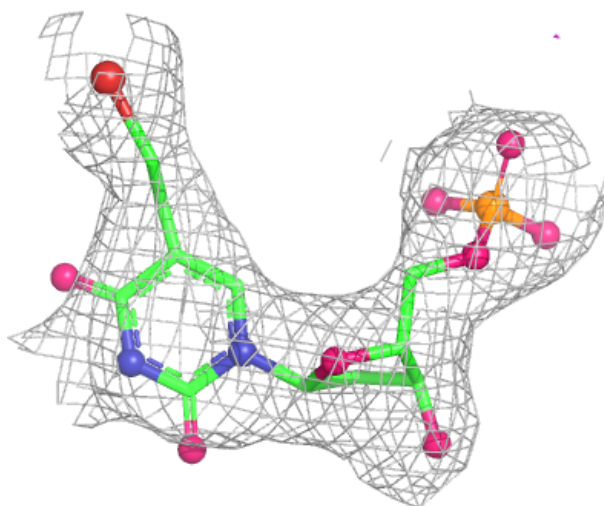
Electron density around BVP A 500:

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



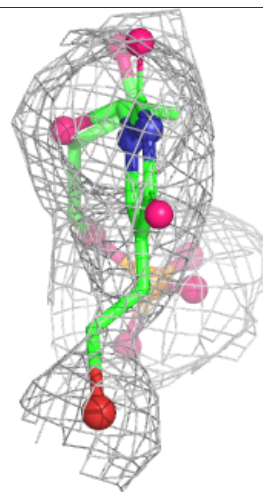
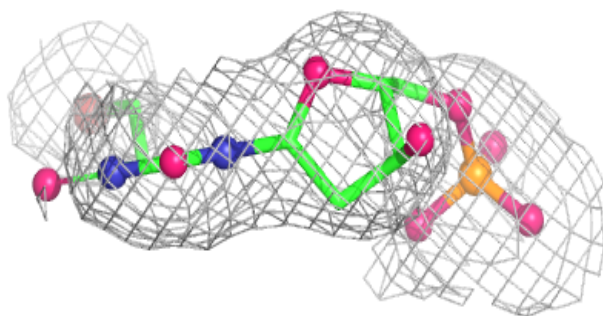
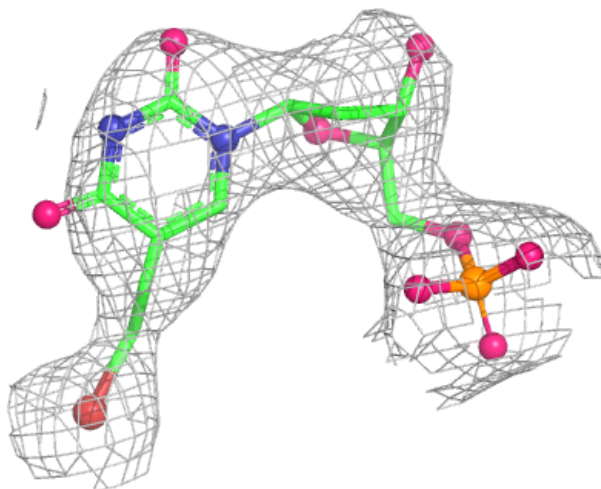
Electron density around BVP B 1500:

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



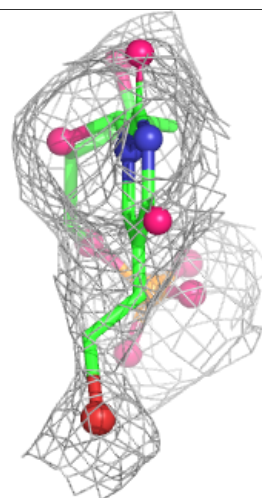
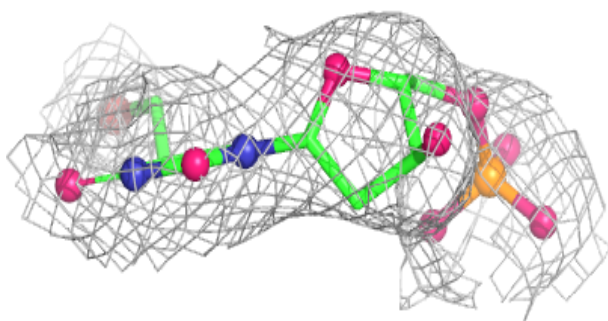
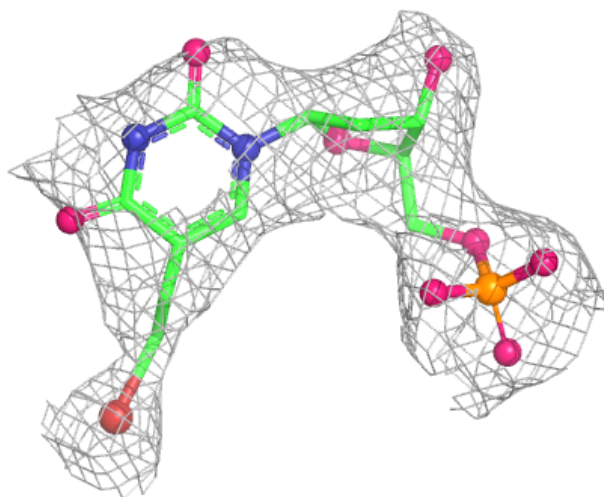
Electron density around BVP C 2500:

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



Electron density around BVP D 3500:

$2mF_o-DF_c$ (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.