



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2023 – 01:00 pm GMT

PDB ID : 8ARP  
Title : Crystal structure of DEAD-box protein Dbp2 in complex with ADP  
Authors : Song, Q.X.; Rety, S.; Xi, X.G.  
Deposited on : 2022-08-17  
Resolution : 3.05 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

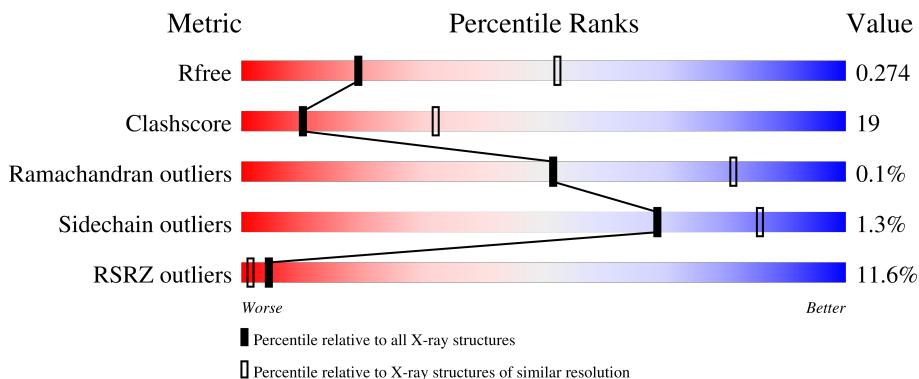
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



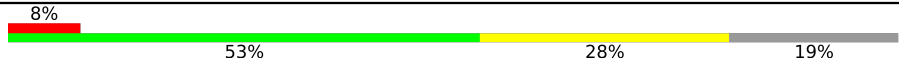
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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  $\geq 3$ , 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	546	
1	B	546	
1	C	546	
1	D	546	
1	E	546	

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Mol	Chain	Length	Quality of chain
1	F	546	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	E	2002	-	-	X	-

## 2 Entry composition [i](#)

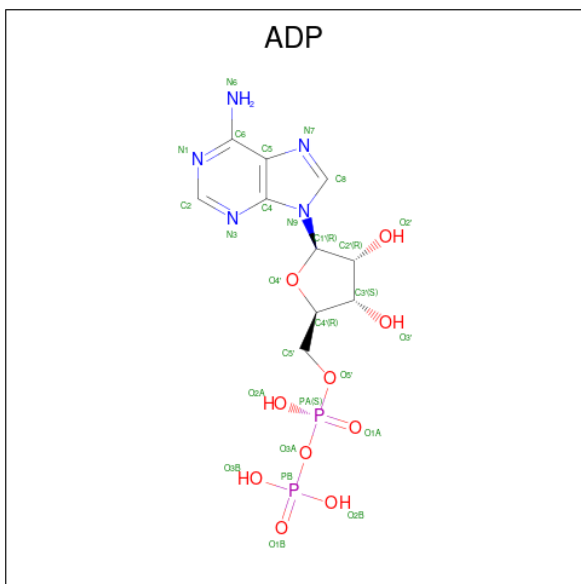
There are 4 unique types of molecules in this entry. The entry contains 21294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DBP2.

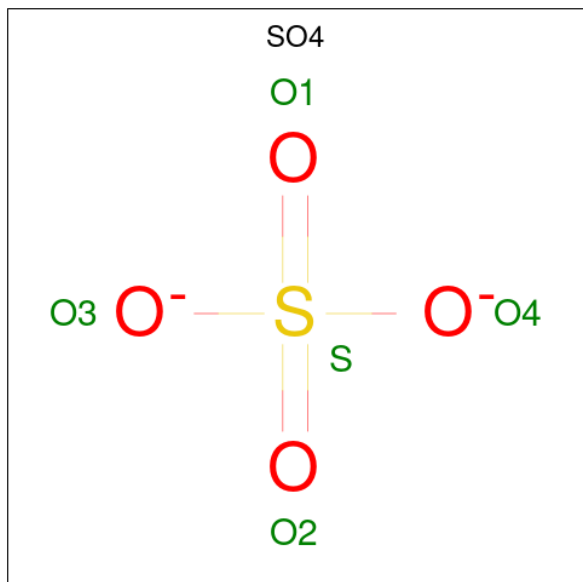
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	Total 3505	C 2202	N 616	O 671	S 16	0	0	0
1	B	444	Total 3516	C 2208	N 620	O 672	S 16	0	0	0
1	C	445	Total 3528	C 2217	N 621	O 674	S 16	0	0	0
1	D	444	Total 3516	C 2208	N 620	O 672	S 16	0	0	0
1	E	444	Total 3516	C 2208	N 620	O 672	S 16	0	0	0
1	F	443	Total 3508	C 2204	N 618	O 670	S 16	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O S		
3	A	1	Total 5	O 4 S 1	0	0
3	B	1	Total 5	O 4 S 1	0	0
3	C	1	Total 5	O 4 S 1	0	0
3	D	1	Total 5	O 4 S 1	0	0
3	E	1	Total 5	O 4 S 1	0	0
3	E	1	Total 5	O 4 S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

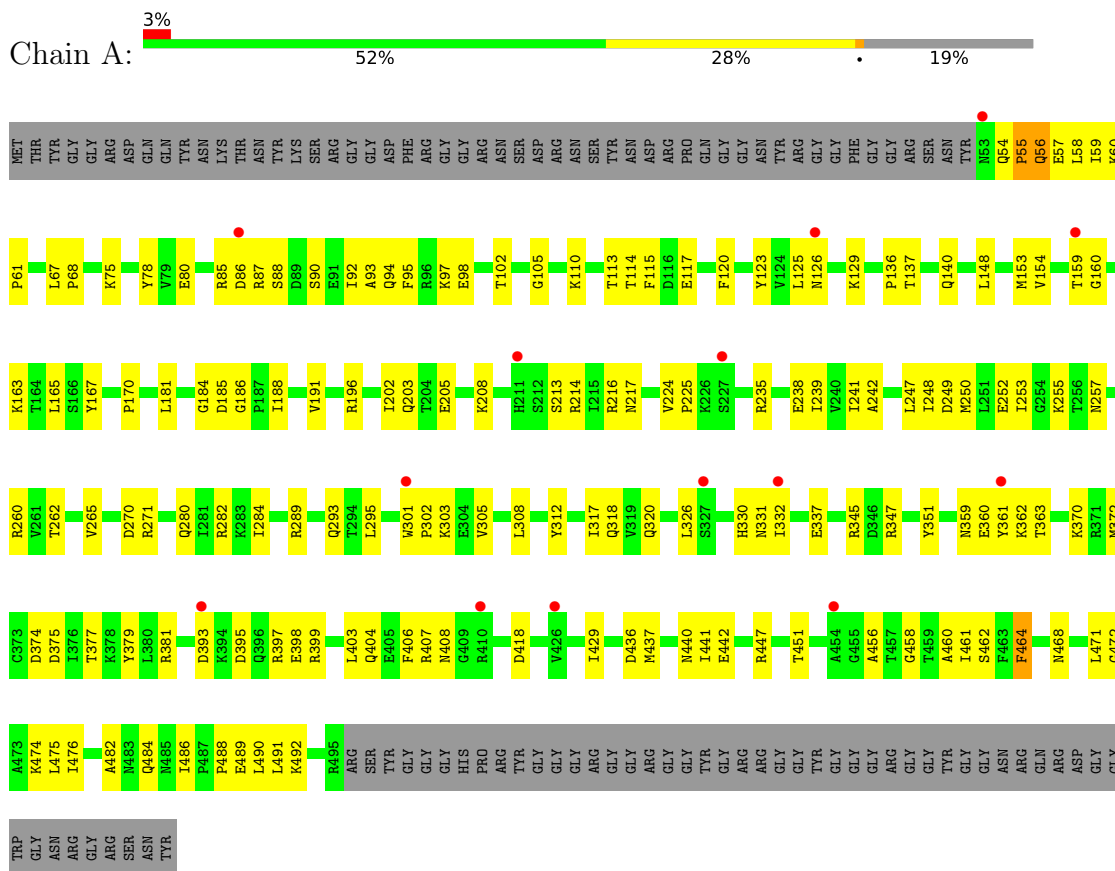
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

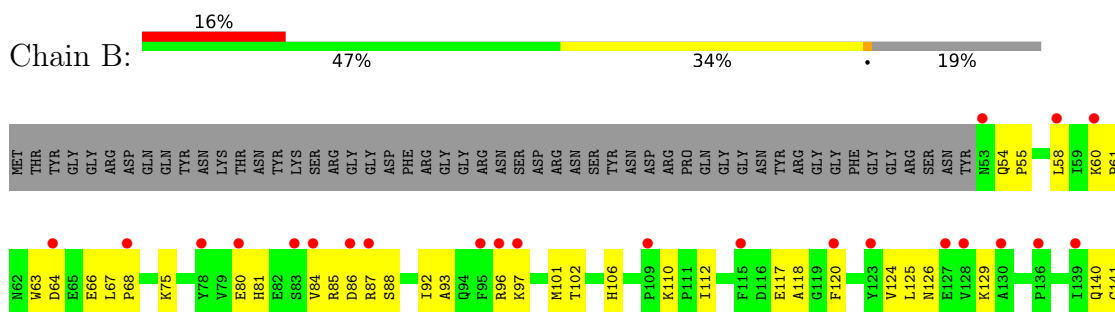
### 3 Residue-property plots

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 DBP2



- Molecule 1: ATP-dependent RNA helicase DBP2











## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.94Å 168.84Å 168.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.40 – 3.05 119.40 – 3.05	Depositor EDS
% Data completeness (in resolution range)	96.2 (119.40-3.05) 96.1 (119.40-3.05)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.223 , 0.270 0.228 , 0.274	Depositor DCC
$R_{free}$ test set	3779 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.6	Xtrriage
Anisotropy	0.481	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 77.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.428 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	21294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, MG, 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	0.28	0/3574	0.60	1/4840 (0.0%)
1	B	0.29	0/3585	0.64	0/4854
1	C	0.29	0/3598	0.66	1/4872 (0.0%)
1	D	0.29	0/3585	0.64	1/4854 (0.0%)
1	E	0.28	0/3585	0.62	0/4854
1	F	0.28	0/3577	0.60	1/4843 (0.0%)
All	All	0.29	0/21504	0.63	4/29117 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	2
1	F	0	2
All	All	0	13

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	PRO	C-N-CA	6.43	137.78	121.70
1	F	380	LEU	CA-CB-CG	6.32	129.84	115.30
1	C	302	PRO	C-N-CA	5.85	136.33	121.70
1	D	119	GLY	C-N-CA	5.30	134.96	121.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	GLN	Peptide
1	A	58	LEU	Peptide
1	B	324	LEU	Peptide
1	B	81	HIS	Peptide
1	C	303	LYS	Peptide
1	C	56	GLN	Peptide
1	D	118	ALA	Peptide
1	D	323	SER	Peptide
1	D	422	ARG	Sidechain
1	E	235	ARG	Sidechain
1	E	85	ARG	Peptide
1	F	324	LEU	Peptide
1	F	56	GLN	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3505	0	3485	111	0
1	B	3516	0	3498	158	0
1	C	3528	0	3508	162	0
1	D	3516	0	3498	171	0
1	E	3516	0	3497	117	0
1	F	3508	0	3493	120	0
2	A	27	0	12	5	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
2	D	27	0	12	2	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	15	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	21294	0	21051	800	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 19.

All (800) 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:D:78:TYR:OH	1:D:110:LYS:NZ	1.95	0.98
1:C:330:HIS:NE2	1:C:481:GLU:OE2	2.08	0.87
1:C:302:PRO:HB2	1:C:304:GLU:H	1.39	0.87
1:C:397:ARG:NH1	1:F:213:SER:O	2.09	0.85
1:E:59:ILE:O	1:E:287:GLN:NE2	2.14	0.80
1:F:57:GLU:OE2	1:F:59:ILE:N	2.15	0.80
1:E:307:GLN:NE2	1:E:311:ASP:OD2	2.15	0.79
1:D:152:ASP:HB3	1:D:313:LEU:HD23	1.65	0.78
1:E:219:CYS:HG	1:E:221:TYR:HE2	1.31	0.78
1:B:60:LYS:NZ	1:B:61:PRO:O	2.15	0.78
1:C:156:ILE:HG21	1:C:301:TRP:HB2	1.65	0.78
1:B:336:VAL:HG11	1:B:490:LEU:HD13	1.64	0.78
1:C:66:GLU:OE1	1:C:69:LYS:NZ	2.17	0.77
1:B:196:ARG:NH2	1:B:393:ASP:OD2	2.17	0.77
1:A:148:LEU:HD22	1:A:170:PRO:HB3	1.66	0.77
1:D:235:ARG:HG3	1:D:235:ARG:HH11	1.50	0.77
1:B:397:ARG:NH1	1:E:214:ARG:O	2.17	0.76
1:A:404:GLN:O	1:A:408:ASN:ND2	2.17	0.76
1:C:390:ILE:HG22	1:C:420:ALA:HB1	1.68	0.76
1:D:426:VAL:HG13	1:D:429:ILE:HD11	1.68	0.76
1:F:57:GLU:OE2	1:F:59:ILE:HG13	1.86	0.76
1:D:87:ARG:HG2	1:D:92:ILE:HG23	1.68	0.75
1:F:380:LEU:HB3	1:F:385:TRP:HB2	1.69	0.75
1:D:196:ARG:NH1	1:D:371:ARG:HD2	2.01	0.75
1:A:440:ASN:ND2	1:A:442:GLU:OE1	2.17	0.75
1:F:127:GLU:OE2	1:F:212:SER:OG	2.05	0.74
1:C:334:GLN:O	1:C:485:ASN:ND2	2.18	0.74
1:E:371:ARG:HG2	1:E:371:ARG:HH11	1.53	0.73
1:A:196:ARG:NH2	1:A:393:ASP:OD2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:ILE:HD11	1:F:461:ILE:HA	1.70	0.73
1:D:139:ILE:HG13	1:D:321:VAL:HG21	1.71	0.73
1:E:267:ASP:HA	1:E:297:TRP:HB2	1.70	0.73
1:B:188:ILE:HD13	1:B:260:ARG:O	1.89	0.73
1:D:175:ILE:HG23	1:D:188:ILE:HD11	1.71	0.72
1:A:105:GLY:HA3	1:A:317:ILE:HG22	1.71	0.72
1:A:476:ILE:HG23	1:A:486:ILE:HG12	1.71	0.72
1:D:171:GLY:HA2	1:D:263:TYR:CE2	2.24	0.72
1:A:203:GLN:HB2	1:A:241:ILE:HD13	1.72	0.71
1:D:296:MET:HE3	1:D:313:LEU:HD11	1.72	0.71
1:D:67:LEU:HD22	1:D:290:PRO:HG2	1.73	0.71
1:F:389:ALA:O	1:F:394:LYS:NZ	2.21	0.71
1:A:160:GLY:HA2	2:A:2001:ADP:O1A	1.92	0.70
1:C:153:MET:HG2	1:C:295:LEU:HD22	1.73	0.70
1:C:182:ALA:HB3	1:C:185:ASP:OD2	1.92	0.70
1:A:332:ILE:HD11	1:A:460:ALA:HB2	1.74	0.69
1:B:358:ASP:OD1	1:B:359:ASN:N	2.25	0.69
1:D:156:ILE:HD11	1:D:320:GLN:HA	1.75	0.69
1:E:424:ILE:HD13	1:E:426:VAL:HG12	1.75	0.69
1:C:436:ASP:O	1:C:447:ARG:NH1	2.23	0.69
1:A:262:THR:HG22	1:A:289:ARG:HD3	1.75	0.69
1:B:407:ARG:HD2	1:B:426:VAL:HG23	1.73	0.69
1:A:205:GLU:OE2	2:A:2001:ADP:H3'	1.92	0.69
1:F:174:HIS:NE2	1:F:262:THR:OG1	2.25	0.68
1:C:484:GLN:HG2	1:C:485:ASN:O	1.92	0.68
1:B:54:GLN:HG2	1:B:253:ILE:HG22	1.76	0.68
1:C:247:LEU:HD23	1:C:284:ILE:HD13	1.75	0.68
1:B:464:PHE:HD1	1:B:465:THR:N	1.92	0.67
1:B:58:LEU:HD21	1:B:251:LEU:HD12	1.75	0.67
1:F:54:GLN:N	1:F:249:ASP:OD1	2.28	0.67
1:F:242:ALA:HB1	1:F:247:LEU:HB2	1.76	0.67
1:B:58:LEU:HD11	1:B:251:LEU:HB2	1.76	0.67
1:F:102:THR:OG1	1:F:320:GLN:NE2	2.27	0.67
1:E:67:LEU:HD23	1:E:70:LEU:HD12	1.77	0.67
1:F:288:ILE:HD13	1:F:292:ARG:HD2	1.78	0.66
1:E:288:ILE:HD13	1:E:292:ARG:HD3	1.75	0.66
1:B:380:LEU:HD11	1:B:387:ALA:HB2	1.76	0.66
1:D:197:GLU:OE2	1:D:392:GLY:N	2.28	0.66
1:C:372:MET:O	1:C:376:ILE:HG13	1.96	0.66
1:C:442:GLU:O	1:C:446:HIS:ND1	2.28	0.66
1:C:78:TYR:HB2	1:C:148:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HB2	1:A:56:GLN:HG3	1.77	0.66
1:B:259:LYS:NZ	1:C:342:PHE:O	2.28	0.66
1:C:377:THR:HG21	1:C:389:ALA:HB2	1.78	0.66
1:F:476:ILE:HG23	1:F:486:ILE:HG12	1.78	0.66
1:F:215:ILE:HG23	1:F:238:GLU:HB2	1.77	0.65
1:D:81:HIS:CD2	1:D:117:GLU:HG2	2.30	0.65
1:E:358:ASP:OD1	1:E:361:TYR:HB3	1.96	0.65
1:A:488:PRO:HA	1:A:491:LEU:HD13	1.79	0.65
1:C:345:ARG:NH2	1:C:379:TYR:O	2.28	0.65
1:A:54:GLN:HB3	1:A:253:ILE:HG22	1.79	0.65
1:B:87:ARG:N	1:B:88:SER:OG	2.24	0.65
1:D:190:LEU:HD11	1:D:258:LEU:HD22	1.77	0.65
1:A:437:MET:SD	1:A:462:SER:OG	2.55	0.64
1:D:427:LYS:HE2	1:D:452:GLY:H	1.62	0.64
1:C:426:VAL:HG13	1:C:429:ILE:HD11	1.78	0.64
1:D:357:GLN:OE1	1:D:357:GLN:N	2.30	0.64
1:C:391:HIS:HE1	1:C:394:LYS:HB2	1.63	0.64
1:C:390:ILE:HD11	1:C:402:VAL:HB	1.79	0.64
1:A:472:GLY:O	1:A:476:ILE:HD12	1.98	0.64
1:B:221:TYR:HE1	1:B:224:VAL:HG11	1.62	0.64
1:F:100:GLU:HG3	1:F:321:VAL:O	1.97	0.64
1:F:182:ALA:HB3	1:F:185:ASP:OD2	1.98	0.63
1:B:215:ILE:HG23	1:B:238:GLU:HB2	1.79	0.63
1:B:165:LEU:HD12	1:B:169:LEU:HD11	1.78	0.63
1:D:467:GLN:OE1	1:D:469:LYS:NZ	2.30	0.63
1:A:440:ASN:OD1	1:A:441:ILE:N	2.32	0.63
1:F:222:GLY:HA2	1:F:246:ARG:HE	1.62	0.63
1:D:442:GLU:O	1:D:446:HIS:ND1	2.32	0.63
1:B:216:ARG:NH1	1:B:235:ARG:O	2.32	0.63
1:C:302:PRO:HB2	1:C:304:GLU:N	2.13	0.63
1:E:264:LEU:HB3	1:E:294:THR:HG22	1.80	0.63
1:F:226:LYS:HG3	1:F:246:ARG:HH11	1.64	0.62
1:C:151:ARG:NH2	1:C:315:ASP:O	2.30	0.62
1:C:103:ILE:HG22	1:C:319:VAL:HG22	1.80	0.62
1:D:196:ARG:HH12	1:D:371:ARG:HD2	1.64	0.62
1:E:188:ILE:HA	1:E:261:VAL:HA	1.81	0.62
1:A:137:THR:N	1:A:140:GLN:OE1	2.32	0.62
1:C:218:THR:HG21	1:C:233:LEU:HD12	1.81	0.62
1:B:203:GLN:HB3	1:B:241:ILE:HG13	1.82	0.62
1:B:214:ARG:O	1:E:397:ARG:NH2	2.33	0.62
1:C:83:SER:OG	1:C:117:GLU:OE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:PHE:HD1	1:D:465:THR:N	1.97	0.62
1:E:271:ARG:HD2	1:E:440:ASN:HB3	1.82	0.62
1:D:427:LYS:NZ	1:D:451:THR:HA	2.15	0.62
1:D:464:PHE:CE1	1:D:468:ASN:HB2	2.34	0.61
1:A:249:ASP:O	1:A:253:ILE:HG23	2.00	0.61
1:D:242:ALA:HB1	1:D:247:LEU:HB2	1.82	0.61
1:A:120:PHE:HE1	1:A:148:LEU:HD21	1.64	0.61
1:A:395:ASP:HA	1:A:398:GLU:HG3	1.83	0.61
1:B:106:HIS:O	1:B:151:ARG:NH2	2.34	0.61
1:C:96:ARG:O	1:C:100:GLU:N	2.34	0.61
1:D:331:ASN:ND2	1:D:456:ALA:HB1	2.16	0.61
1:A:78:TYR:HB2	1:A:148:LEU:HB3	1.83	0.60
1:A:126:ASN:HB2	1:D:130:ALA:HB2	1.83	0.60
1:A:337:GLU:OE2	1:A:351:TYR:OH	2.11	0.60
1:D:118:ALA:O	1:D:120:PHE:N	2.29	0.60
1:C:327:SER:OG	1:C:328:ALA:N	2.35	0.60
1:D:437:MET:HE3	1:D:464:PHE:HB2	1.82	0.60
1:C:101:MET:HB3	1:C:321:VAL:HG22	1.83	0.60
1:C:171:GLY:HA2	1:C:263:TYR:CE2	2.35	0.60
1:D:171:GLY:HA2	1:D:263:TYR:HE2	1.62	0.60
1:E:290:PRO:HA	1:E:292:ARG:NH1	2.17	0.60
1:F:377:THR:HG21	1:F:389:ALA:HB2	1.82	0.60
1:C:216:ARG:NH1	1:C:235:ARG:O	2.35	0.60
1:B:112:ILE:HD11	1:B:145:PRO:HD3	1.84	0.60
1:D:372:MET:O	1:D:376:ILE:HD12	2.01	0.60
1:F:407:ARG:HG2	1:F:426:VAL:HG13	1.84	0.60
1:C:235:ARG:NH1	1:F:393:ASP:O	2.31	0.60
1:D:443:ASP:O	1:D:447:ARG:HG3	2.02	0.60
1:E:424:ILE:HD11	1:E:450:ARG:HD2	1.82	0.60
1:B:54:GLN:N	1:B:55:PRO:HD3	2.18	0.59
1:D:57:GLU:HG3	1:D:252:GLU:HG2	1.84	0.59
1:D:427:LYS:HZ1	1:D:451:THR:HA	1.67	0.59
1:C:230:ILE:HD12	1:C:231:ARG:N	2.18	0.59
1:D:361:TYR:HD2	1:D:363:THR:HG23	1.68	0.59
1:B:92:ILE:HD12	1:B:110:LYS:HG2	1.83	0.59
1:F:60:LYS:HE2	1:F:286:ASP:HB3	1.84	0.59
1:D:78:TYR:HH	1:D:110:LYS:NZ	1.97	0.59
1:A:451:THR:HG22	1:A:458:GLY:HA3	1.84	0.59
1:B:386:PRO:HD3	1:D:386:PRO:HB3	1.84	0.59
1:D:358:ASP:OD1	1:D:361:TYR:HB3	2.03	0.59
1:B:112:ILE:N	1:B:141:CYS:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ALA:HB3	1:D:163:LYS:HD3	1.84	0.59
1:F:269:ALA:N	1:F:298:SER:OG	2.35	0.59
1:A:331:ASN:OD1	1:A:456:ALA:HB1	2.03	0.59
1:D:367:ALA:HA	1:D:436:ASP:HB2	1.84	0.59
1:B:191:VAL:HG12	1:B:265:VAL:HB	1.84	0.58
1:E:464:PHE:CE1	1:E:468:ASN:HB2	2.37	0.58
1:E:127:GLU:OE2	1:E:212:SER:HB2	2.03	0.58
1:B:219:CYS:HG	1:B:221:TYR:HD2	1.52	0.58
1:D:270:ASP:OD1	1:D:271:ARG:N	2.34	0.58
1:A:482:ALA:O	1:A:484:GLN:NE2	2.35	0.58
1:C:475:LEU:HD12	1:C:476:ILE:N	2.19	0.58
1:F:353:GLU:O	1:F:357:GLN:NE2	2.35	0.58
1:E:323:SER:HB3	1:E:325:GLU:HG3	1.86	0.58
1:B:345:ARG:NH2	1:B:379:TYR:O	2.36	0.58
1:B:381:ARG:NH2	1:B:387:ALA:O	2.34	0.58
1:B:120:PHE:CE1	1:B:148:LEU:HD11	2.39	0.57
1:D:226:LYS:O	1:D:230:ILE:HG23	2.04	0.57
1:D:115:PHE:HE2	1:D:134:ASP:HA	1.68	0.57
1:E:189:VAL:HG22	1:E:263:TYR:HB3	1.86	0.57
1:B:87:ARG:HB2	1:B:88:SER:HA	1.85	0.57
1:F:318:GLN:OE1	1:F:318:GLN:N	2.32	0.57
1:B:363:THR:OG1	1:B:431:TYR:O	2.11	0.57
1:C:163:LYS:NZ	1:C:268:GLU:OE2	2.31	0.57
1:D:110:LYS:H	1:D:110:LYS:HD3	1.67	0.57
1:A:395:ASP:O	1:A:399:ARG:HB2	2.03	0.57
1:B:84:VAL:HG22	1:B:117:GLU:OE2	2.04	0.57
1:B:214:ARG:NH2	1:E:208:LYS:NZ	2.53	0.57
1:B:378:LYS:HG2	1:B:381:ARG:HD2	1.86	0.57
1:F:87:ARG:H	1:F:88:SER:HB2	1.69	0.57
1:B:422:ARG:HE	1:B:423:GLY:N	2.03	0.56
1:D:395:ASP:HA	1:D:398:GLU:HB2	1.86	0.56
1:E:381:ARG:NH2	3:E:2002:SO4:O1	2.37	0.56
1:E:99:ASN:HB2	1:E:101:MET:SD	2.45	0.56
1:F:167:TYR:CG	1:F:265:VAL:HG21	2.40	0.56
1:C:159:THR:HG22	1:C:163:LYS:NZ	2.21	0.56
1:A:436:ASP:O	1:A:447:ARG:NH2	2.38	0.56
1:C:54:GLN:HB2	1:C:253:ILE:HG23	1.87	0.56
1:D:299:ALA:HB1	1:D:442:GLU:OE2	2.06	0.56
1:E:371:ARG:HH11	1:E:371:ARG:CG	2.17	0.56
1:E:340:SER:N	1:E:343:GLU:OE2	2.37	0.56
1:B:217:ASN:HA	1:B:239:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:ILE:O	1:F:380:LEU:HD12	2.05	0.56
1:A:92:ILE:HG12	1:A:110:LYS:NZ	2.21	0.55
1:C:221:TYR:HA	1:C:243:THR:HG22	1.87	0.55
1:D:151:ARG:HH11	1:D:317:ILE:HD11	1.71	0.55
1:C:344:LYS:HB3	1:C:435:TYR:CE1	2.41	0.55
1:D:153:MET:HG2	1:D:295:LEU:HD22	1.87	0.55
1:E:288:ILE:HD13	1:E:292:ARG:CD	2.36	0.55
1:D:200:VAL:O	1:D:204:THR:N	2.33	0.55
1:C:388:LEU:HD13	1:C:402:VAL:HG13	1.88	0.55
1:D:427:LYS:NZ	1:D:429:ILE:O	2.40	0.55
1:E:103:ILE:HG22	1:E:108:ILE:HD13	1.89	0.55
1:A:181:LEU:O	1:A:185:ASP:HB2	2.06	0.55
1:B:182:ALA:HA	1:E:401:TRP:CE2	2.42	0.55
1:C:175:ILE:HD12	1:C:238:GLU:HB3	1.89	0.55
1:D:343:GLU:O	1:D:347:ARG:N	2.31	0.55
1:F:99:ASN:O	1:F:101:MET:HG3	2.06	0.55
1:C:87:ARG:H	1:C:88:SER:HA	1.72	0.54
1:B:476:ILE:O	1:B:480:ARG:N	2.35	0.54
1:C:395:ASP:O	1:C:399:ARG:NE	2.41	0.54
1:F:181:LEU:O	1:F:185:ASP:HB2	2.07	0.54
1:A:489:GLU:O	1:A:492:LYS:NZ	2.25	0.54
1:C:375:ASP:HB3	1:C:379:TYR:CZ	2.42	0.54
1:E:492:LYS:N	1:E:492:LYS:HD2	2.22	0.54
1:F:472:GLY:O	1:F:476:ILE:HD12	2.08	0.54
1:A:92:ILE:HG12	1:A:110:LYS:HZ1	1.72	0.54
1:A:429:ILE:O	1:A:451:THR:HG23	2.07	0.54
1:B:380:LEU:HD11	1:B:387:ALA:CB	2.38	0.54
1:C:395:ASP:O	1:C:399:ARG:HG2	2.07	0.54
1:D:436:ASP:O	1:D:447:ARG:NH1	2.40	0.54
1:A:102:THR:HB	1:A:320:GLN:HB3	1.89	0.54
1:A:318:GLN:OE1	1:A:318:GLN:N	2.41	0.54
1:B:96:ARG:HB2	1:B:97:LYS:HD3	1.88	0.54
1:D:424:ILE:H	1:D:450:ARG:HH21	1.55	0.54
1:B:164:THR:HA	1:B:167:TYR:CE2	2.43	0.54
1:B:366:PHE:HB3	1:B:447:ARG:HH21	1.72	0.54
1:D:114:THR:HG22	1:D:116:ASP:H	1.73	0.54
1:D:196:ARG:HH12	1:D:371:ARG:HH11	1.56	0.54
1:D:422:ARG:HH11	2:D:2001:ADP:H4'	1.73	0.54
1:B:380:LEU:HD12	1:B:381:ARG:N	2.22	0.54
1:C:487:PRO:HB2	1:C:490:LEU:HB3	1.89	0.53
1:D:486:ILE:HG23	1:D:490:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:LEU:HB3	1:E:385:TRP:HB2	1.90	0.53
1:E:186:GLY:N	1:E:257:ASN:OD1	2.39	0.53
1:F:363:THR:HG23	1:F:431:TYR:O	2.09	0.53
1:D:347:ARG:HH21	1:D:350:LYS:HD3	1.74	0.53
1:F:142:GLN:HG3	1:F:146:MET:HE3	1.90	0.53
1:F:376:ILE:HG22	1:F:380:LEU:HD11	1.91	0.53
1:B:176:ASN:OD1	1:B:213:SER:OG	2.26	0.53
1:C:480:ARG:HG2	1:C:484:GLN:OE1	2.08	0.53
1:D:191:VAL:HG22	1:D:265:VAL:HB	1.90	0.53
1:A:120:PHE:CE1	1:A:148:LEU:HD21	2.42	0.53
1:C:100:GLU:HG3	1:C:321:VAL:O	2.08	0.53
1:A:381:ARG:HD3	1:F:381:ARG:HB3	1.89	0.53
1:B:174:HIS:HD2	1:B:263:TYR:HB2	1.73	0.53
1:A:253:ILE:HG13	1:A:255:LYS:HG2	1.91	0.53
1:D:182:ALA:HB3	1:D:185:ASP:OD2	2.09	0.53
1:F:152:ASP:OD1	1:F:294:THR:N	2.38	0.53
1:F:273:LEU:HD21	1:F:308:LEU:HD22	1.91	0.53
1:B:151:ARG:NH2	1:B:317:ILE:HG13	2.24	0.53
1:B:398:GLU:OE2	1:E:235:ARG:HD3	2.09	0.53
1:C:96:ARG:HH12	1:C:103:ILE:CD1	2.21	0.53
1:D:345:ARG:O	1:D:349:ASN:ND2	2.42	0.53
1:F:285:VAL:HG11	1:F:312:TYR:CD2	2.44	0.53
1:B:196:ARG:HH22	1:B:371:ARG:HH21	1.55	0.53
1:C:159:THR:HG22	1:C:163:LYS:HZ3	1.72	0.53
1:C:253:ILE:CG2	1:C:255:LYS:NZ	2.72	0.53
1:C:191:VAL:HG22	1:C:265:VAL:HB	1.91	0.52
1:C:233:LEU:HD23	1:C:256:THR:HB	1.91	0.52
1:C:391:HIS:CE1	1:C:394:LYS:HB2	2.42	0.52
1:F:87:ARG:N	1:F:88:SER:HB2	2.24	0.52
1:F:105:GLY:HA3	1:F:317:ILE:HD13	1.91	0.52
1:A:95:PHE:HA	1:A:98:GLU:CD	2.29	0.52
1:C:174:HIS:NE2	1:C:262:THR:OG1	2.30	0.52
1:D:263:TYR:HE1	1:D:295:LEU:HD11	1.74	0.52
1:A:90:SER:O	1:A:94:GLN:HG2	2.09	0.52
1:A:184:GLY:HA3	1:B:345:ARG:NH1	2.25	0.52
1:D:330:HIS:ND1	1:D:482:ALA:HA	2.25	0.52
1:E:434:ASN:HB2	1:E:462:SER:HA	1.90	0.52
1:B:125:LEU:O	1:B:129:LYS:HG3	2.10	0.52
1:C:375:ASP:HB3	1:C:379:TYR:CE2	2.44	0.52
1:C:59:ILE:O	1:C:287:GLN:NE2	2.43	0.52
1:E:125:LEU:O	1:E:129:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD23	1:A:284:ILE:HD13	1.92	0.52
1:C:63:TRP:HZ3	1:C:70:LEU:HD11	1.75	0.52
1:E:221:TYR:HE1	1:E:224:VAL:HG21	1.74	0.52
1:A:224:VAL:HG22	1:A:225:PRO:HD2	1.91	0.52
1:A:238:GLU:OE2	1:D:397:ARG:HD3	2.10	0.52
1:D:57:GLU:CD	1:D:58:LEU:H	2.13	0.52
1:F:152:ASP:HB3	1:F:313:LEU:HD22	1.92	0.52
1:D:127:GLU:OE2	1:D:212:SER:OG	2.23	0.52
1:E:67:LEU:HD21	1:E:289:ARG:HB2	1.93	0.51
1:E:335:ILE:HG23	1:E:461:ILE:HD13	1.90	0.51
1:A:248:ILE:O	1:A:252:GLU:HG3	2.11	0.51
1:C:335:ILE:HD11	1:C:461:ILE:HG23	1.91	0.51
1:C:343:GLU:O	1:C:346:ASP:N	2.42	0.51
1:E:426:VAL:HG13	1:E:429:ILE:HD11	1.91	0.51
1:C:103:ILE:HD12	1:C:108:ILE:HD12	1.92	0.51
1:D:87:ARG:H	1:D:88:SER:HB2	1.76	0.51
1:F:96:ARG:HH21	1:F:111:PRO:HD3	1.75	0.51
1:A:250:MET:HA	1:A:253:ILE:HG12	1.91	0.51
1:D:191:VAL:HG23	1:D:239:ILE:HD11	1.92	0.51
1:B:301:TRP:O	1:B:301:TRP:CG	2.64	0.51
1:F:278:GLU:HA	1:F:281:ILE:HG12	1.93	0.51
1:B:64:ASP:N	1:B:64:ASP:OD1	2.43	0.51
1:B:151:ARG:HH21	1:B:317:ILE:HG13	1.75	0.51
1:C:330:HIS:CE1	1:C:481:GLU:OE2	2.64	0.51
1:B:175:ILE:HD11	1:B:189:VAL:HG23	1.92	0.51
1:B:219:CYS:HA	1:B:241:ILE:HB	1.93	0.51
1:F:226:LYS:HE3	1:F:246:ARG:NH1	2.25	0.51
1:F:244:PRO:HG2	1:F:272:MET:HE1	1.92	0.51
1:F:320:GLN:OE1	1:F:320:GLN:N	2.39	0.51
1:A:270:ASP:OD1	1:A:270:ASP:N	2.43	0.51
1:D:96:ARG:HH21	1:D:97:LYS:NZ	2.09	0.51
1:D:217:ASN:HB3	1:D:239:ILE:HG23	1.92	0.51
1:E:253:ILE:HG22	1:E:255:LYS:HD3	1.93	0.51
1:A:93:ALA:O	1:A:97:LYS:HG2	2.11	0.51
1:C:253:ILE:HG22	1:C:255:LYS:HZ2	1.75	0.51
1:B:171:GLY:O	1:B:175:ILE:HG12	2.10	0.50
1:D:438:PRO:HG3	1:D:443:ASP:HB2	1.93	0.50
1:F:115:PHE:CE1	1:F:136:PRO:HB3	2.46	0.50
1:F:264:LEU:O	1:F:294:THR:HA	2.11	0.50
1:A:377:THR:O	1:A:381:ARG:HG3	2.12	0.50
1:C:91:GLU:HB3	1:C:95:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:NE	1:D:393:ASP:OD2	2.44	0.50
1:D:247:LEU:HD23	1:D:284:ILE:HD13	1.92	0.50
1:F:226:LYS:CG	1:F:246:ARG:HH11	2.24	0.50
1:C:253:ILE:HG22	1:C:255:LYS:NZ	2.26	0.50
1:E:92:ILE:O	1:E:96:ARG:HG3	2.10	0.50
1:D:191:VAL:HG11	1:D:202:ILE:HG21	1.94	0.50
1:A:67:LEU:N	1:A:68:PRO:HD2	2.27	0.50
1:F:427:LYS:HZ1	1:F:452:GLY:HA2	1.75	0.50
1:B:189:VAL:HG22	1:B:263:TYR:HB3	1.93	0.50
1:D:422:ARG:NH2	2:D:2001:ADP:O3B	2.44	0.50
1:E:67:LEU:N	1:E:68:PRO:HD2	2.25	0.50
1:B:198:LEU:HD13	1:B:268:GLU:OE1	2.12	0.50
1:B:495:ARG:HG2	1:B:496:ARG:H	1.77	0.50
1:C:185:ASP:HB3	1:C:260:ARG:HD3	1.94	0.50
1:D:148:LEU:HD12	1:D:170:PRO:HB3	1.94	0.50
1:F:172:ILE:HD12	1:F:215:ILE:HD12	1.94	0.50
1:F:425:ASP:OD1	1:F:453:ARG:NH1	2.44	0.50
1:B:66:GLU:OE2	1:C:339:VAL:HG11	2.12	0.50
1:B:112:ILE:HD13	1:B:118:ALA:HB2	1.94	0.50
1:C:171:GLY:HA2	1:C:263:TYR:HE2	1.76	0.50
1:C:479:MET:HG2	1:C:484:GLN:HB2	1.93	0.50
1:D:55:PRO:HG2	1:D:253:ILE:HA	1.94	0.50
1:D:361:TYR:CD2	1:D:363:THR:HG23	2.47	0.50
1:C:269:ALA:N	1:C:298:SER:OG	2.45	0.50
1:D:93:ALA:HA	1:D:96:ARG:NH1	2.27	0.50
1:D:140:GLN:HG2	1:D:144:TRP:CZ2	2.47	0.50
1:D:395:ASP:O	1:D:399:ARG:NE	2.44	0.50
1:D:464:PHE:HD1	1:D:465:THR:H	1.57	0.50
1:C:289:ARG:O	1:C:292:ARG:HG2	2.11	0.49
1:E:181:LEU:O	1:E:185:ASP:HB2	2.12	0.49
1:F:155:GLY:HA2	1:F:319:VAL:HG22	1.94	0.49
1:B:144:TRP:NE1	1:B:165:LEU:O	2.43	0.49
1:A:351:TYR:CE1	1:A:461:ILE:HG12	2.47	0.49
1:B:67:LEU:N	1:B:68:PRO:HD2	2.27	0.49
1:D:53:ASN:OD1	1:F:371:ARG:NH1	2.45	0.49
1:D:57:GLU:CG	1:D:58:LEU:H	2.25	0.49
1:D:377:THR:HG22	1:D:381:ARG:HH21	1.77	0.49
1:D:386:PRO:O	1:D:413:ILE:HB	2.12	0.49
1:E:56:GLN:HG3	1:E:252:GLU:O	2.12	0.49
1:B:169:LEU:O	1:B:172:ILE:HG13	2.12	0.49
1:C:221:TYR:HE1	1:C:224:VAL:HG11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:ILE:HA	1:C:461:ILE:O	2.12	0.49
1:D:103:ILE:HG21	1:D:108:ILE:HG21	1.93	0.49
1:E:184:GLY:O	1:E:257:ASN:ND2	2.45	0.49
1:A:395:ASP:O	1:A:399:ARG:NE	2.46	0.49
1:B:397:ARG:NE	1:E:214:ARG:HB3	2.27	0.49
1:D:219:CYS:HA	1:D:241:ILE:O	2.12	0.49
1:E:105:GLY:CA	1:E:108:ILE:HD11	2.42	0.49
1:F:378:LYS:O	1:F:382:GLU:HG3	2.11	0.49
1:B:126:ASN:O	1:E:126:ASN:HB3	2.11	0.49
1:B:268:GLU:N	1:B:297:TRP:O	2.46	0.49
1:C:309:ALA:O	1:C:313:LEU:HB2	2.12	0.49
1:D:87:ARG:HB3	1:D:88:SER:HA	1.94	0.49
1:D:96:ARG:HH21	1:D:97:LYS:HZ3	1.59	0.49
1:D:363:THR:HG22	1:D:431:TYR:HB2	1.93	0.49
1:F:144:TRP:NE1	1:F:166:SER:HA	2.27	0.49
1:C:292:ARG:NH1	1:C:294:THR:OG1	2.46	0.49
1:C:224:VAL:H	1:C:246:ARG:NH2	2.11	0.49
1:D:78:TYR:OH	1:D:80:GLU:HG2	2.13	0.49
1:D:137:THR:HB	1:D:140:GLN:HB2	1.95	0.49
1:E:393:ASP:O	1:E:394:LYS:HG3	2.13	0.49
1:B:370:LYS:HD3	1:B:393:ASP:OD2	2.12	0.49
1:A:217:ASN:HA	1:A:239:ILE:O	2.13	0.49
1:A:372:MET:HA	1:A:375:ASP:HB2	1.93	0.49
1:C:395:ASP:HA	1:C:398:GLU:HB2	1.94	0.49
1:D:235:ARG:HH11	1:D:235:ARG:CG	2.24	0.49
1:C:79:VAL:HG12	1:C:79:VAL:O	2.13	0.48
1:E:185:ASP:HA	1:E:257:ASN:HD21	1.77	0.48
1:E:197:GLU:OE2	1:E:370:LYS:HB2	2.13	0.48
1:F:142:GLN:O	1:F:146:MET:HG3	2.13	0.48
1:F:144:TRP:CZ2	1:F:169:LEU:HD12	2.48	0.48
1:B:258:LEU:HB3	1:B:288:ILE:HG22	1.95	0.48
1:D:96:ARG:NH2	1:D:97:LYS:HZ3	2.11	0.48
1:E:188:ILE:HD12	1:E:189:VAL:HG23	1.95	0.48
1:F:313:LEU:HD13	1:F:316:PRO:HB3	1.94	0.48
1:F:335:ILE:CD1	1:F:461:ILE:HA	2.42	0.48
1:A:113:THR:OG1	1:A:117:GLU:OE1	2.26	0.48
1:A:148:LEU:CD2	1:A:170:PRO:HB3	2.41	0.48
1:B:60:LYS:CD	1:B:286:ASP:HB3	2.43	0.48
1:B:101:MET:SD	1:B:321:VAL:HG23	2.53	0.48
1:C:350:LYS:O	1:C:354:THR:HG23	2.14	0.48
1:C:405:GLU:HB3	1:C:410:ARG:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:GLN:HB2	1:E:241:ILE:HD12	1.96	0.48
1:C:465:THR:HG22	1:C:466:GLU:OE1	2.14	0.48
1:F:92:ILE:O	1:F:96:ARG:N	2.42	0.48
1:A:153:MET:HG2	1:A:295:LEU:HD22	1.96	0.48
1:B:214:ARG:O	1:E:397:ARG:NE	2.46	0.48
1:F:159:THR:HG23	1:F:299:ALA:HB2	1.96	0.48
1:A:123:TYR:CE2	1:A:213:SER:HB3	2.48	0.48
1:A:191:VAL:HG11	1:A:202:ILE:HG21	1.96	0.48
1:E:195:THR:OG1	1:E:198:LEU:HD23	2.13	0.48
1:C:175:ILE:HD13	1:C:188:ILE:HB	1.96	0.48
1:C:224:VAL:O	1:C:246:ARG:NH2	2.47	0.48
1:D:263:TYR:CE1	1:D:295:LEU:HD11	2.49	0.48
1:C:370:LYS:HE2	1:C:374:ASP:OD2	2.14	0.48
1:C:475:LEU:HD11	1:C:490:LEU:CD1	2.44	0.48
1:D:84:VAL:HA	1:D:87:ARG:NH2	2.29	0.48
1:F:396:GLN:O	1:F:400:ASP:N	2.46	0.48
1:B:333:THR:OG1	1:B:459:THR:HA	2.14	0.48
1:C:253:ILE:CG2	1:C:255:LYS:HZ2	2.27	0.48
1:D:55:PRO:HG2	1:D:252:GLU:O	2.14	0.47
1:E:215:ILE:HD12	1:E:239:ILE:HD11	1.94	0.47
1:E:399:ARG:O	1:E:403:LEU:HG	2.14	0.47
1:F:81:HIS:ND1	1:F:82:GLU:HG2	2.28	0.47
1:B:75:LYS:HD3	1:B:150:GLY:O	2.13	0.47
1:E:381:ARG:NH2	3:E:2002:SO4:S	2.87	0.47
1:F:87:ARG:HD2	1:F:92:ILE:HD11	1.95	0.47
1:B:102:THR:HB	1:B:320:GLN:HB3	1.96	0.47
1:D:92:ILE:HD12	1:D:96:ARG:HH11	1.79	0.47
1:B:339:VAL:HG12	1:B:340:SER:O	2.14	0.47
1:D:189:VAL:HG22	1:D:263:TYR:HB3	1.95	0.47
1:F:156:ILE:HA	1:F:298:SER:O	2.13	0.47
1:B:140:GLN:NE2	1:B:165:LEU:HB2	2.29	0.47
1:B:142:GLN:O	1:B:146:MET:HG3	2.13	0.47
1:F:223:GLY:H	1:F:246:ARG:HH21	1.63	0.47
1:B:265:VAL:HG22	1:B:295:LEU:HB2	1.96	0.47
1:C:113:THR:N	1:C:117:GLU:OE1	2.31	0.47
1:E:207:SER:OG	1:E:217:ASN:ND2	2.46	0.47
1:E:359:ASN:HA	1:E:360:GLU:HA	1.56	0.47
1:F:67:LEU:N	1:F:68:PRO:HD2	2.30	0.47
1:A:345:ARG:CZ	1:A:379:TYR:HB3	2.44	0.47
1:A:362:LYS:NZ	1:A:406:PHE:O	2.36	0.47
1:B:188:ILE:HD11	1:B:260:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASP:OD1	1:B:271:ARG:N	2.46	0.47
1:B:339:VAL:HG12	1:B:340:SER:N	2.30	0.47
1:B:397:ARG:NH1	1:E:238:GLU:CD	2.67	0.47
1:C:63:TRP:O	1:C:67:LEU:HG	2.14	0.47
1:C:197:GLU:HG2	1:C:370:LYS:HB3	1.97	0.47
1:C:397:ARG:HD2	1:F:214:ARG:O	2.15	0.47
1:D:216:ARG:NH1	1:D:238:GLU:OE2	2.47	0.47
1:D:345:ARG:NH2	1:D:383:ASP:OD1	2.46	0.47
1:E:367:ALA:HA	1:E:436:ASP:HB2	1.95	0.47
1:E:464:PHE:CD1	1:E:468:ASN:HB2	2.48	0.47
1:F:147:ALA:HB2	1:F:153:MET:HE1	1.95	0.47
1:F:270:ASP:OD1	1:F:271:ARG:N	2.45	0.47
1:F:334:GLN:OE1	1:F:479:MET:HG2	2.15	0.47
1:A:159:THR:HA	1:A:163:LYS:NZ	2.29	0.47
1:A:216:ARG:NH1	1:A:235:ARG:O	2.47	0.47
1:A:397:ARG:NH1	1:D:214:ARG:HA	2.30	0.47
1:A:471:LEU:HD12	1:A:475:LEU:HB2	1.96	0.47
1:B:152:ASP:HB3	1:B:313:LEU:HD23	1.97	0.47
1:D:101:MET:HE1	1:D:142:GLN:HB2	1.96	0.47
1:E:386:PRO:O	1:E:413:ILE:HB	2.14	0.47
1:F:153:MET:CE	1:F:295:LEU:HD23	2.44	0.47
1:B:80:GLU:OE2	1:B:84:VAL:HB	2.15	0.47
1:B:124:VAL:CG2	1:B:169:LEU:HD23	2.44	0.47
1:C:181:LEU:O	1:C:185:ASP:HB2	2.15	0.47
1:C:224:VAL:H	1:C:246:ARG:HH21	1.63	0.47
1:E:407:ARG:HG3	1:E:426:VAL:HG23	1.96	0.47
1:F:476:ILE:O	1:F:480:ARG:N	2.45	0.47
1:A:181:LEU:HD21	1:A:238:GLU:HG3	1.96	0.47
1:C:197:GLU:HG2	1:C:370:LYS:CB	2.44	0.47
1:F:285:VAL:HG11	1:F:312:TYR:HD2	1.78	0.47
1:A:114:THR:HG22	1:A:117:GLU:HG3	1.97	0.46
1:A:381:ARG:HB3	1:F:381:ARG:HD3	1.96	0.46
1:C:63:TRP:CZ3	1:C:70:LEU:HD11	2.50	0.46
1:D:278:GLU:OE1	1:D:282:ARG:NH2	2.47	0.46
1:D:348:LEU:HD21	1:D:352:LEU:HD12	1.97	0.46
1:D:476:ILE:O	1:D:480:ARG:HG3	2.14	0.46
1:F:127:GLU:OE1	1:F:209:PHE:HA	2.14	0.46
1:F:203:GLN:HG3	1:F:219:CYS:HB2	1.97	0.46
1:B:345:ARG:NH2	1:B:383:ASP:OD1	2.48	0.46
1:C:294:THR:O	1:C:295:LEU:HD23	2.15	0.46
1:D:474:LYS:N	1:D:474:LYS:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ARG:HG3	1:E:294:THR:HG23	1.96	0.46
1:C:484:GLN:CG	1:C:485:ASN:N	2.79	0.46
1:D:289:ARG:NH1	1:D:291:ASP:OD1	2.49	0.46
1:E:390:ILE:HD12	1:E:420:ALA:HB1	1.96	0.46
1:F:427:LYS:HD2	1:F:427:LYS:HA	1.73	0.46
1:B:101:MET:HA	1:B:320:GLN:O	2.15	0.46
1:A:78:TYR:HB2	1:A:148:LEU:CB	2.44	0.46
1:A:140:GLN:HE21	1:A:165:LEU:HG	1.81	0.46
1:A:395:ASP:HA	1:A:398:GLU:CG	2.45	0.46
1:B:466:GLU:O	1:B:469:LYS:HG2	2.15	0.46
1:D:302:PRO:HB2	1:D:304:GLU:H	1.79	0.46
1:D:424:ILE:H	1:D:450:ARG:NH2	2.14	0.46
1:F:250:MET:HA	1:F:253:ILE:HG22	1.97	0.46
1:B:164:THR:HA	1:B:167:TYR:CZ	2.50	0.46
1:B:282:ARG:HA	1:B:285:VAL:HG22	1.98	0.46
1:C:398:GLU:OE2	1:F:235:ARG:O	2.33	0.46
1:E:103:ILE:CG2	1:E:108:ILE:HD13	2.45	0.46
1:A:163:LYS:N	2:A:2001:ADP:O3B	2.46	0.46
1:C:85:ARG:HA	1:C:86:ASP:HA	1.65	0.46
1:C:127:GLU:OE1	1:C:209:PHE:HA	2.15	0.46
1:C:171:GLY:O	1:C:175:ILE:HG12	2.15	0.46
1:E:242:ALA:HB1	1:E:247:LEU:HB2	1.96	0.46
1:B:396:GLN:HA	1:B:399:ARG:NH2	2.31	0.46
1:C:340:SER:O	1:C:344:LYS:HG3	2.16	0.46
1:C:359:ASN:OD1	1:C:360:GLU:HA	2.16	0.46
1:E:174:HIS:NE2	1:E:262:THR:OG1	2.33	0.46
1:E:336:VAL:HG22	1:E:462:SER:HB2	1.97	0.46
1:A:75:LYS:HD2	1:A:293:GLN:HB2	1.97	0.46
1:A:160:GLY:HA2	2:A:2001:ADP:PA	2.56	0.46
1:B:154:VAL:HG23	1:B:296:MET:HB3	1.98	0.46
1:B:390:ILE:HD11	1:B:421:ALA:HB2	1.98	0.46
1:F:394:LYS:HB3	1:F:399:ARG:HG3	1.98	0.46
1:A:418:ASP:OD1	1:A:447:ARG:NH1	2.37	0.46
1:C:105:GLY:HA3	1:C:317:ILE:HD12	1.97	0.46
1:C:464:PHE:CZ	1:C:469:LYS:HA	2.51	0.46
1:F:147:ALA:HB2	1:F:153:MET:CE	2.46	0.46
1:F:191:VAL:HB	1:F:265:VAL:HG13	1.98	0.46
1:A:359:ASN:OD1	1:A:359:ASN:N	2.49	0.45
1:C:285:VAL:HG13	1:C:292:ARG:HH21	1.81	0.45
1:D:81:HIS:HD2	1:D:117:GLU:HG2	1.76	0.45
1:F:291:ASP:OD1	1:F:291:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LEU:O	1:D:185:ASP:HB2	2.17	0.45
1:D:441:ILE:HB	1:D:471:LEU:HD11	1.98	0.45
1:F:57:GLU:O	1:F:58:LEU:HD12	2.15	0.45
1:A:85:ARG:HA	1:A:86:ASP:HA	1.54	0.45
1:D:103:ILE:HG21	1:D:108:ILE:HG13	1.98	0.45
1:D:344:LYS:HB3	1:D:435:TYR:CE1	2.52	0.45
1:D:443:ASP:O	1:D:447:ARG:N	2.39	0.45
1:A:125:LEU:HD21	1:A:129:LYS:NZ	2.32	0.45
1:A:303:LYS:HD3	1:A:303:LYS:N	2.32	0.45
1:C:226:LYS:HD3	1:C:226:LYS:H	1.81	0.45
1:D:281:ILE:O	1:D:285:VAL:HG23	2.16	0.45
1:E:120:PHE:CE1	1:E:148:LEU:HD11	2.52	0.45
1:F:181:LEU:HD12	1:F:181:LEU:HA	1.82	0.45
1:F:200:VAL:O	1:F:204:THR:HG23	2.15	0.45
1:A:60:LYS:HD2	1:A:61:PRO:HD2	1.98	0.45
1:C:144:TRP:NE1	1:C:166:SER:HA	2.32	0.45
1:A:59:ILE:HD12	1:B:340:SER:HB2	1.98	0.45
1:C:156:ILE:HA	1:C:298:SER:O	2.17	0.45
1:C:220:VAL:HG11	1:C:233:LEU:HD11	1.98	0.45
1:C:305:VAL:O	1:C:309:ALA:N	2.30	0.45
1:C:332:ILE:HG12	1:C:451:THR:HG23	1.99	0.45
1:B:102:THR:O	1:B:319:VAL:HA	2.17	0.45
1:C:246:ARG:O	1:C:246:ARG:HG2	2.16	0.45
1:E:200:VAL:O	1:E:204:THR:HG23	2.17	0.45
1:B:157:ALA:HB3	1:B:163:LYS:CG	2.47	0.45
1:C:270:ASP:OD1	1:C:271:ARG:N	2.48	0.45
1:C:403:LEU:O	1:C:407:ARG:HG3	2.17	0.45
1:A:359:ASN:HA	1:A:360:GLU:HA	1.66	0.45
1:B:182:ALA:HB3	1:B:185:ASP:OD2	2.17	0.45
1:E:77:PHE:HE2	1:E:174:HIS:HA	1.80	0.45
1:E:188:ILE:CD1	1:E:189:VAL:HG23	2.47	0.45
1:D:78:TYR:HB2	1:D:148:LEU:HB3	1.98	0.45
1:D:96:ARG:NH2	1:D:97:LYS:NZ	2.64	0.45
1:E:109:PRO:HG3	1:E:146:MET:HA	1.98	0.45
1:E:161:SER:HB2	1:E:163:LYS:HG3	1.98	0.45
1:D:117:GLU:HA	1:D:117:GLU:OE1	2.16	0.44
1:D:305:VAL:O	1:D:309:ALA:N	2.43	0.44
1:B:80:GLU:OE2	1:B:85:ARG:HG3	2.18	0.44
1:B:180:LEU:HB2	1:E:401:TRP:HD1	1.82	0.44
1:C:365:ILE:HB	1:C:415:VAL:HG22	1.98	0.44
1:D:87:ARG:HG3	1:D:91:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:ASN:HA	1:F:360:GLU:HA	1.57	0.44
1:A:326:LEU:HD11	1:A:442:GLU:HG3	1.99	0.44
1:B:464:PHE:HE2	1:B:472:GLY:HA2	1.82	0.44
1:C:81:HIS:O	1:C:84:VAL:HG12	2.17	0.44
1:C:313:LEU:HB3	1:C:316:PRO:HB3	1.99	0.44
1:C:381:ARG:HG3	1:C:387:ALA:HB3	2.00	0.44
1:D:407:ARG:HG2	1:D:426:VAL:HG23	1.99	0.44
1:E:192:LEU:HB2	1:E:266:LEU:HD13	1.99	0.44
1:B:93:ALA:HA	1:B:96:ARG:HG3	2.00	0.44
1:E:144:TRP:NE1	1:E:165:LEU:O	2.32	0.44
1:E:99:ASN:O	1:E:100:GLU:HG2	2.17	0.44
1:F:328:ALA:HB2	1:F:478:ILE:HG23	1.98	0.44
1:A:242:ALA:HB1	1:A:247:LEU:HB2	2.00	0.44
1:B:203:GLN:HG2	1:B:219:CYS:HB2	1.99	0.44
1:C:340:SER:HB3	1:C:344:LYS:HG2	1.99	0.44
1:C:397:ARG:HD3	1:F:238:GLU:OE2	2.16	0.44
1:C:448:ILE:O	1:C:451:THR:HG22	2.18	0.44
1:C:492:LYS:HB2	1:C:493:TYR:CE1	2.52	0.44
1:D:67:LEU:N	1:D:68:PRO:HD2	2.32	0.44
1:D:156:ILE:HD12	1:D:156:ILE:O	2.18	0.44
1:E:56:GLN:N	1:E:252:GLU:O	2.37	0.44
1:E:103:ILE:HG21	1:E:108:ILE:HG21	1.99	0.44
1:A:56:GLN:C	1:A:57:GLU:HG3	2.38	0.44
1:C:78:TYR:HB2	1:C:148:LEU:HD23	1.99	0.44
1:E:127:GLU:OE1	1:E:209:PHE:HA	2.18	0.44
1:E:443:ASP:O	1:E:447:ARG:N	2.47	0.44
1:F:341:ASP:OD1	1:F:342:PHE:N	2.51	0.44
1:A:205:GLU:HA	1:A:208:LYS:HD3	1.99	0.44
1:C:164:THR:HG23	2:C:2001:ADP:O1B	2.18	0.44
1:E:85:ARG:HA	1:E:110:LYS:NZ	2.33	0.44
1:E:391:HIS:NE2	1:E:394:LYS:HB2	2.33	0.44
1:F:220:VAL:HG13	1:F:229:GLN:OE1	2.18	0.44
1:A:308:LEU:O	1:A:312:TYR:HD1	2.00	0.44
1:B:85:ARG:HA	1:B:86:ASP:HA	1.67	0.44
1:B:433:ILE:HG23	1:B:461:ILE:HB	1.99	0.44
1:D:164:THR:HA	1:D:167:TYR:CE2	2.53	0.44
1:D:465:THR:HG22	1:D:466:GLU:H	1.83	0.44
1:A:154:VAL:HG11	1:A:301:TRP:HZ3	1.82	0.43
1:A:186:GLY:N	1:A:257:ASN:OD1	2.50	0.43
1:B:190:LEU:O	1:B:264:LEU:HD12	2.18	0.43
1:B:308:LEU:HD13	1:B:312:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:THR:HB	1:C:302:PRO:HD3	2.00	0.43
1:D:87:ARG:N	1:D:88:SER:HB2	2.32	0.43
1:F:153:MET:HB2	1:F:317:ILE:O	2.18	0.43
1:A:403:LEU:O	1:A:407:ARG:HG3	2.18	0.43
1:C:316:PRO:O	1:C:317:ILE:HD13	2.19	0.43
1:D:156:ILE:HA	1:D:298:SER:O	2.18	0.43
1:E:235:ARG:HG2	1:E:235:ARG:HH11	1.82	0.43
1:E:311:ASP:C	1:E:312:TYR:HD1	2.21	0.43
1:B:353:GLU:OE2	1:B:385:TRP:HZ2	2.00	0.43
1:D:101:MET:HA	1:D:320:GLN:O	2.18	0.43
1:D:156:ILE:HD11	1:D:320:GLN:HG2	1.99	0.43
1:F:336:VAL:HG22	1:F:462:SER:OG	2.18	0.43
1:B:301:TRP:O	1:B:301:TRP:CD2	2.70	0.43
1:D:419:VAL:O	1:D:422:ARG:HB2	2.19	0.43
1:B:337:GLU:OE2	1:B:351:TYR:OH	2.29	0.43
1:C:84:VAL:HG22	1:C:87:ARG:NH2	2.33	0.43
1:C:87:ARG:NH1	1:C:92:ILE:HG12	2.33	0.43
1:C:484:GLN:HG3	1:C:485:ASN:N	2.33	0.43
1:E:222:GLY:HA2	1:E:246:ARG:HD3	1.99	0.43
1:E:261:VAL:HB	1:E:288:ILE:HG22	2.00	0.43
1:E:351:TYR:CE2	1:E:461:ILE:HD12	2.53	0.43
1:A:337:GLU:OE1	1:A:347:ARG:NE	2.50	0.43
1:B:362:LYS:NZ	1:B:406:PHE:O	2.39	0.43
1:C:154:VAL:HG23	1:C:296:MET:CB	2.49	0.43
1:C:182:ALA:HA	1:F:401:TRP:NE1	2.33	0.43
1:D:139:ILE:HD12	1:D:139:ILE:H	1.83	0.43
1:E:144:TRP:NE1	1:E:166:SER:HA	2.32	0.43
1:F:85:ARG:HA	1:F:86:ASP:HA	1.53	0.43
1:A:163:LYS:HB2	2:A:2001:ADP:O3B	2.18	0.43
1:B:395:ASP:HA	1:B:398:GLU:CG	2.49	0.43
1:C:92:ILE:O	1:C:96:ARG:HG2	2.19	0.43
1:C:140:GLN:NE2	1:C:162:GLY:HA3	2.33	0.43
1:D:306:LYS:HA	1:D:309:ALA:HB3	2.01	0.43
1:D:347:ARG:CZ	1:D:351:TYR:HE1	2.32	0.43
1:A:361:TYR:HD2	1:A:363:THR:HG23	1.83	0.43
1:B:354:THR:O	1:B:357:GLN:HG2	2.18	0.43
1:B:397:ARG:NH1	1:E:214:ARG:C	2.72	0.43
1:C:335:ILE:HD12	1:C:335:ILE:O	2.19	0.43
1:C:345:ARG:CZ	1:C:379:TYR:HB3	2.49	0.43
1:C:352:LEU:HD21	1:C:363:THR:HG21	2.00	0.43
1:C:434:ASN:OD1	1:C:447:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:LYS:HD2	1:D:97:LYS:N	2.34	0.43
1:D:412:PRO:HG2	1:D:413:ILE:HD12	2.00	0.43
1:E:328:ALA:HB2	1:E:478:ILE:HD12	2.01	0.43
1:F:84:VAL:O	1:F:87:ARG:HG3	2.18	0.43
1:D:441:ILE:O	1:D:445:VAL:HG22	2.18	0.43
1:A:87:ARG:N	1:A:88:SER:HB2	2.34	0.43
1:A:92:ILE:HG21	1:A:110:LYS:HE3	2.01	0.43
1:A:464:PHE:CE1	1:A:468:ASN:HB2	2.54	0.43
1:A:474:LYS:HD2	1:A:474:LYS:N	2.33	0.43
1:B:144:TRP:CZ2	1:B:169:LEU:HD13	2.54	0.43
1:D:67:LEU:HD12	1:D:67:LEU:HA	1.91	0.43
1:D:407:ARG:NE	1:D:425:ASP:O	2.48	0.43
1:D:435:TYR:HD1	1:D:435:TYR:O	2.01	0.43
1:F:86:ASP:HB3	1:F:88:SER:HB2	2.00	0.43
1:B:211:HIS:CE1	1:E:211:HIS:CE1	3.06	0.42
1:B:331:ASN:HD21	1:B:456:ALA:C	2.23	0.42
1:B:381:ARG:HB3	1:D:381:ARG:HD2	2.00	0.42
1:C:407:ARG:HG2	1:C:426:VAL:HG23	2.00	0.42
1:D:53:ASN:HD21	1:F:371:ARG:HH11	1.67	0.42
1:D:131:GLU:HG3	1:D:209:PHE:CE1	2.54	0.42
1:E:247:LEU:O	1:E:251:LEU:HD23	2.19	0.42
1:B:362:LYS:HG2	1:B:429:ILE:HG12	2.00	0.42
1:D:347:ARG:NH2	1:D:351:TYR:HE1	2.17	0.42
1:B:186:GLY:N	1:B:257:ASN:OD1	2.51	0.42
1:D:398:GLU:O	1:D:402:VAL:HG23	2.18	0.42
1:F:258:LEU:HB3	1:F:288:ILE:HG22	2.00	0.42
1:B:390:ILE:HG13	1:B:390:ILE:O	2.20	0.42
1:B:427:LYS:HE2	1:B:452:GLY:HA2	2.01	0.42
1:C:475:LEU:HD11	1:C:490:LEU:HD13	2.02	0.42
1:D:296:MET:HE1	1:D:308:LEU:HD23	2.01	0.42
1:F:396:GLN:NE2	1:F:400:ASP:OD1	2.50	0.42
1:B:294:THR:OG1	1:B:313:LEU:HG	2.19	0.42
1:C:273:LEU:CD1	1:C:278:GLU:HB2	2.50	0.42
1:D:289:ARG:O	1:D:292:ARG:NE	2.53	0.42
1:F:269:ALA:H	1:F:298:SER:HG	1.67	0.42
1:A:80:GLU:OE2	1:A:85:ARG:HB2	2.19	0.42
1:B:199:ALA:O	1:B:241:ILE:HG21	2.19	0.42
1:B:258:LEU:HB3	1:B:288:ILE:CG2	2.49	0.42
1:B:359:ASN:HA	1:B:360:GLU:HA	1.52	0.42
1:B:381:ARG:HB3	1:D:381:ARG:HH11	1.84	0.42
1:C:87:ARG:HD2	1:C:92:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ASN:O	1:F:126:ASN:HB3	2.19	0.42
1:C:181:LEU:HD12	1:C:181:LEU:HA	1.79	0.42
1:E:76:ASN:O	1:E:77:PHE:HD1	2.02	0.42
1:B:157:ALA:HB3	1:B:163:LYS:HG2	2.02	0.42
1:C:62:ASN:O	1:C:66:GLU:HG2	2.19	0.42
1:C:302:PRO:HA	1:C:303:LYS:HB3	2.01	0.42
1:F:136:PRO:HA	2:F:2001:ADP:N6	2.34	0.42
1:B:181:LEU:HA	1:B:260:ARG:HH12	1.84	0.42
1:B:278:GLU:N	1:B:279:PRO:HD2	2.35	0.42
1:D:266:LEU:HD11	1:D:296:MET:HE2	2.02	0.42
1:E:330:HIS:CE1	1:E:482:ALA:HA	2.55	0.42
1:A:302:PRO:O	1:A:305:VAL:HG22	2.20	0.42
1:B:337:GLU:O	1:B:339:VAL:HG23	2.20	0.42
1:B:389:ALA:HA	1:B:415:VAL:O	2.20	0.42
1:B:450:ARG:HD3	1:B:450:ARG:N	2.34	0.42
1:D:344:LYS:HE2	1:D:435:TYR:CD1	2.55	0.42
1:B:96:ARG:O	1:B:101:MET:HG2	2.20	0.42
1:B:407:ARG:CD	1:B:426:VAL:HG23	2.47	0.42
1:C:372:MET:HA	1:C:375:ASP:HB2	2.01	0.42
1:E:219:CYS:SG	1:E:221:TYR:HE2	2.37	0.42
1:D:53:ASN:HD21	1:F:371:ARG:HD2	1.84	0.41
1:E:464:PHE:HD2	1:E:490:LEU:HD12	1.85	0.41
1:F:154:VAL:O	1:F:318:GLN:HA	2.21	0.41
1:A:280:GLN:O	1:A:284:ILE:HG13	2.20	0.41
1:A:301:TRP:HA	1:A:305:VAL:HG21	2.03	0.41
1:A:370:LYS:HE2	1:A:374:ASP:OD2	2.20	0.41
1:C:105:GLY:N	1:C:108:ILE:HD11	2.35	0.41
1:C:112:ILE:HD11	1:C:144:TRP:HE3	1.85	0.41
1:C:201:GLN:O	1:C:205:GLU:HG2	2.20	0.41
1:C:296:MET:HG3	1:C:313:LEU:HD11	2.01	0.41
1:C:427:LYS:HE3	1:C:450:ARG:HA	2.02	0.41
1:E:356:SER:HA	1:E:361:TYR:CE1	2.55	0.41
1:F:464:PHE:HZ	1:F:469:LYS:HA	1.84	0.41
1:B:282:ARG:HD3	1:B:286:ASP:OD2	2.21	0.41
1:C:376:ILE:HG12	1:C:435:TYR:CE2	2.56	0.41
1:C:476:ILE:HA	1:C:479:MET:HB3	2.02	0.41
1:C:486:ILE:O	1:C:488:PRO:HD2	2.20	0.41
1:D:154:VAL:HG13	1:D:296:MET:HB3	2.02	0.41
1:D:303:LYS:H	1:D:303:LYS:HD2	1.85	0.41
1:D:364:LEU:HD22	1:D:366:PHE:CE2	2.56	0.41
1:D:438:PRO:HD3	1:D:447:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:ALA:HA	1:E:96:ARG:NE	2.35	0.41
1:E:175:ILE:CD1	1:E:238:GLU:HB3	2.49	0.41
1:E:278:GLU:N	1:E:279:PRO:HD2	2.35	0.41
1:E:464:PHE:HD1	1:E:465:THR:H	1.66	0.41
1:A:188:ILE:HA	1:A:260:ARG:O	2.21	0.41
1:B:174:HIS:CD2	1:B:263:TYR:HB2	2.53	0.41
1:B:397:ARG:HD3	1:E:216:ARG:HD3	2.02	0.41
1:B:426:VAL:HG13	1:B:429:ILE:HD12	2.03	0.41
1:C:359:ASN:HA	1:C:360:GLU:HA	1.57	0.41
1:E:77:PHE:CE2	1:E:174:HIS:HA	2.56	0.41
1:F:222:GLY:HA2	1:F:246:ARG:HH21	1.84	0.41
1:B:481:GLU:OE1	1:B:481:GLU:HA	2.20	0.41
1:D:290:PRO:HA	1:D:292:ARG:NH2	2.36	0.41
1:E:156:ILE:HA	1:E:298:SER:O	2.21	0.41
1:F:223:GLY:N	1:F:246:ARG:HH21	2.18	0.41
1:A:57:GLU:HA	1:A:252:GLU:HG2	2.02	0.41
1:A:102:THR:N	1:A:320:GLN:O	2.52	0.41
1:B:304:GLU:O	1:B:308:LEU:HB2	2.20	0.41
1:C:490:LEU:HA	1:C:493:TYR:CD2	2.56	0.41
1:D:226:LYS:H	1:D:226:LYS:HG2	1.72	0.41
1:B:235:ARG:O	1:E:398:GLU:OE2	2.39	0.41
1:B:401:TRP:O	1:B:404:GLN:HG2	2.21	0.41
1:B:441:ILE:HG13	1:B:441:ILE:O	2.21	0.41
1:D:102:THR:OG1	1:D:320:GLN:HB3	2.21	0.41
1:D:402:VAL:HG12	1:D:414:MET:CE	2.51	0.41
1:B:60:LYS:NZ	1:B:63:TRP:CD1	2.84	0.41
1:B:260:ARG:O	1:B:262:THR:HG23	2.21	0.41
1:B:331:ASN:OD1	1:B:456:ALA:HA	2.21	0.41
1:B:397:ARG:CZ	1:E:214:ARG:HB3	2.51	0.41
1:D:94:GLN:O	1:D:98:GLU:N	2.45	0.41
1:F:81:HIS:O	1:F:84:VAL:HG22	2.21	0.41
1:A:330:HIS:ND1	1:A:482:ALA:HA	2.36	0.41
1:B:157:ALA:HB2	1:B:321:VAL:HG12	2.02	0.41
1:C:243:THR:HG23	1:C:246:ARG:H	1.85	0.41
1:C:336:VAL:HG13	1:C:462:SER:O	2.21	0.41
1:D:139:ILE:HD13	1:D:161:SER:OG	2.21	0.41
1:D:390:ILE:O	1:D:390:ILE:HG13	2.20	0.41
1:F:187:PRO:HB3	1:F:240:VAL:HG23	2.02	0.41
1:F:339:VAL:HG21	1:F:463:PHE:HB3	2.03	0.41
1:A:115:PHE:CE1	1:A:136:PRO:HB3	2.57	0.40
1:A:167:TYR:CE2	1:A:265:VAL:HG11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:HB3	1:A:260:ARG:HG3	2.02	0.40
1:B:208:LYS:O	1:B:211:HIS:HE1	2.05	0.40
1:B:397:ARG:HD3	1:E:216:ARG:CD	2.51	0.40
1:B:495:ARG:HG2	1:B:496:ARG:N	2.36	0.40
1:C:169:LEU:HD23	1:C:169:LEU:HA	1.91	0.40
1:C:284:ILE:O	1:C:288:ILE:HG13	2.21	0.40
1:D:92:ILE:O	1:D:96:ARG:HG3	2.21	0.40
1:D:231:ARG:O	1:D:234:SER:OG	2.39	0.40
1:D:444:TYR:O	1:D:448:ILE:HG13	2.21	0.40
1:E:350:LYS:HA	1:E:350:LYS:HD3	1.79	0.40
1:F:87:ARG:H	1:F:88:SER:CB	2.33	0.40
1:F:277:PHE:O	1:F:281:ILE:HG23	2.21	0.40
1:F:284:ILE:HD12	1:F:285:VAL:HG23	2.03	0.40
1:A:490:LEU:HD23	1:A:490:LEU:H	1.86	0.40
1:B:112:ILE:CG2	1:B:117:GLU:HB3	2.51	0.40
1:D:233:LEU:HD23	1:D:256:THR:HB	2.03	0.40
1:E:226:LYS:NZ	3:E:2004:SO4:O1	2.55	0.40
1:E:422:ARG:NH2	1:E:443:ASP:OD1	2.54	0.40
1:F:226:LYS:HG3	1:F:246:ARG:NH1	2.32	0.40
1:C:464:PHE:HZ	1:C:469:LYS:HA	1.85	0.40
1:D:110:LYS:HD3	1:D:110:LYS:N	2.35	0.40
1:D:114:THR:HG22	1:D:115:PHE:N	2.37	0.40
1:E:67:LEU:N	1:E:68:PRO:CD	2.84	0.40
1:F:257:ASN:HB2	1:F:259:LYS:HD3	2.03	0.40
1:B:126:ASN:HD22	1:E:130:ALA:HA	1.86	0.40
1:B:396:GLN:CD	1:B:396:GLN:H	2.25	0.40
1:E:175:ILE:HD11	1:E:238:GLU:HB3	2.03	0.40
1:B:386:PRO:O	1:B:413:ILE:HB	2.22	0.40
1:C:97:LYS:HA	1:C:100:GLU:HA	2.03	0.40
1:D:103:ILE:CG2	1:D:108:ILE:HG13	2.51	0.40
1:D:438:PRO:HG2	1:D:440:ASN:O	2.22	0.40
1:F:185:ASP:HB3	1:F:260:ARG:HD3	2.04	0.40
1:F:443:ASP:O	1:F:447:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/546 (81%)	437 (99%)	4 (1%)	0	100	100
1	B	442/546 (81%)	440 (100%)	1 (0%)	1 (0%)	47	77
1	C	443/546 (81%)	432 (98%)	10 (2%)	1 (0%)	47	77
1	D	442/546 (81%)	437 (99%)	4 (1%)	1 (0%)	47	77
1	E	442/546 (81%)	439 (99%)	3 (1%)	0	100	100
1	F	441/546 (81%)	437 (99%)	4 (1%)	0	100	100
All	All	2651/3276 (81%)	2622 (99%)	26 (1%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	80	GLU
1	C	327	SER
1	B	324	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/450 (85%)	379 (99%)	4 (1%)	76	89
1	B	384/450 (85%)	377 (98%)	7 (2%)	59	80
1	C	385/450 (86%)	378 (98%)	7 (2%)	59	80
1	D	384/450 (85%)	377 (98%)	7 (2%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	384/450 (85%)	382 (100%)	2 (0%)	88	94
1	F	383/450 (85%)	380 (99%)	3 (1%)	81	91
All	All	2303/2700 (85%)	2273 (99%)	30 (1%)	69	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ARG
1	A	271	ARG
1	A	282	ARG
1	A	464	PHE
1	B	196	ARG
1	B	292	ARG
1	B	318	GLN
1	B	410	ARG
1	B	435	TYR
1	B	450	ARG
1	B	464	PHE
1	C	214	ARG
1	C	231	ARG
1	C	263	TYR
1	C	292	ARG
1	C	399	ARG
1	C	435	TYR
1	C	493	TYR
1	D	110	LYS
1	D	151	ARG
1	D	301	TRP
1	D	320	GLN
1	D	422	ARG
1	D	435	TYR
1	D	464	PHE
1	E	101	MET
1	E	492	LYS
1	F	280	GLN
1	F	292	ARG
1	F	370	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	126	ASN
1	C	391	HIS
1	D	331	ASN
1	E	330	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	SO4	F	2002	-	4,4,4	0.15	0	6,6,6	0.06	0
2	ADP	C	2001	4	24,29,29	0.94	1 (4%)	29,45,45	1.61	3 (10%)
3	SO4	A	2002	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	D	2002	-	4,4,4	0.14	0	6,6,6	0.08	0
2	ADP	B	2001	1	24,29,29	0.97	1 (4%)	29,45,45	1.63	5 (17%)
2	ADP	E	2001	1	24,29,29	0.98	1 (4%)	29,45,45	1.60	5 (17%)
2	ADP	D	2001	1	24,29,29	0.94	1 (4%)	29,45,45	1.64	6 (20%)
3	SO4	B	2002	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	E	2002	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	E	2003	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	E	2004	-	4,4,4	0.13	0	6,6,6	0.08	0
2	ADP	F	2001	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	5 (17%)
2	ADP	A	2001	4,1	24,29,29	1.00	1 (4%)	29,45,45	1.50	5 (17%)
3	SO4	C	2002	-	4,4,4	0.14	0	6,6,6	0.14	0

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	C	2001	4	-	5/12/32/32	0/3/3/3
2	ADP	B	2001	1	-	5/12/32/32	0/3/3/3
2	ADP	E	2001	1	-	4/12/32/32	0/3/3/3
2	ADP	D	2001	1	-	5/12/32/32	0/3/3/3
2	ADP	F	2001	-	-	4/12/32/32	0/3/3/3
2	ADP	A	2001	4,1	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2001	ADP	C5-C4	2.58	1.47	1.40
2	A	2001	ADP	C5-C4	2.57	1.47	1.40
2	B	2001	ADP	C5-C4	2.56	1.47	1.40
2	D	2001	ADP	C5-C4	2.56	1.47	1.40
2	F	2001	ADP	C5-C4	2.47	1.47	1.40
2	C	2001	ADP	C5-C4	2.40	1.47	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	ADP	PA-O3A-PB	-5.35	114.47	132.83
2	D	2001	ADP	PA-O3A-PB	-4.56	117.17	132.83
2	E	2001	ADP	PA-O3A-PB	-4.52	117.31	132.83
2	A	2001	ADP	PA-O3A-PB	-4.47	117.48	132.83
2	B	2001	ADP	PA-O3A-PB	-4.29	118.09	132.83
2	F	2001	ADP	PA-O3A-PB	-3.83	119.68	132.83
2	F	2001	ADP	C4-C5-N7	-3.16	106.10	109.40
2	C	2001	ADP	C4-C5-N7	-3.10	106.17	109.40
2	C	2001	ADP	N3-C2-N1	-3.10	123.84	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	ADP	C3'-C2'-C1'	3.09	105.62	100.98
2	F	2001	ADP	N3-C2-N1	-3.03	123.94	128.68
2	E	2001	ADP	C3'-C2'-C1'	3.00	105.50	100.98
2	E	2001	ADP	N3-C2-N1	-2.98	124.02	128.68
2	B	2001	ADP	N3-C2-N1	-2.98	124.03	128.68
2	A	2001	ADP	N3-C2-N1	-2.93	124.10	128.68
2	D	2001	ADP	C4-C5-N7	-2.86	106.42	109.40
2	A	2001	ADP	C4-C5-N7	-2.84	106.44	109.40
2	D	2001	ADP	C3'-C2'-C1'	2.78	105.16	100.98
2	B	2001	ADP	C4-C5-N7	-2.77	106.51	109.40
2	D	2001	ADP	N3-C2-N1	-2.76	124.36	128.68
2	E	2001	ADP	C4-C5-N7	-2.73	106.55	109.40
2	A	2001	ADP	C3'-C2'-C1'	2.55	104.81	100.98
2	B	2001	ADP	O2A-PA-O1A	2.44	124.31	112.24
2	D	2001	ADP	O5'-PA-O1A	-2.37	99.80	109.07
2	E	2001	ADP	O2A-PA-O1A	2.20	123.10	112.24
2	D	2001	ADP	O2A-PA-O1A	2.07	122.46	112.24
2	A	2001	ADP	O3B-PB-O2B	2.03	115.39	107.64
2	F	2001	ADP	O3B-PB-O2B	2.01	115.33	107.64
2	F	2001	ADP	C5'-C4'-C3'	-2.01	107.64	115.18

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	ADP	C5'-O5'-PA-O1A
2	A	2001	ADP	C4'-C5'-O5'-PA
2	A	2001	ADP	O4'-C4'-C5'-O5'
2	A	2001	ADP	C3'-C4'-C5'-O5'
2	B	2001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C3'-C4'-C5'-O5'
2	C	2001	ADP	PA-O3A-PB-O2B
2	C	2001	ADP	PA-O3A-PB-O3B
2	D	2001	ADP	C5'-O5'-PA-O3A
2	D	2001	ADP	O4'-C4'-C5'-O5'
2	D	2001	ADP	C3'-C4'-C5'-O5'
2	E	2001	ADP	C5'-O5'-PA-O1A
2	E	2001	ADP	O4'-C4'-C5'-O5'
2	E	2001	ADP	C3'-C4'-C5'-O5'
2	F	2001	ADP	PA-O3A-PB-O2B
2	F	2001	ADP	PA-O3A-PB-O3B
2	F	2001	ADP	C3'-C4'-C5'-O5'

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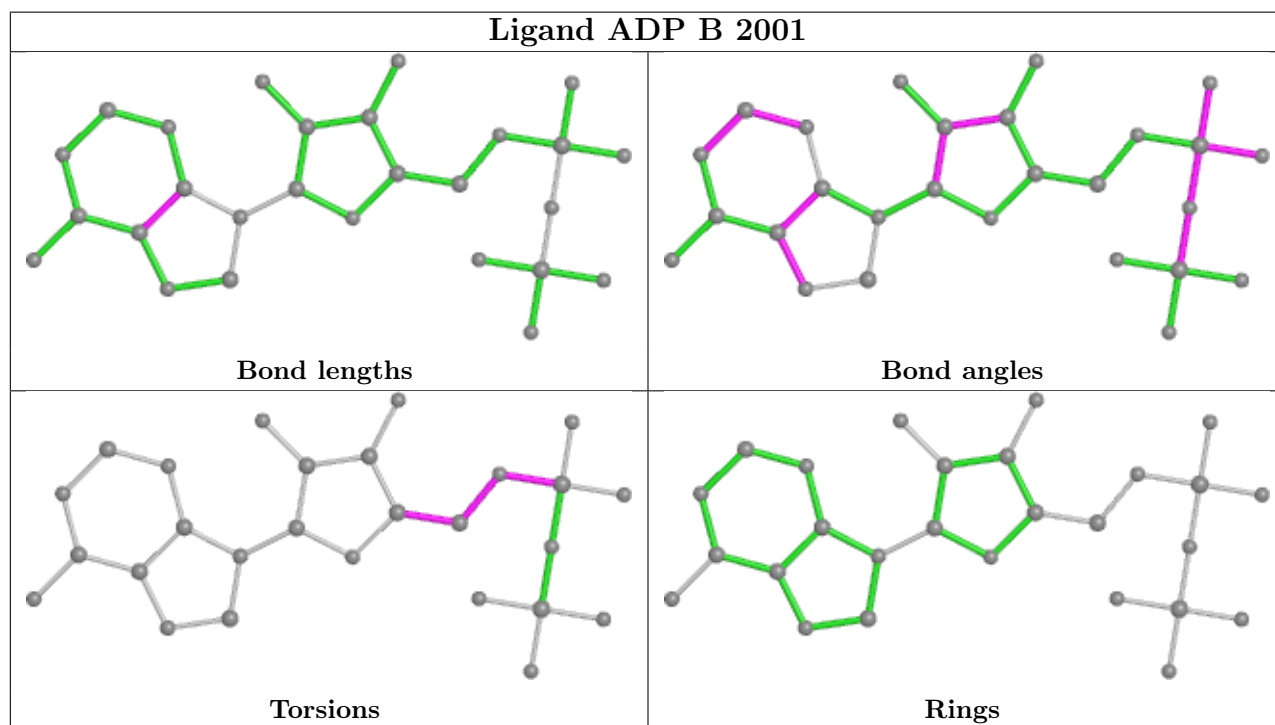
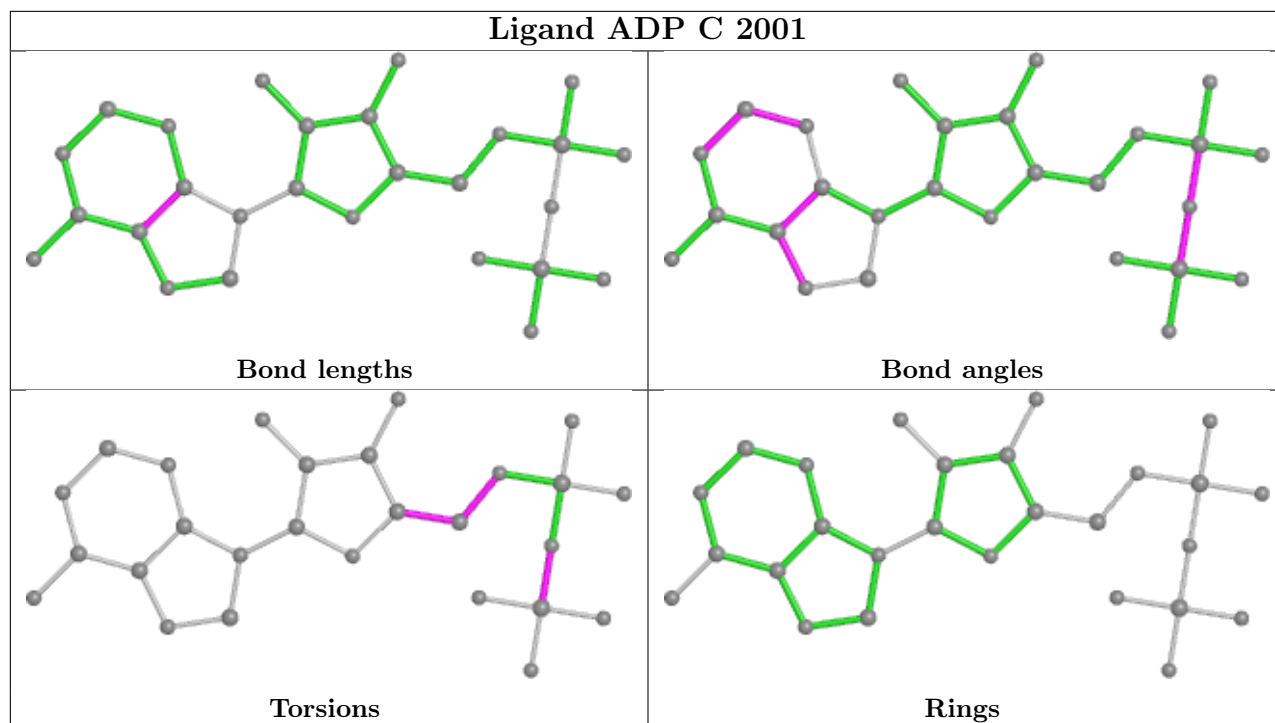
Mol	Chain	Res	Type	Atoms
2	B	2001	ADP	O4'-C4'-C5'-O5'
2	C	2001	ADP	O4'-C4'-C5'-O5'
2	C	2001	ADP	C3'-C4'-C5'-O5'
2	F	2001	ADP	O4'-C4'-C5'-O5'
2	B	2001	ADP	C4'-C5'-O5'-PA
2	C	2001	ADP	C4'-C5'-O5'-PA
2	E	2001	ADP	C4'-C5'-O5'-PA
2	D	2001	ADP	C4'-C5'-O5'-PA
2	D	2001	ADP	C5'-O5'-PA-O2A
2	B	2001	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

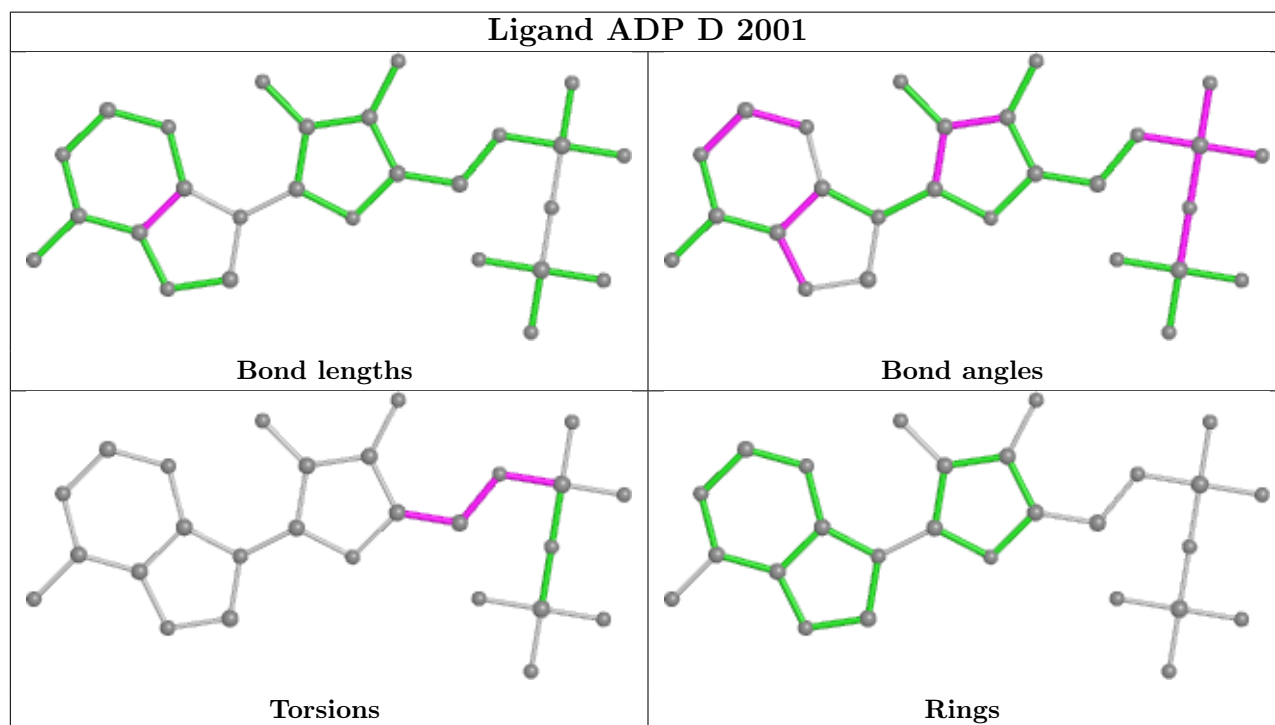
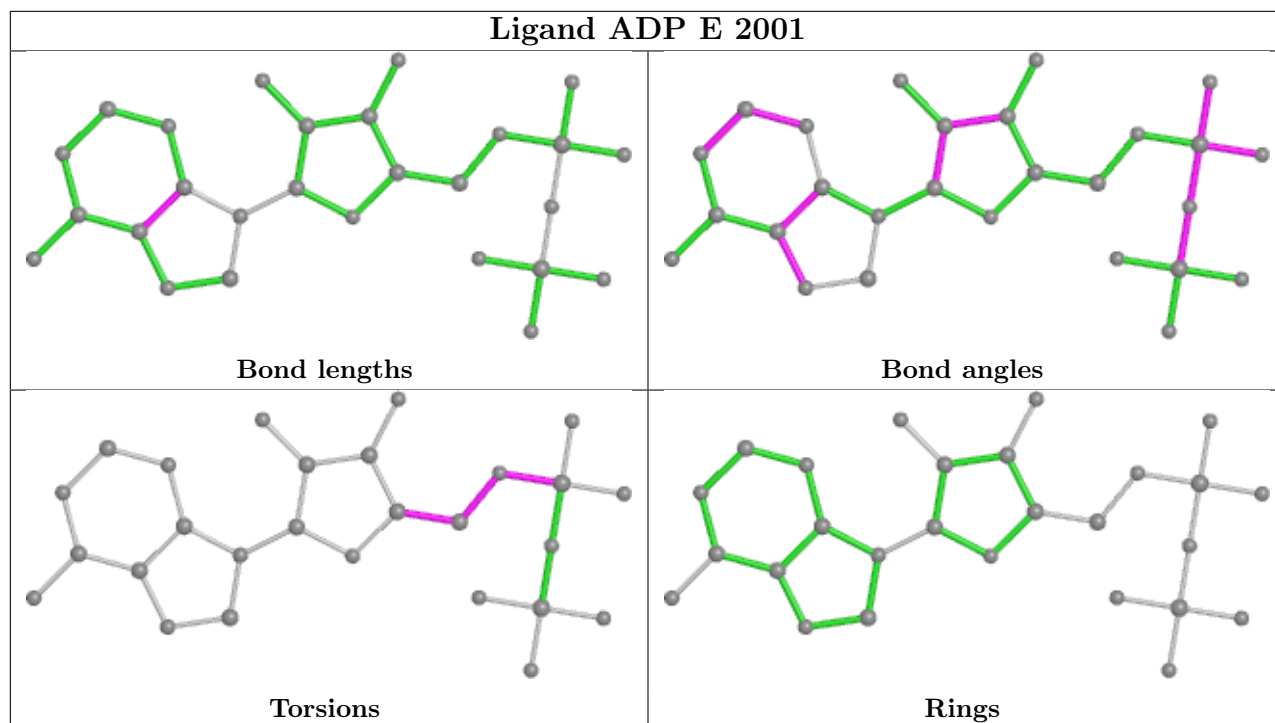
6 monomers are involved in 12 short contacts:

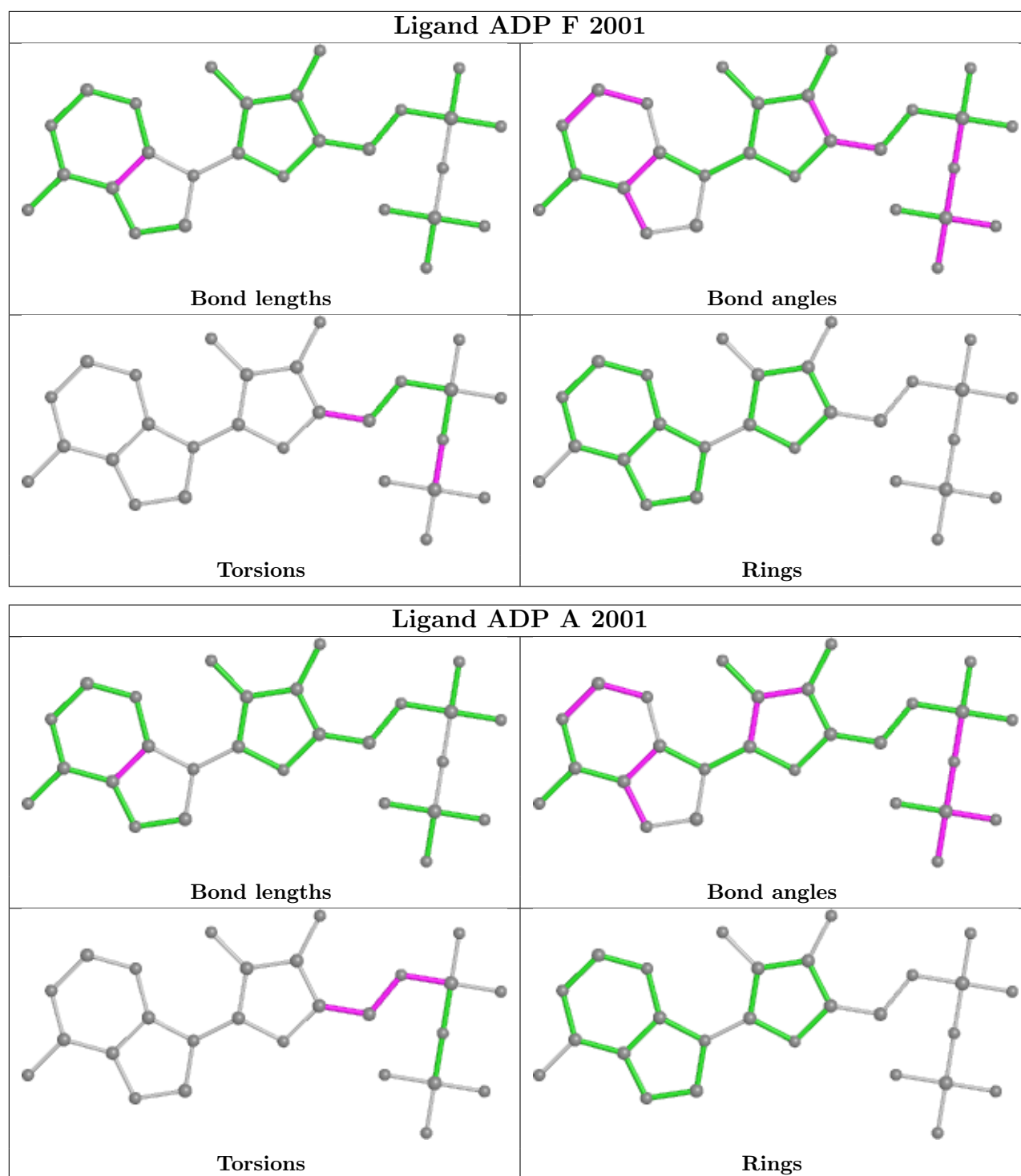
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	ADP	1	0
2	D	2001	ADP	2	0
3	E	2002	SO4	2	0
3	E	2004	SO4	1	0
2	F	2001	ADP	1	0
2	A	2001	ADP	5	0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	443/546 (81%)	0.48	14 (3%) 47 24	44, 79, 135, 213	0
1	B	444/546 (81%)	1.12	89 (20%) 1 0	81, 127, 188, 295	0
1	C	445/546 (81%)	0.96	67 (15%) 2 1	47, 104, 181, 267	0
1	D	444/546 (81%)	0.91	57 (12%) 3 1	69, 118, 174, 280	0
1	E	444/546 (81%)	0.80	40 (9%) 9 3	53, 106, 166, 274	0
1	F	443/546 (81%)	0.75	41 (9%) 8 3	46, 93, 164, 266	0
All	All	2663/3276 (81%)	0.83	308 (11%) 4 1	44, 106, 175, 295	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	454	ALA	11.5
1	C	155	GLY	10.4
1	E	81	HIS	10.2
1	B	115	PHE	10.0
1	E	359	ASN	9.2
1	F	54	GLN	8.3
1	D	298	SER	7.6
1	C	441	ILE	6.8
1	D	393	ASP	6.3
1	F	455	GLY	6.2
1	F	330	HIS	6.2
1	D	363	THR	6.0
1	B	451	THR	6.0
1	D	455	GLY	5.9
1	D	488	PRO	5.9
1	F	456	ALA	5.9
1	C	327	SER	5.8
1	B	423	GLY	5.7
1	A	301	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	119	GLY	5.5
1	B	429	ILE	5.4
1	E	84	VAL	5.4
1	B	78	TYR	5.4
1	C	442	GLU	5.3
1	C	337	GLU	5.2
1	F	454	ALA	5.2
1	B	95	PHE	5.2
1	C	275	MET	5.2
1	C	489	GLU	5.1
1	E	190	LEU	5.1
1	E	80	GLU	5.1
1	C	316	PRO	5.1
1	B	455	GLY	5.0
1	B	322	GLY	5.0
1	A	454	ALA	5.0
1	B	426	VAL	4.9
1	C	94	GLN	4.9
1	D	434	ASN	4.9
1	D	385	TRP	4.8
1	D	99	ASN	4.8
1	B	156	ILE	4.7
1	C	325	GLU	4.7
1	C	84	VAL	4.6
1	A	393	ASP	4.6
1	B	325	GLU	4.6
1	B	378	LYS	4.6
1	C	326	LEU	4.5
1	B	96	ARG	4.5
1	C	464	PHE	4.4
1	E	395	ASP	4.4
1	C	87	ARG	4.4
1	D	495	ARG	4.3
1	C	340	SER	4.2
1	E	147	ALA	4.2
1	B	97	LYS	4.2
1	B	148	LEU	4.1
1	E	210	GLY	4.1
1	B	326	LEU	4.1
1	C	328	ALA	4.0
1	B	58	LEU	4.0
1	E	134	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	456	ALA	4.0
1	B	123	TYR	4.0
1	F	222	GLY	4.0
1	B	448	ILE	3.9
1	B	462	SER	3.9
1	F	490	LEU	3.8
1	F	428	GLY	3.8
1	B	144	TRP	3.8
1	B	419	VAL	3.8
1	B	323	SER	3.7
1	E	64	ASP	3.7
1	C	78	TYR	3.7
1	C	456	ALA	3.7
1	D	491	LEU	3.7
1	F	434	ASN	3.7
1	D	440	ASN	3.7
1	A	227	SER	3.6
1	D	166	SER	3.6
1	B	463	PHE	3.6
1	B	496	ARG	3.6
1	D	471	LEU	3.5
1	E	120	PHE	3.5
1	C	111	PRO	3.5
1	E	112	ILE	3.5
1	B	155	GLY	3.5
1	B	314	ASN	3.5
1	A	327	SER	3.5
1	B	68	PRO	3.4
1	D	236	GLY	3.4
1	B	269	ALA	3.4
1	C	253	ILE	3.4
1	D	439	GLY	3.4
1	B	235	ARG	3.4
1	B	159	THR	3.4
1	B	438	PRO	3.3
1	C	143	GLY	3.3
1	E	155	GLY	3.3
1	F	79	VAL	3.3
1	B	87	ARG	3.3
1	B	53	ASN	3.2
1	E	318	GLN	3.2
1	F	103	ILE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	159	THR	3.2
1	D	327	SER	3.2
1	F	441	ILE	3.2
1	C	373	CYS	3.2
1	E	310	ALA	3.2
1	B	424	ILE	3.2
1	D	456	ALA	3.2
1	F	468	ASN	3.2
1	B	151	ARG	3.2
1	F	442	GLU	3.2
1	B	454	ALA	3.1
1	B	162	GLY	3.1
1	B	296	MET	3.1
1	F	466	GLU	3.1
1	B	393	ASP	3.1
1	D	296	MET	3.1
1	B	166	SER	3.1
1	F	495	ARG	3.1
1	D	128	VAL	3.1
1	C	156	ILE	3.0
1	F	327	SER	3.0
1	E	496	ARG	3.0
1	D	486	ILE	3.0
1	B	453	ARG	3.0
1	D	78	TYR	3.0
1	B	490	LEU	3.0
1	B	84	VAL	2.9
1	C	277	PHE	2.9
1	C	483	ASN	2.9
1	B	418	ASP	2.9
1	B	427	LYS	2.9
1	D	55	PRO	2.9
1	A	426	VAL	2.9
1	B	297	TRP	2.8
1	F	416	ALA	2.8
1	B	279	PRO	2.8
1	C	480	ARG	2.8
1	D	332	ILE	2.8
1	B	284	ILE	2.8
1	C	66	GLU	2.8
1	E	227	SER	2.8
1	D	364	LEU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	431	TYR	2.7
1	B	470	GLY	2.7
1	B	430	ASN	2.7
1	D	254	GLY	2.7
1	E	262	THR	2.7
1	F	464	PHE	2.7
1	E	79	VAL	2.7
1	C	486	ILE	2.7
1	C	67	LEU	2.7
1	F	359	ASN	2.7
1	B	366	PHE	2.7
1	D	476	ILE	2.7
1	A	361	TYR	2.7
1	B	226	LYS	2.7
1	C	344	LYS	2.6
1	E	495	ARG	2.6
1	B	363	THR	2.6
1	D	133	PHE	2.6
1	D	229	GLN	2.6
1	F	97	LYS	2.6
1	D	111	PRO	2.6
1	C	336	VAL	2.6
1	C	368	SER	2.6
1	D	451	THR	2.6
1	D	426	VAL	2.6
1	C	399	ARG	2.6
1	B	190	LEU	2.6
1	B	263	TYR	2.6
1	F	304	GLU	2.6
1	E	54	GLN	2.6
1	F	274	ASP	2.6
1	D	294	THR	2.6
1	B	444	TYR	2.6
1	D	306	LYS	2.6
1	B	109	PRO	2.5
1	E	175	ILE	2.5
1	D	147	ALA	2.5
1	E	189	VAL	2.5
1	B	120	PHE	2.5
1	D	347	ARG	2.5
1	E	246	ARG	2.5
1	C	390	ILE	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	394	LYS	2.5
1	E	164	THR	2.5
1	F	197	GLU	2.5
1	D	86	ASP	2.5
1	B	348	LEU	2.4
1	F	155	GLY	2.4
1	B	139	ILE	2.4
1	E	78	TYR	2.4
1	F	108	ILE	2.4
1	C	471	LEU	2.4
1	C	494	ASP	2.4
1	B	136	PRO	2.4
1	F	379	TYR	2.4
1	E	211	HIS	2.4
1	B	64	ASP	2.4
1	D	77	PHE	2.4
1	B	130	ALA	2.4
1	B	199	ALA	2.4
1	A	86	ASP	2.4
1	C	403	LEU	2.4
1	B	461	ILE	2.3
1	B	83	SER	2.3
1	D	329	SER	2.3
1	F	154	VAL	2.3
1	D	317	ILE	2.3
1	F	271	ARG	2.3
1	B	319	VAL	2.3
1	C	107	ASP	2.3
1	F	427	LYS	2.3
1	C	445	VAL	2.3
1	B	450	ARG	2.3
1	C	408	ASN	2.3
1	C	485	ASN	2.3
1	D	431	TYR	2.3
1	C	388	LEU	2.3
1	C	267	ASP	2.3
1	F	461	ILE	2.3
1	F	336	VAL	2.2
1	B	434	ASN	2.2
1	C	465	THR	2.2
1	D	178	GLN	2.2
1	E	74	GLU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	426	VAL	2.2
1	F	363	THR	2.2
1	E	178	GLN	2.2
1	E	491	LEU	2.2
1	C	154	VAL	2.2
1	A	410	ARG	2.2
1	C	481	GLU	2.2
1	D	142	GLN	2.2
1	B	154	VAL	2.2
1	A	126	ASN	2.2
1	D	351	TYR	2.2
1	F	143	GLY	2.2
1	C	448	ILE	2.2
1	C	93	ALA	2.2
1	B	471	LEU	2.2
1	C	491	LEU	2.2
1	D	139	ILE	2.2
1	D	156	ILE	2.2
1	B	80	GLU	2.2
1	D	481	GLU	2.2
1	D	482	ALA	2.2
1	D	266	LEU	2.2
1	C	75	LYS	2.2
1	D	159	THR	2.2
1	C	479	MET	2.2
1	E	353	GLU	2.2
1	C	493	TYR	2.2
1	B	169	LEU	2.2
1	C	416	ALA	2.2
1	F	484	GLN	2.2
1	A	332	ILE	2.2
1	B	295	LEU	2.1
1	D	154	VAL	2.1
1	B	86	ASP	2.1
1	C	439	GLY	2.1
1	F	392	GLY	2.1
1	D	124	VAL	2.1
1	F	55	PRO	2.1
1	A	53	ASN	2.1
1	B	332	ILE	2.1
1	C	451	THR	2.1
1	E	380	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	104	SER	2.1
1	C	495	ARG	2.1
1	D	397	ARG	2.1
1	C	444	TYR	2.1
1	C	125	LEU	2.1
1	E	94	GLN	2.1
1	F	322	GLY	2.1
1	C	147	ALA	2.1
1	C	212	SER	2.1
1	D	335	ILE	2.1
1	E	291	ASP	2.1
1	A	159	THR	2.1
1	B	60	LYS	2.1
1	C	370	LYS	2.1
1	B	128	VAL	2.1
1	B	327	SER	2.1
1	E	168	CYS	2.1
1	C	225	PRO	2.1
1	F	242	ALA	2.1
1	B	175	ILE	2.1
1	E	172	ILE	2.1
1	E	105	GLY	2.1
1	D	132	GLY	2.0
1	D	404	GLN	2.0
1	C	118	ALA	2.0
1	E	263	TYR	2.0
1	D	230	ILE	2.0
1	A	211	HIS	2.0
1	B	197	GLU	2.0
1	F	86	ASP	2.0
1	B	218	THR	2.0
1	B	307	GLN	2.0
1	C	110	LYS	2.0
1	B	342	PHE	2.0
1	E	87	ARG	2.0
1	B	127	GLU	2.0
1	B	289	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

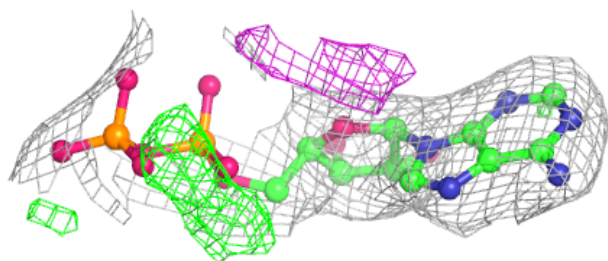
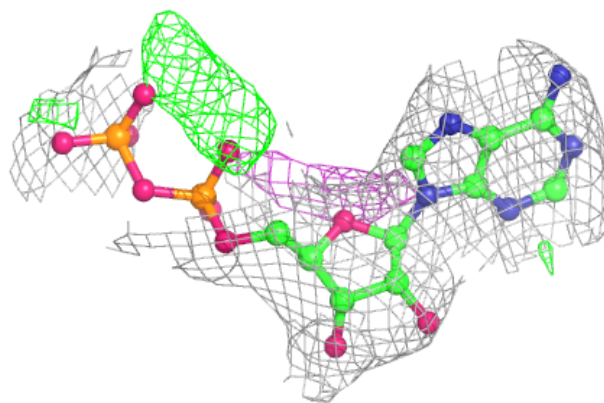
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	SO4	B	2002	5/5	0.78	0.31	98,99,110,123	0
3	SO4	E	2003	5/5	0.85	0.20	116,119,133,138	0
3	SO4	E	2004	5/5	0.86	0.16	89,106,119,140	0
2	ADP	D	2001	27/27	0.87	0.20	78,95,129,132	0
2	ADP	B	2001	27/27	0.88	0.17	76,105,130,146	0
3	SO4	E	2002	5/5	0.88	0.22	79,81,85,85	0
4	MG	E	2005	1/1	0.89	0.13	88,88,88,88	0
2	ADP	A	2001	27/27	0.92	0.25	56,72,87,92	0
3	SO4	A	2002	5/5	0.93	0.20	62,94,101,154	0
2	ADP	E	2001	27/27	0.93	0.19	81,94,101,103	0
3	SO4	F	2002	5/5	0.93	0.16	52,63,70,72	0
4	MG	C	2003	1/1	0.93	0.09	141,141,141,141	0
2	ADP	F	2001	27/27	0.93	0.24	62,74,86,86	0
2	ADP	C	2001	27/27	0.94	0.24	71,91,108,111	0
3	SO4	C	2002	5/5	0.94	0.20	51,65,87,94	0
3	SO4	D	2002	5/5	0.96	0.14	62,74,81,84	0
4	MG	A	2003	1/1	0.96	0.24	47,47,47,47	0

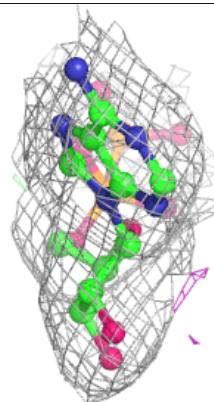
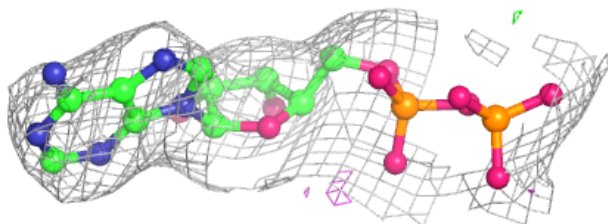
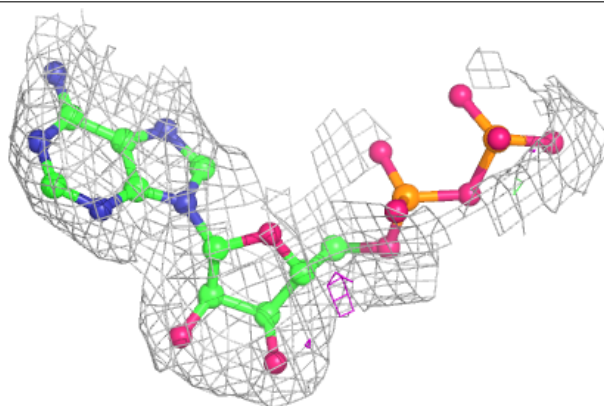
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

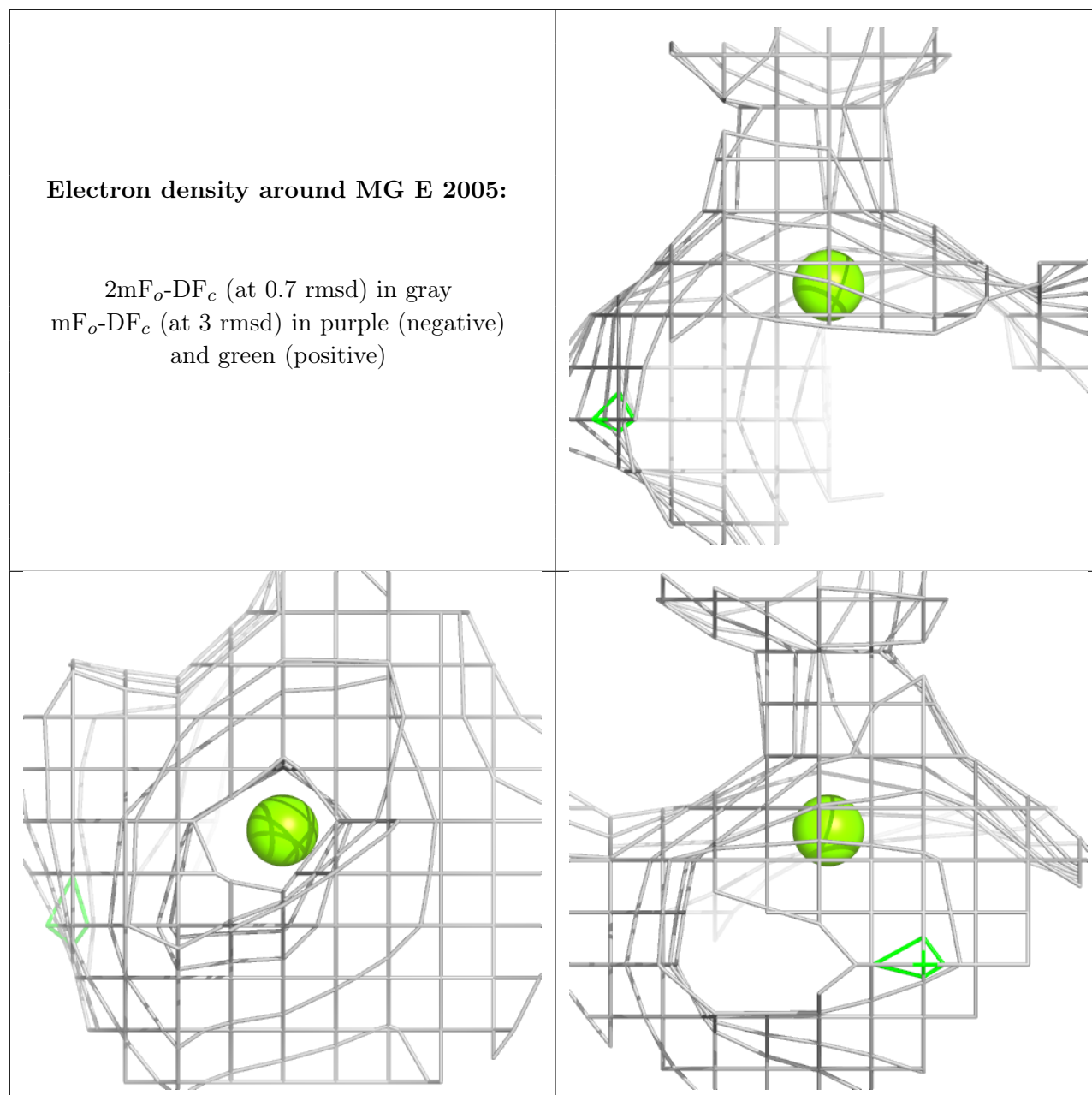
**Electron density around ADP D 2001:**

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

**Electron density around ADP B 2001:**

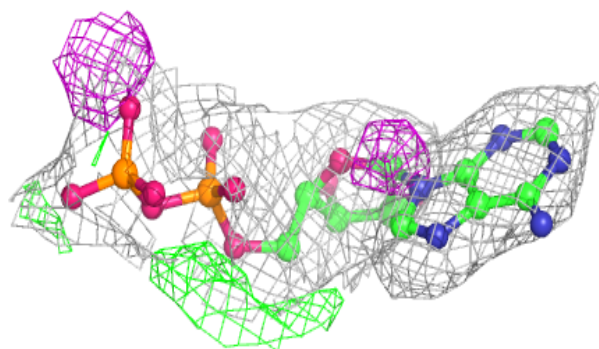
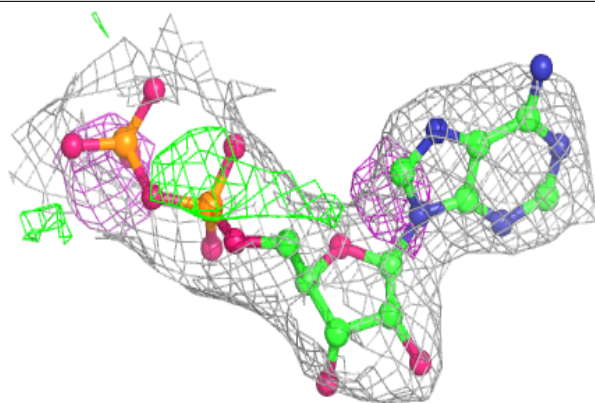
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



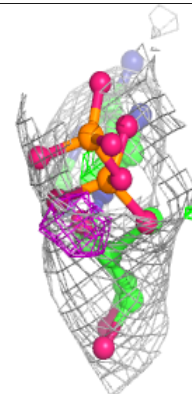
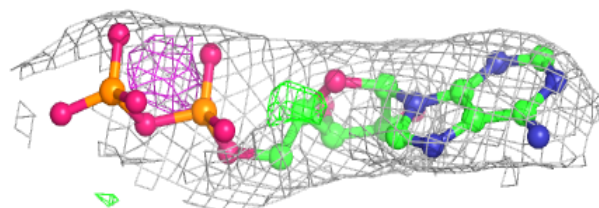
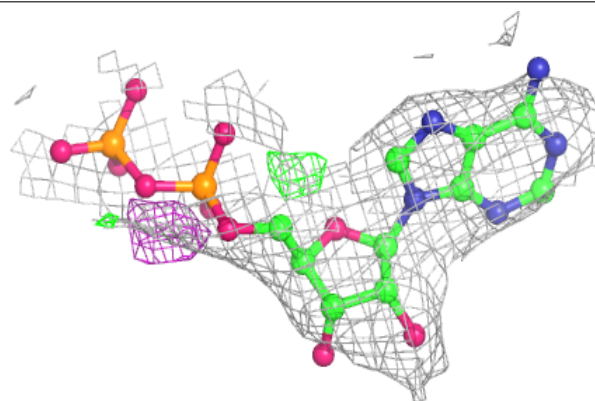


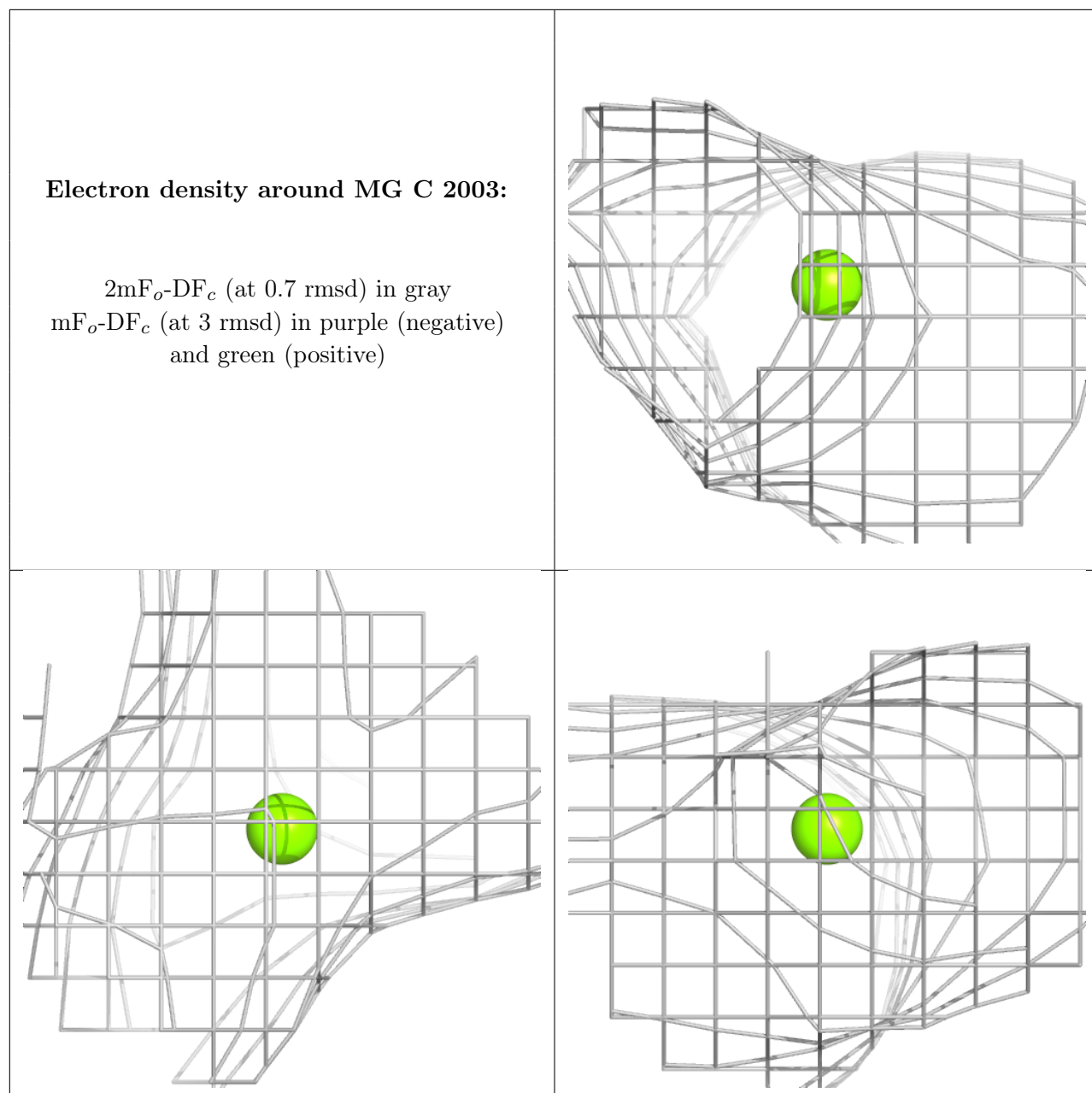
**Electron density around ADP A 2001:**

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

**Electron density around ADP E 2001:**

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

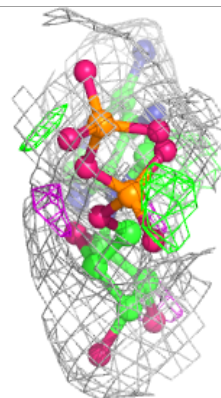
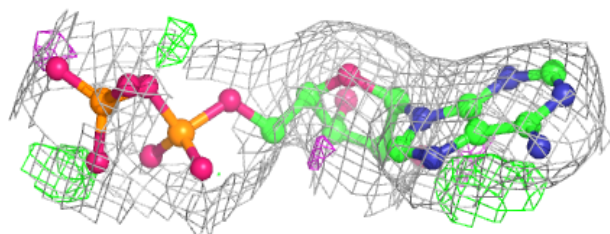
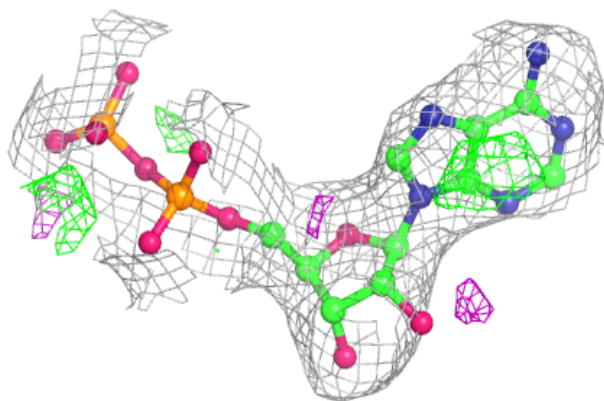




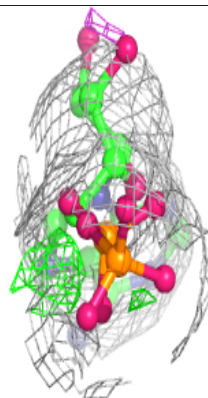
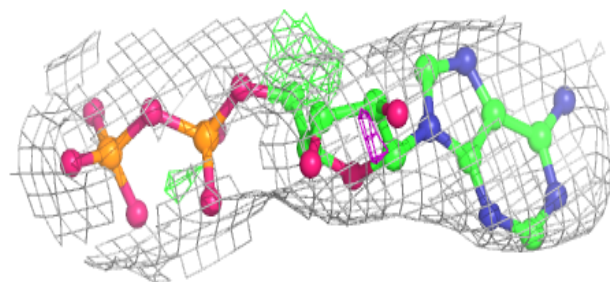
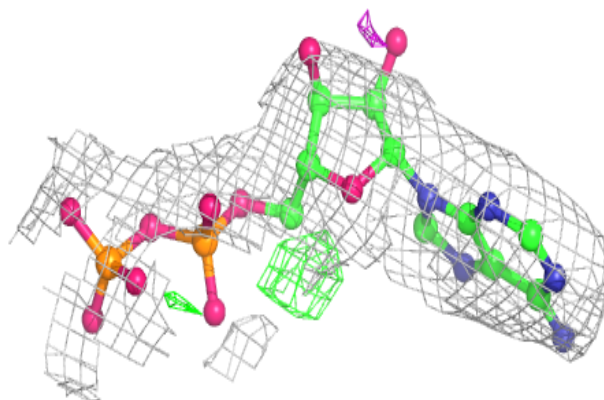


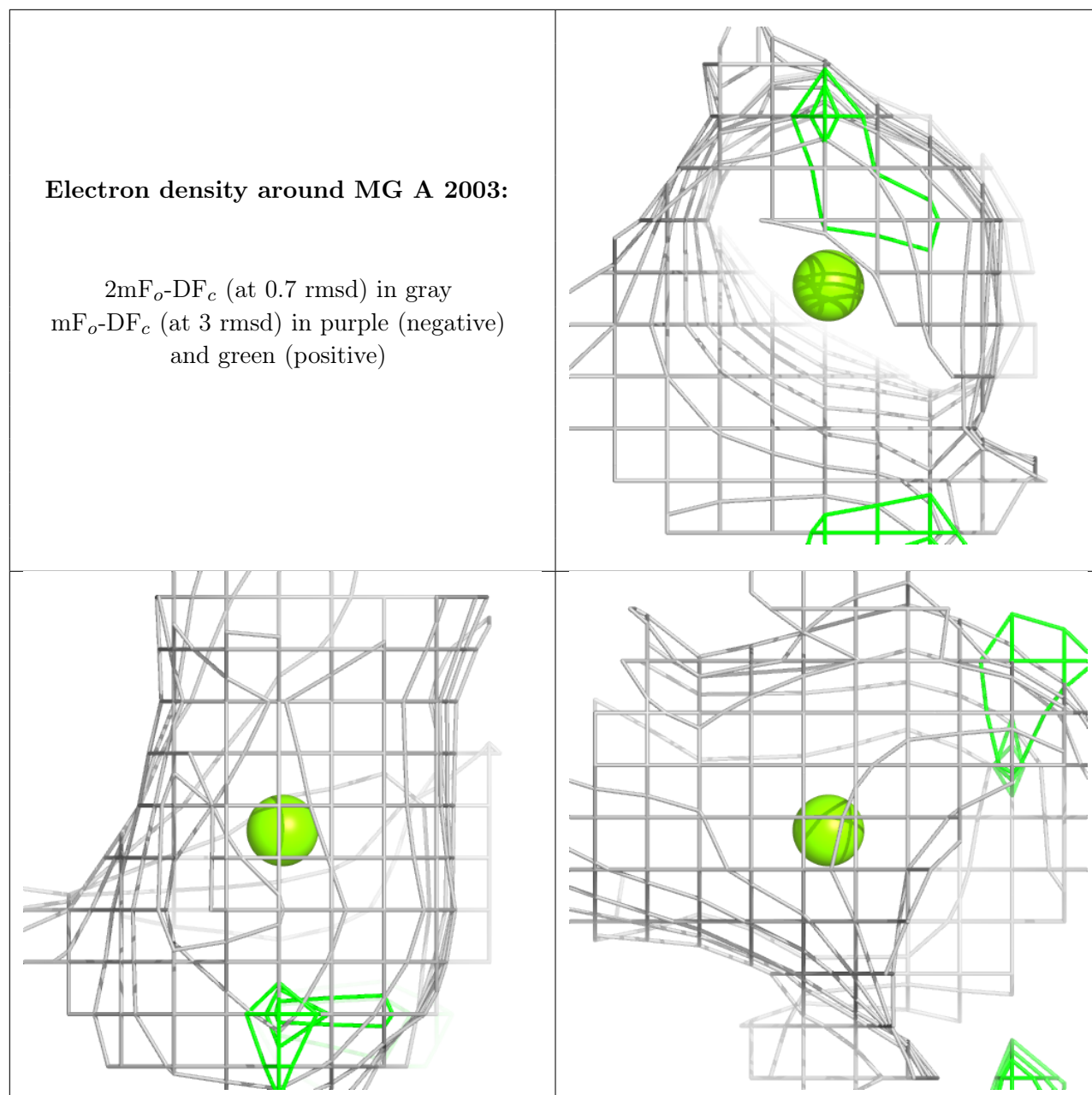
**Electron density around ADP F 2001:**

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

**Electron density around ADP C 2001:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.