



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 12:36 PM JST

PDB ID : 9ILZ / pdb_00009ilz
EMDB ID : EMD-60677
Title : The Cryo-EM structure of MPXV E5 in complex with ssDNA
Authors : Cheng, Y.X.; Han, P.; Wang, H.
Deposited on : 2024-07-01
Resolution : 2.95 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

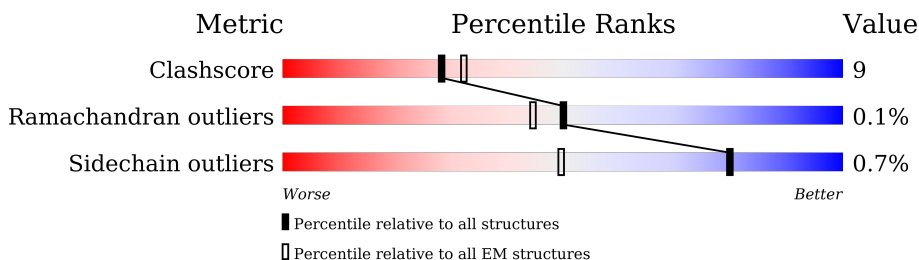
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	785	
1	B	785	
1	C	785	
1	D	785	
1	E	785	
1	F	785	
2	X	7	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27776 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Primase D5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	768	Total	C	N	O	S	0	0
			6218	3964	1054	1168	32		
1	B	465	Total	C	N	O	S	0	0
			3764	2410	632	705	17		
1	C	464	Total	C	N	O	S	0	0
			3756	2404	631	704	17		
1	D	465	Total	C	N	O	S	0	0
			3764	2410	632	705	17		
1	E	691	Total	C	N	O	S	0	0
			5599	3559	947	1063	30		
1	F	546	Total	C	N	O	S	0	0
			4414	2828	746	820	20		

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*T)-3').

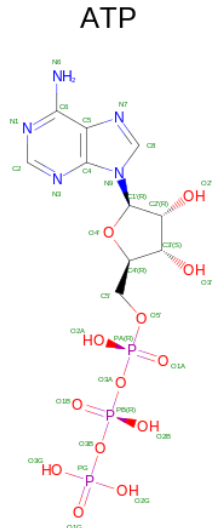
Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	7	Total	C	N	O	P	0	0
			140	70	14	49	7		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

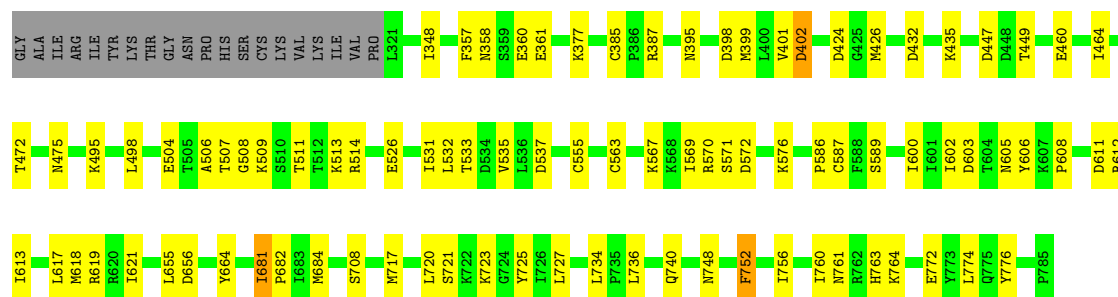
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0

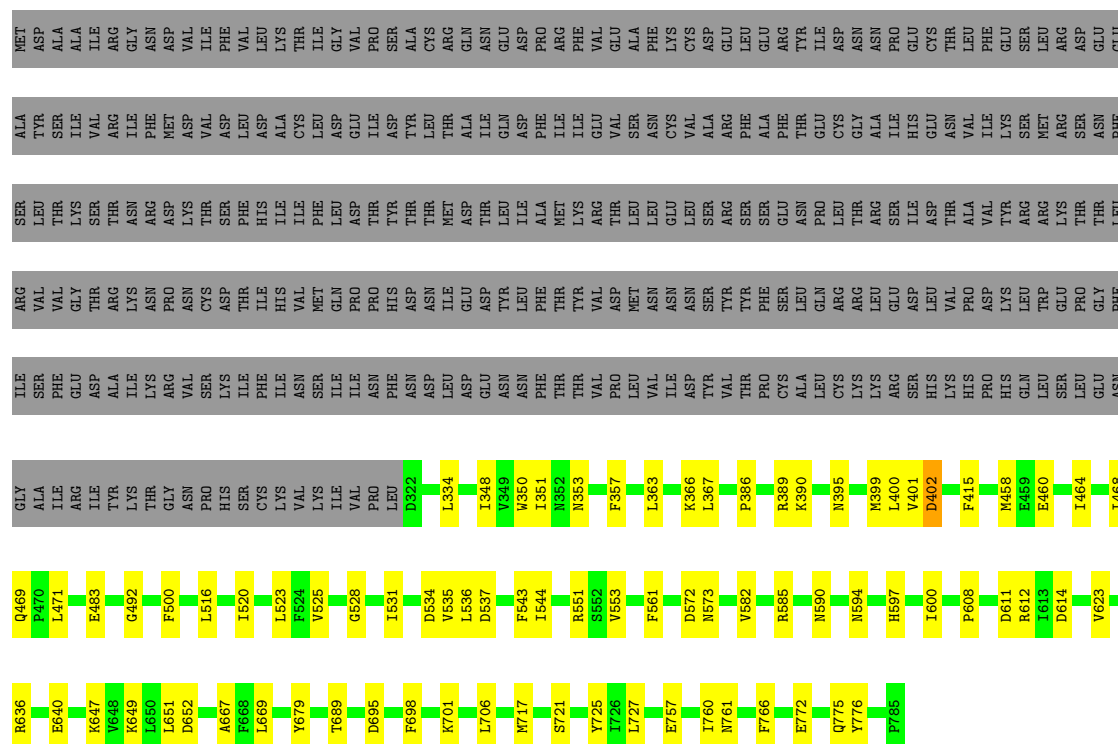
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	F	1	Total	Zn	0
			1	1	



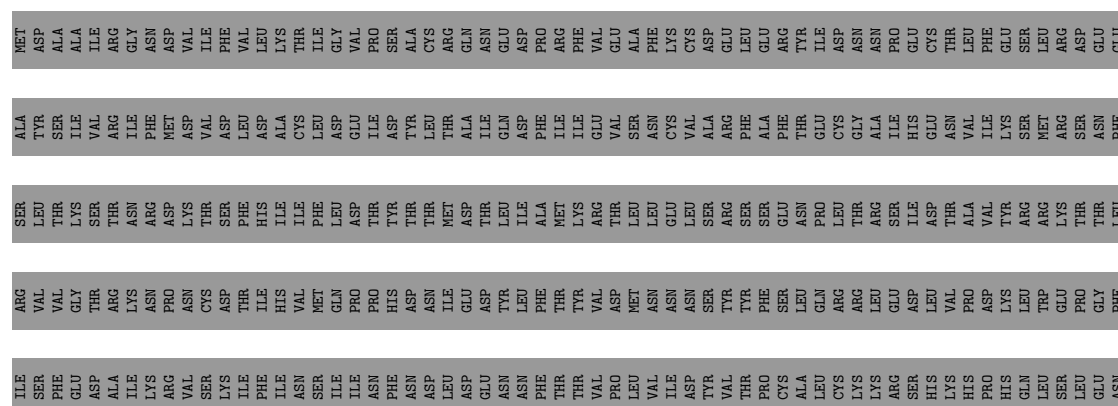
• Molecule 1: Primase D5

Chain C: 49% 10% 41%



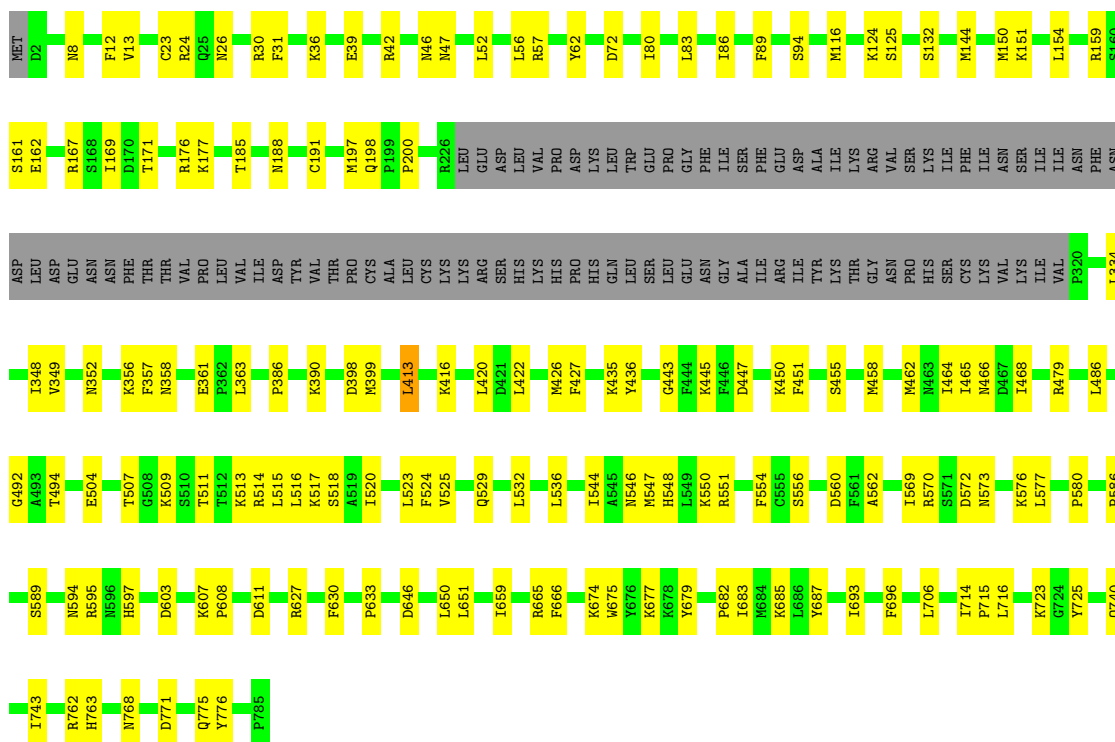
• Molecule 1: Primase D5

Chain D: 46% 12% 41%

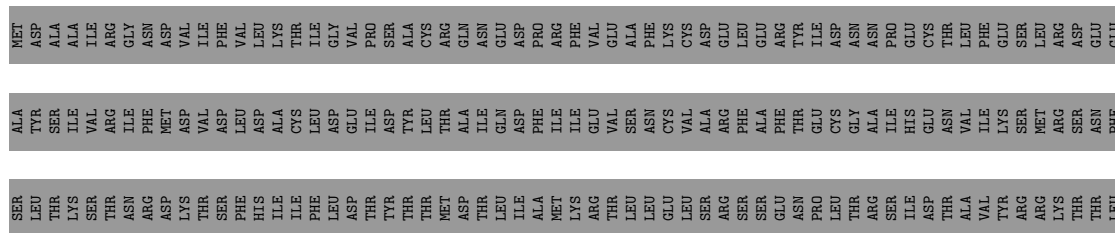


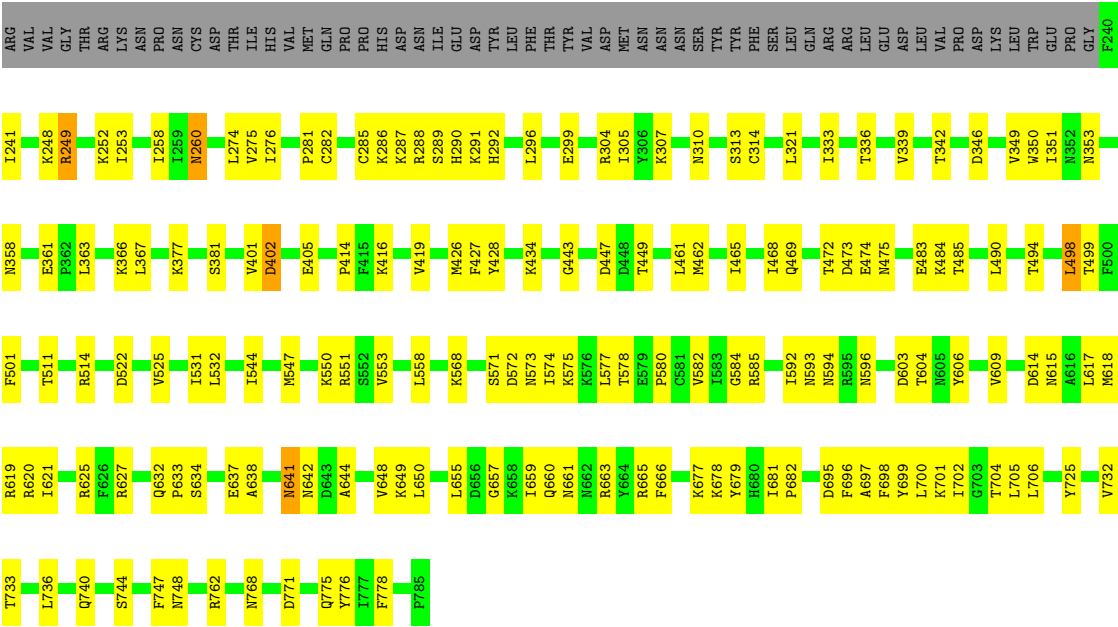


- Molecule 1: Primase D5

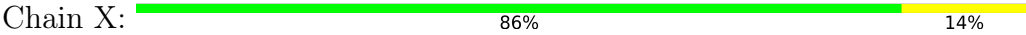


- Molecule 1: Primase D5





● Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*T)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	339072	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, ZN

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	0.14	0/6349	0.38	3/8586 (0.0%)
1	B	0.11	0/3845	0.33	0/5193
1	C	0.10	0/3837	0.30	0/5182
1	D	0.11	0/3845	0.31	0/5193
1	E	0.11	0/5713	0.30	0/7723
1	F	0.12	0/4511	0.35	0/6096
2	X	0.14	0/153	0.44	0/234
All	All	0.12	0/28253	0.33	3/38207 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	PRO	CA-N-CD	-5.81	103.86	112.00
1	A	115	SER	CA-C-N	-5.04	115.07	122.83
1	A	115	SER	C-N-CA	-5.04	115.07	122.83

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	6218	0	6216	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3764	0	3785	62	0
1	C	3756	0	3774	49	0
1	D	3764	0	3785	67	0
1	E	5599	0	5577	103	0
1	F	4414	0	4448	114	0
2	X	140	0	85	1	0
3	A	27	0	12	4	0
4	A	31	0	12	1	0
4	B	31	0	12	2	0
4	C	31	0	12	2	0
5	F	1	0	0	0	0
All	All	27776	0	27718	515	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 9.

All (515) 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:657:GLY:HA2	1:F:660:GLN:HE21	1.44	0.83
1:B:681:ILE:HG13	1:B:682:PRO:HD3	1.62	0.81
1:A:681:ILE:HD12	1:A:682:PRO:HD3	1.63	0.80
1:A:618:MET:H	1:A:618:MET:HE3	1.48	0.79
1:F:740:GLN:HA	1:F:744:SER:HB3	1.65	0.77
1:E:546:ASN:O	1:E:550:LYS:NZ	2.19	0.76
1:F:290:HIS:CD2	1:F:314:CYS:SG	2.78	0.75
1:D:652:ASP:HB3	1:D:655:LEU:HD23	1.70	0.74
1:B:555:CYS:HB2	1:B:602:ILE:HG12	1.70	0.74
1:A:361:GLU:OE2	1:A:361:GLU:N	2.18	0.73
1:F:258:ILE:HG22	1:F:276:ILE:HG22	1.70	0.73
1:E:462:MET:O	1:E:466:ASN:ND2	2.22	0.72
1:A:692:GLU:HG2	1:A:693:ILE:HG12	1.71	0.72
1:F:260:ASN:OD1	1:F:260:ASN:N	2.21	0.71
1:E:518:SER:O	1:E:665:ARG:NH1	2.25	0.70
1:B:717:MET:HG2	1:B:727:LEU:HD12	1.75	0.69
1:A:197:MET:HA	1:A:197:MET:HE2	1.74	0.69
1:E:494:THR:HG21	1:E:580:PRO:HA	1.74	0.69
1:A:21:SER:HA	1:A:24:ARG:HE	1.58	0.69
1:E:447:ASP:HB3	1:E:450:LYS:HE2	1.75	0.68
1:F:292:HIS:HB2	1:F:307:LYS:HE2	1.76	0.68
1:A:684:MET:HE2	1:A:684:MET:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:GLN:O	1:C:775:GLN:NE2	2.27	0.68
1:F:405:GLU:OE1	1:F:405:GLU:N	2.19	0.67
1:F:681:ILE:HG13	1:F:682:PRO:HD3	1.75	0.67
1:F:573:ASN:O	1:F:577:LEU:HB2	1.96	0.66
1:A:417:ASN:HD21	1:A:446:PHE:HB3	1.62	0.65
1:E:560:ASP:OD2	1:F:762:ARG:NH2	2.30	0.65
1:E:576:LYS:HG3	1:E:577:LEU:HD12	1.76	0.65
1:F:604:THR:HG22	1:F:606:TYR:H	1.61	0.65
1:C:721:SER:HA	1:C:725:TYR:HB3	1.78	0.65
1:A:570:ARG:HB2	1:A:573:ASN:HB2	1.79	0.64
1:B:514:ARG:NH2	1:B:656:ASP:OD1	2.31	0.64
1:E:524:PHE:HE1	1:E:554:PHE:HB3	1.62	0.64
1:A:116:MET:O	1:A:117:ARG:NH1	2.31	0.64
1:F:287:LYS:HD3	1:F:288:ARG:H	1.62	0.64
1:A:223:LEU:HD12	1:A:227:LEU:HD21	1.78	0.64
1:A:490:LEU:O	1:A:551:ARG:NH1	2.30	0.64
1:A:214:MET:HE3	1:A:214:MET:HA	1.79	0.64
1:A:348:ILE:HG22	1:A:357:PHE:HB3	1.80	0.63
1:A:69:MET:HA	1:A:69:MET:HE3	1.80	0.63
1:E:334:LEU:HD12	1:E:399:MET:HE3	1.80	0.63
1:E:198:GLN:HG3	1:E:200:PRO:HD2	1.79	0.63
1:B:720:LEU:HD13	1:B:723:LYS:HD2	1.80	0.63
1:E:24:ARG:NH2	1:E:56:LEU:O	2.31	0.63
1:B:507:THR:OG1	1:B:509:LYS:NZ	2.32	0.62
1:A:677:LYS:HD3	1:A:681:ILE:HG12	1.81	0.62
1:D:426:MET:HE1	1:D:428:TYR:CZ	2.35	0.62
1:D:660:GLN:CD	1:D:660:GLN:H	2.07	0.62
1:F:725:TYR:HD2	1:F:732:VAL:HB	1.65	0.62
1:A:119:ASN:ND2	1:A:139:ASP:OD2	2.32	0.62
1:A:144:MET:HE3	1:A:144:MET:O	2.00	0.62
1:D:531:ILE:O	1:D:573:ASN:ND2	2.33	0.62
1:F:377:LYS:O	1:F:377:LYS:NZ	2.32	0.62
1:D:717:MET:HE3	1:D:717:MET:HA	1.82	0.61
1:E:511:THR:O	1:E:515:LEU:HG	2.00	0.61
1:F:490:LEU:O	1:F:551:ARG:NH1	2.31	0.61
1:F:568:LYS:HE3	1:F:609:VAL:HG13	1.82	0.61
1:B:426:MET:HE3	1:B:426:MET:H	1.65	0.61
1:F:657:GLY:CA	1:F:660:GLN:HE21	2.11	0.61
1:D:697:ALA:HA	1:D:700:LEU:HD23	1.82	0.61
1:F:584:GLY:O	1:F:594:ASN:ND2	2.34	0.61
1:C:572:ASP:OD2	1:C:573:ASN:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:757:GLU:O	1:C:761:ASN:ND2	2.34	0.61
1:D:531:ILE:HA	1:D:536:LEU:HD21	1.83	0.61
1:F:657:GLY:O	1:F:660:GLN:NE2	2.34	0.61
1:D:763:HIS:O	1:D:775:GLN:NE2	2.29	0.60
1:A:248:LYS:O	1:A:252:LYS:HG3	2.01	0.60
1:E:159:ARG:O	1:E:167:ARG:NH1	2.33	0.60
1:F:426:MET:HE2	1:F:426:MET:HA	1.83	0.60
1:B:531:ILE:HG13	1:B:532:LEU:HD12	1.83	0.60
1:D:695:ASP:OD1	1:D:695:ASP:N	2.33	0.60
1:A:499:THR:HB	1:A:601:ILE:HG12	1.83	0.60
1:E:633:PRO:HG3	1:E:650:LEU:HD21	1.84	0.60
1:E:529:GLN:NE2	1:E:556:SER:O	2.35	0.59
1:D:342:THR:OG1	1:D:346:ASP:OD1	2.20	0.59
1:E:573:ASN:HA	1:E:576:LYS:HG2	1.85	0.59
1:C:401:VAL:O	1:C:402:ASP:HB2	2.02	0.59
1:D:615:ASN:HA	1:D:618:MET:HG3	1.83	0.59
1:D:492:GLY:O	1:D:597:HIS:ND1	2.34	0.59
1:A:618:MET:H	1:A:618:MET:CE	2.16	0.58
1:C:582:VAL:HG23	1:C:594:ASN:HB2	1.83	0.58
1:F:582:VAL:HG12	1:F:594:ASN:HB2	1.83	0.58
1:B:395:ASN:O	1:B:399:MET:HG3	2.02	0.58
1:F:572:ASP:HA	1:F:575:LYS:HG2	1.84	0.58
1:E:455:SER:HB2	1:E:458:MET:SD	2.43	0.58
1:A:113:ILE:O	1:A:117:ARG:HG2	2.03	0.58
1:D:723:LYS:HE2	1:D:782:ILE:HG22	1.84	0.58
1:D:469:GLN:O	1:D:479:ARG:NH1	2.37	0.58
1:A:249:ARG:HA	1:A:252:LYS:HE2	1.84	0.58
1:B:348:ILE:HG22	1:B:357:PHE:HB3	1.85	0.58
1:C:492:GLY:O	1:C:597:HIS:ND1	2.37	0.58
1:D:548:HIS:HE1	1:D:595:ARG:HG3	1.69	0.57
1:A:285:CYS:C	1:A:286:LYS:HE2	2.29	0.57
1:C:483:GLU:HG3	1:C:679:TYR:HE2	1.69	0.57
1:C:500:PHE:HB2	1:C:623:VAL:HG22	1.86	0.57
1:E:413:LEU:HD23	1:E:422:LEU:HD21	1.85	0.57
1:A:281:PRO:HA	1:A:288:ARG:HH22	1.69	0.57
1:E:706:LEU:HD21	1:E:776:TYR:HD1	1.69	0.57
1:A:236:TRP:O	1:A:236:TRP:CE3	2.57	0.57
1:A:507:THR:N	3:A:801:ADP:O1B	2.36	0.57
1:E:685:LYS:HB3	1:E:687:TYR:HE2	1.68	0.57
1:B:424:ASP:HB2	1:B:426:MET:HE1	1.87	0.57
1:B:736:LEU:HD21	1:B:772:GLU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TRP:O	1:A:236:TRP:HE3	1.88	0.56
1:A:286:LYS:HE2	1:A:286:LYS:N	2.20	0.56
1:E:462:MET:HE3	1:E:462:MET:HA	1.87	0.56
1:F:333:ILE:O	1:F:336:THR:OG1	2.23	0.56
1:F:638:ALA:O	1:F:642:ASN:ND2	2.38	0.56
1:A:40:LEU:HD11	1:A:204:ILE:HG21	1.86	0.56
1:F:627:ARG:NH2	1:F:644:ALA:O	2.39	0.56
1:A:288:ARG:CZ	1:A:288:ARG:HA	2.35	0.56
1:F:285:CYS:SG	1:F:290:HIS:HE1	2.27	0.56
1:C:395:ASN:O	1:C:399:MET:HG3	2.05	0.56
1:A:71:VAL:O	1:A:132:SER:HA	2.05	0.56
1:A:720:LEU:HD12	1:A:723:LYS:HD2	1.85	0.56
1:B:495:LYS:HD2	1:B:684:MET:HE1	1.87	0.56
1:A:570:ARG:H	1:A:570:ARG:HD3	1.71	0.55
1:B:426:MET:H	1:B:426:MET:CE	2.19	0.55
1:E:536:LEU:HD13	1:E:544:ILE:HG13	1.87	0.55
1:C:706:LEU:HD12	1:C:776:TYR:HB3	1.87	0.55
1:D:523:LEU:HD13	1:D:551:ARG:HD2	1.88	0.55
1:F:514:ARG:NH1	1:F:514:ARG:HB2	2.22	0.55
1:E:124:LYS:NZ	1:E:197:MET:O	2.40	0.55
1:C:334:LEU:HD11	1:C:400:LEU:HD13	1.89	0.55
1:F:641:ASN:OD1	1:F:641:ASN:N	2.40	0.55
1:F:706:LEU:HD22	1:F:776:TYR:HB3	1.87	0.55
1:A:681:ILE:HD12	1:A:682:PRO:CD	2.34	0.55
1:E:151:LYS:HG3	1:E:171:THR:HB	1.88	0.55
1:F:282:CYS:SG	1:F:290:HIS:CD2	2.89	0.54
1:B:506:ALA:N	4:B:901:ATP:O1B	2.40	0.54
1:F:414:PRO:HA	1:F:419:VAL:HG22	1.90	0.54
1:A:532:LEU:HB3	1:A:569:ILE:HD12	1.89	0.54
1:C:523:LEU:HD13	1:C:551:ARG:HD2	1.89	0.54
1:E:504:GLU:O	1:E:509:LYS:NZ	2.39	0.54
1:F:462:MET:HE2	1:F:462:MET:N	2.22	0.54
1:A:483:GLU:OE1	1:A:678:LYS:NZ	2.36	0.54
1:A:706:LEU:HD22	1:A:778:PHE:HA	1.89	0.54
1:D:498:LEU:HD22	1:D:600:ILE:HB	1.90	0.54
1:D:562:ALA:HB1	1:E:762:ARG:HD3	1.90	0.54
1:E:525:VAL:HB	1:E:550:LYS:HD2	1.89	0.54
1:F:248:LYS:O	1:F:252:LYS:HG2	2.08	0.54
1:E:586:PRO:HB2	1:E:589:SER:HB3	1.89	0.54
1:F:547:MET:O	1:F:547:MET:HE2	2.08	0.54
1:C:585:ARG:NH1	2:X:3:DT:OP1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:447:ASP:OD2	1:F:449:THR:OG1	2.24	0.54
1:A:591:LYS:O	1:A:593:ASN:N	2.40	0.54
1:E:386:PRO:O	1:E:390:LYS:HG2	2.08	0.54
1:E:514:ARG:HD3	1:E:659:ILE:HG21	1.89	0.53
1:B:464:ILE:HD13	1:B:655:LEU:HD11	1.89	0.53
1:B:618:MET:SD	1:B:619:ARG:HG3	2.49	0.53
1:D:348:ILE:HG22	1:D:357:PHE:HB3	1.90	0.53
1:E:547:MET:HE2	1:E:547:MET:O	2.08	0.53
1:D:709:SER:HA	1:D:713:HIS:HD2	1.73	0.53
1:D:759:PHE:HA	1:D:763:HIS:CE1	2.43	0.53
1:F:402:ASP:OD2	1:F:402:ASP:N	2.35	0.53
1:E:420:LEU:HD23	1:E:427:PHE:HB2	1.91	0.53
1:F:260:ASN:HD21	1:F:275:VAL:HG12	1.74	0.53
1:F:473:ASP:OD1	1:F:474:GLU:N	2.41	0.53
1:A:124:LYS:HB3	1:A:196:VAL:HB	1.91	0.52
1:E:125:SER:HG	1:E:132:SER:HG	1.57	0.52
1:F:531:ILE:HD12	1:F:532:LEU:N	2.24	0.52
1:D:358:ASN:ND2	1:D:361:GLU:OE1	2.42	0.52
1:B:533:THR:HA	1:B:567:LYS:HZ1	1.74	0.52
1:F:472:THR:OG1	1:F:475:ASN:ND2	2.36	0.52
1:B:734:LEU:HD23	1:B:774:LEU:HB3	1.92	0.52
1:A:71:VAL:O	1:A:132:SER:CA	2.58	0.52
1:A:514:ARG:NH2	1:A:660:GLN:OE1	2.43	0.52
1:D:586:PRO:HG2	1:D:589:SER:HB3	1.92	0.52
1:F:733:THR:HG21	1:F:775:GLN:HA	1.92	0.52
1:E:458:MET:O	1:E:462:MET:HG2	2.10	0.52
1:B:533:THR:HA	1:B:567:LYS:NZ	2.25	0.51
1:E:775:GLN:CD	1:E:775:GLN:H	2.18	0.51
1:B:736:LEU:O	1:B:740:GLN:HG2	2.11	0.51
1:E:520:ILE:HD11	1:E:524:PHE:HB2	1.91	0.51
1:A:66:ARG:HE	1:A:141:TYR:HE1	1.57	0.51
1:B:611:ASP:OD1	1:B:611:ASP:N	2.43	0.51
1:E:39:GLU:HB2	1:E:42:ARG:HH21	1.74	0.51
1:C:471:LEU:HD23	1:C:471:LEU:H	1.75	0.51
1:E:176:ARG:HE	1:E:177:LYS:HG2	1.74	0.51
1:F:342:THR:OG1	1:F:346:ASP:OD1	2.28	0.51
1:A:304:ARG:HD3	1:E:80:ILE:HG21	1.93	0.51
1:C:348:ILE:HG22	1:C:357:PHE:HB3	1.92	0.51
1:F:637:GLU:H	1:F:637:GLU:CD	2.17	0.51
1:C:698:PHE:O	1:C:701:LYS:HG2	2.10	0.51
1:A:262:ASN:OD1	1:A:262:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:MET:O	1:B:721:SER:N	2.44	0.51
1:B:760:ILE:O	1:B:764:LYS:N	2.43	0.51
1:A:260:ASN:HD22	1:A:274:LEU:HA	1.76	0.51
1:B:535:VAL:HG12	1:B:537:ASP:H	1.76	0.51
1:D:611:ASP:OD1	1:D:611:ASP:N	2.44	0.51
1:D:726:ILE:O	1:D:733:THR:OG1	2.26	0.51
1:A:299:GLU:HG2	1:A:300:ASN:OD1	2.11	0.50
1:A:442:THR:O	1:A:521:GLY:HA3	2.10	0.50
1:E:150:MET:HG2	1:E:154:LEU:HD13	1.92	0.50
1:E:627:ARG:NH2	1:E:646:ASP:OD1	2.43	0.50
1:A:95:ASN:O	1:A:99:ARG:HG3	2.12	0.50
1:A:117:ARG:CZ	1:A:117:ARG:HA	2.41	0.50
1:A:757:GLU:HA	1:A:760:ILE:HG12	1.92	0.50
1:D:522:ASP:OD2	1:D:522:ASP:N	2.33	0.50
1:E:348:ILE:HG22	1:E:357:PHE:HB3	1.92	0.50
1:A:3:ALA:O	1:A:5:ILE:N	2.41	0.50
1:B:752:PHE:HB2	1:B:756:ILE:HD13	1.93	0.50
1:D:735:PRO:HB2	1:D:738:THR:HG22	1.92	0.50
1:D:548:HIS:CE1	1:D:595:ARG:HG3	2.47	0.50
1:E:492:GLY:O	1:E:597:HIS:ND1	2.44	0.50
1:E:675:TRP:O	1:E:679:TYR:HB2	2.12	0.50
1:A:402:ASP:OD1	1:A:402:ASP:N	2.35	0.50
1:B:447:ASP:OD2	1:B:449:THR:OG1	2.21	0.50
1:A:237:GLU:HB2	1:A:298:LEU:HD22	1.94	0.50
1:A:461:LEU:HD11	1:A:664:TYR:HB3	1.93	0.50
1:A:574:ILE:HD11	1:A:617:LEU:HD11	1.93	0.50
1:D:389:ARG:NH1	1:E:398:ASP:OD2	2.44	0.50
1:E:532:LEU:HG	1:E:569:ILE:HD12	1.93	0.50
1:F:514:ARG:HB2	1:F:514:ARG:HH11	1.76	0.50
1:A:344:ARG:HD3	1:A:591:LYS:HE3	1.93	0.49
1:F:618:MET:HE3	1:F:618:MET:N	2.27	0.49
1:A:99:ARG:NH1	1:A:99:ARG:HB2	2.27	0.49
1:A:555:CYS:HB2	1:A:602:ILE:HG12	1.93	0.49
1:F:544:ILE:HD11	1:F:582:VAL:HG11	1.95	0.49
1:F:310:ASN:O	1:F:313:SER:OG	2.27	0.49
1:F:483:GLU:OE2	1:F:484:LYS:NZ	2.34	0.49
1:F:615:ASN:O	1:F:619:ARG:NH1	2.45	0.49
1:A:153:THR:O	1:A:156:GLU:HG3	2.12	0.49
1:A:334:LEU:HD22	1:A:399:MET:HE3	1.95	0.49
1:B:621:ILE:HD12	1:B:621:ILE:O	2.12	0.49
1:F:648:VAL:O	1:F:649:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:GLU:O	1:B:509:LYS:NZ	2.45	0.49
1:C:536:LEU:HD22	1:C:544:ILE:HD13	1.93	0.49
1:A:63:SER:HB2	1:A:144:MET:HB3	1.95	0.49
1:A:71:VAL:O	1:A:132:SER:N	2.46	0.49
1:A:153:THR:O	1:A:157:LEU:HG	2.12	0.49
1:C:647:LYS:HE2	1:C:649:LYS:HE3	1.94	0.49
1:E:161:SER:OG	1:E:162:GLU:N	2.46	0.49
1:A:124:LYS:HD2	1:A:133:PHE:HE1	1.78	0.48
1:E:682:PRO:HB2	1:E:683:ILE:HD12	1.95	0.48
1:F:416:LYS:NZ	1:F:443:GLY:O	2.46	0.48
1:F:578:THR:HG22	1:F:620:ARG:HH21	1.78	0.48
1:A:593:ASN:C	1:A:594:ASN:HD22	2.21	0.48
1:A:172:ALA:H	1:F:252:LYS:HZ3	1.60	0.48
1:F:532:LEU:HD23	1:F:532:LEU:H	1.78	0.48
1:E:23:CYS:HA	1:E:26:ASN:HB2	1.95	0.48
1:A:699:TYR:HA	1:A:702:ILE:HG12	1.95	0.48
1:B:763:HIS:O	1:B:763:HIS:ND1	2.47	0.48
1:D:657:GLY:HA2	1:D:660:GLN:HE22	1.78	0.48
1:F:577:LEU:O	1:F:596:ASN:ND2	2.47	0.48
1:B:424:ASP:CB	1:B:426:MET:HE1	2.43	0.48
1:E:517:LYS:NZ	1:E:517:LYS:O	2.46	0.48
1:F:291:LYS:HG3	1:F:292:HIS:ND1	2.29	0.48
1:E:504:GLU:O	1:E:507:THR:OG1	2.31	0.48
1:F:363:LEU:HD23	1:F:366:LYS:HE2	1.96	0.48
1:F:377:LYS:NZ	1:F:381:SER:OG	2.38	0.48
1:C:689:THR:O	1:C:689:THR:OG1	2.28	0.48
1:F:701:LYS:O	1:F:704:THR:OG1	2.29	0.48
1:B:508:GLY:O	1:B:511:THR:OG1	2.30	0.48
1:C:652:ASP:H	4:C:801:ATP:H8	1.62	0.48
1:A:66:ARG:HD2	1:A:209:PHE:HA	1.95	0.47
1:D:529:GLN:NE2	1:D:556:SER:O	2.47	0.47
1:E:607:LYS:HD3	1:E:608:PRO:HD2	1.95	0.47
1:C:757:GLU:HA	1:C:760:ILE:HG12	1.95	0.47
1:D:536:LEU:HD13	1:D:576:LYS:NZ	2.29	0.47
1:F:603:ASP:OD1	1:F:603:ASP:N	2.46	0.47
1:B:748:ASN:OD1	1:B:748:ASN:N	2.47	0.47
1:A:650:LEU:HD22	1:A:651:LEU:H	1.78	0.47
1:D:553:VAL:HB	1:D:600:ILE:HD13	1.96	0.47
1:D:734:LEU:HD23	1:D:774:LEU:HD12	1.95	0.47
1:B:401:VAL:O	1:B:402:ASP:HB2	2.14	0.47
1:C:458:MET:HE2	1:C:667:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:CD1	1:A:181:ARG:HA	2.50	0.47
1:A:63:SER:O	1:A:144:MET:N	2.48	0.47
1:A:108:ILE:HD12	1:A:109:HIS:H	1.80	0.47
1:A:651:LEU:HD12	3:A:801:ADP:H1'	1.95	0.47
1:E:465:ILE:HD13	1:E:479:ARG:HH22	1.80	0.47
1:F:461:LEU:HB3	1:F:462:MET:HE2	1.97	0.47
1:F:462:MET:HA	1:F:465:ILE:HG22	1.97	0.47
1:C:636:ARG:NH1	1:C:640:GLU:OE2	2.45	0.47
1:C:458:MET:HE2	1:C:458:MET:HA	1.97	0.47
1:A:424:ASP:OD1	1:A:424:ASP:N	2.42	0.46
1:B:426:MET:HE3	1:B:426:MET:N	2.30	0.46
1:D:658:LYS:HD2	1:D:663:ARG:HD3	1.97	0.46
1:D:742:LYS:O	1:D:745:LYS:NZ	2.48	0.46
1:F:426:MET:SD	1:F:427:PHE:N	2.88	0.46
1:A:535:VAL:HA	1:A:570:ARG:HH22	1.79	0.46
1:D:514:ARG:HH21	1:D:659:ILE:HD12	1.80	0.46
1:E:352:ASN:HB2	1:E:356:LYS:HZ3	1.80	0.46
1:F:522:ASP:O	1:F:550:LYS:NZ	2.31	0.46
1:F:661:ASN:HD21	1:F:663:ARG:HB2	1.80	0.46
1:A:14:LEU:HD23	1:A:32:VAL:HG22	1.97	0.46
1:C:651:LEU:HD12	4:C:801:ATP:H1'	1.98	0.46
1:D:532:LEU:HD23	1:D:532:LEU:H	1.79	0.46
1:E:36:LYS:H	1:E:39:GLU:CD	2.24	0.46
1:E:548:HIS:CE1	1:E:595:ARG:H	2.33	0.46
1:F:485:THR:HG21	1:F:499:THR:HG21	1.97	0.46
1:A:41:GLU:HA	1:A:44:ILE:HG12	1.97	0.46
1:D:709:SER:HA	1:D:713:HIS:CD2	2.49	0.46
1:E:723:LYS:HE3	1:E:725:TYR:HE2	1.81	0.46
1:F:655:LEU:O	1:F:659:ILE:HG12	2.14	0.46
1:C:528:GLY:H	1:C:543:PHE:HD2	1.63	0.46
1:E:548:HIS:CE1	1:E:594:ASN:HA	2.51	0.46
1:F:287:LYS:HD2	1:F:290:HIS:HD1	1.80	0.46
1:A:269:PHE:C	1:A:269:PHE:CD1	2.93	0.46
1:A:535:VAL:HG12	1:A:537:ASP:H	1.81	0.46
1:C:415:PHE:HZ	1:C:669:LEU:HD21	1.80	0.46
1:A:285:CYS:HB3	1:A:315:LYS:HD3	1.97	0.46
1:D:477:LYS:HE2	1:D:477:LYS:HB2	1.85	0.46
1:F:494:THR:HG21	1:F:580:PRO:HA	1.98	0.46
1:C:389:ARG:NH2	1:D:398:ASP:OD2	2.39	0.46
1:D:535:VAL:HG22	1:D:570:ARG:HH12	1.80	0.46
1:E:562:ALA:HB3	1:F:762:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:THR:HG21	4:B:901:ATP:H8	1.80	0.46
1:B:603:ASP:OD1	1:B:603:ASP:N	2.44	0.46
1:E:693:ILE:HG13	1:E:696:PHE:HB2	1.98	0.46
1:A:292:HIS:HB2	1:A:307:LYS:HE2	1.96	0.45
1:A:738:THR:HG22	1:A:742:LYS:HE3	1.98	0.45
1:C:766:PHE:HB3	1:C:772:GLU:HG2	1.98	0.45
1:D:636:ARG:O	1:D:636:ARG:NH1	2.48	0.45
1:F:241:ILE:HD11	1:F:321:LEU:HD22	1.98	0.45
1:B:432:ASP:O	1:B:435:LYS:NZ	2.38	0.45
1:E:451:PHE:HE1	1:E:666:PHE:HB3	1.80	0.45
1:A:145:ASP:OD1	1:A:145:ASP:N	2.49	0.45
1:B:684:MET:HE2	1:B:684:MET:HB3	1.85	0.45
1:F:426:MET:HG3	1:F:428:TYR:CE1	2.52	0.45
1:A:296:LEU:HD13	1:A:305:ILE:HG12	1.97	0.45
1:B:535:VAL:HG22	1:B:570:ARG:HH12	1.81	0.45
1:D:343:GLU:OE2	1:D:343:GLU:N	2.43	0.45
1:D:426:MET:HE1	1:D:428:TYR:CE1	2.51	0.45
1:D:748:ASN:HB2	1:D:751:LEU:HB2	1.97	0.45
1:E:72:ASP:OD1	1:E:72:ASP:N	2.50	0.45
1:A:150:MET:N	1:A:150:MET:HE3	2.32	0.45
1:A:170:ASP:OD1	1:A:170:ASP:N	2.49	0.45
1:A:187:LYS:NZ	4:A:802:ATP:O1G	2.49	0.45
1:A:112:VAL:HG13	1:A:116:MET:HE1	1.99	0.45
1:A:282:CYS:HB2	1:A:285:CYS:O	2.17	0.45
1:F:296:LEU:HD22	1:F:305:ILE:HG12	1.97	0.45
1:B:606:TYR:OH	1:C:614:ASP:OD2	2.30	0.45
1:A:701:LYS:HD2	1:A:702:ILE:HG23	1.99	0.45
1:B:460:GLU:OE2	1:B:664:TYR:OH	2.34	0.45
1:B:586:PRO:HG2	1:B:589:SER:HB3	1.99	0.45
1:C:531:ILE:O	1:C:573:ASN:ND2	2.49	0.45
1:D:701:LYS:O	1:D:705:LEU:HG	2.17	0.45
1:E:8:ASN:HB2	1:E:62:TYR:CE2	2.52	0.45
1:E:36:LYS:N	1:E:39:GLU:OE2	2.48	0.45
1:F:736:LEU:O	1:F:740:GLN:NE2	2.40	0.45
1:B:720:LEU:HD12	1:B:725:TYR:HE2	1.82	0.44
1:D:544:ILE:HG21	1:D:584:GLY:HA3	1.99	0.44
1:F:571:SER:O	1:F:574:ILE:HG13	2.17	0.44
1:A:754:HIS:O	1:A:757:GLU:HG3	2.17	0.44
1:B:708:SER:HA	1:B:776:TYR:HA	1.99	0.44
1:C:561:PHE:HE2	1:C:608:PRO:HA	1.82	0.44
1:D:759:PHE:HD1	1:D:763:HIS:HD1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:VAL:HG21	1:E:52:LEU:HD23	1.99	0.44
1:E:445:LYS:HA	1:E:445:LYS:HE2	1.99	0.44
1:F:525:VAL:HG23	1:F:553:VAL:HG12	1.99	0.44
1:B:385:CYS:SG	1:B:387:ARG:NH2	2.91	0.44
1:D:334:LEU:HD11	1:D:400:LEU:HD13	1.99	0.44
1:F:614:ASP:OD1	1:F:617:LEU:HD23	2.18	0.44
1:D:458:MET:HE2	1:D:458:MET:HA	2.00	0.44
1:E:188:ASN:HB2	1:E:191:CYS:HB2	1.99	0.44
1:F:705:LEU:HB2	1:F:778:PHE:CE1	2.52	0.44
1:B:612:ARG:HE	1:B:613:ILE:H	1.64	0.44
1:D:462:MET:C	1:D:462:MET:HE3	2.42	0.44
1:F:575:LYS:O	1:F:620:ARG:NH2	2.40	0.44
1:D:490:LEU:O	1:D:551:ARG:NH1	2.51	0.44
1:F:558:LEU:HD23	1:F:604:THR:OG1	2.18	0.44
1:F:625:ARG:H	1:F:625:ARG:HD3	1.83	0.44
1:A:524:PHE:HE1	1:A:554:PHE:HB2	1.83	0.44
1:B:472:THR:HG23	1:B:475:ASN:H	1.83	0.44
1:C:468:ILE:HG22	1:C:469:GLN:HG2	1.99	0.44
1:D:471:LEU:HG	1:D:479:ARG:NH1	2.33	0.44
1:D:658:LYS:HB3	1:D:663:ARG:HD3	2.00	0.44
1:E:486:LEU:HD23	1:E:675:TRP:HZ3	1.83	0.44
1:A:6:ARG:HH22	1:A:62:TYR:HD1	1.66	0.43
1:A:655:LEU:O	1:A:659:ILE:HG12	2.18	0.43
1:B:358:ASN:ND2	1:B:361:GLU:OE1	2.51	0.43
1:E:523:LEU:HD13	1:E:551:ARG:HG3	1.99	0.43
1:A:104:GLU:OE1	1:A:225:ARG:NH1	2.51	0.43
1:C:535:VAL:HG12	1:C:537:ASP:H	1.83	0.43
1:E:513:LYS:C	1:E:513:LYS:HD2	2.43	0.43
1:F:696:PHE:HA	1:F:699:TYR:CD2	2.53	0.43
1:A:361:GLU:H	1:A:361:GLU:CD	2.20	0.43
1:B:587:CYS:HB2	1:C:590:ASN:HD21	1.82	0.43
1:C:363:LEU:HD23	1:C:366:LYS:HD2	2.00	0.43
1:F:678:LYS:HE3	1:F:679:TYR:OH	2.17	0.43
1:C:386:PRO:O	1:C:390:LYS:HG2	2.18	0.43
1:D:743:ILE:HA	1:D:746:TYR:HD2	1.84	0.43
1:E:674:LYS:O	1:E:677:LYS:HG3	2.19	0.43
1:F:281:PRO:HG3	1:F:286:LYS:NZ	2.34	0.43
1:B:572:ASP:OD2	1:B:576:LYS:NZ	2.44	0.43
1:C:516:LEU:O	1:C:520:ILE:HG12	2.18	0.43
1:E:435:LYS:HE2	1:E:436:TYR:CZ	2.53	0.43
1:A:41:GLU:HG2	1:A:42:ARG:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:MET:C	1:A:426:MET:HE2	2.44	0.43
1:A:498:LEU:HG	1:A:600:ILE:HB	2.01	0.43
1:E:52:LEU:HB2	1:E:185:THR:HG21	2.00	0.43
1:E:451:PHE:CE1	1:E:666:PHE:HB3	2.54	0.43
1:F:358:ASN:OD1	1:F:361:GLU:N	2.51	0.43
1:A:122:LEU:HB3	1:A:198:GLN:HG2	2.01	0.43
1:C:351:ILE:HD11	1:C:367:LEU:HA	2.00	0.43
1:D:614:ASP:OD1	1:D:614:ASP:N	2.50	0.43
1:D:736:LEU:HG	1:D:740:GLN:OE1	2.19	0.43
1:E:89:PHE:HE1	1:E:169:ILE:HD11	1.84	0.43
1:E:83:LEU:O	1:E:86:ILE:HG22	2.19	0.43
1:E:570:ARG:HG2	1:E:572:ASP:H	1.84	0.43
1:E:630:PHE:HB3	1:E:651:LEU:HD12	2.01	0.43
1:F:593:ASN:OD1	1:F:593:ASN:N	2.50	0.43
1:F:677:LYS:HA	1:F:681:ILE:HG23	2.01	0.43
1:F:768:ASN:HB3	1:F:771:ASP:HB2	2.01	0.43
1:A:687:TYR:CD1	1:A:688:PRO:HD2	2.54	0.43
1:B:569:ILE:HD11	1:B:608:PRO:HB2	2.00	0.43
1:D:424:ASP:OD1	1:D:424:ASP:N	2.51	0.43
1:E:511:THR:O	1:E:514:ARG:HG2	2.19	0.43
1:F:351:ILE:HD11	1:F:367:LEU:HA	2.01	0.43
1:F:511:THR:HA	1:F:514:ARG:NH1	2.34	0.43
1:F:585:ARG:HD2	1:F:592:ILE:HG23	2.01	0.43
1:F:698:PHE:O	1:F:702:ILE:HG12	2.18	0.43
1:B:571:SER:HB3	1:B:617:LEU:HD21	2.01	0.42
1:F:748:ASN:OD1	1:F:748:ASN:N	2.52	0.42
1:B:360:GLU:HB2	1:B:361:GLU:OE2	2.19	0.42
1:F:697:ALA:HA	1:F:700:LEU:HG	1.99	0.42
1:B:498:LEU:HG	1:B:600:ILE:HB	2.00	0.42
1:B:618:MET:O	1:B:618:MET:HE2	2.18	0.42
1:E:8:ASN:HB2	1:E:62:TYR:HE2	1.84	0.42
1:E:464:ILE:O	1:E:468:ILE:HG13	2.19	0.42
1:E:516:LEU:O	1:E:520:ILE:HG12	2.20	0.42
1:F:299:GLU:OE2	1:F:304:ARG:NE	2.42	0.42
1:F:511:THR:HA	1:F:514:ARG:HH12	1.84	0.42
1:B:507:THR:HG1	1:B:509:LYS:NZ	2.16	0.42
1:E:176:ARG:HG3	1:E:177:LYS:HG2	2.02	0.42
1:E:349:VAL:HG11	1:E:363:LEU:HB3	2.01	0.42
1:E:518:SER:O	1:E:665:ARG:HG3	2.19	0.42
1:A:96:CYS:HA	1:A:99:ARG:NE	2.34	0.42
1:A:508:GLY:N	3:A:801:ADP:O1B	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LYS:HD2	1:A:679:TYR:CE1	2.54	0.42
1:B:513:LYS:NZ	1:B:526:GLU:OE2	2.52	0.42
1:C:460:GLU:O	1:C:464:ILE:HG12	2.19	0.42
1:E:556:SER:HA	1:E:603:ASP:HB3	2.00	0.42
1:A:152:ARG:O	1:A:155:LEU:HG	2.20	0.42
1:A:723:LYS:NZ	1:A:781:ASP:OD2	2.53	0.42
1:E:416:LYS:HD3	1:E:443:GLY:HA2	2.01	0.42
1:A:117:ARG:HA	1:A:117:ARG:NE	2.35	0.42
1:A:748:ASN:OD1	1:A:748:ASN:N	2.53	0.42
1:C:717:MET:HE3	1:C:727:LEU:HD13	2.01	0.42
1:D:503:GLY:O	1:D:605:ASN:HA	2.19	0.42
1:E:42:ARG:HE	1:E:42:ARG:HB3	1.69	0.42
1:C:706:LEU:HD13	1:C:706:LEU:HA	1.95	0.42
1:D:761:ASN:OD1	1:D:762:ARG:N	2.53	0.42
1:E:358:ASN:ND2	1:E:361:GLU:OE1	2.53	0.42
1:E:426:MET:SD	1:E:427:PHE:N	2.93	0.42
1:F:349:VAL:HG12	1:F:351:ILE:HG12	2.02	0.42
1:A:255:ILE:HD12	1:A:256:ASN:N	2.35	0.42
1:A:411:ASP:OD2	1:A:412:LYS:NZ	2.47	0.42
1:D:680:HIS:HB3	1:D:684:MET:HB2	2.02	0.42
1:E:768:ASN:HB2	1:E:771:ASP:HB2	2.02	0.42
1:C:400:LEU:HD12	1:C:400:LEU:HA	1.81	0.41
1:D:604:THR:OG1	1:D:606:TYR:O	2.35	0.41
1:F:291:LYS:HG3	1:F:292:HIS:HD1	1.84	0.41
1:A:90:ILE:HG21	1:A:117:ARG:HH22	1.85	0.41
1:A:469:GLN:HB3	1:A:479:ARG:HD3	2.01	0.41
1:D:520:ILE:HD11	1:D:524:PHE:HB2	2.02	0.41
1:F:468:ILE:HG22	1:F:469:GLN:HG2	2.02	0.41
1:A:40:LEU:HD21	1:A:204:ILE:HD12	2.01	0.41
1:A:156:GLU:OE1	1:A:159:ARG:NH2	2.53	0.41
1:C:350:TRP:CZ2	1:C:353:ASN:HA	2.55	0.41
1:E:716:LEU:H	1:E:716:LEU:HD23	1.85	0.41
1:A:17:ILE:HG23	1:A:53:PHE:HE2	1.85	0.41
1:A:144:MET:HE3	1:A:144:MET:C	2.46	0.41
1:A:350:TRP:CZ2	1:A:353:ASN:HA	2.56	0.41
1:B:377:LYS:HD2	1:B:377:LYS:N	2.35	0.41
1:B:567:LYS:HD3	1:B:567:LYS:C	2.45	0.41
1:A:175:ARG:NH1	1:A:176:ARG:O	2.53	0.41
1:F:350:TRP:CD2	1:F:434:LYS:HD2	2.56	0.41
1:F:531:ILE:H	1:F:531:ILE:HG13	1.68	0.41
1:A:652:ASP:H	3:A:801:ADP:H8	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:VAL:HB	1:C:600:ILE:HD13	2.02	0.41
1:E:144:MET:HE3	1:E:144:MET:O	2.21	0.41
1:E:413:LEU:HD23	1:E:422:LEU:HD11	2.03	0.41
1:E:416:LYS:HB2	1:E:443:GLY:HA2	2.01	0.41
1:F:632:GLN:HG2	1:F:634:SER:H	1.85	0.41
1:F:744:SER:OG	1:F:747:PHE:O	2.38	0.41
1:A:689:THR:HA	1:A:690:PRO:HD3	1.89	0.41
1:A:719:ASP:OD1	1:A:720:LEU:N	2.53	0.41
1:F:498:LEU:HB3	1:F:621:ILE:HD13	2.02	0.41
1:A:718:THR:O	1:A:721:SER:OG	2.30	0.41
1:C:611:ASP:OD1	1:C:611:ASP:N	2.52	0.41
1:E:30:ARG:HG3	1:E:31:PHE:CD2	2.55	0.41
1:E:46:ASN:OD1	1:E:47:ASN:N	2.54	0.41
1:F:665:ARG:HG2	1:F:666:PHE:CD2	2.55	0.41
1:D:359:SER:OG	1:D:360:GLU:OE1	2.31	0.41
1:E:12:PHE:CD2	1:E:57:ARG:HB3	2.55	0.41
1:F:604:THR:HG22	1:F:606:TYR:N	2.32	0.41
1:F:249:ARG:O	1:F:253:ILE:HG12	2.19	0.40
1:F:350:TRP:CZ2	1:F:353:ASN:HA	2.55	0.40
1:F:501:PHE:HB2	1:F:603:ASP:HB3	2.03	0.40
1:A:389:ARG:NH2	1:B:398:ASP:OD2	2.45	0.40
1:A:417:ASN:ND2	1:A:446:PHE:HB3	2.34	0.40
1:A:741:GLN:O	1:A:745:LYS:HG3	2.21	0.40
1:E:547:MET:HE2	1:E:547:MET:C	2.46	0.40
1:E:740:GLN:HA	1:E:743:ILE:HG12	2.03	0.40
1:F:288:ARG:HE	1:F:289:SER:N	2.19	0.40
1:A:163:ASN:HB2	1:A:166:THR:OG1	2.21	0.40
1:C:612:ARG:HD2	1:C:612:ARG:HA	1.82	0.40
1:E:714:ILE:N	1:E:715:PRO:HD2	2.37	0.40
1:F:350:TRP:CE2	1:F:434:LYS:HD2	2.56	0.40
1:F:574:ILE:HD11	1:F:617:LEU:HD11	2.02	0.40
1:A:225:ARG:HH22	1:A:231:VAL:HG23	1.87	0.40
1:A:255:ILE:HD12	1:A:255:ILE:C	2.46	0.40
1:B:761:ASN:HA	1:B:764:LYS:HG2	2.03	0.40
1:D:529:GLN:HE21	1:D:558:LEU:HA	1.87	0.40
1:F:547:MET:HE2	1:F:547:MET:C	2.46	0.40
1:A:89:PHE:O	1:A:93:VAL:HG22	2.22	0.40
1:A:316:VAL:HG23	1:E:83:LEU:HD23	2.03	0.40
1:C:534:ASP:OD1	1:C:535:VAL:N	2.55	0.40
1:D:662:ASN:HD22	1:D:665:ARG:NH2	2.19	0.40
1:E:94:SER:HA	1:E:116:MET:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:633:PRO:HG3	1:F:650:LEU:HD12	2.03	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 PDB entries followed by that with respect to all EM entries.

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	762/785 (97%)	723 (95%)	37 (5%)	2 (0%)	37	60
1	B	463/785 (59%)	455 (98%)	7 (2%)	1 (0%)	44	67
1	C	462/785 (59%)	451 (98%)	10 (2%)	1 (0%)	44	67
1	D	463/785 (59%)	454 (98%)	9 (2%)	0	100	100
1	E	687/785 (88%)	672 (98%)	15 (2%)	0	100	100
1	F	544/785 (69%)	527 (97%)	16 (3%)	1 (0%)	44	67
All	All	3381/4710 (72%)	3282 (97%)	94 (3%)	5 (0%)	50	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	690	PRO
1	B	402	ASP
1	F	695	ASP
1	C	402	ASP
1	A	693	ILE

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 PDB entries followed by that with respect to all EM entries.

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	709/725 (98%)	706 (100%)	3 (0%)	89	95
1	B	427/725 (59%)	423 (99%)	4 (1%)	75	86
1	C	426/725 (59%)	424 (100%)	2 (0%)	86	93
1	D	427/725 (59%)	425 (100%)	2 (0%)	86	93
1	E	637/725 (88%)	634 (100%)	3 (0%)	86	93
1	F	503/725 (69%)	495 (98%)	8 (2%)	58	77
All	All	3129/4350 (72%)	3107 (99%)	22 (1%)	80	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	687	TYR
1	A	689	THR
1	B	563	CYS
1	B	605	ASN
1	B	681	ILE
1	B	752	PHE
1	C	525	VAL
1	C	695	ASP
1	D	684	MET
1	D	695	ASP
1	E	413	LEU
1	E	611	ASP
1	E	763	HIS
1	F	249	ARG
1	F	260	ASN
1	F	274	LEU
1	F	339	VAL
1	F	401	VAL
1	F	402	ASP
1	F	498	LEU
1	F	641	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	256	ASN
1	A	328	ASN
1	A	478	ASN
1	A	546	ASN
1	A	662	ASN
1	B	324	ASN
1	B	328	ASN
1	B	596	ASN
1	B	730	ASN
1	C	478	ASN
1	C	541	ASN
1	C	548	HIS
1	C	590	ASN
1	C	629	HIS
1	D	324	ASN
1	D	328	ASN
1	D	463	ASN
1	D	594	ASN
1	D	629	HIS
1	D	748	ASN
1	E	111	ASN
1	E	201	HIS
1	F	660	GLN
1	F	775	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADP	A	801	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	4 (13%)
4	ATP	B	901	-	26,33,33	0.61	0	31,52,52	0.74	2 (6%)
4	ATP	C	801	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
4	ATP	A	802	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	801	-	-	5/12/32/32	0/3/3/3
4	ATP	B	901	-	-	8/18/38/38	0/3/3/3
4	ATP	C	801	-	-	6/18/38/38	0/3/3/3
4	ATP	A	802	-	-	8/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ADP	C5-C4	2.50	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ADP	PA-O3A-PB	-3.46	120.96	132.83
3	A	801	ADP	N3-C2-N1	-3.10	123.84	128.68
3	A	801	ADP	C3'-C2'-C1'	2.50	104.75	100.98
3	A	801	ADP	C4-C5-N7	-2.49	106.81	109.40
4	B	901	ATP	C5-C6-N6	2.29	123.84	120.35
4	A	802	ATP	C5-C6-N6	2.28	123.82	120.35
4	C	801	ATP	C5-C6-N6	2.26	123.78	120.35
4	B	901	ATP	PB-O3B-PG	2.04	139.84	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	ATP	PB-O3B-PG	2.04	139.82	132.83
4	C	801	ATP	PB-O3B-PG	2.02	139.76	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	ATP	PB-O3B-PG-O2G
4	A	802	ATP	PB-O3B-PG-O3G
4	A	802	ATP	C5'-O5'-PA-O3A
4	A	802	ATP	O4'-C4'-C5'-O5'
4	B	901	ATP	C5'-O5'-PA-O1A
4	B	901	ATP	C5'-O5'-PA-O3A
4	C	801	ATP	C5'-O5'-PA-O1A
4	C	801	ATP	C5'-O5'-PA-O2A
4	C	801	ATP	C5'-O5'-PA-O3A
4	C	801	ATP	C4'-C5'-O5'-PA
4	C	801	ATP	O4'-C4'-C5'-O5'
4	C	801	ATP	C3'-C4'-C5'-O5'
4	B	901	ATP	O4'-C4'-C5'-O5'
4	B	901	ATP	C3'-C4'-C5'-O5'
4	A	802	ATP	C4'-C5'-O5'-PA
4	A	802	ATP	PB-O3A-PA-O5'
3	A	801	ADP	PB-O3A-PA-O1A
4	B	901	ATP	PA-O3A-PB-O2B
4	A	802	ATP	C5'-O5'-PA-O1A
4	A	802	ATP	C3'-C4'-C5'-O5'
3	A	801	ADP	PB-O3A-PA-O2A
4	B	901	ATP	PB-O3B-PG-O1G
4	B	901	ATP	C4'-C5'-O5'-PA
3	A	801	ADP	O4'-C4'-C5'-O5'
3	A	801	ADP	C5'-O5'-PA-O3A
4	B	901	ATP	PA-O3A-PB-O1B
3	A	801	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 9 short contacts:

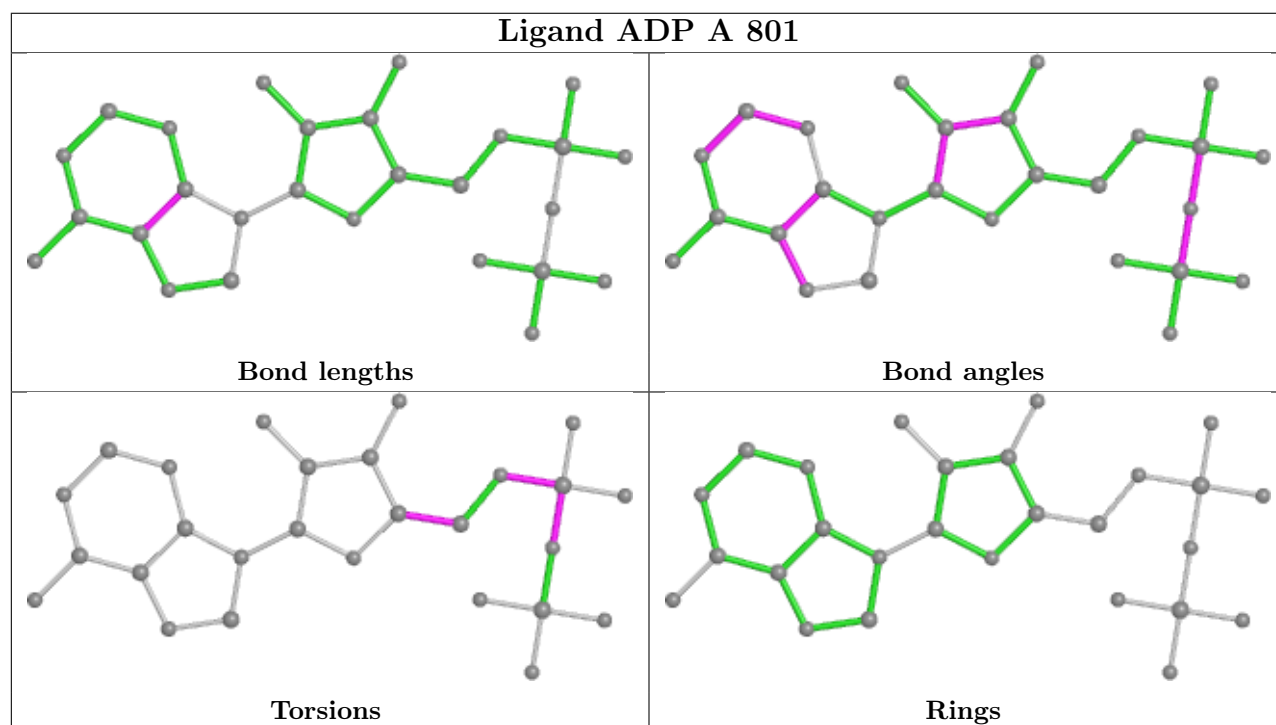
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	ADP	4	0
4	B	901	ATP	2	0

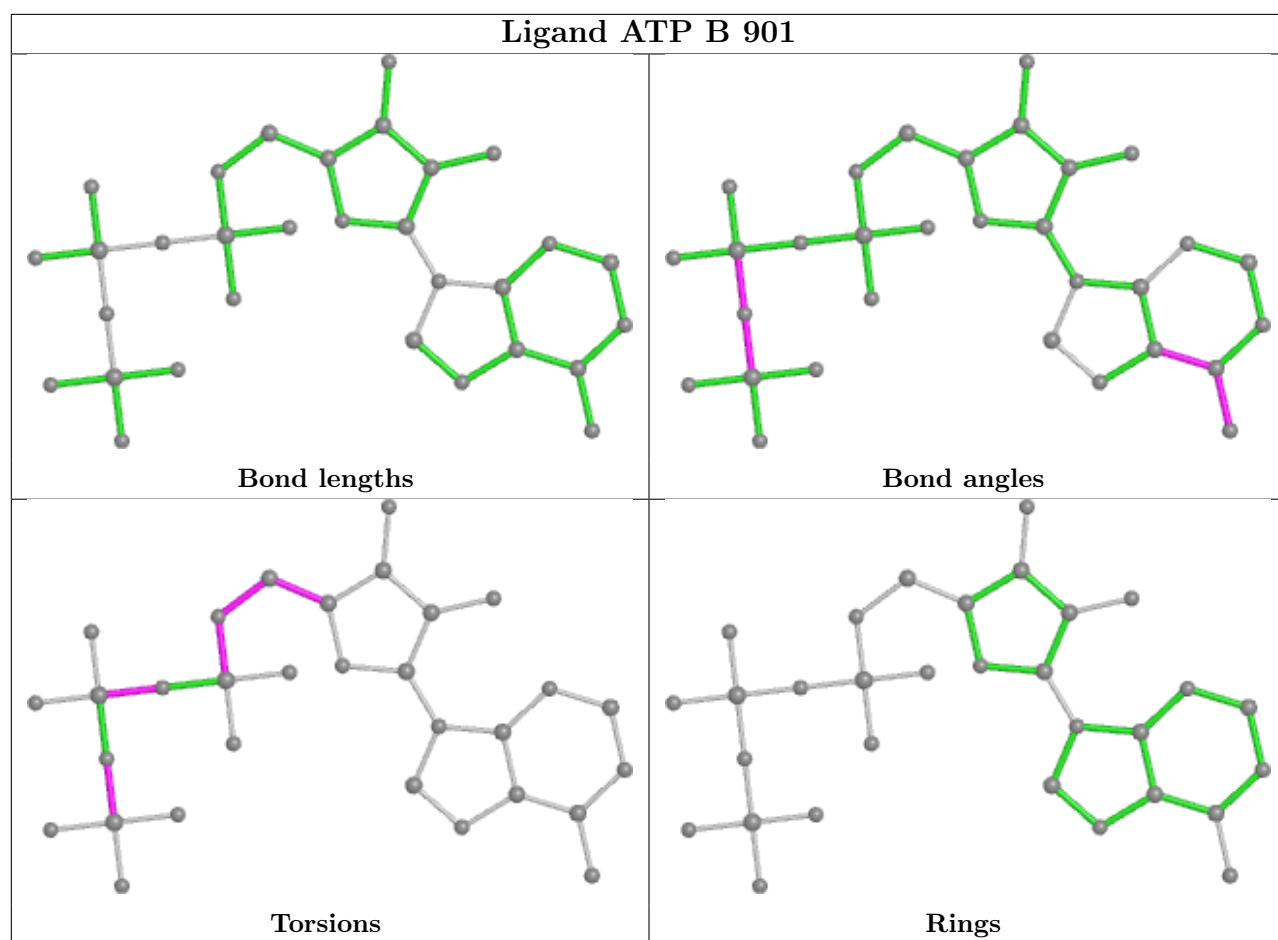
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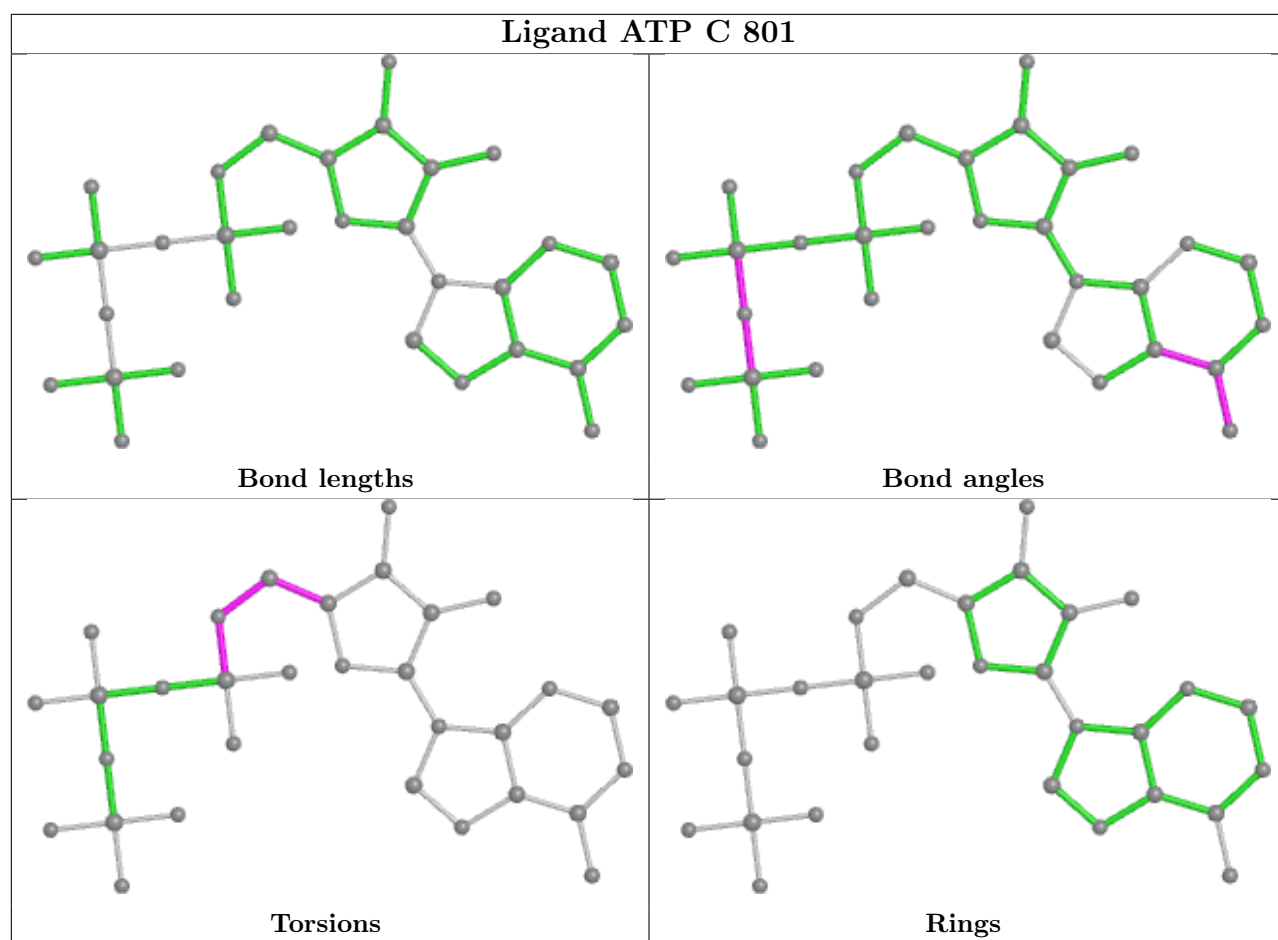
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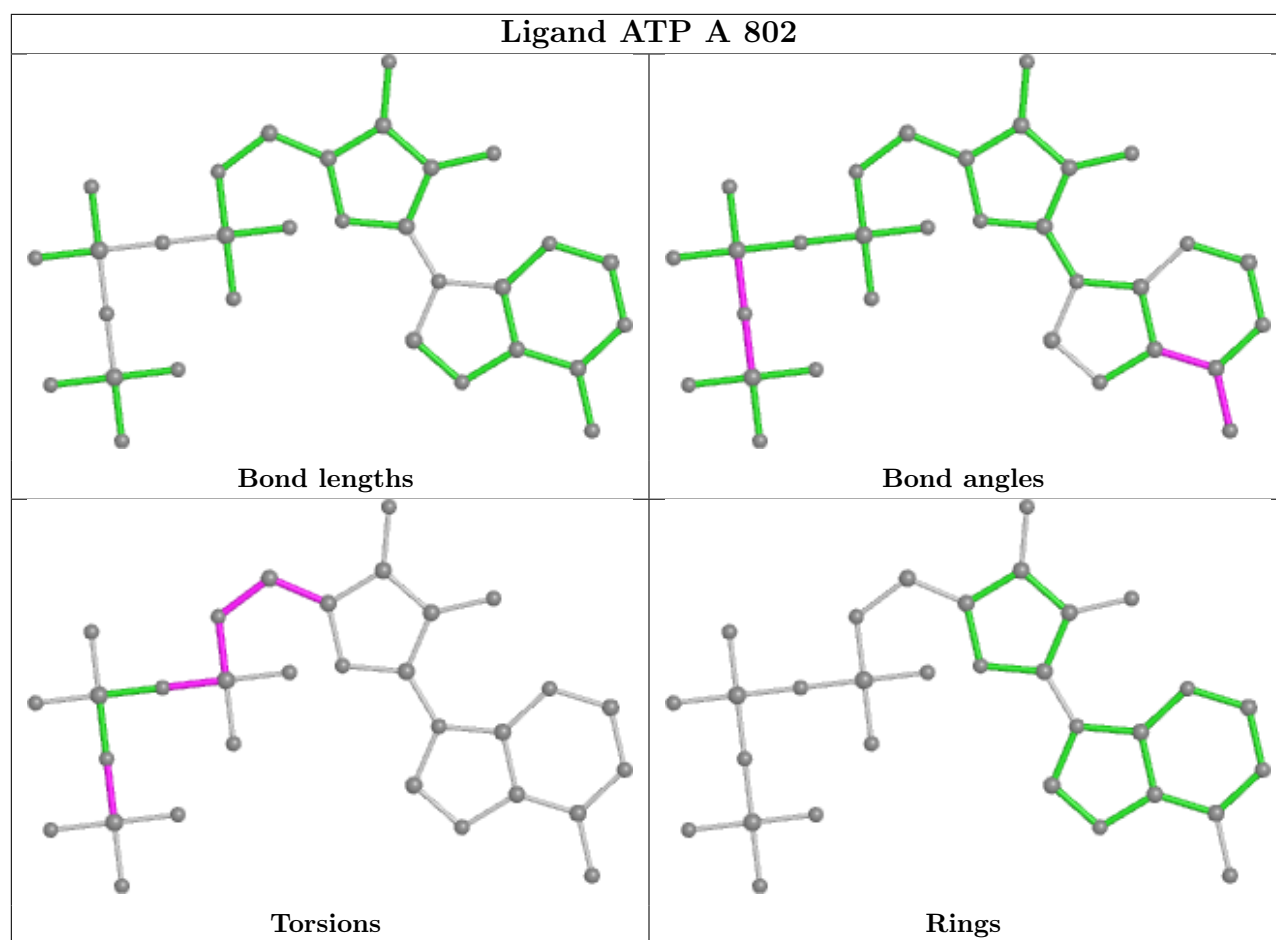
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	801	ATP	2	0
4	A	802	ATP	1	0

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.