



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 2VSO / pdb_00002vso
Title : Crystal Structure of a Translation Initiation Complex
Authors : Schutz, P.; Bumann, M.; Oberholzer, A.E.; Bieniossek, C.; Altmann, M.; Trachsel, H.; Baumann, U.
Deposited on : 2008-04-28
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

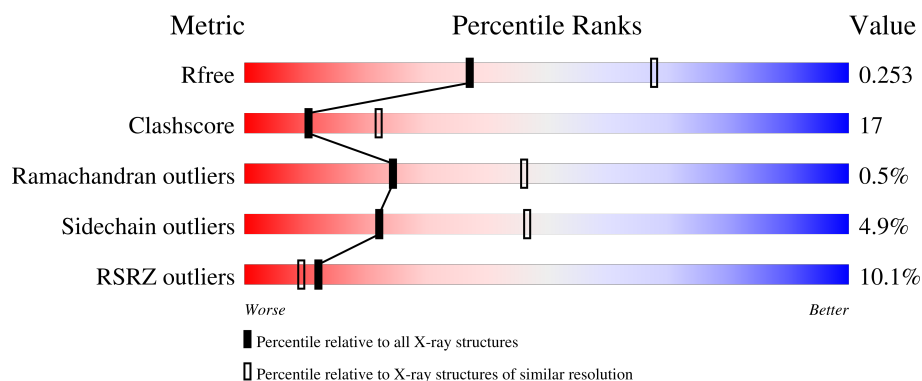
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	395	10% 61% 28% • 7%
1	B	395	9% 62% 28% •• 7%
2	E	284	9% 57% 23% • 16%
2	F	284	7% 56% 24% • 17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9694 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

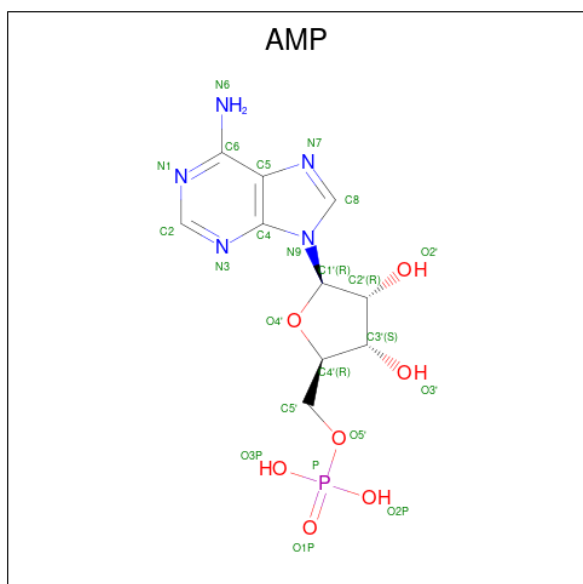
- Molecule 1 is a protein called ATP-DEPENDENT RNA HELICASE EIF4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2907	1846	490	557	14			
1	B	366	Total	C	N	O	S	0	0	0
			2907	1846	490	557	14			

- Molecule 2 is a protein called EUKARYOTIC INITIATION FACTOR 4F SUBUNIT P150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	239	Total	C	N	O	S	0	0	0
			1887	1205	319	353	10			
2	F	237	Total	C	N	O	S	0	0	0
			1871	1197	316	348	10			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

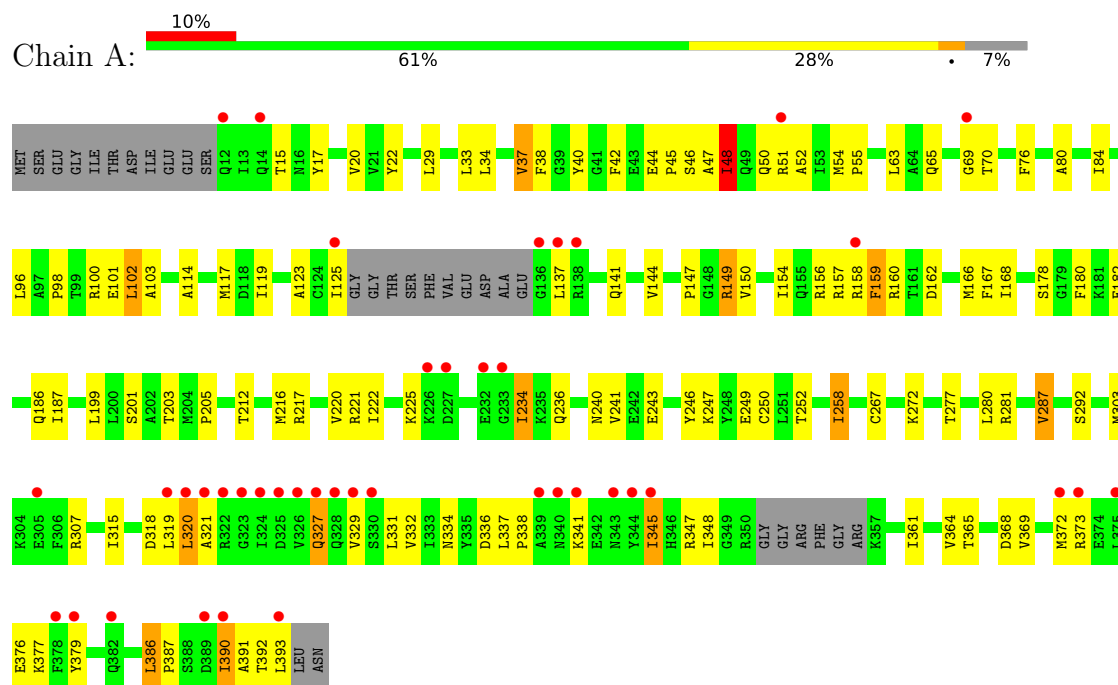
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	28	Total	O	0	0
			28	28		
4	E	14	Total	O	0	0
			14	14		
4	F	11	Total	O	0	0
			11	11		

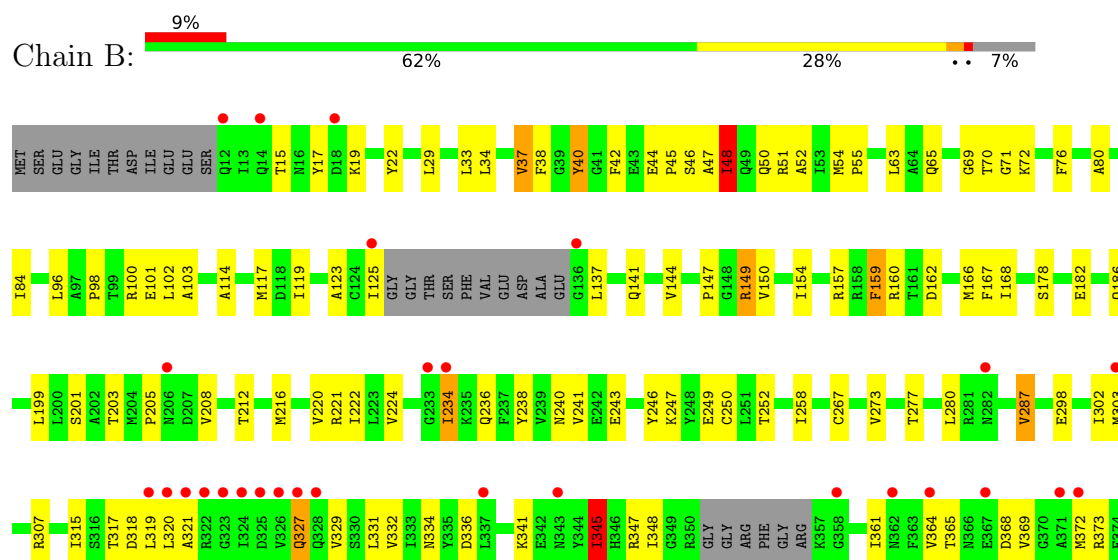
3 Residue-property plots

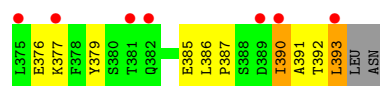
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-DEPENDENT RNA HELICASE EIF4A

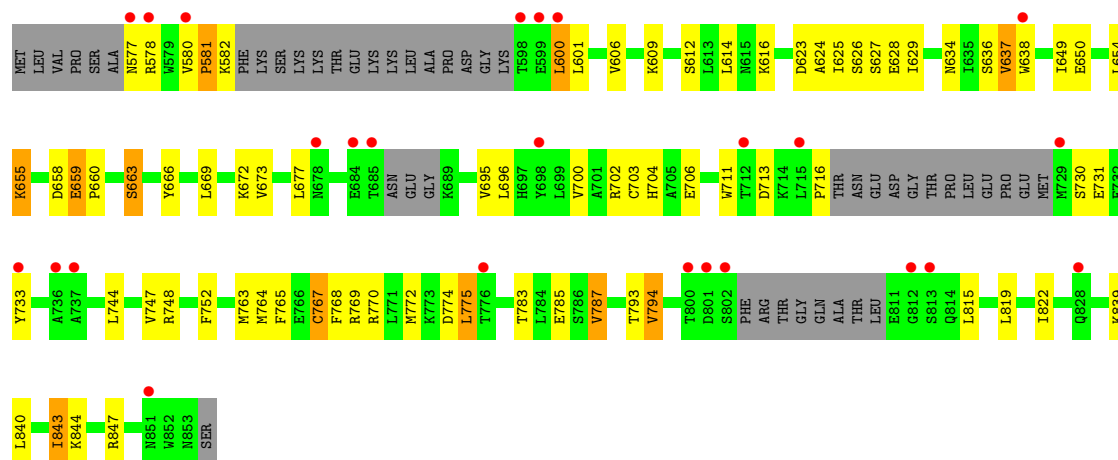


• Molecule 1: ATP-DEPENDENT RNA HELICASE EIF4A

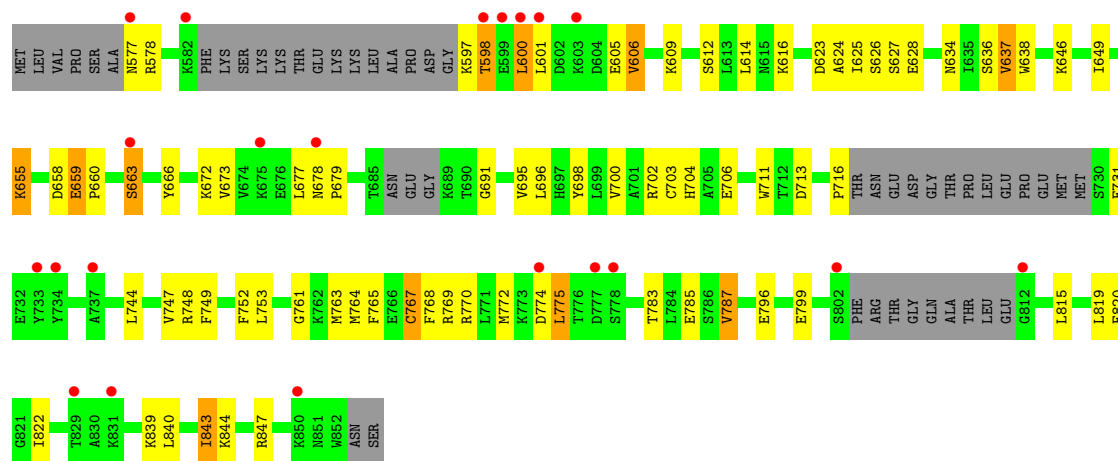




● Molecule 2: EUKARYOTIC INITIATION FACTOR 4F SUBUNIT P150



● Molecule 2: EUKARYOTIC INITIATION FACTOR 4F SUBUNIT P150



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.26Å 69.80Å 101.97Å 91.70° 102.01° 115.30°	Depositor
Resolution (Å)	48.01 – 2.60 48.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (48.01-2.60) 94.3 (48.01-2.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.214 , 0.260 0.212 , 0.253	Depositor DCC
R_{free} test set	1314 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9694	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.92% 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: AMP

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	0.53	0/2949	0.88	7/3985 (0.2%)
1	B	0.54	0/2949	0.88	10/3985 (0.3%)
2	E	0.49	0/1915	0.87	3/2578 (0.1%)
2	F	0.46	0/1899	0.87	5/2556 (0.2%)
All	All	0.51	0/9712	0.88	25/13104 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	716	PRO	N-CA-CB	7.30	111.03	103.00
2	F	716	PRO	N-CA-CB	7.15	110.87	103.00
1	A	48	ILE	CB-CA-C	-6.94	103.00	111.88
1	B	48	ILE	CB-CA-C	-6.69	103.32	111.88
2	F	659	GLU	CA-C-N	6.55	126.78	119.32
2	F	659	GLU	C-N-CA	6.55	126.78	119.32
2	E	659	GLU	CA-C-N	6.49	126.72	119.32
2	E	659	GLU	C-N-CA	6.49	126.72	119.32
1	A	234	ILE	N-CA-C	5.55	117.31	108.87
1	B	386	LEU	CA-C-N	5.49	125.25	119.76
1	B	386	LEU	C-N-CA	5.49	125.25	119.76
1	A	159	PHE	N-CA-C	5.48	117.36	108.26
1	B	321	ALA	N-CA-C	-5.42	106.64	113.20
1	B	234	ILE	N-CA-C	5.40	117.08	108.87
1	B	40	TYR	N-CA-C	-5.30	107.47	114.31
1	A	321	ALA	N-CA-C	-5.29	106.80	113.20
2	F	691	GLY	CA-C-N	5.28	124.60	118.85
2	F	691	GLY	C-N-CA	5.28	124.60	118.85
1	B	345	ILE	CB-CA-C	-5.21	103.83	112.26
1	A	292	SER	N-CA-C	5.20	116.76	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	LEU	CA-C-N	5.10	125.00	119.85
1	A	386	LEU	C-N-CA	5.10	125.00	119.85
1	B	44	GLU	CA-C-N	5.09	125.01	119.76
1	B	44	GLU	C-N-CA	5.09	125.01	119.76
1	B	159	PHE	N-CA-C	5.04	117.61	108.69

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	2907	0	2935	105	0
1	B	2907	0	2935	101	0
2	E	1887	0	1882	59	0
2	F	1871	0	1866	59	0
3	A	23	0	12	1	0
3	B	23	0	12	1	0
4	A	23	0	0	2	0
4	B	28	0	0	4	0
4	E	14	0	0	0	0
4	F	11	0	0	0	0
All	All	9694	0	9642	324	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 17.

All (324) 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:69:GLY:HA2	3:B:1394:AMP:H5'1	1.23	1.09
1:B:341:LYS:H	1:B:341:LYS:HD2	1.17	1.08
1:A:341:LYS:H	1:A:341:LYS:HD2	1.18	1.08
1:A:114:ALA:HA	1:A:117:MET:HE2	1.53	0.91
1:A:69:GLY:HA2	3:A:1394:AMP:H5'1	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ALA:HA	1:B:117:MET:HE2	1.51	0.89
1:B:63:LEU:HD13	1:B:216:MET:HE1	1.60	0.83
1:A:63:LEU:HD13	1:A:216:MET:HE1	1.65	0.78
1:B:96:LEU:HD11	1:B:150:VAL:HG11	1.66	0.77
1:A:96:LEU:HD11	1:A:150:VAL:HG11	1.68	0.73
1:B:258:ILE:HG22	1:B:391:ALA:HA	1.71	0.73
1:B:243:GLU:HB2	1:B:246:TYR:CD1	2.25	0.72
1:B:345:ILE:HG12	1:B:379:TYR:CE1	2.24	0.72
1:A:243:GLU:HB2	1:A:246:TYR:CD1	2.27	0.70
1:A:345:ILE:HG12	1:A:379:TYR:OH	1.93	0.69
1:A:258:ILE:HG22	1:A:391:ALA:HA	1.74	0.69
2:F:600:LEU:C	2:F:600:LEU:HD23	2.18	0.69
1:A:345:ILE:HG12	1:A:379:TYR:CE1	2.28	0.69
1:A:37:VAL:HG23	1:A:42:PHE:HB2	1.75	0.68
1:B:46:SER:O	1:B:50:GLN:HG3	1.93	0.68
2:E:772:MET:HE1	2:E:815:LEU:HD11	1.74	0.68
1:B:341:LYS:HD2	1:B:341:LYS:N	2.01	0.68
2:E:844:LYS:O	2:E:844:LYS:HD3	1.94	0.68
2:E:600:LEU:C	2:E:600:LEU:HD23	2.19	0.67
2:F:772:MET:HE1	2:F:815:LEU:HD11	1.76	0.67
2:E:577:ASN:O	2:E:578:ARG:HD3	1.95	0.67
1:A:119:ILE:HA	1:A:141:GLN:OE1	1.94	0.67
2:E:765:PHE:O	2:E:769:ARG:HB2	1.95	0.67
1:B:345:ILE:HG12	1:B:379:TYR:OH	1.93	0.66
1:B:37:VAL:HG23	1:B:42:PHE:HB2	1.76	0.66
2:E:730:SER:HB3	2:E:733:TYR:CB	2.26	0.66
1:B:327:GLN:HG3	1:B:329:VAL:HG23	1.78	0.66
2:F:765:PHE:O	2:F:769:ARG:HB2	1.95	0.65
1:A:327:GLN:HG3	1:A:329:VAL:HG23	1.78	0.65
2:F:844:LYS:O	2:F:844:LYS:HD3	1.97	0.65
1:A:114:ALA:HA	1:A:117:MET:CE	2.26	0.64
1:B:332:VAL:HG11	1:B:348:ILE:HG22	1.80	0.64
1:A:46:SER:O	1:A:50:GLN:HG3	1.98	0.64
2:F:703:CYS:HB2	2:F:763:MET:HE3	1.81	0.63
1:B:119:ILE:HA	1:B:141:GLN:OE1	1.98	0.63
2:F:775:LEU:HB3	2:F:822:ILE:HG21	1.80	0.62
2:F:783:THR:O	2:F:787:VAL:HG23	1.99	0.62
1:A:332:VAL:HG11	1:A:348:ILE:HG22	1.80	0.62
2:E:783:THR:O	2:E:787:VAL:HG23	1.99	0.61
2:E:655:LYS:HE2	2:E:659:GLU:OE1	2.00	0.61
1:A:369:VAL:O	1:A:373:ARG:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HA	1:A:149:ARG:HG3	1.82	0.61
1:B:345:ILE:HG12	1:B:379:TYR:CZ	2.35	0.61
2:E:577:ASN:C	2:E:578:ARG:HD3	2.26	0.61
2:E:775:LEU:HB3	2:E:822:ILE:HG21	1.82	0.61
2:F:612:SER:O	2:F:616:LYS:HG3	1.99	0.61
1:B:369:VAL:O	1:B:373:ARG:HG2	2.00	0.61
1:B:34:LEU:HG	1:B:38:PHE:CE1	2.36	0.60
2:E:614:LEU:HB3	2:E:655:LYS:HG3	1.82	0.60
1:A:345:ILE:HG12	1:A:379:TYR:CZ	2.37	0.59
2:F:658:ASP:C	2:F:660:PRO:HD3	2.26	0.59
2:E:634:ASN:O	2:E:637:VAL:HG13	2.02	0.59
2:E:730:SER:HB3	2:E:733:TYR:HB2	1.84	0.59
2:E:703:CYS:HB2	2:E:763:MET:HE3	1.84	0.59
2:F:704:HIS:CG	2:F:763:MET:HE1	2.38	0.59
2:F:616:LYS:HB2	2:F:625:ILE:HD13	1.84	0.58
1:B:125:ILE:HA	1:B:149:ARG:HG3	1.85	0.58
1:B:48:ILE:HD11	1:B:70:THR:C	2.28	0.58
2:F:634:ASN:O	2:F:637:VAL:HG13	2.03	0.58
1:B:17:TYR:CE2	1:B:55:PRO:HG3	2.39	0.57
2:F:840:LEU:HA	2:F:843:ILE:HD11	1.85	0.57
1:B:150:VAL:O	1:B:154:ILE:HG13	2.03	0.57
2:E:616:LYS:HB2	2:E:625:ILE:HD13	1.85	0.57
1:A:17:TYR:CE2	1:A:55:PRO:HG3	2.39	0.57
1:B:114:ALA:HA	1:B:117:MET:CE	2.28	0.57
2:E:658:ASP:C	2:E:660:PRO:HD3	2.29	0.57
1:A:22:TYR:O	1:A:45:PRO:HD2	2.05	0.57
1:B:243:GLU:HB2	1:B:246:TYR:HD1	1.70	0.56
2:F:713:ASP:HB2	2:F:774:ASP:OD2	2.05	0.56
1:A:137:LEU:HG	1:A:159:PHE:HB3	1.87	0.56
2:F:614:LEU:HB3	2:F:655:LYS:HG3	1.86	0.56
2:F:655:LYS:HE2	2:F:659:GLU:OE1	2.04	0.56
1:A:150:VAL:O	1:A:154:ILE:HG13	2.06	0.56
1:B:182:GLU:O	1:B:186:GLN:HG2	2.05	0.56
1:A:341:LYS:H	1:A:341:LYS:CD	2.04	0.56
1:A:149:ARG:NH1	1:A:149:ARG:HA	2.22	0.55
1:A:182:GLU:O	1:A:186:GLN:HG2	2.06	0.55
2:F:577:ASN:O	2:F:578:ARG:HD3	2.05	0.55
1:B:137:LEU:HG	1:B:159:PHE:HB3	1.86	0.55
1:B:319:LEU:HD13	4:B:2021:HOH:O	2.05	0.55
2:E:612:SER:O	2:E:616:LYS:HG3	2.05	0.55
1:B:17:TYR:HB2	1:B:220:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:O	1:A:159:PHE:HB2	2.06	0.55
1:A:240:ASN:HA	1:A:364:VAL:HG13	1.88	0.55
1:B:137:LEU:O	1:B:159:PHE:HB2	2.07	0.55
1:A:48:ILE:HD11	1:A:70:THR:C	2.31	0.55
2:F:844:LYS:HD3	2:F:844:LYS:C	2.31	0.55
1:A:15:THR:HA	1:A:221:ARG:O	2.07	0.54
1:B:47:ALA:HB1	1:B:51:ARG:HH21	1.72	0.54
1:A:212:THR:HG23	1:A:216:MET:HE3	1.89	0.54
1:B:303:MET:O	1:B:307:ARG:HG3	2.08	0.54
2:E:844:LYS:HD3	2:E:844:LYS:C	2.30	0.54
2:F:744:LEU:O	2:F:747:VAL:HG22	2.07	0.54
1:A:303:MET:O	1:A:307:ARG:HG3	2.07	0.54
2:E:713:ASP:HB2	2:E:774:ASP:OD2	2.07	0.54
2:F:704:HIS:CD2	2:F:763:MET:HE1	2.43	0.54
2:E:744:LEU:O	2:E:747:VAL:HG22	2.08	0.54
2:F:659:GLU:N	2:F:660:PRO:HD3	2.22	0.54
1:B:319:LEU:HD12	1:B:319:LEU:H	1.73	0.53
2:E:704:HIS:CG	2:E:763:MET:HE1	2.43	0.53
1:B:15:THR:HA	1:B:221:ARG:O	2.08	0.53
1:B:22:TYR:O	1:B:45:PRO:HD2	2.08	0.53
1:B:240:ASN:HA	1:B:364:VAL:HG13	1.90	0.53
1:A:149:ARG:HA	1:A:149:ARG:CZ	2.39	0.53
2:F:702:ARG:O	2:F:706:GLU:HG2	2.09	0.53
1:B:341:LYS:H	1:B:341:LYS:CD	2.02	0.53
1:B:392:THR:OG1	1:B:393:LEU:HD23	2.09	0.53
2:F:637:VAL:HG22	2:F:638:TRP:CD1	2.44	0.53
1:A:96:LEU:HD22	1:A:167:PHE:CE1	2.43	0.52
2:E:840:LEU:HA	2:E:843:ILE:HD11	1.91	0.52
1:A:234:ILE:HD12	1:A:234:ILE:O	2.09	0.52
1:A:243:GLU:HB2	1:A:246:TYR:HD1	1.72	0.52
1:B:345:ILE:HG12	1:B:379:TYR:HE1	1.75	0.52
2:E:655:LYS:HE2	2:E:659:GLU:CD	2.33	0.52
2:E:702:ARG:O	2:E:706:GLU:HG2	2.10	0.52
2:F:600:LEU:HD23	2:F:601:LEU:N	2.24	0.52
2:F:772:MET:HG2	2:F:819:LEU:HD13	1.92	0.52
1:A:52:ALA:HB2	1:A:222:ILE:HD12	1.92	0.52
1:A:341:LYS:HD2	1:A:341:LYS:N	2.02	0.52
1:B:149:ARG:NH1	1:B:149:ARG:HA	2.24	0.52
1:A:52:ALA:HB2	1:A:222:ILE:CD1	2.38	0.52
1:B:96:LEU:HD22	1:B:167:PHE:CE1	2.44	0.52
1:A:47:ALA:HB1	1:A:51:ARG:HH21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:772:MET:HG2	2:E:819:LEU:HD13	1.92	0.52
2:F:764:MET:HE3	2:F:764:MET:HA	1.92	0.52
1:B:80:ALA:O	1:B:84:ILE:HG12	2.09	0.52
2:E:696:LEU:O	2:E:700:VAL:HG23	2.09	0.52
2:E:764:MET:HE3	2:E:764:MET:HA	1.92	0.52
2:E:659:GLU:N	2:E:660:PRO:HD3	2.24	0.51
1:A:331:LEU:HD11	1:A:361:ILE:HD12	1.91	0.51
2:E:730:SER:HB3	2:E:733:TYR:HB3	1.92	0.51
1:A:203:THR:C	1:A:205:PRO:HD3	2.36	0.51
2:E:793:THR:HG22	2:E:794:VAL:HG23	1.92	0.51
2:F:655:LYS:HE2	2:F:659:GLU:CD	2.36	0.51
1:A:33:LEU:O	1:A:37:VAL:HG12	2.10	0.51
2:E:768:PHE:O	2:E:772:MET:HG3	2.11	0.51
1:A:241:VAL:HG12	1:A:250:CYS:SG	2.51	0.51
1:B:33:LEU:O	1:B:37:VAL:HG12	2.10	0.51
1:B:149:ARG:HA	1:B:149:ARG:CZ	2.41	0.51
1:A:319:LEU:HD12	1:A:319:LEU:H	1.75	0.50
1:A:280:LEU:HD12	1:A:315:ILE:HD11	1.93	0.50
1:A:34:LEU:HG	1:A:38:PHE:CE1	2.47	0.50
1:B:76:PHE:HB2	1:B:168:ILE:HD13	1.93	0.50
2:E:614:LEU:HD13	2:E:655:LYS:HG3	1.93	0.50
1:B:331:LEU:HD11	1:B:361:ILE:HD12	1.92	0.50
2:E:600:LEU:HD23	2:E:601:LEU:N	2.26	0.50
2:E:704:HIS:CD2	2:E:763:MET:HE1	2.46	0.50
2:F:696:LEU:O	2:F:700:VAL:HG23	2.11	0.50
1:A:80:ALA:O	1:A:84:ILE:HG12	2.11	0.50
2:E:637:VAL:HG22	2:E:638:TRP:CD1	2.46	0.49
1:A:52:ALA:C	1:A:55:PRO:HD2	2.37	0.49
2:F:614:LEU:HD13	2:F:655:LYS:HG3	1.93	0.49
1:B:241:VAL:HG12	1:B:250:CYS:SG	2.52	0.49
2:F:601:LEU:HD21	2:F:609:LYS:NZ	2.28	0.49
1:B:52:ALA:C	1:B:55:PRO:HD2	2.37	0.49
2:E:655:LYS:HD2	2:E:666:TYR:OH	2.13	0.48
2:F:655:LYS:HD2	2:F:666:TYR:OH	2.13	0.48
2:F:663:SER:HB3	2:F:752:PHE:HD1	1.77	0.48
1:B:212:THR:CG2	4:B:2015:HOH:O	2.61	0.48
1:B:212:THR:HG23	1:B:216:MET:HE3	1.95	0.48
1:A:17:TYR:HB2	1:A:220:VAL:HG13	1.94	0.48
2:E:772:MET:CE	2:E:815:LEU:HD11	2.43	0.48
1:B:205:PRO:HG3	4:B:2008:HOH:O	2.13	0.48
2:E:601:LEU:HD21	2:E:609:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:677:LEU:HD22	2:F:695:VAL:CG2	2.43	0.48
2:E:601:LEU:HB2	2:E:606:VAL:HG23	1.95	0.48
1:B:390:ILE:C	1:B:392:THR:N	2.71	0.48
1:B:234:ILE:HD12	1:B:234:ILE:O	2.14	0.47
2:E:677:LEU:HD22	2:E:695:VAL:CG2	2.45	0.47
2:E:744:LEU:HD23	2:E:744:LEU:HA	1.69	0.47
2:F:616:LYS:CB	2:F:625:ILE:HD13	2.45	0.47
1:A:63:LEU:CD1	1:A:199:LEU:HD22	2.45	0.47
1:A:80:ALA:HA	1:A:166:MET:HE1	1.96	0.47
1:B:52:ALA:HB2	1:B:222:ILE:CD1	2.44	0.47
1:B:387:PRO:O	1:B:390:ILE:HG12	2.15	0.47
1:A:277:THR:HG23	1:A:287:VAL:CG2	2.44	0.47
1:B:212:THR:HG22	4:B:2015:HOH:O	2.14	0.47
1:A:241:VAL:HG21	1:A:247:LYS:HG3	1.97	0.47
1:B:45:PRO:HB2	1:B:50:GLN:HG2	1.96	0.47
2:E:626:SER:OG	2:E:672:LYS:HD2	2.15	0.47
1:A:100:ARG:HB3	1:A:125:ILE:HG12	1.97	0.46
1:A:373:ARG:O	1:A:377:LYS:HG2	2.15	0.46
1:B:100:ARG:HB3	1:B:125:ILE:HG12	1.96	0.46
1:B:234:ILE:CD1	1:B:348:ILE:HD12	2.45	0.46
1:B:63:LEU:CD1	1:B:199:LEU:HD22	2.46	0.46
1:A:117:MET:HB2	1:A:117:MET:HE3	1.79	0.46
1:A:387:PRO:O	1:A:390:ILE:HG12	2.15	0.46
2:F:626:SER:OG	2:F:672:LYS:HD2	2.15	0.46
1:A:390:ILE:C	1:A:392:THR:N	2.72	0.46
2:E:623:ASP:O	2:E:627:SER:HB3	2.16	0.46
2:F:601:LEU:HB2	2:F:606:VAL:HG23	1.97	0.46
2:F:772:MET:CE	2:F:815:LEU:HD11	2.45	0.46
1:A:29:LEU:HD12	1:A:34:LEU:HD13	1.96	0.46
2:E:616:LYS:CB	2:E:625:ILE:HD13	2.45	0.46
1:B:364:VAL:HG23	1:B:368:ASP:CB	2.46	0.46
1:B:96:LEU:HD22	1:B:167:PHE:HE1	1.81	0.46
1:B:373:ARG:O	1:B:377:LYS:HG2	2.15	0.46
2:F:623:ASP:O	2:F:627:SER:HB3	2.16	0.46
1:A:327:GLN:CG	1:A:329:VAL:HG23	2.44	0.46
1:B:203:THR:C	1:B:205:PRO:HD3	2.41	0.45
1:A:364:VAL:HG23	1:A:368:ASP:CB	2.47	0.45
1:A:348:ILE:O	1:A:348:ILE:HG13	2.17	0.45
1:A:101:GLU:H	1:A:101:GLU:CD	2.24	0.45
1:B:280:LEU:HD12	1:B:315:ILE:HD11	1.97	0.45
1:B:327:GLN:CG	1:B:329:VAL:HG23	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD22	1:A:167:PHE:HE1	1.81	0.45
2:E:601:LEU:HD21	2:E:609:LYS:HZ2	1.82	0.45
1:B:234:ILE:HD11	1:B:348:ILE:HD12	1.99	0.45
1:B:365:THR:H	1:B:368:ASP:HB2	1.80	0.45
2:F:768:PHE:O	2:F:772:MET:HG3	2.17	0.45
1:A:65:GLN:HA	1:A:201:SER:O	2.16	0.45
2:F:796:GLU:O	2:F:799:GLU:HB2	2.16	0.45
1:A:54:MET:N	1:A:55:PRO:CD	2.80	0.44
1:B:80:ALA:HA	1:B:166:MET:HE1	1.98	0.44
2:E:663:SER:HB3	2:E:752:PHE:HD1	1.82	0.44
2:F:601:LEU:CB	2:F:606:VAL:HG23	2.47	0.44
1:A:318:ASP:O	1:A:319:LEU:C	2.61	0.44
2:F:600:LEU:C	2:F:600:LEU:CD2	2.88	0.44
1:A:243:GLU:OE2	1:A:243:GLU:HA	2.18	0.44
2:E:581:PRO:HB2	2:E:582:LYS:H	1.60	0.44
1:B:137:LEU:H	1:B:137:LEU:HD23	1.83	0.44
1:A:334:ASN:OD1	1:A:347:ARG:HD3	2.18	0.44
1:A:365:THR:H	1:A:368:ASP:HB2	1.83	0.44
1:A:44:GLU:HA	1:A:45:PRO:HD3	1.85	0.44
2:F:673:VAL:O	2:F:677:LEU:HB2	2.18	0.44
2:F:843:ILE:H	2:F:843:ILE:HG13	1.62	0.44
2:E:600:LEU:C	2:E:600:LEU:CD2	2.90	0.44
1:B:101:GLU:CD	1:B:101:GLU:H	2.26	0.43
1:B:277:THR:HG23	1:B:287:VAL:CG2	2.48	0.43
2:F:785:GLU:OE1	2:F:839:LYS:HE2	2.17	0.43
1:B:123:ALA:HA	1:B:144:VAL:O	2.18	0.43
1:B:52:ALA:HB2	1:B:222:ILE:HD12	1.99	0.43
1:B:38:PHE:C	1:B:40:TYR:H	2.26	0.43
2:F:624:ALA:O	2:F:628:GLU:HG3	2.18	0.43
1:A:258:ILE:HG22	1:A:391:ALA:CA	2.47	0.43
1:B:267:CYS:HA	1:B:336:ASP:HB2	2.00	0.43
2:E:747:VAL:HG23	2:E:748:ARG:N	2.33	0.43
2:F:597:LYS:O	2:F:598:THR:C	2.61	0.43
1:A:225:LYS:HE2	1:A:225:LYS:HB3	1.80	0.43
1:B:29:LEU:HD12	1:B:34:LEU:HD13	2.01	0.43
2:E:711:TRP:O	2:E:770:ARG:NH2	2.52	0.43
1:A:47:ALA:HB1	1:A:51:ARG:NH2	2.34	0.43
1:A:217:ARG:O	1:A:217:ARG:HG2	2.19	0.43
1:B:98:PRO:HD2	1:B:102:LEU:HD13	1.99	0.43
1:B:334:ASN:OD1	1:B:347:ARG:HD3	2.19	0.43
1:A:137:LEU:HD23	1:A:137:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASP:C	1:A:320:LEU:N	2.76	0.43
1:A:234:ILE:CD1	1:A:348:ILE:HD12	2.49	0.43
1:A:372:MET:O	1:A:372:MET:HG2	2.18	0.43
1:B:205:PRO:HD2	1:B:208:VAL:HB	2.00	0.43
1:A:123:ALA:HA	1:A:144:VAL:O	2.19	0.43
1:B:65:GLN:HA	1:B:201:SER:O	2.19	0.43
2:E:624:ALA:O	2:E:628:GLU:HG3	2.19	0.43
2:F:764:MET:HE3	2:F:767:CYS:HB3	2.00	0.43
2:F:775:LEU:HD12	2:F:775:LEU:HA	1.88	0.43
1:A:147:PRO:HA	1:A:150:VAL:HG12	2.02	0.42
1:B:103:ALA:HB1	1:B:144:VAL:HG12	2.01	0.42
1:B:241:VAL:HG21	1:B:247:LYS:HG3	2.02	0.42
1:B:199:LEU:C	1:B:199:LEU:HD23	2.45	0.42
2:F:601:LEU:HD21	2:F:609:LYS:HZ2	1.83	0.42
1:A:212:THR:CG2	4:A:2015:HOH:O	2.67	0.42
1:A:272:LYS:HE3	1:A:272:LYS:HB2	1.81	0.42
1:B:147:PRO:HA	1:B:150:VAL:HG12	2.02	0.42
1:B:373:ARG:O	1:B:376:GLU:HB3	2.18	0.42
2:E:785:GLU:OE1	2:E:839:LYS:HE2	2.19	0.42
1:A:160:ARG:CG	1:A:162:ASP:OD2	2.68	0.42
2:E:601:LEU:CB	2:E:606:VAL:HG23	2.48	0.42
2:F:646:LYS:HG3	2:F:698:TYR:CE2	2.54	0.42
2:F:678:ASN:HA	2:F:679:PRO:HD3	1.91	0.42
1:A:267:CYS:HA	1:A:336:ASP:HB2	2.02	0.42
1:B:54:MET:N	1:B:55:PRO:CD	2.82	0.42
1:A:150:VAL:HG13	1:A:187:ILE:HD11	2.01	0.42
1:B:238:TYR:CZ	1:B:385:GLU:HB2	2.54	0.42
1:B:318:ASP:O	1:B:319:LEU:C	2.62	0.42
2:F:601:LEU:HD22	2:F:605:GLU:HB3	2.02	0.42
1:A:45:PRO:HB2	1:A:50:GLN:HG2	2.02	0.42
2:E:764:MET:HE3	2:E:767:CYS:HB3	2.02	0.42
2:F:711:TRP:O	2:F:770:ARG:NH2	2.53	0.42
1:A:373:ARG:O	1:A:376:GLU:HB3	2.19	0.42
1:A:103:ALA:HB1	1:A:144:VAL:HG12	2.02	0.42
1:B:160:ARG:CG	1:B:162:ASP:OD2	2.68	0.42
1:B:348:ILE:O	1:B:348:ILE:HG13	2.20	0.42
1:B:241:VAL:O	1:B:243:GLU:N	2.52	0.41
1:B:273:VAL:HG21	1:B:317:THR:HG23	2.02	0.41
2:E:650:GLU:O	2:E:654:LEU:HG	2.20	0.41
1:A:199:LEU:HD23	1:A:199:LEU:C	2.45	0.41
1:A:147:PRO:HG2	1:A:180:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:CD1	1:B:71:GLY:C	2.93	0.41
1:B:258:ILE:HG22	1:B:391:ALA:CA	2.45	0.41
1:A:234:ILE:HD11	1:A:348:ILE:HD12	2.02	0.41
2:E:580:VAL:HA	2:E:581:PRO:HD3	1.89	0.41
2:E:629:ILE:HD13	2:E:669:LEU:HD21	2.02	0.41
2:F:744:LEU:HD23	2:F:744:LEU:HA	1.70	0.41
1:B:72:LYS:HB3	1:B:72:LYS:HE3	1.93	0.41
1:B:298:GLU:O	1:B:302:ILE:HG12	2.21	0.41
1:A:20:VAL:HG13	1:A:50:GLN:HB3	2.03	0.41
2:E:775:LEU:HD12	2:E:775:LEU:HA	1.86	0.41
1:A:38:PHE:C	1:A:40:TYR:H	2.28	0.41
1:A:98:PRO:HD2	1:A:102:LEU:HD13	2.01	0.41
2:F:749:PHE:O	2:F:753:LEU:HG	2.21	0.41
1:A:386:LEU:HA	1:A:387:PRO:HD3	1.84	0.41
2:F:747:VAL:HG23	2:F:748:ARG:N	2.36	0.41
1:A:156:ARG:HD3	1:A:158:ARG:NH2	2.36	0.40
1:A:212:THR:HG21	4:A:2015:HOH:O	2.21	0.40
2:F:761:GLY:O	2:F:765:PHE:HD1	2.04	0.40
1:A:234:ILE:HD12	1:A:234:ILE:C	2.46	0.40
1:A:372:MET:HE2	1:A:372:MET:HB3	1.85	0.40
1:B:102:LEU:HD23	1:B:102:LEU:O	2.21	0.40
1:A:277:THR:O	1:A:281:ARG:HG3	2.22	0.40
1:A:386:LEU:HD11	1:A:390:ILE:HG21	2.03	0.40
1:B:224:VAL:O	1:B:224:VAL:HG23	2.21	0.40
1:B:372:MET:HE2	1:B:372:MET:HB3	1.85	0.40
2:E:673:VAL:O	2:E:677:LEU:HB2	2.21	0.40
2:F:820:PHE:CE1	2:F:847:ARG:HD3	2.55	0.40
1:A:337:LEU:HA	1:A:338:PRO:HD3	1.90	0.40
1:B:17:TYR:CE2	1:B:19:LYS:HB2	2.57	0.40
1:A:48:ILE:H	1:A:48:ILE:HG13	1.65	0.40
1:A:76:PHE:HB2	1:A:168:ILE:HD13	2.03	0.40
1:B:372:MET:O	1:B:372:MET:HG2	2.21	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	360/395 (91%)	338 (94%)	21 (6%)	1 (0%)	36	58
1	B	360/395 (91%)	340 (94%)	19 (5%)	1 (0%)	36	58
2	E	229/284 (81%)	217 (95%)	10 (4%)	2 (1%)	14	30
2	F	227/284 (80%)	214 (94%)	11 (5%)	2 (1%)	14	30
All	All	1176/1358 (87%)	1109 (94%)	61 (5%)	6 (0%)	24	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	581	PRO
2	E	731	GLU
1	A	327	GLN
1	B	327	GLN
2	F	598	THR
2	F	731	GLU

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	322/348 (92%)	307 (95%)	15 (5%)	23	48
1	B	322/348 (92%)	309 (96%)	13 (4%)	28	55
2	E	203/253 (80%)	191 (94%)	12 (6%)	18	38
2	F	200/253 (79%)	189 (94%)	11 (6%)	19	41
All	All	1047/1202 (87%)	996 (95%)	51 (5%)	22	47

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	48	ILE
1	A	102	LEU
1	A	149	ARG
1	A	157	ARG
1	A	178	SER
1	A	236	GLN
1	A	249	GLU
1	A	252	THR
1	A	258	ILE
1	A	287	VAL
1	A	320	LEU
1	A	345	ILE
1	A	390	ILE
1	A	393	LEU
1	B	37	VAL
1	B	48	ILE
1	B	149	ARG
1	B	157	ARG
1	B	178	SER
1	B	236	GLN
1	B	249	GLU
1	B	252	THR
1	B	287	VAL
1	B	320	LEU
1	B	345	ILE
1	B	390	ILE
1	B	393	LEU
2	E	600	LEU
2	E	636	SER
2	E	637	VAL
2	E	649	ILE
2	E	655	LYS
2	E	663	SER
2	E	767	CYS
2	E	775	LEU
2	E	787	VAL
2	E	794	VAL
2	E	843	ILE
2	E	847	ARG
2	F	600	LEU
2	F	606	VAL
2	F	636	SER

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Mol	Chain	Res	Type
2	F	637	VAL
2	F	649	ILE
2	F	655	LYS
2	F	663	SER
2	F	767	CYS
2	F	775	LEU
2	F	787	VAL
2	F	843	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	641	ASN
2	E	697	HIS
2	F	641	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
3	AMP	A	1394	-	25,25,25	1.49	4 (16%)	37,38,38	1.98	11 (29%)
3	AMP	B	1394	-	25,25,25	1.46	4 (16%)	37,38,38	2.03	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	A	1394	-	-	5/10/26/26	0/3/3/3
3	AMP	B	1394	-	-	0/10/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1394	AMP	C5-C4	4.93	1.47	1.39
3	B	1394	AMP	C5-C4	4.45	1.47	1.39
3	B	1394	AMP	C5-C6	2.91	1.49	1.41
3	A	1394	AMP	C8-N7	2.66	1.36	1.31
3	A	1394	AMP	C5-C6	2.52	1.48	1.41
3	A	1394	AMP	C5-N7	-2.47	1.34	1.39
3	B	1394	AMP	C8-N7	2.35	1.36	1.31
3	B	1394	AMP	C5-N7	-2.03	1.35	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1394	AMP	C5-C4-N3	-6.20	118.18	126.72
3	B	1394	AMP	C5-C4-N3	-5.93	118.55	126.72
3	B	1394	AMP	N3-C4-N9	4.50	134.82	127.17
3	A	1394	AMP	N3-C4-N9	4.26	134.42	127.17
3	B	1394	AMP	C2-N3-C4	4.05	121.73	111.83
3	A	1394	AMP	C2-N3-C4	3.94	121.46	111.83
3	A	1394	AMP	C4-C5-N7	-3.70	106.35	110.58
3	B	1394	AMP	C4-C5-N7	-3.68	106.37	110.58
3	B	1394	AMP	N3-C2-N1	-3.65	123.05	128.58
3	A	1394	AMP	N3-C2-N1	-3.33	123.53	128.58
3	A	1394	AMP	O2P-P-O5'	-2.80	99.37	106.67
3	B	1394	AMP	C5-N7-C8	2.62	107.57	103.45
3	B	1394	AMP	C4-N9-C8	2.53	108.39	105.74
3	B	1394	AMP	C6-C5-N7	2.49	136.89	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1394	AMP	O3P-P-O2P	2.42	116.89	107.80
3	A	1394	AMP	C5-N7-C8	2.37	107.18	103.45
3	A	1394	AMP	C6-C5-N7	2.21	136.35	132.09
3	B	1394	AMP	C2'-C3'-C4'	2.20	106.86	102.61
3	A	1394	AMP	C2'-C3'-C4'	2.08	106.63	102.61
3	A	1394	AMP	C2-N1-C6	2.05	122.09	118.73
3	B	1394	AMP	N9-C8-N7	-2.05	111.03	113.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

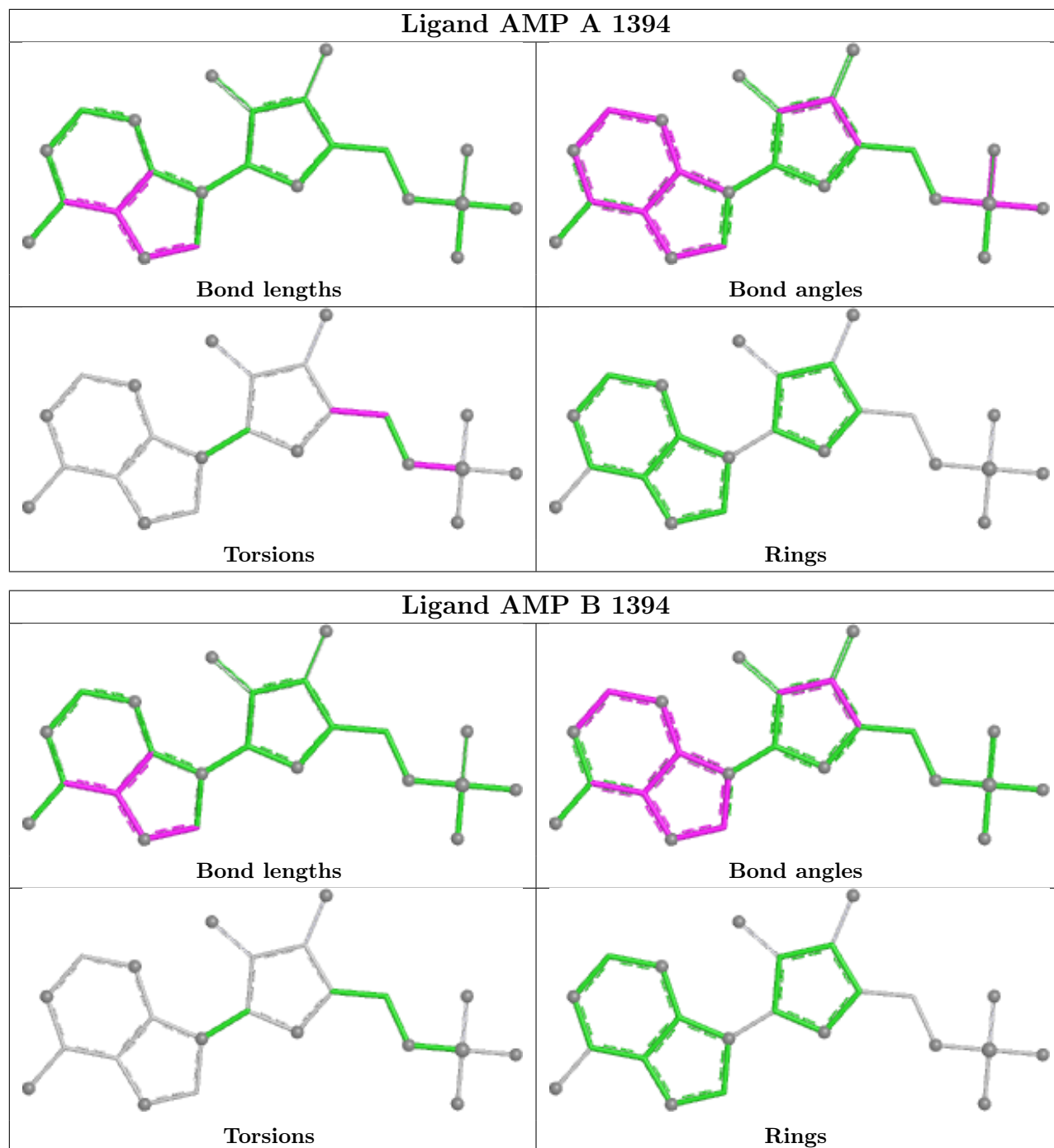
Mol	Chain	Res	Type	Atoms
3	A	1394	AMP	C5'-O5'-P-O2P
3	A	1394	AMP	C5'-O5'-P-O3P
3	A	1394	AMP	O4'-C4'-C5'-O5'
3	A	1394	AMP	C5'-O5'-P-O1P
3	A	1394	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1394	AMP	1	0
3	B	1394	AMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	366/395 (92%)	0.53	41 (11%) 10 8	31, 59, 119, 171	0
1	B	366/395 (92%)	0.47	35 (9%) 13 10	30, 58, 118, 171	0
2	E	239/284 (84%)	0.76	25 (10%) 11 9	35, 64, 107, 147	0
2	F	237/284 (83%)	0.62	21 (8%) 15 12	42, 69, 106, 142	0
All	All	1208/1358 (88%)	0.58	122 (10%) 12 9	30, 62, 113, 171	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	LEU	6.1
1	A	319	LEU	5.5
1	A	324	ILE	5.2
1	B	324	ILE	4.9
2	E	598	THR	4.3
1	B	372	MET	4.2
1	A	321	ALA	4.1
1	B	322	ARG	4.0
1	A	390	ILE	3.9
1	B	321	ALA	3.8
1	A	393	LEU	3.8
1	A	136	GLY	3.7
1	A	325	ASP	3.7
1	A	320	LEU	3.6
1	B	325	ASP	3.6
2	F	600	LEU	3.6
2	E	851	ASN	3.5
1	A	323	GLY	3.5
2	E	813	SER	3.5
1	B	136	GLY	3.5
1	B	125	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	802	SER	3.5
2	E	638	TRP	3.4
1	A	341	LYS	3.4
2	E	684	GLU	3.3
1	A	326	VAL	3.3
2	E	737	ALA	3.2
2	E	577	ASN	3.2
1	B	389	ASP	3.2
1	A	322	ARG	3.2
1	A	382	GLN	3.2
1	A	379	TYR	3.2
1	B	371	ALA	3.1
1	B	233	GLY	3.1
2	F	598	THR	3.1
2	E	729	MET	3.1
2	F	812	GLY	3.0
1	B	206	ASN	3.0
1	B	326	VAL	3.0
2	F	802	SER	3.0
1	B	343	ASN	3.0
2	F	777	ASP	2.9
2	F	829	THR	2.9
2	F	582	LYS	2.9
2	F	577	ASN	2.9
1	A	125	ILE	2.9
2	E	800	THR	2.9
2	F	599	GLU	2.9
1	A	69	GLY	2.9
1	A	327	GLN	2.9
1	A	232	GLU	2.8
2	F	778	SER	2.8
2	E	580	VAL	2.8
1	B	328	GLN	2.8
2	E	678	ASN	2.8
2	E	733	TYR	2.8
1	A	389	ASP	2.7
1	B	320	LEU	2.7
1	B	327	GLN	2.7
1	A	227	ASP	2.7
1	B	337	LEU	2.7
1	B	375	LEU	2.7
1	A	373	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	340	ASN	2.6
2	E	715	LEU	2.6
1	A	226	LYS	2.6
2	E	736	ALA	2.6
1	B	12	GLN	2.5
2	F	850	LYS	2.5
2	F	733	TYR	2.5
1	B	234	ILE	2.5
2	E	698	TYR	2.5
1	A	158	ARG	2.4
1	B	390	ILE	2.4
1	B	393	LEU	2.4
2	E	600	LEU	2.4
2	E	801	ASP	2.4
2	E	776	THR	2.4
1	A	330	SER	2.4
1	B	18	ASP	2.4
1	A	14	GLN	2.4
1	A	372	MET	2.3
2	E	812	GLY	2.3
1	B	367	GLU	2.3
2	E	599	GLU	2.3
1	B	382	GLN	2.3
2	E	578	ARG	2.3
1	A	343	ASN	2.3
1	A	138	ARG	2.3
2	E	828	GLN	2.3
2	F	737	ALA	2.3
2	F	734	TYR	2.3
1	B	282	ASN	2.3
1	A	378	PHE	2.3
2	F	678	ASN	2.2
1	B	323	GLY	2.2
2	E	685	THR	2.2
1	A	12	GLN	2.2
2	F	675	LYS	2.2
2	F	831	LYS	2.2
1	A	339	ALA	2.2
1	A	137	LEU	2.2
2	F	601	LEU	2.2
2	E	712	THR	2.2
1	A	375	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	663	SER	2.2
1	B	14	GLN	2.1
1	B	358	GLY	2.1
1	A	329	VAL	2.1
2	F	774	ASP	2.1
2	F	603	LYS	2.1
1	B	303	MET	2.1
1	A	233	GLY	2.1
1	A	344	TYR	2.1
1	A	51	ARG	2.1
1	B	381	THR	2.1
1	A	345	ILE	2.1
1	B	377	LYS	2.0
1	A	328	GLN	2.0
1	B	362	ASN	2.0
1	A	305	GLU	2.0
1	B	364	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

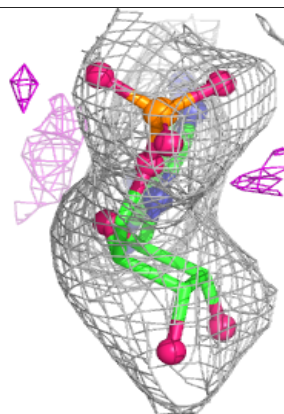
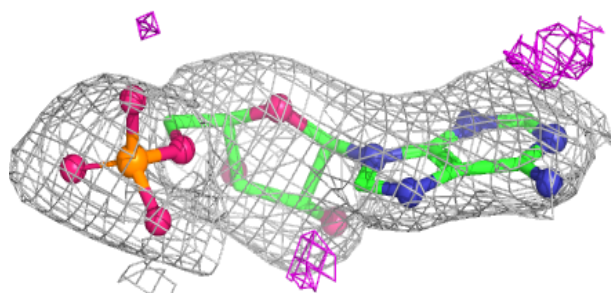
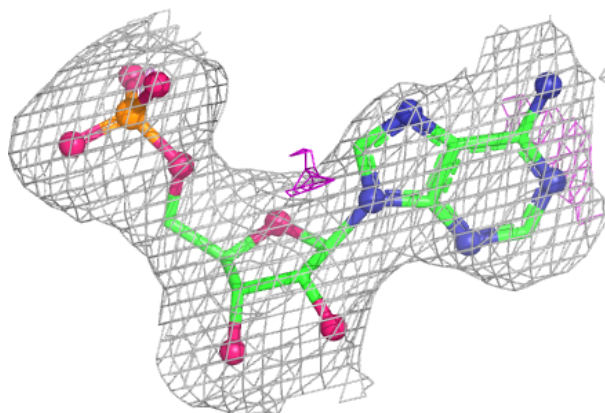
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	A	1394	23/23	0.93	0.11	38,56,75,78	0
3	AMP	B	1394	23/23	0.94	0.12	34,67,73,89	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.

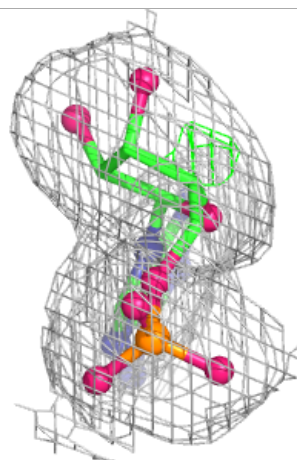
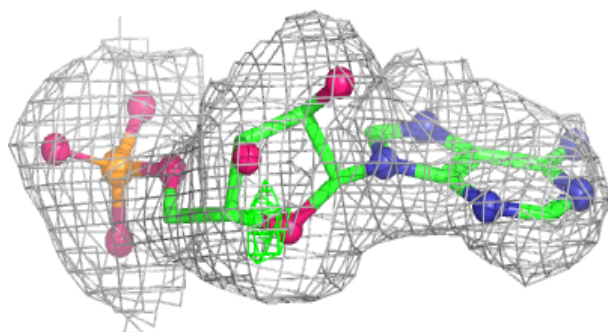
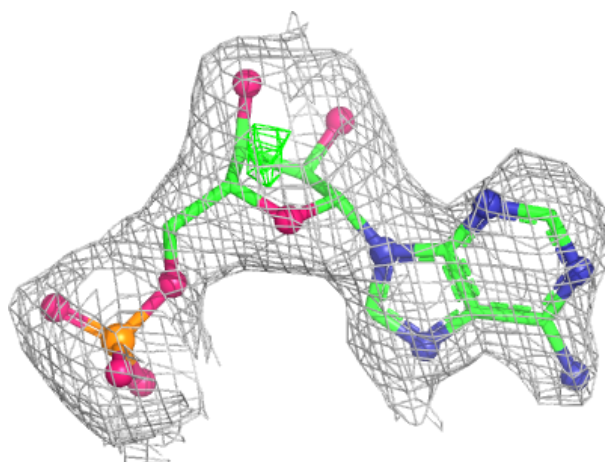
Electron density around AMP A 1394:

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



Electron density around AMP B 1394:

$2mF_o-DF_c$ (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.