



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2025 – 02:12 PM JST

PDB ID : 8IGV
Title : Hexameric Ring Complex of Engineered V1-ATPase bound to 5 ADPs: A3(D
e)3_(ADP-Pi)1cat(ADP)2cat,2non-cat
Authors : Kosugi, T.; Tanabe, M.; Koga, N.
Deposited on : 2023-02-21
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

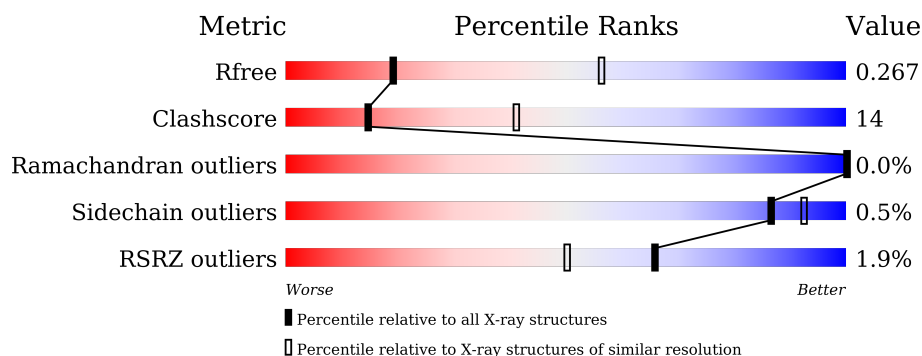
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	596	<div> <div>70%</div> <div>28%</div> <div>.</div> </div>
1	B	596	<div> <div>6%</div> <div>65%</div> <div>33%</div> <div>..</div> </div>
1	C	596	<div> <div>71%</div> <div>27%</div> <div>.</div> </div>
2	D	458	<div> <div>2%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
2	E	458	<div> <div>3%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
2	F	458	<div> <div>6%</div> <div>65%</div> <div>29%</div> <div>5%</div> </div>

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
5	PO4	A	602	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24267 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4571	2871	767	907	26			
1	B	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	C	584	Total	C	N	O	S	0	0	0
			4549	2858	764	901	26			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

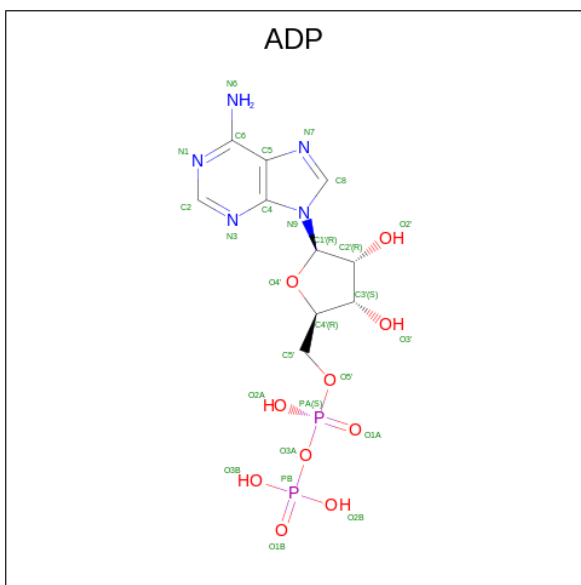
- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	444	Total	C	N	O	S	0	0	0
			3471	2196	596	665	14			
2	E	440	Total	C	N	O	S	0	0	0
			3450	2186	592	658	14			
2	F	433	Total	C	N	O	S	0	1	0
			3402	2154	586	648	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLY	SER	engineered mutation	UNP Q08637
D	152	PRO	GLY	engineered mutation	UNP Q08637
D	153	PRO	SER	engineered mutation	UNP Q08637
D	155	ALA	LEU	engineered mutation	UNP Q08637
D	156	GLY	PRO	engineered mutation	UNP Q08637
D	157	LYS	HIS	engineered mutation	UNP Q08637
D	158	SER	LYS	engineered mutation	UNP Q08637
D	159	ALA	GLU	engineered mutation	UNP Q08637
D	248	GLU	THR	engineered mutation	UNP Q08637
D	339	SER	GLN	engineered mutation	UNP Q08637
E	151	GLY	SER	engineered mutation	UNP Q08637
E	152	PRO	GLY	engineered mutation	UNP Q08637
E	153	PRO	SER	engineered mutation	UNP Q08637
E	155	ALA	LEU	engineered mutation	UNP Q08637
E	156	GLY	PRO	engineered mutation	UNP Q08637
E	157	LYS	HIS	engineered mutation	UNP Q08637
E	158	SER	LYS	engineered mutation	UNP Q08637
E	159	ALA	GLU	engineered mutation	UNP Q08637
E	248	GLU	THR	engineered mutation	UNP Q08637
E	339	SER	GLN	engineered mutation	UNP Q08637
F	151	GLY	SER	engineered mutation	UNP Q08637
F	152	PRO	GLY	engineered mutation	UNP Q08637
F	153	PRO	SER	engineered mutation	UNP Q08637
F	155	ALA	LEU	engineered mutation	UNP Q08637
F	156	GLY	PRO	engineered mutation	UNP Q08637
F	157	LYS	HIS	engineered mutation	UNP Q08637
F	158	SER	LYS	engineered mutation	UNP Q08637
F	159	ALA	GLU	engineered mutation	UNP Q08637
F	248	GLU	THR	engineered mutation	UNP Q08637
F	339	SER	GLN	engineered mutation	UNP Q08637

- Molecule 3 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).

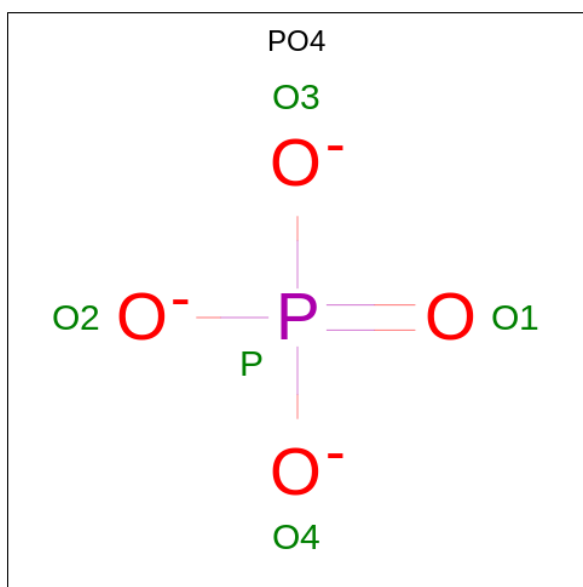


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0

- 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	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

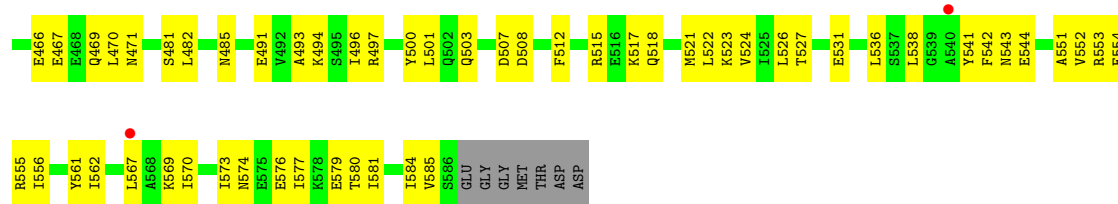
- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



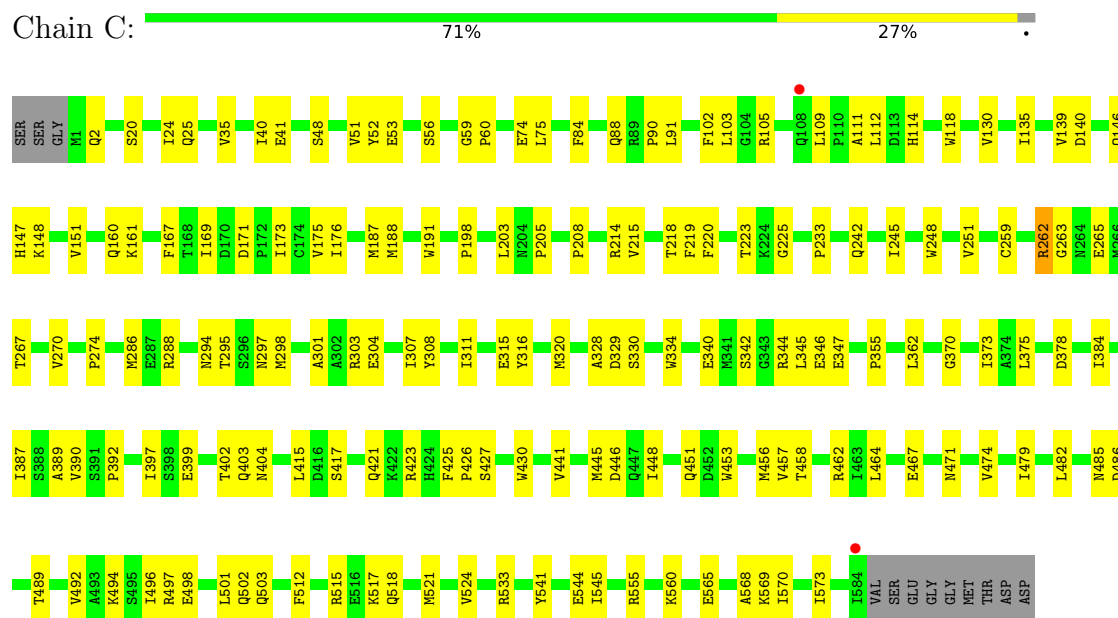
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

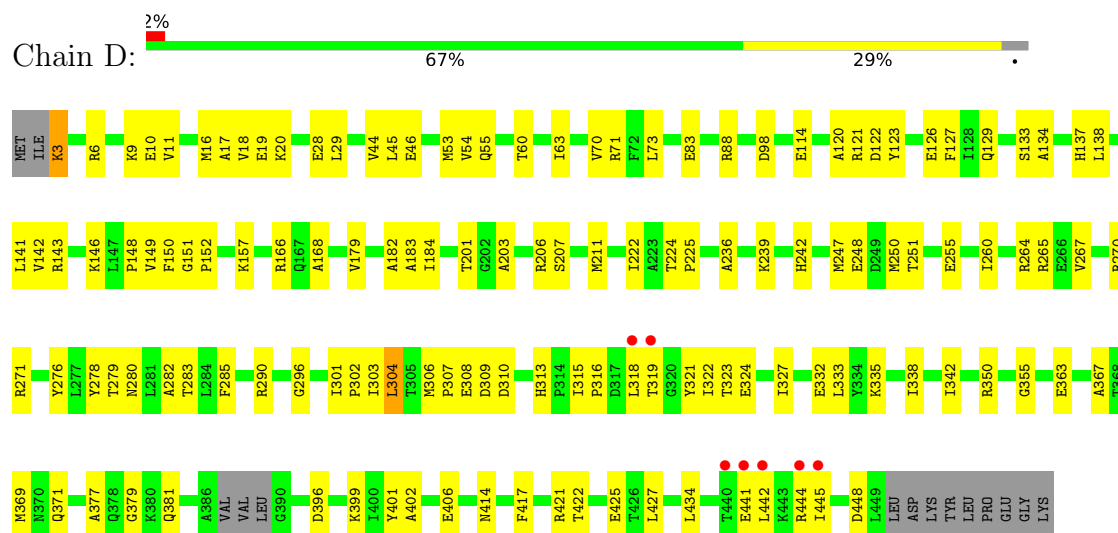
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	12	Total	O	0	0
			12	12		
6	C	30	Total	O	0	0
			30	30		
6	D	21	Total	O	0	0
			21	21		
6	E	11	Total	O	0	0
			11	11		
6	F	11	Total	O	0	0
			11	11		



• Molecule 1: V-type sodium ATPase catalytic subunit A

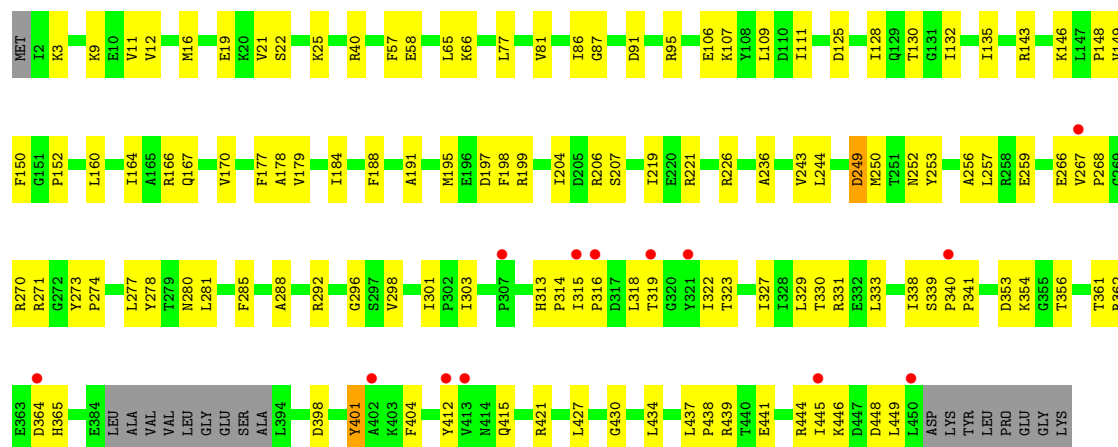


• Molecule 2: V-type sodium ATPase subunit B

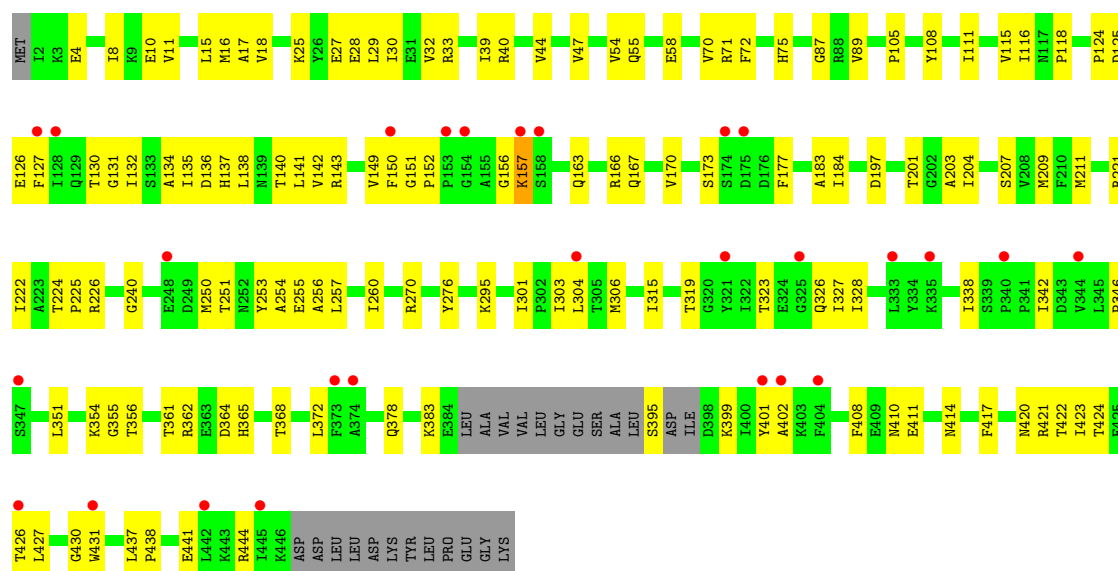


• Molecule 2: V-type sodium ATPase subunit B





• Molecule 2: V-type sodium ATPase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.67Å 126.74Å 123.65Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	48.38 – 3.15 48.38 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.38-3.15) 99.9 (48.38-3.15)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.211 , 0.268 0.211 , 0.267	Depositor DCC
R_{free} test set	3154 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24267	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ADP, MG

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	0.37	0/4647	0.59	1/6287 (0.0%)
1	B	0.29	0/4638	0.53	2/6275 (0.0%)
1	C	0.29	0/4625	0.52	0/6257
2	D	0.30	0/3531	0.58	6/4770 (0.1%)
2	E	0.30	0/3510	0.56	1/4742 (0.0%)
2	F	0.29	0/3461	0.54	1/4673 (0.0%)
All	All	0.31	0/24412	0.55	11/33004 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	444	ARG	NE-CZ-NH1	7.83	124.22	120.30
2	E	266	GLU	N-CA-C	-7.12	91.78	111.00
2	F	156	GLY	O-C-N	-7.01	111.48	122.70
2	D	444	ARG	CA-CB-CG	6.04	126.70	113.40
1	B	410	LYS	CB-CG-CD	-5.95	96.12	111.60
2	D	444	ARG	CB-CG-CD	-5.86	96.36	111.60
2	D	307	PRO	N-CA-C	-5.66	97.38	112.10
1	A	170	ASP	C-N-CA	5.57	135.63	121.70
2	D	309	ASP	CB-CA-C	5.52	121.43	110.40
2	D	304	LEU	CA-CB-CG	5.04	126.88	115.30
1	B	278	ASP	CB-CG-OD1	5.02	122.81	118.30

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	4571	0	4533	128	0
1	B	4562	0	4527	140	0
1	C	4549	0	4511	116	0
2	D	3471	0	3484	101	0
2	E	3450	0	3470	102	0
2	F	3402	0	3418	101	0
3	A	27	0	12	4	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	2	0
6	A	32	0	0	1	0
6	B	12	0	0	1	0
6	C	30	0	0	2	0
6	D	21	0	0	1	0
6	E	11	0	0	0	0
6	F	11	0	0	1	0
All	All	24267	0	24003	661	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 14.

All (661) 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)
2:F:140:THR:HG21	2:F:356:THR:HG23	1.58	0.84
2:E:130:THR:HG23	2:E:132:ILE:H	1.44	0.82
2:D:445:ILE:HG23	2:D:448:ASP:HB3	1.60	0.82
2:F:338:ILE:HG23	2:F:414:ASN:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:ARG:HD2	2:F:201:THR:OG1	1.81	0.80
1:C:426:PRO:HD3	1:C:503:GLN:HB3	1.61	0.80
2:F:361:THR:HG23	2:F:362:ARG:H	1.47	0.80
2:E:339:SER:HB2	2:E:340:PRO:HD3	1.66	0.77
2:D:308:GLU:OE1	2:D:308:GLU:N	2.15	0.77
1:B:260:GLY:HA3	1:B:303:ARG:HD2	1.67	0.76
1:C:445:MET:SD	1:C:515:ARG:NH1	2.59	0.75
2:E:132:ILE:HA	2:E:415:GLN:HE22	1.51	0.75
1:C:35:VAL:HG13	1:C:53:GLU:HB2	1.67	0.74
1:A:34:GLY:O	1:A:108:GLN:NE2	2.20	0.74
2:D:44:VAL:HG12	2:D:54:VAL:HG12	1.69	0.74
1:B:25:GLN:NE2	1:B:38:GLU:OE1	2.22	0.73
2:E:11:VAL:HG12	2:E:16:MET:HG2	1.70	0.73
2:D:250:MET:HB2	2:D:304:LEU:HD23	1.71	0.72
2:D:371:GLN:HB2	2:D:442:LEU:HD21	1.70	0.72
2:D:371:GLN:HG3	2:D:434:LEU:HD11	1.70	0.72
1:A:261:GLU:OE2	1:A:330:SER:N	2.22	0.72
2:E:149:VAL:HG22	2:E:327:ILE:HB	1.72	0.72
1:B:574:ASN:HA	1:B:577:ILE:HD12	1.71	0.71
1:A:243:HIS:O	1:A:247:LYS:HG3	1.90	0.71
2:E:221:ARG:HE	2:E:256:ALA:HB2	1.55	0.71
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.71	0.71
2:D:45:LEU:HD13	2:D:264:ARG:HG2	1.72	0.71
2:E:128:ILE:HG13	2:E:143:ARG:HG2	1.73	0.71
1:A:44:GLN:NE2	2:E:9:LYS:HE3	2.06	0.70
1:A:199:ILE:HG21	1:A:318:ARG:HH12	1.54	0.70
1:C:494:LYS:HG2	1:C:497:ARG:HH12	1.56	0.70
2:F:201:THR:HG23	2:F:203:ALA:H	1.56	0.70
1:A:230:VAL:HG22	1:A:413:TRP:HE3	1.55	0.70
2:D:166:ARG:NH1	2:D:417:PHE:O	2.24	0.70
2:F:166:ARG:CD	2:F:201:THR:OG1	2.40	0.70
1:A:237:GLY:HA3	3:A:600:ADP:H2	1.57	0.69
2:F:140:THR:HG21	2:F:356:THR:CG2	2.22	0.69
1:B:148:LYS:HD2	1:B:320:MET:HB3	1.75	0.69
2:F:44:VAL:HG12	2:F:54:VAL:HG12	1.74	0.69
1:C:267:THR:HA	1:C:270:VAL:HG22	1.75	0.69
2:F:364:ASP:HB2	2:F:431:TRP:HE1	1.58	0.69
2:E:353:ASP:HA	2:E:356:THR:HG22	1.75	0.69
2:F:11:VAL:HG22	2:F:16:MET:HG2	1.73	0.69
2:E:277:LEU:HG	2:E:318:LEU:HD21	1.75	0.67
2:D:55:GLN:OE1	2:D:264:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:HH11	1:A:513:THR:HG21	1.60	0.67
1:B:194:ARG:NH2	1:B:304:GLU:OE1	2.27	0.67
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.76	0.67
2:D:126:GLU:OE1	2:D:143:ARG:NH1	2.28	0.67
2:E:130:THR:HG21	2:E:135:ILE:HB	1.77	0.67
1:B:43:ARG:HG2	2:F:10:GLU:HG3	1.76	0.67
2:E:288:ALA:HA	2:E:298:VAL:HG13	1.77	0.66
1:A:555:ARG:NH2	1:A:572:SER:OG	2.28	0.66
1:B:51:VAL:HG21	1:B:55:THR:HG23	1.77	0.66
1:A:315:GLU:HA	1:A:318:ARG:HE	1.61	0.66
2:E:281:LEU:HD12	2:E:318:LEU:HD13	1.77	0.66
2:D:422:THR:HG23	2:D:425:GLU:H	1.61	0.66
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.78	0.65
2:E:226:ARG:NH2	2:E:253:TYR:OH	2.30	0.65
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.79	0.65
1:A:555:ARG:HE	1:A:573:ILE:HG12	1.61	0.65
1:C:245:ILE:HD13	1:C:387:ILE:HD13	1.78	0.65
1:B:175:VAL:HG22	1:B:184:GLU:HG3	1.78	0.64
2:D:278:TYR:CE1	2:D:322:ILE:HD11	2.32	0.64
1:C:517:LYS:O	1:C:521:MET:HG3	1.97	0.64
1:C:251:VAL:O	1:C:288:ARG:NH1	2.31	0.63
1:C:161:LYS:HB3	1:C:175:VAL:HG12	1.78	0.63
2:D:338:ILE:HG23	2:D:414:ASN:HB2	1.78	0.63
2:E:57:PHE:CG	2:E:219:ILE:HG21	2.33	0.63
2:E:333:LEU:HB3	2:E:338:ILE:HD11	1.80	0.63
1:B:90:PRO:HB2	1:B:93:THR:HB	1.79	0.63
2:D:168:ALA:O	2:D:206:ARG:NH2	2.31	0.62
2:E:412:TYR:O	2:E:421:ARG:NH1	2.32	0.62
1:C:342:SER:OG	1:C:347:GLU:OE1	2.13	0.62
1:A:391:SER:O	2:D:321:TYR:OH	2.15	0.62
2:F:4:GLU:HG2	2:F:71:ARG:HD3	1.81	0.62
2:F:328:ILE:HD13	2:F:346:PRO:HB2	1.81	0.62
1:A:40:ILE:HD13	1:A:50:GLN:HG2	1.82	0.62
2:D:379:GLY:HA2	2:D:401:TYR:HB3	1.80	0.62
2:E:444:ARG:HG3	2:E:446:LYS:O	2.00	0.62
1:B:271:ASN:OD1	2:E:292:ARG:NH2	2.31	0.62
2:D:122:ASP:HB3	2:D:290:ARG:HB2	1.82	0.62
1:A:230:VAL:HG22	1:A:413:TRP:CE3	2.35	0.62
1:C:242:GLN:NE2	1:C:328:ALA:O	2.31	0.62
2:F:411:GLU:O	2:F:421:ARG:NH2	2.33	0.61
1:B:87:ILE:HG13	1:B:89:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ILE:HD13	1:C:187:MET:HG2	1.81	0.61
2:D:367:ALA:HB1	2:D:442:LEU:HD22	1.82	0.61
2:F:126:GLU:H	2:F:142:VAL:HG13	1.65	0.61
1:A:124:ILE:HD12	1:A:159:VAL:HG21	1.82	0.61
1:B:238:LYS:HG3	1:B:389:ALA:HB1	1.81	0.61
2:D:129:GLN:NE2	2:D:422:THR:HA	2.15	0.61
1:A:340:GLU:OE2	2:D:279:THR:OG1	2.20	0.60
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.67	0.60
1:A:55:THR:HA	1:A:58:ILE:HD12	1.82	0.60
1:A:203:LEU:HD11	1:A:373:ILE:HG13	1.81	0.60
1:C:311:ILE:O	1:C:315:GLU:HG3	2.01	0.60
1:A:582:GLN:O	1:A:585:VAL:HG22	2.01	0.60
1:B:523:LYS:O	1:B:527:THR:HG23	2.01	0.60
1:C:214:ARG:HG3	1:C:503:GLN:NE2	2.16	0.60
2:F:378:GLN:HB3	2:F:401:TYR:CE2	2.37	0.60
2:F:150:PHE:HA	2:F:304:LEU:O	2.02	0.60
1:B:281:THR:HG23	1:B:283:GLU:H	1.67	0.59
1:C:533:ARG:O	1:C:533:ARG:NH2	2.35	0.59
2:E:398:ASP:HB3	2:E:401:TYR:H	1.67	0.59
2:E:11:VAL:CG2	2:E:65:LEU:HD11	2.33	0.59
1:A:556:ILE:HG22	1:A:573:ILE:HG21	1.85	0.59
1:C:479:ILE:HA	1:C:482:LEU:HD13	1.85	0.59
1:A:189:GLN:OE1	1:A:197:ARG:NH2	2.36	0.59
1:B:333:ARG:NH2	1:B:336:GLU:OE1	2.33	0.59
1:A:263:GLY:O	1:A:267:THR:HG23	2.03	0.58
1:A:406:LEU:O	3:E:600:ADP:O2'	2.19	0.58
2:E:87:GLY:HA2	2:E:204:ILE:HG22	1.84	0.58
2:E:448:ASP:OD1	2:E:449:LEU:N	2.31	0.58
1:B:318:ARG:HG2	1:B:384:ILE:HG13	1.85	0.58
2:D:315:ILE:HB	2:D:316:PRO:HD3	1.84	0.58
2:E:445:ILE:HG23	2:E:446:LYS:HD3	1.86	0.58
2:D:278:TYR:HE1	2:D:322:ILE:HD11	1.67	0.58
1:B:244:GLN:HE21	1:B:248:TRP:HD1	1.50	0.58
1:B:454:SER:O	1:B:457:VAL:HG22	2.04	0.58
1:C:346:GLU:O	2:D:265:ARG:NH2	2.30	0.58
2:E:257:LEU:HG	2:E:274:PRO:HG2	1.86	0.58
2:F:437:LEU:HD12	2:F:438:PRO:HD2	1.85	0.58
1:B:247:LYS:HD3	1:B:276:LEU:HD22	1.86	0.57
1:B:555:ARG:NH1	1:B:576:GLU:OE1	2.37	0.57
2:E:149:VAL:HB	2:E:303:ILE:HD12	1.86	0.57
1:B:538:LEU:HD12	1:B:585:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:MET:HA	1:C:448:ILE:HG22	1.86	0.57
1:B:199:ILE:HG22	1:B:318:ARG:HH12	1.69	0.57
1:B:243:HIS:NE2	1:B:269:VAL:HG12	2.19	0.57
1:C:90:PRO:HD2	1:C:109:LEU:HD23	1.85	0.57
2:D:88:ARG:HH21	2:D:98:ASP:HB2	1.69	0.57
1:A:194:ARG:NH1	1:A:304:GLU:OE2	2.37	0.57
1:A:333:ARG:HH22	5:A:602:PO4:P	2.28	0.57
1:B:203:LEU:HD13	1:B:371:ARG:HE	1.68	0.57
2:D:45:LEU:H	2:D:45:LEU:HD23	1.70	0.57
2:D:152:PRO:O	2:D:157:LYS:NZ	2.38	0.57
2:E:278:TYR:CD2	2:E:318:LEU:HD23	2.39	0.57
1:A:197:ARG:NH1	1:A:319:ASP:OD2	2.38	0.57
1:B:331:THR:OG1	1:B:390:VAL:HG12	2.05	0.57
1:A:241:VAL:O	1:A:245:ILE:HG12	2.04	0.56
1:B:173:ILE:HD13	1:B:187:MET:HG3	1.87	0.56
2:E:11:VAL:HG21	2:E:65:LEU:HD11	1.87	0.56
2:F:167:GLN:NE2	2:F:420:ASN:HA	2.20	0.56
1:B:206:ASP:OD1	1:B:371:ARG:NH1	2.38	0.56
1:B:212:GLY:HA3	1:B:512:PHE:CD1	2.40	0.56
1:B:485:ASN:HB2	1:B:536:LEU:HD13	1.87	0.56
2:D:138:LEU:HA	2:D:369:MET:HG3	1.87	0.56
2:E:81:VAL:O	2:E:106:GLU:N	2.38	0.56
2:E:412:TYR:HA	2:E:421:ARG:HH12	1.70	0.56
1:A:581:ILE:HA	1:A:584:ILE:HD12	1.85	0.56
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.86	0.56
2:D:306:MET:O	2:D:306:MET:HG3	2.05	0.56
1:C:167:PHE:HB3	1:C:171:ASP:HB2	1.88	0.56
2:E:166:ARG:HG3	2:E:167:GLN:HG3	1.87	0.56
2:F:127:PHE:HB2	2:F:355:GLY:O	2.06	0.56
1:B:543:ASN:OD1	1:B:544:GLU:N	2.39	0.55
2:D:260:ILE:HG23	2:D:264:ARG:HH11	1.71	0.55
2:D:318:LEU:O	2:D:322:ILE:HG12	2.06	0.55
1:B:392:PRO:HG3	1:B:402:THR:HG21	1.86	0.55
1:C:453:TRP:HA	1:C:456:MET:HE3	1.89	0.55
1:B:79:ILE:HD11	1:B:313:ILE:HD13	1.89	0.55
1:B:552:VAL:CG2	1:B:577:ILE:HG12	2.36	0.55
1:C:295:THR:OG1	1:C:298:MET:HG3	2.07	0.55
1:C:541:TYR:O	1:C:545:ILE:HG13	2.07	0.55
1:C:35:VAL:CG1	1:C:53:GLU:HB2	2.36	0.55
2:D:83:GLU:OE2	2:D:239:LYS:HD2	2.06	0.55
1:B:144:ILE:HD13	1:B:287:GLU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:SER:O	1:C:105:ARG:NH2	2.30	0.55
1:B:178:THR:N	1:B:181:GLY:O	2.40	0.55
2:D:260:ILE:HG23	2:D:264:ARG:NH1	2.22	0.55
1:A:80:ILE:HA	1:A:290:VAL:HG22	1.89	0.55
1:A:174:CYS:HB3	1:A:185:LEU:HB2	1.88	0.55
1:C:91:LEU:HD13	2:F:118:PRO:HD2	1.87	0.55
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.89	0.55
1:A:144:ILE:HG13	1:A:145:ILE:HG13	1.89	0.54
1:B:55:THR:HA	1:B:58:ILE:HD12	1.89	0.54
1:B:390:VAL:HG21	1:B:402:THR:HG22	1.88	0.54
1:B:118:TRP:HZ3	1:B:141:GLU:HA	1.73	0.54
1:B:562:ILE:HD13	1:B:569:LYS:HB2	1.88	0.54
2:F:135:ILE:O	2:F:140:THR:HA	2.08	0.54
1:A:463:ILE:HD11	1:A:496:ILE:HD12	1.90	0.54
1:C:486:ASP:O	1:C:489:THR:OG1	2.21	0.54
2:E:315:ILE:HA	2:E:318:LEU:HD12	1.90	0.54
1:B:481:SER:OG	1:B:482:LEU:HD12	2.06	0.54
2:D:127:PHE:HB2	2:D:355:GLY:O	2.07	0.54
1:B:577:ILE:O	1:B:581:ILE:HD12	2.07	0.54
1:A:148:LYS:HD2	1:A:320:MET:HB3	1.89	0.54
1:C:118:TRP:HB3	1:C:139:VAL:HG21	1.89	0.54
1:C:415:LEU:HA	1:C:427:SER:O	2.08	0.54
2:F:15:LEU:HD12	2:F:55:GLN:HG3	1.90	0.54
1:B:73:VAL:HG23	1:B:193:VAL:HG22	1.89	0.54
1:A:102:PHE:HB3	2:D:114:GLU:HB3	1.89	0.54
2:D:143:ARG:HH11	2:D:242:HIS:CE1	2.26	0.54
2:E:313:HIS:HB3	2:E:316:PRO:HD2	1.90	0.54
1:A:205:PRO:HB2	1:A:223:THR:OG1	2.09	0.53
1:A:232:GLY:HA3	1:A:415:LEU:HB2	1.90	0.53
1:B:318:ARG:NH1	1:B:319:ASP:OD1	2.41	0.53
2:E:444:ARG:HA	2:E:444:ARG:NE	2.23	0.53
1:B:214:ARG:HA	1:B:518:GLN:OE1	2.07	0.53
1:C:570:ILE:HD12	1:C:570:ILE:H	1.72	0.53
2:D:250:MET:HB2	2:D:304:LEU:CD2	2.38	0.53
2:E:184:ILE:HG21	2:E:253:TYR:HB2	1.89	0.53
2:E:81:VAL:HB	2:E:107:LYS:O	2.08	0.53
1:A:472:GLU:OE2	1:A:475:ARG:NH1	2.40	0.53
1:B:90:PRO:HG3	1:B:111:ALA:HA	1.90	0.53
2:D:285:PHE:HE2	2:D:319:THR:HG22	1.72	0.53
2:F:32:VAL:HG22	2:F:70:VAL:HG12	1.90	0.53
2:F:138:LEU:HD11	2:F:408:PHE:HZ	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:HA3	3:A:600:ADP:C2	2.43	0.53
2:E:361:THR:OG1	2:E:362:ARG:N	2.41	0.53
2:D:129:GLN:HE22	2:D:422:THR:HA	1.74	0.53
2:E:438:PRO:HB2	2:E:441:GLU:HB2	1.90	0.53
2:F:378:GLN:HB3	2:F:401:TYR:HE2	1.74	0.53
1:A:94:PHE:CD2	1:A:109:LEU:HD12	2.44	0.53
1:A:238:LYS:HG3	1:A:415:LEU:HD12	1.91	0.53
1:B:440:GLU:OE1	1:B:443:ARG:NH2	2.42	0.53
2:D:143:ARG:HD3	2:D:242:HIS:ND1	2.23	0.53
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.45	0.52
1:C:24:ILE:HG13	2:D:11:VAL:HG11	1.90	0.52
1:C:103:LEU:HD12	2:F:115:VAL:HG13	1.92	0.52
1:A:215:VAL:HG22	1:A:501:LEU:HD22	1.90	0.52
1:B:191:TRP:CD2	1:B:192:PRO:HD2	2.44	0.52
1:B:491:GLU:HG3	1:B:542:PHE:HZ	1.74	0.52
2:E:267:VAL:HG23	2:E:267:VAL:O	2.09	0.52
1:A:267:THR:CG2	2:D:121:ARG:HB3	2.39	0.52
1:A:318:ARG:HD3	1:A:384:ILE:HG13	1.89	0.52
1:B:410:LYS:HG2	1:B:436:LEU:HD12	1.91	0.52
1:A:555:ARG:NE	1:A:573:ILE:HG12	2.23	0.52
1:A:80:ILE:HD11	1:A:142:THR:HG23	1.92	0.52
2:E:339:SER:HB2	2:E:340:PRO:CD	2.38	0.52
2:E:191:ALA:O	2:E:195:MET:HG2	2.08	0.52
1:B:454:SER:O	1:B:458:THR:HG23	2.10	0.52
1:C:445:MET:HE1	6:C:717:HOH:O	2.09	0.52
1:B:149:ILE:HG21	1:B:173:ILE:HD11	1.92	0.52
1:C:378:ASP:OD1	1:C:378:ASP:N	2.41	0.52
2:E:107:LYS:HE3	2:E:109:LEU:HD11	1.92	0.52
2:F:149:VAL:HG22	2:F:327:ILE:HB	1.92	0.52
1:C:471:ASN:O	1:C:474:VAL:HG12	2.10	0.51
2:D:45:LEU:CD1	2:D:264:ARG:HG2	2.38	0.51
1:B:6:ILE:HG22	1:B:60:PRO:HA	1.93	0.51
1:A:339:ARG:NH1	1:A:352:GLU:O	2.43	0.51
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.46	0.51
1:A:534:LYS:O	1:A:538:LEU:HB2	2.10	0.51
1:B:553:ARG:HA	1:B:556:ILE:HG12	1.93	0.51
2:D:248:GLU:O	2:D:303:ILE:HB	2.11	0.51
1:A:237:GLY:HA2	3:A:600:ADP:O1A	2.11	0.51
1:B:248:TRP:HB3	1:B:512:PHE:CD1	2.45	0.51
1:C:262:ARG:HB2	1:C:265:GLU:HG3	1.93	0.51
1:C:294:ASN:HD22	1:C:303:ARG:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:322:ILE:HG13	2:E:323:THR:N	2.24	0.51
1:B:491:GLU:HG3	1:B:542:PHE:CZ	2.45	0.51
2:F:130:THR:HG22	2:F:136:ASP:OD1	2.10	0.51
1:A:347:GLU:OE2	1:A:357:TYR:OH	2.19	0.51
2:D:141:LEU:HD22	2:D:301:ILE:HD11	1.92	0.51
2:E:111:ILE:HG22	2:E:226:ARG:HB3	1.93	0.51
1:A:318:ARG:NH1	1:A:372:VAL:HG21	2.26	0.51
2:E:253:TYR:OH	2:E:280:ASN:OD1	2.22	0.51
1:A:573:ILE:O	1:A:577:ILE:HG13	2.10	0.51
1:B:133:GLY:O	1:B:380:ARG:NH2	2.27	0.51
1:B:496:ILE:HD12	1:B:500:TYR:HB3	1.93	0.51
1:B:425:PHE:C	1:B:427:SER:H	2.14	0.51
1:C:90:PRO:HG3	1:C:111:ALA:O	2.11	0.51
1:C:135:ILE:HD13	1:C:148:LYS:HD2	1.92	0.51
2:F:10:GLU:HB3	2:F:17:ALA:HB3	1.91	0.51
2:D:46:GLU:HB3	2:D:53:MET:HB2	1.93	0.50
2:D:304:LEU:HD11	2:D:319:THR:HG21	1.93	0.50
2:D:222:ILE:HD12	2:D:260:ILE:HG13	1.94	0.50
1:B:51:VAL:HG21	1:B:55:THR:CG2	2.42	0.50
2:F:319:THR:O	2:F:323:THR:HG22	2.12	0.50
1:A:285:LEU:HD13	1:A:288:ARG:HH21	1.76	0.50
1:B:209:MET:SD	1:B:249:SER:OG	2.69	0.50
1:C:471:ASN:HA	1:C:474:VAL:HG12	1.94	0.50
1:C:205:PRO:HB2	1:C:223:THR:OG1	2.12	0.50
1:C:315:GLU:HA	1:C:384:ILE:HD11	1.93	0.50
1:C:397:ILE:O	1:C:403:GLN:NE2	2.42	0.50
1:C:423:ARG:O	1:C:423:ARG:HG2	2.11	0.50
1:B:210:ILE:N	1:B:250:ASP:OD1	2.38	0.50
2:D:149:VAL:HG23	2:D:327:ILE:HG13	1.94	0.50
1:A:132:ALA:HB1	1:A:153:ASN:HA	1.94	0.50
1:A:338:LEU:HD11	1:A:357:TYR:HE1	1.76	0.50
1:B:238:LYS:CG	1:B:389:ALA:HB1	2.41	0.50
1:C:148:LYS:HB2	1:C:320:MET:HG2	1.94	0.49
2:E:86:ILE:HD12	2:E:86:ILE:H	1.77	0.49
1:A:44:GLN:CD	2:E:9:LYS:HE3	2.32	0.49
1:B:248:TRP:CZ3	1:B:278:ASP:HB2	2.47	0.49
1:C:340:GLU:HB3	1:C:344:ARG:HH11	1.77	0.49
2:F:301:ILE:HG13	2:F:301:ILE:O	2.12	0.49
2:F:383:LYS:HB2	2:F:402:ALA:HB1	1.94	0.49
1:B:497:ARG:HA	1:B:501:LEU:HB2	1.93	0.49
2:D:396:ASP:HA	2:D:399:LYS:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HG13	1:B:41:GLU:HG3	1.95	0.49
1:B:466:GLU:O	1:B:470:LEU:HG	2.12	0.49
1:B:467:GLU:O	1:B:471:ASN:ND2	2.31	0.49
2:E:244:LEU:HD11	2:E:301:ILE:HG13	1.94	0.49
2:E:315:ILE:HA	2:E:318:LEU:CD1	2.43	0.49
2:F:89:VAL:HG22	2:F:209:MET:HB2	1.92	0.49
1:A:513:THR:HB	1:A:517:LYS:HD3	1.95	0.49
1:B:133:GLY:HA2	1:B:150:MET:HE2	1.94	0.49
1:B:218:THR:HG21	1:B:500:TYR:OH	2.12	0.49
1:B:413:TRP:HB3	1:B:428:ILE:HG12	1.93	0.49
2:E:150:PHE:CZ	2:E:319:THR:HB	2.48	0.49
1:B:517:LYS:O	1:B:521:MET:HG3	2.13	0.49
1:C:218:THR:HA	1:C:453:TRP:CZ2	2.47	0.49
1:A:214:ARG:NH1	1:A:513:THR:HG21	2.27	0.49
1:B:497:ARG:HA	1:B:501:LEU:HD12	1.95	0.49
1:C:102:PHE:CE1	2:F:116:ILE:HG12	2.48	0.49
2:E:438:PRO:HB2	2:E:441:GLU:CB	2.43	0.49
2:F:126:GLU:HB3	2:F:143:ARG:NE	2.28	0.49
1:C:140:ASP:OD1	1:C:146:GLN:HG2	2.13	0.49
1:C:340:GLU:OE2	2:F:276:TYR:HA	2.12	0.48
2:F:422:THR:O	2:F:426:THR:HG23	2.13	0.48
1:A:333:ARG:NH2	5:A:602:PO4:O3	2.46	0.48
1:C:24:ILE:HG22	1:C:25:GLN:HG2	1.94	0.48
1:B:225:GLY:O	1:B:370:GLY:HA2	2.12	0.48
2:D:201:THR:HG23	2:D:203:ALA:H	1.76	0.48
1:A:260:GLY:H	1:A:294:ASN:HB2	1.78	0.48
1:A:552:VAL:O	1:A:556:ILE:HG23	2.13	0.48
1:C:214:ARG:HG2	1:C:518:GLN:HG2	1.95	0.48
2:F:27:GLU:H	2:F:44:VAL:HG23	1.77	0.48
2:F:163:GLN:HG3	2:F:417:PHE:O	2.13	0.48
1:B:425:PHE:C	1:B:427:SER:N	2.67	0.48
2:E:170:VAL:HG12	2:E:177:PHE:HB2	1.94	0.48
2:E:81:VAL:HG21	2:E:109:LEU:HD12	1.94	0.48
2:F:197:ASP:O	2:F:201:THR:HG22	2.13	0.48
2:E:160:LEU:O	2:E:164:ILE:HG13	2.13	0.48
1:B:467:GLU:HG2	1:B:471:ASN:HD21	1.78	0.48
1:B:507:ASP:OD1	1:B:508:ASP:N	2.46	0.48
2:D:236:ALA:O	2:D:296:GLY:HA3	2.14	0.48
2:F:424:THR:HA	2:F:427:LEU:HD12	1.95	0.48
1:B:12:PRO:HB2	1:B:50:GLN:NE2	2.29	0.48
2:E:249:ASP:O	2:E:252:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:HD2	2:E:188:PHE:CD2	2.49	0.48
1:B:92:ASP:OD1	1:B:93:THR:N	2.47	0.48
1:B:399:GLU:HG2	1:B:400:PRO:HD2	1.94	0.48
2:D:60:THR:HA	2:D:63:ILE:HD12	1.96	0.48
2:E:3:LYS:NZ	2:E:22:SER:O	2.36	0.48
1:A:95:MET:SD	2:D:120:ALA:HB2	2.54	0.47
1:B:419:LEU:HB3	1:B:424:HIS:HB3	1.94	0.47
2:D:28:GLU:N	2:D:44:VAL:HG22	2.29	0.47
2:D:271:ARG:HH22	2:D:310:ASP:HB3	1.78	0.47
2:F:395:SER:HA	2:F:399:LYS:HA	1.96	0.47
1:B:277:ILE:HD11	1:B:282:GLY:O	2.14	0.47
1:B:552:VAL:HG21	1:B:577:ILE:HG12	1.96	0.47
2:D:308:GLU:H	2:D:308:GLU:CD	2.09	0.47
1:C:198:PRO:HB2	1:C:375:LEU:HD11	1.95	0.47
2:F:30:ILE:HG13	2:F:54:VAL:HG11	1.96	0.47
2:F:138:LEU:HD11	2:F:408:PHE:CZ	2.49	0.47
1:A:120:PHE:CE1	1:A:137:GLY:HA3	2.49	0.47
1:B:522:LEU:O	1:B:526:LEU:HG	2.15	0.47
1:C:75:LEU:HB3	1:C:316:TYR:CE2	2.50	0.47
1:C:425:PHE:HB3	3:C:600:ADP:C6	2.49	0.47
2:D:251:THR:O	2:D:255:GLU:HG2	2.14	0.47
1:A:486:ASP:O	1:A:489:THR:OG1	2.27	0.47
1:B:493:ALA:HA	1:B:496:ILE:HG22	1.97	0.47
1:A:178:THR:OG1	1:A:181:GLY:O	2.17	0.47
1:A:233:PRO:O	1:A:238:LYS:NZ	2.42	0.47
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.95	0.47
1:C:215:VAL:HG23	1:C:501:LEU:HD22	1.97	0.47
1:C:399:GLU:OE2	1:C:402:THR:N	2.43	0.47
2:E:77:LEU:O	2:E:111:ILE:HG12	2.15	0.47
1:A:517:LYS:HE2	1:A:521:MET:HE1	1.97	0.47
2:E:285:PHE:CE2	2:E:322:ILE:HD13	2.50	0.47
1:A:318:ARG:HH11	1:A:372:VAL:HG21	1.80	0.47
1:B:203:LEU:HD11	1:B:373:ILE:HG13	1.97	0.47
1:A:315:GLU:O	1:A:318:ARG:HG2	2.15	0.47
1:B:467:GLU:HG2	1:B:471:ASN:ND2	2.29	0.47
2:F:131:GLY:HA3	2:F:167:GLN:HE21	1.80	0.47
2:F:170:VAL:HG22	2:F:177:PHE:HB2	1.97	0.47
1:C:297:ASN:ND2	2:F:115:VAL:HG23	2.30	0.46
2:E:271:ARG:HA	2:E:271:ARG:HD3	1.82	0.46
3:C:600:ADP:H5'1	3:C:600:ADP:H8	1.80	0.46
2:D:184:ILE:HD13	2:D:250:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:ASP:OD2	2:E:95:ARG:NH2	2.47	0.46
2:E:365:HIS:HA	2:E:427:LEU:HD21	1.97	0.46
1:C:225:GLY:O	1:C:370:GLY:HA2	2.16	0.46
2:F:141:LEU:HD12	2:F:142:VAL:H	1.81	0.46
1:A:410:LYS:HG2	1:A:436:LEU:HD12	1.98	0.46
2:E:148:PRO:HB2	2:E:150:PHE:HE1	1.81	0.46
2:E:268:PRO:HB2	2:E:273:TYR:O	2.15	0.46
2:F:25:LYS:O	2:F:44:VAL:HG21	2.15	0.46
2:F:33:ARG:HA	2:F:39:ILE:HD13	1.97	0.46
2:F:410:ASN:O	2:F:414:ASN:HB3	2.15	0.46
1:A:173:ILE:HD13	1:A:187:MET:HG2	1.97	0.46
1:A:210:ILE:HD11	1:A:515:ARG:CZ	2.46	0.46
1:A:252:ASP:O	1:A:288:ARG:HG3	2.15	0.46
1:B:124:ILE:CG1	1:B:136:ILE:HA	2.45	0.46
1:B:253:LEU:HD22	1:B:317:PHE:CG	2.50	0.46
2:E:314:PRO:O	2:E:318:LEU:HG	2.15	0.46
1:B:205:PRO:HB2	1:B:223:THR:OG1	2.16	0.46
2:D:137:HIS:HB3	2:D:138:LEU:HD12	1.97	0.46
2:E:199:ARG:HG3	2:E:204:ILE:HD11	1.96	0.46
2:F:362:ARG:HD3	2:F:427:LEU:HD13	1.97	0.46
2:D:282:ALA:HA	2:D:322:ILE:HG21	1.97	0.46
2:F:142:VAL:HG21	2:F:351:LEU:O	2.16	0.46
1:A:2:GLN:OE1	1:A:21:GLU:HB2	2.16	0.46
1:C:498:GLU:HA	1:C:502:GLN:HG3	1.98	0.46
1:A:319:ASP:O	1:A:380:ARG:NH1	2.47	0.46
2:F:40:ARG:HD3	2:F:58:GLU:HB2	1.98	0.46
2:F:105:PRO:HG3	2:F:108:TYR:CZ	2.51	0.46
1:A:138:TYR:CD2	1:A:146:GLN:HG2	2.51	0.46
1:C:467:GLU:OE2	1:C:497:ARG:NH2	2.49	0.46
2:F:134:ALA:HB3	2:F:342:ILE:CD1	2.46	0.46
1:A:72:SER:HA	1:A:192:PRO:HA	1.97	0.45
1:A:474:VAL:HG22	1:A:479:ILE:HA	1.97	0.45
1:C:248:TRP:HB3	1:C:512:PHE:CD2	2.50	0.45
1:A:479:ILE:HG13	1:A:487:ARG:NH1	2.31	0.45
1:C:446:ASP:HA	1:C:451:GLN:O	2.16	0.45
2:D:9:LYS:HA	2:D:9:LYS:HD3	1.70	0.45
2:D:313:HIS:HB3	2:D:316:PRO:HD2	1.99	0.45
2:E:329:LEU:HA	2:E:341:PRO:O	2.16	0.45
2:F:362:ARG:HG2	2:F:427:LEU:HD13	1.98	0.45
1:A:356:ALA:HB1	2:E:259:GLU:HA	1.98	0.45
1:A:489:THR:HG23	1:A:533:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:THR:HA	1:C:453:TRP:HZ2	1.80	0.45
2:E:270:ARG:O	2:E:273:TYR:HB2	2.16	0.45
1:A:549:THR:O	1:A:553:ARG:HG3	2.17	0.45
1:B:272:GLU:O	1:B:276:LEU:HG	2.17	0.45
1:C:203:LEU:HD11	1:C:373:ILE:HG13	1.98	0.45
1:C:464:LEU:O	1:C:467:GLU:HB3	2.16	0.45
1:B:89:ARG:HB3	1:B:94:PHE:HE2	1.81	0.45
1:B:228:ALA:HA	1:B:411:VAL:HB	1.99	0.45
1:C:307:ILE:HG13	1:C:308:TYR:N	2.31	0.45
1:C:75:LEU:HB3	1:C:316:TYR:CD2	2.51	0.45
2:D:150:PHE:CE1	2:D:304:LEU:HD12	2.51	0.45
1:B:120:PHE:HA	1:B:139:VAL:HG12	1.98	0.45
2:D:137:HIS:NE2	2:D:427:LEU:HD23	2.32	0.45
1:B:75:LEU:HD13	1:B:316:TYR:HB2	1.99	0.45
1:B:342:SER:CB	1:B:355:PRO:HG3	2.47	0.45
1:B:466:GLU:O	1:B:469:GLN:HG2	2.16	0.45
1:C:220:PHE:HZ	1:C:430:TRP:HA	1.82	0.45
1:C:485:ASN:O	1:C:489:THR:HG23	2.17	0.45
1:C:524:VAL:HG12	1:C:573:ILE:HG13	1.98	0.45
2:F:30:ILE:HD11	2:F:72:PHE:CD2	2.52	0.45
2:F:257:LEU:O	2:F:260:ILE:HG12	2.16	0.45
1:A:262:ARG:NH1	1:A:265:GLU:OE1	2.46	0.45
1:C:214:ARG:HG3	1:C:503:GLN:HE21	1.80	0.45
1:C:492:VAL:O	1:C:496:ILE:HG13	2.17	0.45
2:D:19:GLU:HG2	2:D:20:LYS:H	1.81	0.45
2:E:125:ASP:HA	2:E:354:LYS:HB3	1.99	0.45
1:A:536:LEU:HD12	1:A:537:SER:N	2.32	0.45
1:B:215:VAL:HG11	1:B:428:ILE:HB	1.99	0.45
1:B:242:GLN:NE2	1:B:327:MET:HB3	2.32	0.45
1:C:52:TYR:HA	1:C:301:ALA:HB3	1.99	0.45
1:C:390:VAL:O	1:C:392:PRO:HD3	2.17	0.45
2:D:133:SER:OG	2:D:421:ARG:HD2	2.17	0.45
2:E:330:THR:OG1	2:E:333:LEU:HD13	2.17	0.45
2:F:124:PRO:HB3	2:F:143:ARG:O	2.17	0.45
1:A:473:ILE:HG21	1:A:482:LEU:HD21	1.99	0.44
2:D:333:LEU:HD22	2:D:338:ILE:HD12	1.99	0.44
2:F:137:HIS:HA	2:F:365:HIS:CE1	2.52	0.44
2:F:221:ARG:HD2	2:F:256:ALA:HB2	1.99	0.44
1:B:26:ASP:HB2	1:B:39:ILE:HD12	1.99	0.44
1:B:199:ILE:HG22	1:B:318:ARG:NH1	2.31	0.44
1:C:139:VAL:HG12	1:C:147:HIS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:THR:HG23	2:F:132:ILE:H	1.82	0.44
2:F:18:VAL:HG11	2:F:70:VAL:HG21	2.00	0.44
1:A:566:GLU:HB3	1:A:569:LYS:HE3	1.99	0.44
1:B:124:ILE:HG12	1:B:136:ILE:HA	1.99	0.44
1:B:494:LYS:HA	1:B:497:ARG:HE	1.83	0.44
1:C:130:VAL:CG2	1:C:151:VAL:HG21	2.47	0.44
1:C:498:GLU:O	1:C:560:LYS:NZ	2.39	0.44
2:D:222:ILE:O	2:D:225:PRO:HD2	2.18	0.44
1:B:177:GLU:HA	1:B:182:LEU:HA	1.99	0.44
1:C:565:GLU:OE2	1:C:565:GLU:N	2.46	0.44
2:D:402:ALA:O	2:D:406:GLU:HG2	2.17	0.44
2:E:401:TYR:CE2	2:E:437:LEU:HD22	2.53	0.44
2:F:30:ILE:HD11	2:F:72:PHE:CE2	2.53	0.44
2:F:136:ASP:HB3	2:F:423:ILE:HD13	2.00	0.44
1:A:297:ASN:OD1	2:D:283:THR:HA	2.17	0.44
1:B:570:ILE:HA	1:B:573:ILE:HG13	1.98	0.44
1:B:576:GLU:O	1:B:579:GLU:HG2	2.18	0.44
1:A:346:GLU:HG3	2:D:267:VAL:HG21	2.00	0.44
2:D:11:VAL:HG22	2:D:16:MET:HG2	2.00	0.44
2:D:278:TYR:HB2	2:D:318:LEU:HD22	2.00	0.44
1:C:169:ILE:HB	1:C:188:MET:HB2	2.00	0.44
2:D:29:LEU:HD23	2:D:73:LEU:HD12	2.00	0.44
2:D:148:PRO:HB3	2:D:302:PRO:HD2	1.98	0.44
2:D:183:ALA:HB3	2:D:211:MET:HA	1.99	0.44
2:E:111:ILE:HG22	2:E:226:ARG:CB	2.48	0.44
2:F:183:ALA:HB3	2:F:211:MET:HA	2.00	0.44
2:F:361:THR:HG23	2:F:362:ARG:N	2.25	0.44
1:A:240:VAL:HG23	3:A:600:ADP:O1A	2.17	0.44
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.90	0.44
1:C:130:VAL:HG11	1:C:176:ILE:HD12	1.98	0.44
2:E:398:ASP:HB2	2:E:401:TYR:HB2	1.99	0.44
1:A:24:ILE:HG22	1:A:25:GLN:HG2	2.00	0.43
1:C:160:GLN:HB3	1:C:175:VAL:HG13	1.99	0.43
2:D:179:VAL:O	2:D:207:SER:HA	2.18	0.43
2:F:8:ILE:HG12	2:F:16:MET:HE1	1.99	0.43
1:A:575:GLU:O	1:A:578:LYS:HG3	2.18	0.43
1:C:524:VAL:HG12	1:C:573:ILE:CG1	2.47	0.43
2:D:332:GLU:O	2:D:335:LYS:HG2	2.17	0.43
1:B:259:CYS:O	1:B:260:GLY:C	2.57	0.43
1:B:364:GLU:O	1:B:368:ARG:HG3	2.18	0.43
1:C:569:LYS:HB2	1:C:569:LYS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:445:ILE:CG2	2:D:448:ASP:HB3	2.40	0.43
2:F:28:GLU:OE2	2:F:72:PHE:HB3	2.18	0.43
1:B:507:ASP:OD2	1:B:561:TYR:HE1	2.02	0.43
1:C:60:PRO:HD3	2:F:47:VAL:HG13	2.00	0.43
1:C:245:ILE:HG21	1:C:387:ILE:CD1	2.48	0.43
2:E:146:LYS:CD	2:E:285:PHE:HB3	2.48	0.43
2:F:152:PRO:HG3	2:F:306:MET:CE	2.48	0.43
1:A:20:SER:O	2:E:66:LYS:HE3	2.18	0.43
1:A:90:PRO:HD3	1:A:111:ALA:HA	2.01	0.43
1:A:221:PRO:HG3	1:A:441:VAL:HG11	2.01	0.43
1:A:267:THR:HG21	2:D:121:ARG:HB3	1.99	0.43
1:B:144:ILE:HD12	1:B:144:ILE:H	1.84	0.43
1:A:225:GLY:O	1:A:370:GLY:HA2	2.18	0.43
1:C:417:SER:O	1:C:421:GLN:HG3	2.18	0.43
2:F:151:GLY:HA2	2:F:152:PRO:HD3	1.89	0.43
1:B:378:ASP:N	1:B:378:ASP:OD1	2.51	0.43
2:D:3:LYS:HZ3	2:D:71:ARG:HE	1.67	0.43
2:E:40:ARG:HD3	2:E:58:GLU:HB2	1.99	0.43
2:F:44:VAL:HG12	2:F:54:VAL:CG1	2.46	0.43
2:F:326:GLN:O	2:F:327:ILE:HD13	2.18	0.43
2:F:354:LYS:NZ	6:F:502:HOH:O	2.51	0.43
2:F:437:LEU:HD21	2:F:441:GLU:HG3	1.99	0.43
1:A:315:GLU:CA	1:A:318:ARG:HE	2.30	0.43
1:C:51:VAL:HG12	1:C:53:GLU:H	1.84	0.43
1:B:371:ARG:NH2	6:B:702:HOH:O	2.52	0.42
1:C:362:LEU:HD12	1:C:404:ASN:HB3	2.01	0.42
2:D:379:GLY:CA	2:D:401:TYR:HB3	2.49	0.42
2:E:57:PHE:CD1	2:E:219:ILE:HG21	2.53	0.42
2:E:339:SER:CB	2:E:340:PRO:HD3	2.45	0.42
1:B:73:VAL:HG13	1:B:88:GLN:NE2	2.34	0.42
1:B:244:GLN:NE2	1:B:248:TRP:CD1	2.83	0.42
1:B:327:MET:SD	1:B:387:ILE:HB	2.59	0.42
1:C:263:GLY:O	1:C:267:THR:HG23	2.19	0.42
1:C:453:TRP:HA	1:C:456:MET:CE	2.49	0.42
1:C:458:THR:O	1:C:462:ARG:HG2	2.19	0.42
2:D:371:GLN:OE1	2:D:441:GLU:HG2	2.19	0.42
2:F:365:HIS:O	2:F:368:THR:OG1	2.37	0.42
2:F:87:GLY:HA2	2:F:204:ILE:HG13	2.00	0.42
1:A:88:GLN:O	1:A:88:GLN:HG2	2.19	0.42
1:B:425:PHE:HB3	3:B:600:ADP:C5	2.54	0.42
2:E:285:PHE:CD2	2:E:322:ILE:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:GLY:HA2	2:F:204:ILE:O	2.20	0.42
2:F:250:MET:O	2:F:253:TYR:HB3	2.20	0.42
1:B:237:GLY:C	1:B:239:THR:H	2.23	0.42
2:D:151:GLY:O	2:D:306:MET:N	2.45	0.42
2:F:224:THR:HB	2:F:225:PRO:HD3	2.01	0.42
1:A:247:LYS:HD2	1:A:276:LEU:CD1	2.49	0.42
1:B:569:LYS:O	1:B:573:ILE:HG13	2.19	0.42
1:C:208:PRO:HG3	1:C:441:VAL:HG13	2.01	0.42
1:C:541:TYR:HB2	1:C:544:GLU:HB3	2.02	0.42
2:E:206:ARG:HD2	2:E:206:ARG:N	2.34	0.42
2:F:111:ILE:O	2:F:226:ARG:HB3	2.20	0.42
1:B:580:THR:O	1:B:584:ILE:HD12	2.19	0.42
2:F:8:ILE:HG12	2:F:16:MET:CE	2.49	0.42
2:F:364:ASP:O	2:F:427:LEU:HD22	2.19	0.42
1:A:454:SER:HA	1:A:457:VAL:HG22	2.01	0.42
1:A:507:ASP:HB3	1:A:510:ASP:HB3	2.02	0.42
1:C:74:GLU:HG2	1:C:188:MET:SD	2.60	0.42
2:D:224:THR:HB	2:D:225:PRO:HD3	2.02	0.42
2:E:277:LEU:HG	2:E:318:LEU:HD11	2.02	0.42
1:A:272:GLU:HG3	2:D:123:TYR:OH	2.20	0.42
1:B:527:THR:O	1:B:531:GLU:HG2	2.20	0.42
2:E:362:ARG:NH2	2:E:364:ASP:OD2	2.37	0.42
2:F:240:GLY:HA3	2:F:295:LYS:HE3	2.02	0.42
1:A:361:ARG:NH1	6:A:708:HOH:O	2.53	0.42
2:D:142:VAL:HG12	2:D:355:GLY:HA3	2.02	0.42
2:D:146:LYS:O	2:D:323:THR:HB	2.20	0.42
2:E:281:LEU:HB3	2:E:285:PHE:CE2	2.55	0.42
1:A:336:GLU:OE2	1:A:339:ARG:NH2	2.51	0.41
1:B:215:VAL:HG22	1:B:501:LEU:HD23	2.01	0.41
1:C:59:GLY:HA3	2:F:25:LYS:HD3	2.01	0.41
1:C:220:PHE:CZ	1:C:430:TRP:HA	2.55	0.41
2:D:45:LEU:HD23	2:D:53:MET:O	2.20	0.41
2:E:132:ILE:HA	2:E:415:GLN:NE2	2.27	0.41
2:F:125:ASP:O	2:F:126:GLU:HG3	2.19	0.41
1:A:156:LYS:O	1:A:178:THR:HG22	2.19	0.41
1:A:173:ILE:HD13	1:A:187:MET:CG	2.51	0.41
1:A:230:VAL:CG2	1:A:413:TRP:HE3	2.27	0.41
1:B:541:TYR:O	1:B:544:GLU:HB2	2.20	0.41
1:C:218:THR:HG23	1:C:457:VAL:HG22	2.02	0.41
2:E:166:ARG:NH1	2:E:197:ASP:OD2	2.53	0.41
2:E:315:ILE:O	2:E:319:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:254:ALA:CB	2:F:315:ILE:HG12	2.50	0.41
1:A:41:GLU:HG2	2:E:12:VAL:HA	2.01	0.41
1:A:254:VAL:O	1:A:289:THR:HA	2.20	0.41
1:A:463:ILE:HD11	1:A:496:ILE:CD1	2.50	0.41
1:B:232:GLY:HA3	1:B:415:LEU:HB2	2.02	0.41
1:B:426:PRO:HG2	1:B:503:GLN:H	1.84	0.41
1:B:517:LYS:HG3	1:B:567:LEU:CD2	2.49	0.41
1:B:551:ALA:HA	1:B:554:GLU:OE1	2.19	0.41
1:C:139:VAL:CG1	1:C:147:HIS:HB3	2.50	0.41
2:F:29:LEU:HD12	2:F:75:HIS:CE1	2.55	0.41
1:B:193:VAL:HG12	1:B:308:TYR:HB3	2.01	0.41
2:E:19:GLU:O	2:E:21:VAL:HG23	2.20	0.41
2:F:372:LEU:HD21	2:F:430:GLY:CA	2.50	0.41
1:A:479:ILE:HG13	1:A:487:ARG:HH12	1.85	0.41
1:C:304:GLU:HA	1:C:334:TRP:CD1	2.56	0.41
2:D:18:VAL:HG11	2:D:70:VAL:HG21	2.03	0.41
2:E:132:ILE:HG12	2:E:415:GLN:NE2	2.35	0.41
2:E:152:PRO:HG3	2:E:331:ARG:HB2	2.01	0.41
2:E:178:ALA:O	2:E:243:VAL:HA	2.21	0.41
2:F:204:ILE:HD12	2:F:204:ILE:HA	1.95	0.41
2:F:251:THR:O	2:F:255:GLU:HG2	2.20	0.41
1:A:161:LYS:HE2	1:A:163:GLU:HG3	2.03	0.41
1:A:294:ASN:ND2	1:A:306:SER:HB3	2.35	0.41
1:A:581:ILE:O	1:A:584:ILE:HB	2.21	0.41
1:C:330:SER:HB2	1:C:389:ALA:O	2.21	0.41
2:E:198:PHE:HB3	2:E:204:ILE:CG1	2.51	0.41
2:F:222:ILE:HD11	2:F:257:LEU:N	2.36	0.41
1:A:473:ILE:O	1:A:477:VAL:HG22	2.21	0.41
1:B:221:PRO:CG	1:B:441:VAL:HG21	2.51	0.41
1:B:229:ALA:O	1:B:231:PRO:HD3	2.21	0.41
1:C:274:PRO:HG3	1:C:286:MET:HG3	2.03	0.41
2:E:179:VAL:O	2:E:207:SER:HA	2.20	0.41
1:A:267:THR:HG22	2:D:121:ARG:HB3	2.01	0.41
1:C:2:GLN:HE22	1:C:20:SER:H	1.69	0.41
1:C:259:CYS:N	1:C:329:ASP:O	2.51	0.41
1:C:555:ARG:HH22	1:C:568:ALA:HB1	1.86	0.41
2:E:250:MET:O	2:E:253:TYR:HB3	2.21	0.41
2:F:184:ILE:HD11	2:F:225:PRO:HG3	2.03	0.41
1:A:84:PHE:HB3	1:A:88:GLN:HA	2.02	0.41
1:B:191:TRP:CZ2	1:B:198:PRO:HD3	2.55	0.41
1:B:493:ALA:O	1:B:497:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:VAL:HG12	1:B:574:ASN:HB3	2.03	0.41
2:D:137:HIS:HE1	2:D:369:MET:N	2.19	0.41
2:D:143:ARG:HH11	2:D:242:HIS:HE1	1.69	0.41
2:D:363:GLU:HG3	6:D:715:HOH:O	2.20	0.41
2:D:377:ALA:O	2:D:381:GLN:HG2	2.21	0.41
2:E:313:HIS:HB3	2:E:316:PRO:CD	2.51	0.41
1:C:40:ILE:HD12	1:C:345:LEU:HD11	2.03	0.41
1:C:208:PRO:HG3	1:C:441:VAL:HG22	2.03	0.41
1:C:219:PHE:CE2	1:C:501:LEU:HD21	2.56	0.41
1:C:342:SER:HB2	1:C:355:PRO:HG3	2.03	0.41
2:D:134:ALA:HB3	2:D:342:ILE:HD12	2.02	0.41
2:D:324:GLU:HA	2:D:350:ARG:HD2	2.03	0.41
2:E:277:LEU:HG	2:E:318:LEU:CD2	2.47	0.41
2:F:444:ARG:HA	2:F:444:ARG:HD2	1.82	0.41
1:B:118:TRP:CZ3	1:B:141:GLU:HA	2.54	0.40
1:B:276:LEU:O	1:B:285:LEU:HB2	2.21	0.40
1:C:130:VAL:HG22	1:C:151:VAL:HG21	2.02	0.40
2:E:236:ALA:O	2:E:296:GLY:HA3	2.21	0.40
2:E:319:THR:O	2:E:323:THR:HG23	2.20	0.40
1:A:247:LYS:HD2	1:A:276:LEU:HD13	2.02	0.40
1:B:426:PRO:HG2	1:B:503:GLN:N	2.36	0.40
3:D:600:ADP:N3	3:D:600:ADP:H2'	2.36	0.40
2:E:430:GLY:O	2:E:434:LEU:HB2	2.22	0.40
2:F:30:ILE:HD13	2:F:30:ILE:HA	1.89	0.40
2:F:130:THR:O	2:F:167:GLN:HB2	2.22	0.40
1:A:348:MET:HE2	2:E:267:VAL:HA	2.04	0.40
1:A:454:SER:O	1:A:457:VAL:HG22	2.21	0.40
1:B:62:GLU:OE2	2:E:25:LYS:HE3	2.21	0.40
2:D:276:TYR:O	2:D:280:ASN:HB2	2.21	0.40
2:D:278:TYR:CD1	2:D:318:LEU:HD22	2.56	0.40
2:F:157:LYS:HG3	2:F:303:ILE:HG21	2.02	0.40
1:A:214:ARG:NE	1:A:500:TYR:O	2.47	0.40
1:A:329:ASP:HA	1:A:330:SER:HA	1.68	0.40
1:C:112:LEU:O	1:C:114:HIS:HD2	2.05	0.40
1:C:233:PRO:HG3	1:C:417:SER:HB3	2.04	0.40
1:A:29:LEU:HD22	1:A:108:GLN:NE2	2.35	0.40
1:B:120:PHE:CZ	1:B:173:ILE:HD12	2.57	0.40
1:B:251:VAL:HG23	1:B:323:ASP:HB3	2.03	0.40
1:B:555:ARG:NH2	1:B:569:LYS:O	2.54	0.40
1:C:191:TRP:CZ2	1:C:198:PRO:HD3	2.57	0.40
1:C:445:MET:CE	6:C:717:HOH:O	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:204:ILE:HA	2:F:207:SER:HB2	2.04	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	585/596 (98%)	572 (98%)	13 (2%)	0	100	100
1	B	584/596 (98%)	562 (96%)	21 (4%)	1 (0%)	44	72
1	C	582/596 (98%)	568 (98%)	14 (2%)	0	100	100
2	D	440/458 (96%)	424 (96%)	16 (4%)	0	100	100
2	E	436/458 (95%)	413 (95%)	23 (5%)	0	100	100
2	F	429/458 (94%)	411 (96%)	18 (4%)	0	100	100
All	All	3056/3162 (97%)	2950 (96%)	105 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	GLY

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	503/509 (99%)	502 (100%)	1 (0%)	92	96
1	B	502/509 (99%)	501 (100%)	1 (0%)	92	96
1	C	500/509 (98%)	499 (100%)	1 (0%)	92	96
2	D	367/380 (97%)	364 (99%)	3 (1%)	79	89
2	E	366/380 (96%)	362 (99%)	4 (1%)	70	84
2	F	360/380 (95%)	357 (99%)	3 (1%)	79	89
All	All	2598/2667 (97%)	2585 (100%)	13 (0%)	86	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	578	LYS
1	B	515	ARG
1	C	262	ARG
2	D	3	LYS
2	D	6	ARG
2	D	270	ARG
2	E	249	ASP
2	E	401	TYR
2	E	404	PHE
2	E	439	ARG
2	F	157	LYS
2	F	173	SER
2	F	270	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	264	ASN
1	C	244	GLN
1	C	503	GLN
2	E	48	GLN
2	E	414	ASN
2	E	415	GLN
2	F	163	GLN
2	F	167	GLN
2	F	326	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	600	4	24,29,29	0.99	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	C	600	4	24,29,29	0.95	1 (4%)	29,45,45	1.34	4 (13%)
3	ADP	B	600	4	24,29,29	0.99	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	D	600	4	24,29,29	1.02	1 (4%)	29,45,45	1.34	4 (13%)
5	PO4	A	602	4	4,4,4	0.96	0	6,6,6	0.48	0
3	ADP	E	600	4	24,29,29	0.97	1 (4%)	29,45,45	1.32	4 (13%)

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	600	4	-	1/12/32/32	0/3/3/3
3	ADP	C	600	4	-	1/12/32/32	0/3/3/3
3	ADP	B	600	4	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	600	4	-	2/12/32/32	0/3/3/3
3	ADP	E	600	4	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	ADP	C5-C4	2.67	1.48	1.40
3	A	600	ADP	C5-C4	2.59	1.47	1.40
3	E	600	ADP	C5-C4	2.59	1.47	1.40
3	B	600	ADP	C5-C4	2.54	1.47	1.40
3	C	600	ADP	C5-C4	2.52	1.47	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	ADP	PA-O3A-PB	-3.23	121.74	132.83
3	B	600	ADP	N3-C2-N1	-3.19	123.69	128.68
3	D	600	ADP	C3'-C2'-C1'	3.18	105.77	100.98
3	D	600	ADP	N3-C2-N1	-3.17	123.72	128.68
3	C	600	ADP	PA-O3A-PB	-3.13	122.09	132.83
3	C	600	ADP	N3-C2-N1	-3.09	123.85	128.68
3	E	600	ADP	N3-C2-N1	-3.02	123.95	128.68
3	A	600	ADP	N3-C2-N1	-2.96	124.05	128.68
3	B	600	ADP	C3'-C2'-C1'	2.87	105.30	100.98
3	B	600	ADP	PA-O3A-PB	-2.85	123.04	132.83
3	E	600	ADP	PA-O3A-PB	-2.83	123.10	132.83
3	A	600	ADP	C3'-C2'-C1'	2.80	105.20	100.98
3	E	600	ADP	C3'-C2'-C1'	2.76	105.14	100.98
3	B	600	ADP	C4-C5-N7	-2.72	106.57	109.40
3	C	600	ADP	C4-C5-N7	-2.52	106.78	109.40
3	A	600	ADP	C4-C5-N7	-2.48	106.81	109.40
3	D	600	ADP	C4-C5-N7	-2.46	106.84	109.40
3	E	600	ADP	C4-C5-N7	-2.39	106.91	109.40
3	C	600	ADP	C3'-C2'-C1'	2.36	104.53	100.98
3	D	600	ADP	PA-O3A-PB	-2.17	125.39	132.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	600	ADP	C5'-O5'-PA-O1A

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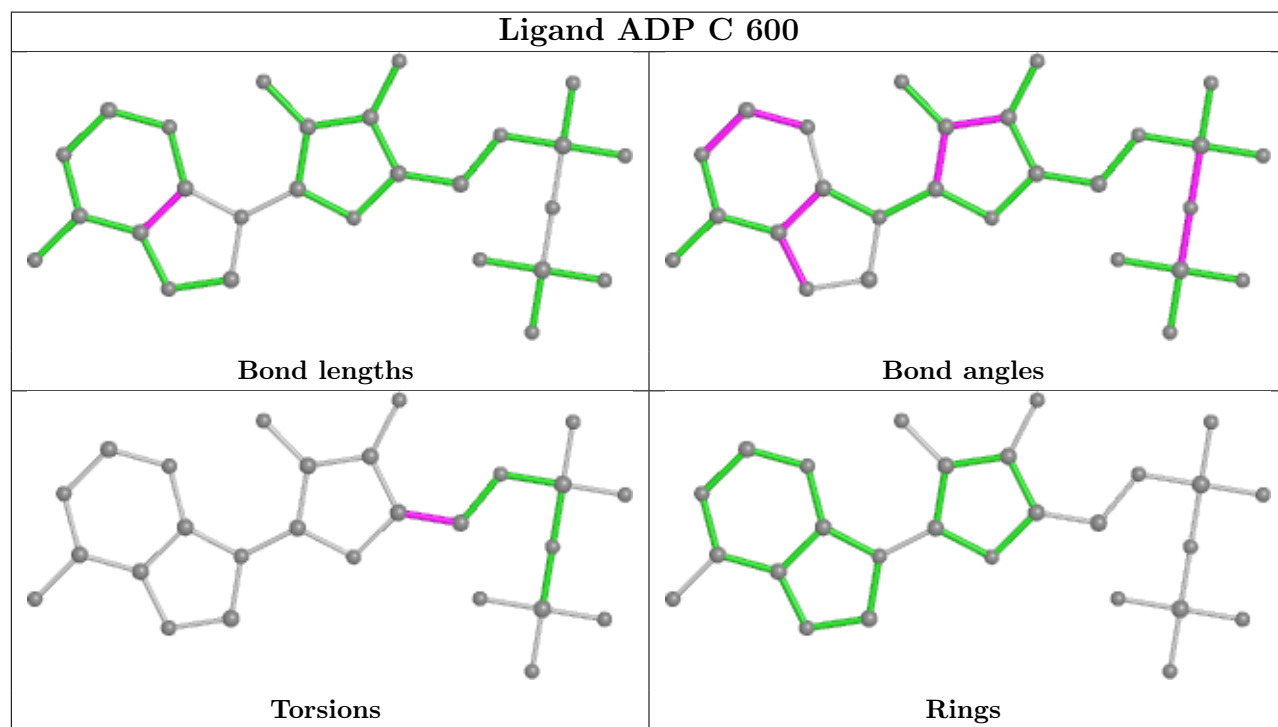
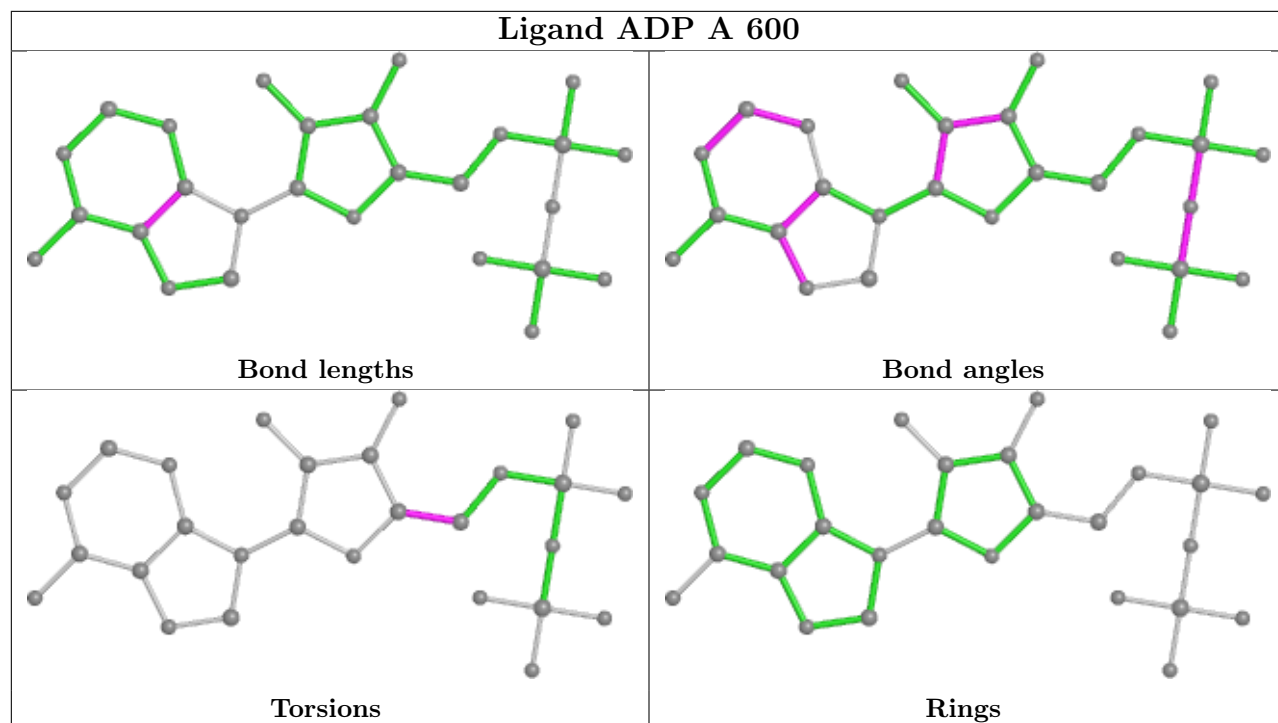
Mol	Chain	Res	Type	Atoms
3	B	600	ADP	C5'-O5'-PA-O2A
3	B	600	ADP	O4'-C4'-C5'-O5'
3	B	600	ADP	C3'-C4'-C5'-O5'
3	E	600	ADP	O4'-C4'-C5'-O5'
3	E	600	ADP	C3'-C4'-C5'-O5'
3	E	600	ADP	PB-O3A-PA-O5'
3	B	600	ADP	C5'-O5'-PA-O3A
3	D	600	ADP	C5'-O5'-PA-O3A
3	D	600	ADP	C5'-O5'-PA-O2A
3	A	600	ADP	O4'-C4'-C5'-O5'
3	C	600	ADP	O4'-C4'-C5'-O5'

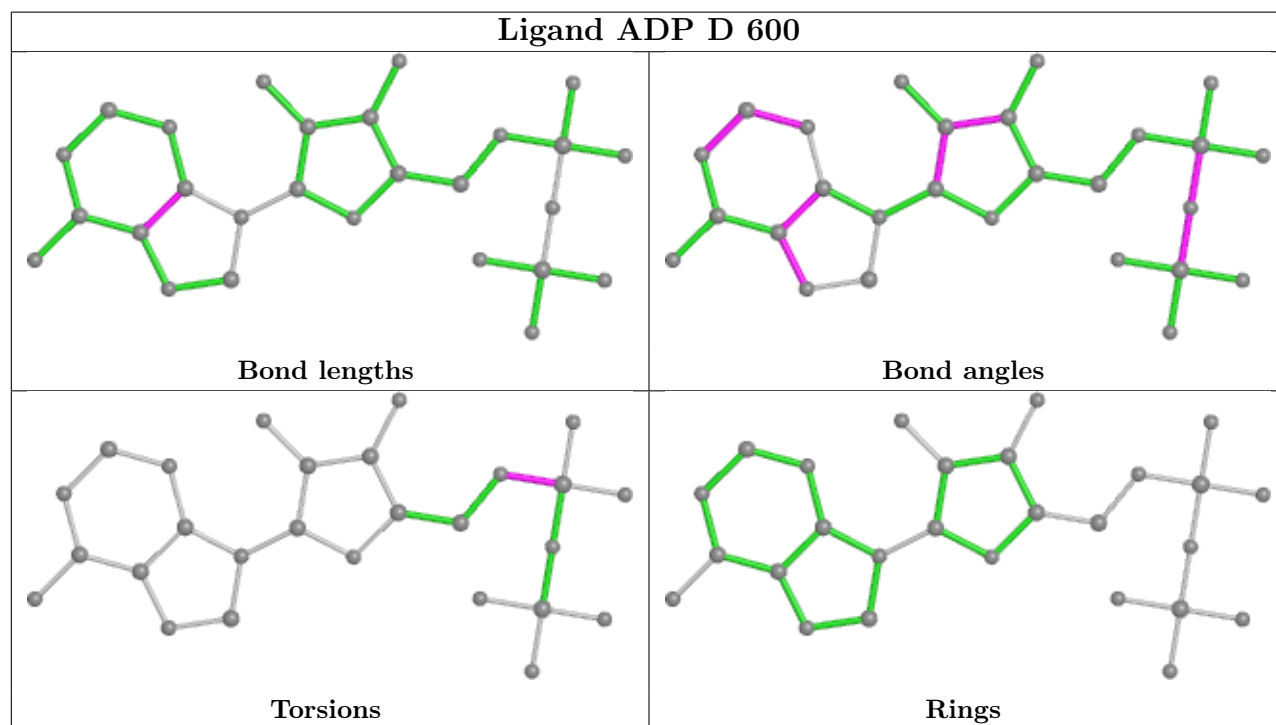
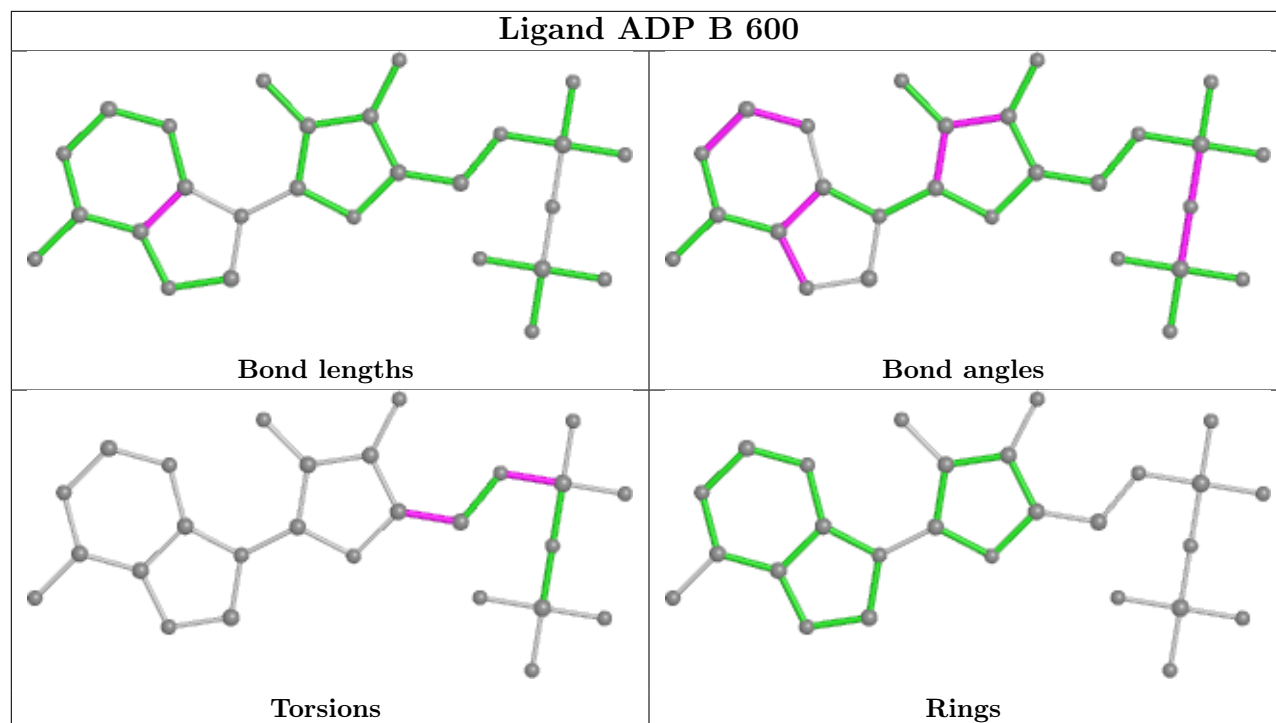
There are no ring outliers.

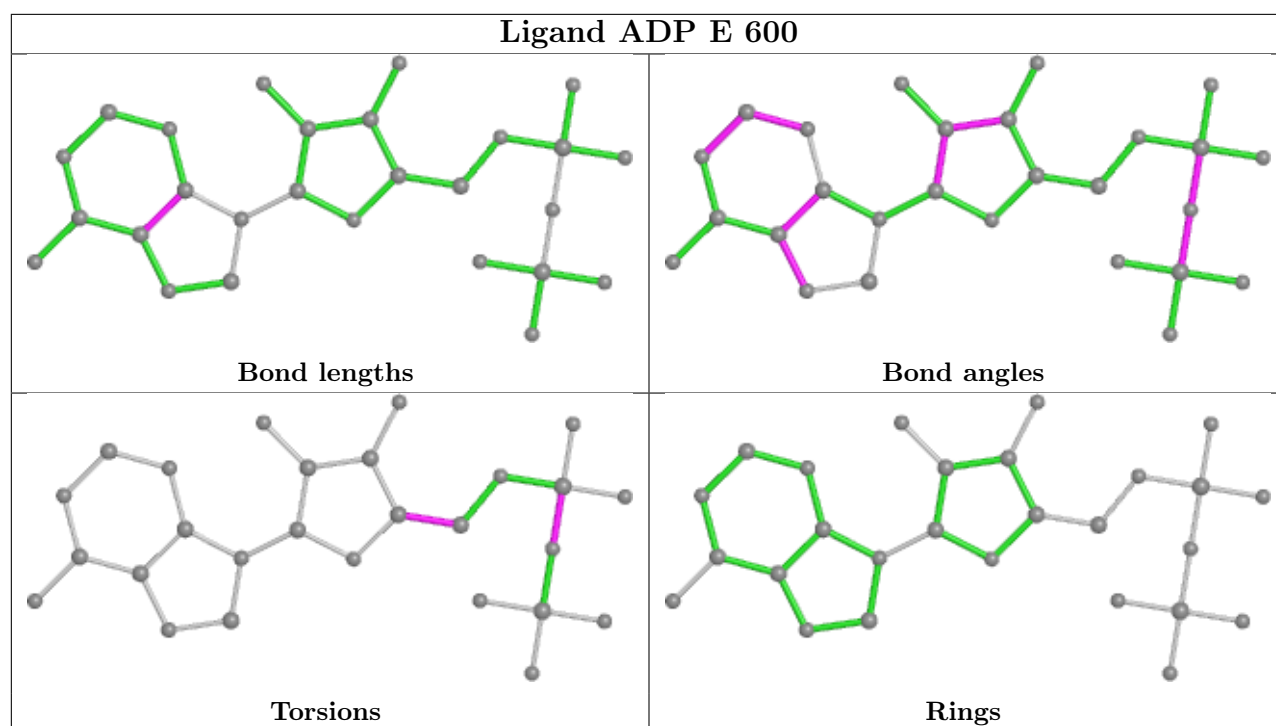
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	ADP	4	0
3	C	600	ADP	2	0
3	B	600	ADP	1	0
3	D	600	ADP	1	0
5	A	602	PO4	2	0
3	E	600	ADP	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	587/596 (98%)	-0.32	1 (0%) 92 87	22, 41, 73, 100	0
1	B	586/596 (98%)	0.00	8 (1%) 73 58	28, 61, 103, 128	0
1	C	584/596 (97%)	-0.23	2 (0%) 90 83	19, 39, 99, 123	0
2	D	444/458 (96%)	-0.23	7 (1%) 70 55	20, 36, 84, 109	0
2	E	440/458 (96%)	0.30	13 (2%) 52 37	26, 71, 118, 136	0
2	F	433/458 (94%)	0.27	27 (6%) 28 18	20, 58, 123, 138	1 (0%)
All	All	3074/3162 (97%)	-0.06	58 (1%) 66 50	19, 50, 106, 138	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	315	ILE	3.4
1	B	425	PHE	3.3
2	D	441	GLU	3.3
2	F	153	PRO	3.1
2	F	157	LYS	3.1
1	B	282	GLY	3.0
2	F	442	LEU	3.0
2	F	347	SER	3.0
2	F	128	ILE	2.9
2	F	174	SER	2.9
2	D	442	LEU	2.8
2	F	373	PHE	2.8
2	E	445	ILE	2.8
2	E	450	LEU	2.7
2	F	150	PHE	2.7
2	E	319	THR	2.7
2	E	412	TYR	2.7
2	E	364	ASP	2.6
2	F	431	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	304	LEU	2.6
2	F	426	THR	2.5
1	B	540	ALA	2.5
2	F	248	GLU	2.5
1	B	293	ALA	2.5
2	F	325	GLY	2.4
2	E	267	VAL	2.4
2	F	321	TYR	2.4
2	F	344	VAL	2.4
1	C	584	ILE	2.3
1	A	1	MET	2.3
2	D	440	THR	2.3
1	C	108	GLN	2.3
2	D	444	ARG	2.3
2	E	316	PRO	2.3
2	F	340	PRO	2.3
1	B	427	SER	2.3
2	F	402	ALA	2.3
2	F	158	SER	2.3
2	D	445	ILE	2.2
2	F	175	ASP	2.2
2	E	402	ALA	2.2
2	E	307	PRO	2.2
2	E	321	TYR	2.2
2	F	374	ALA	2.2
1	B	463	ILE	2.2
1	B	567	LEU	2.1
2	D	318	LEU	2.1
2	F	404	PHE	2.1
2	E	340	PRO	2.1
2	F	154	GLY	2.1
2	F	127	PHE	2.1
2	F	335	LYS	2.1
2	F	445	ILE	2.1
2	F	401	TYR	2.1
2	E	413	VAL	2.1
1	B	238	LYS	2.0
2	D	319	THR	2.0
2	F	333	LEU	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

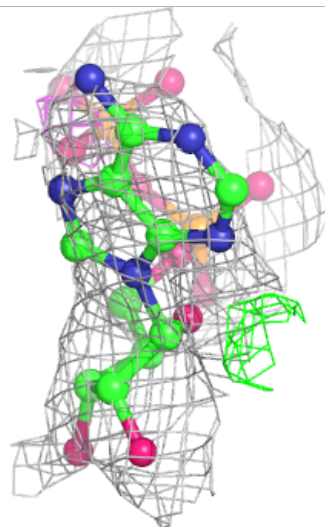
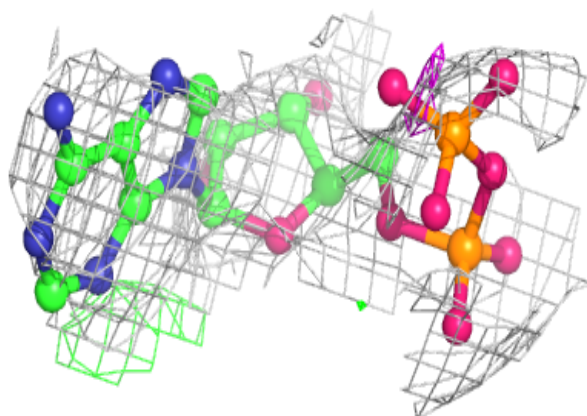
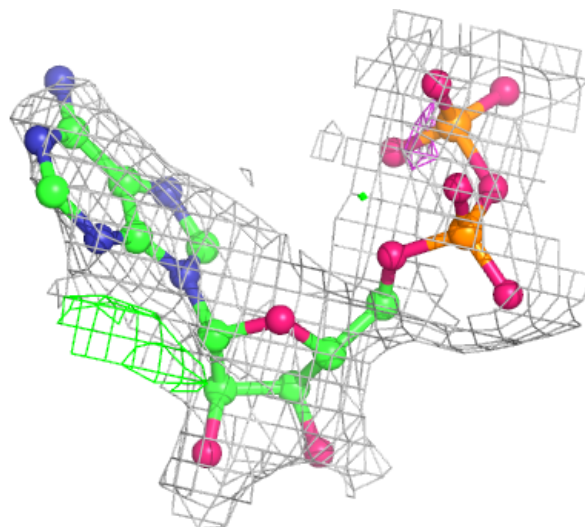
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	E	600	27/27	0.76	0.13	65,86,111,120	0
4	MG	E	601	1/1	0.81	0.09	91,91,91,91	0
3	ADP	D	600	27/27	0.87	0.11	44,52,67,71	0
4	MG	B	601	1/1	0.88	0.15	58,58,58,58	0
4	MG	C	601	1/1	0.89	0.26	39,39,39,39	0
4	MG	A	601	1/1	0.89	0.23	28,28,28,28	0
3	ADP	C	600	27/27	0.91	0.12	44,55,64,67	0
3	ADP	B	600	27/27	0.93	0.09	56,66,72,75	0
3	ADP	A	600	27/27	0.93	0.10	30,38,45,50	0
5	PO4	A	602	5/5	0.95	0.07	39,40,42,44	0
4	MG	D	601	1/1	0.98	0.04	50,50,50,50	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.

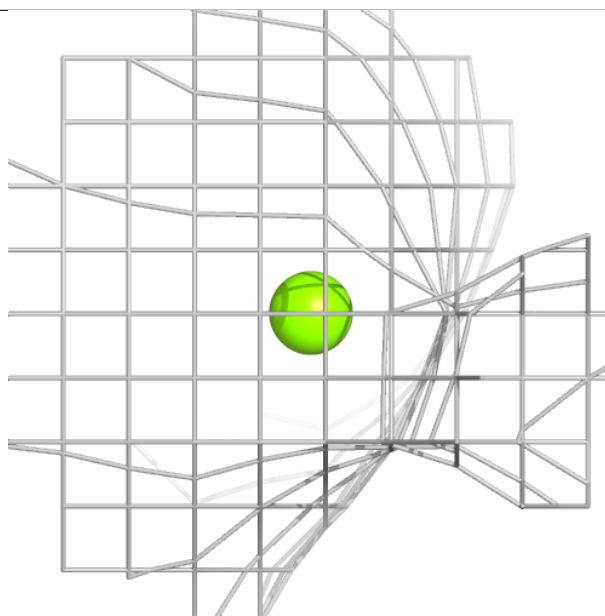
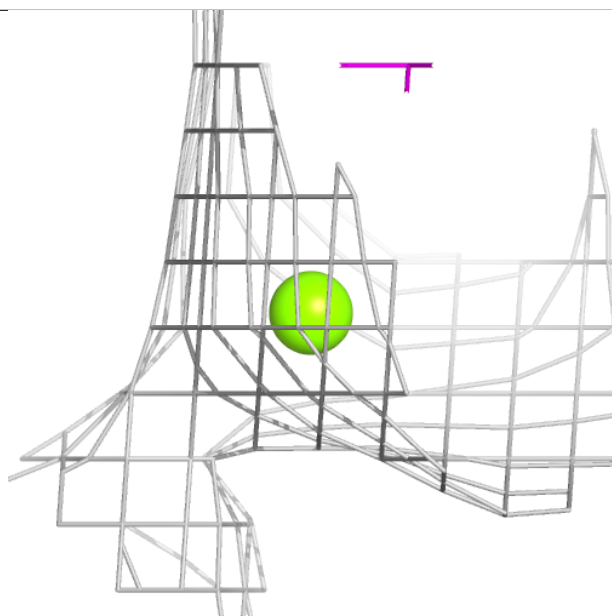
Electron density around ADP E 600:

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



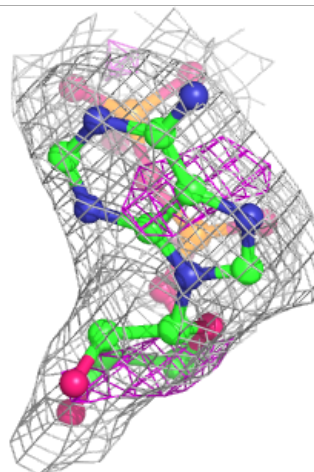
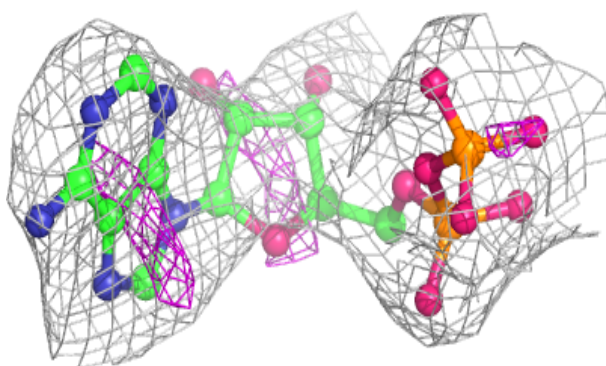
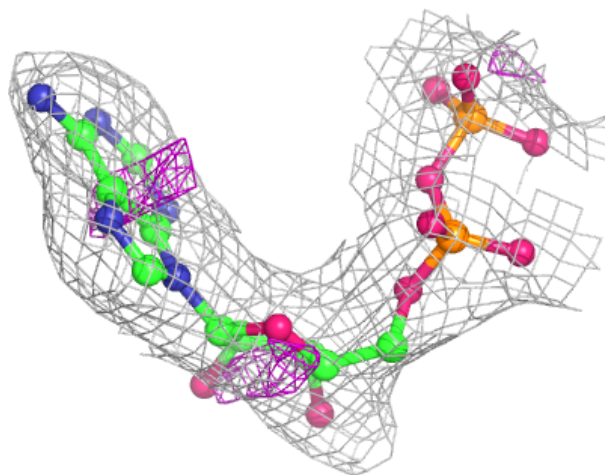
Electron density around MG E 601:

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



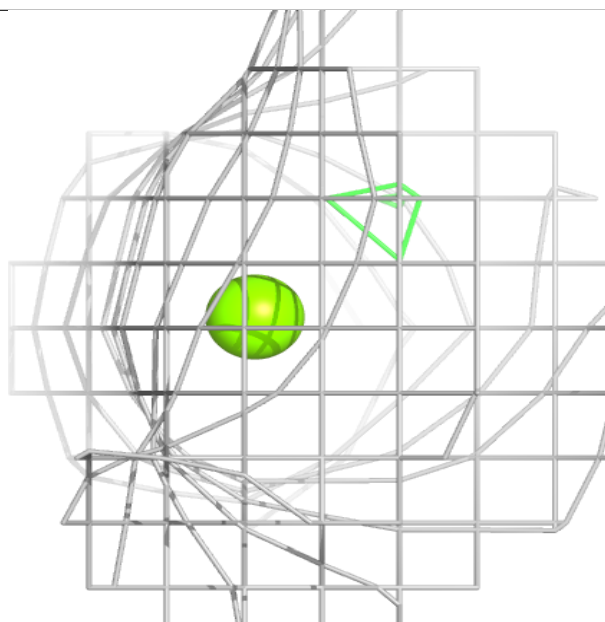
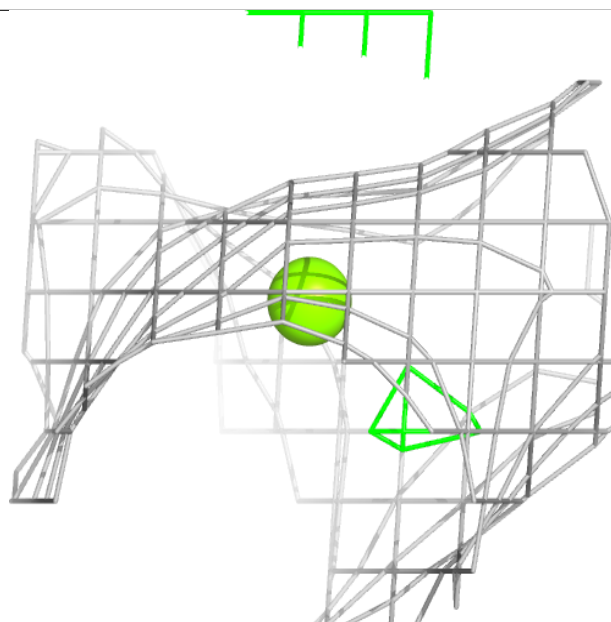
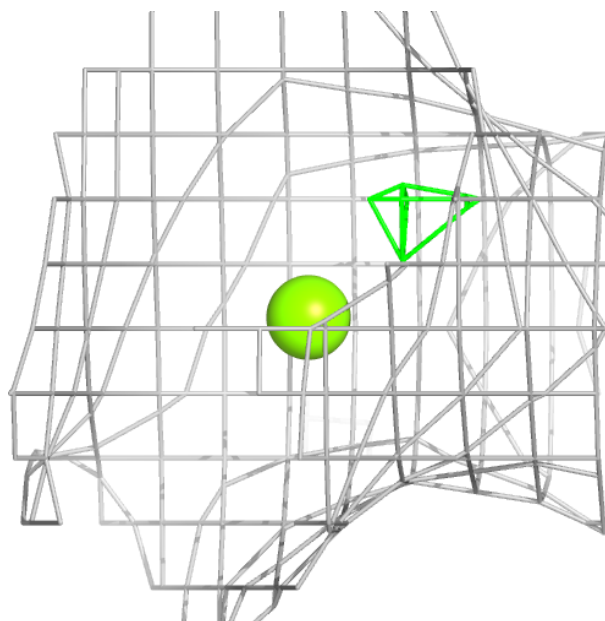
Electron density around ADP D 600:

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



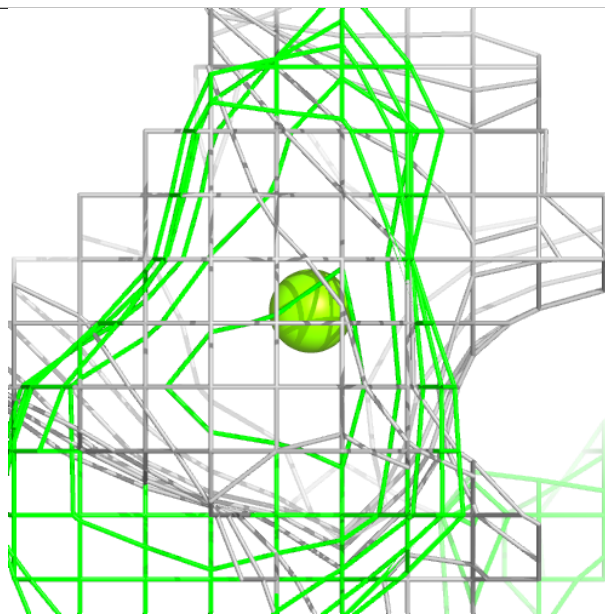
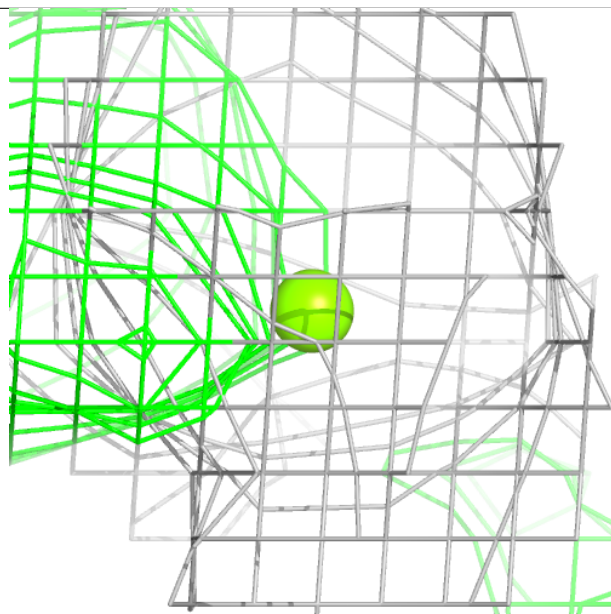
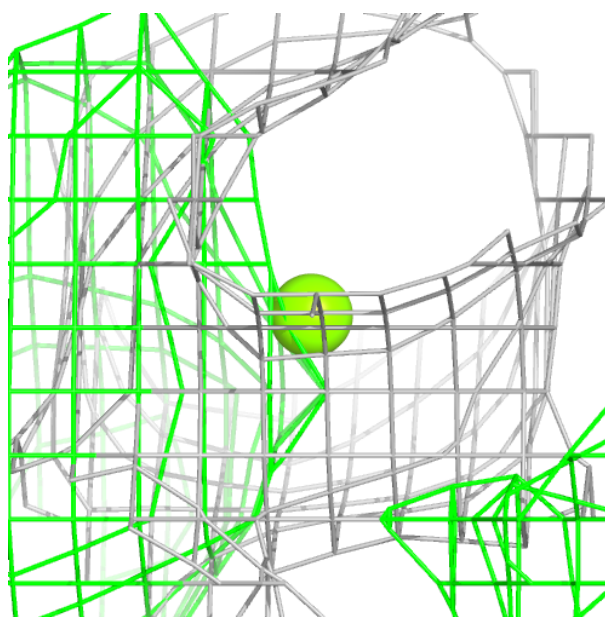
Electron density around MG B 601:

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



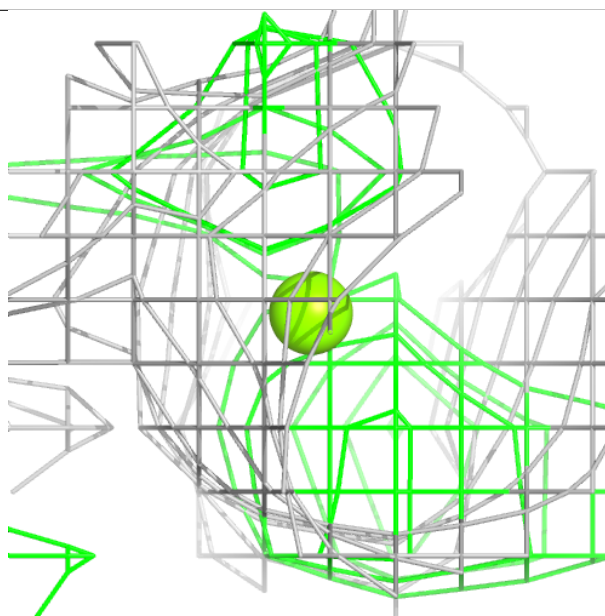
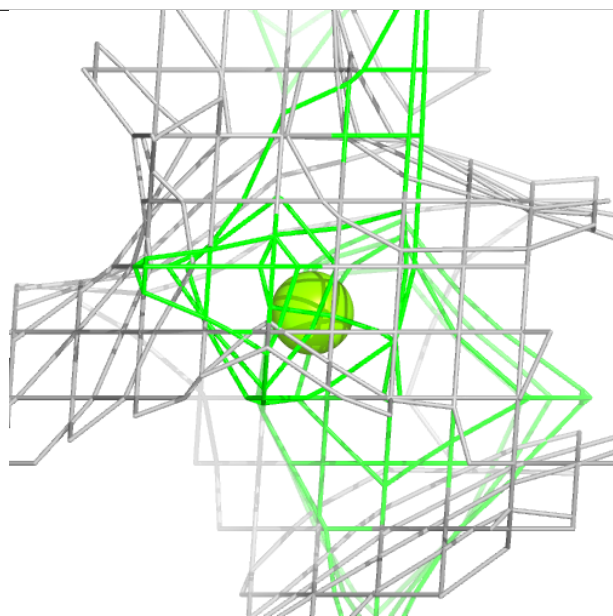
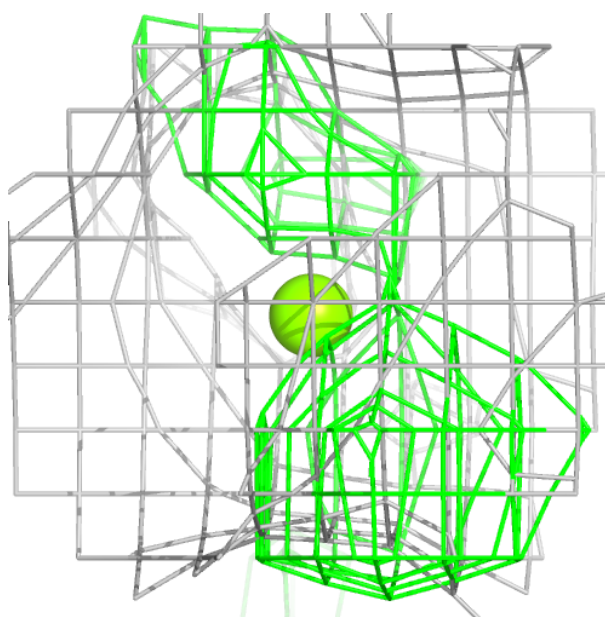
Electron density around MG C 601:

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



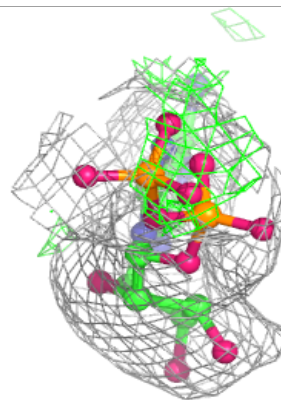
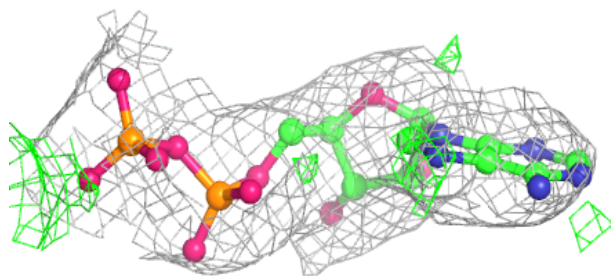
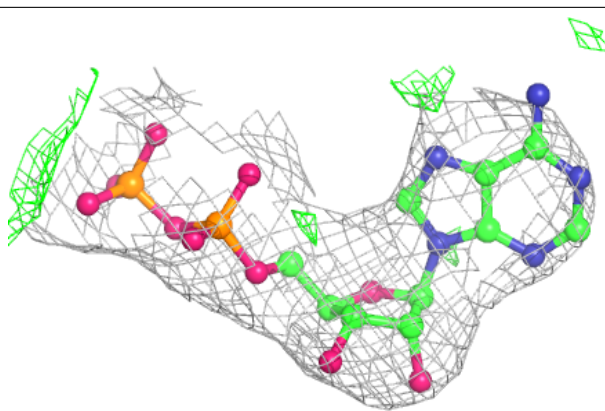
Electron density around MG A 601:

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

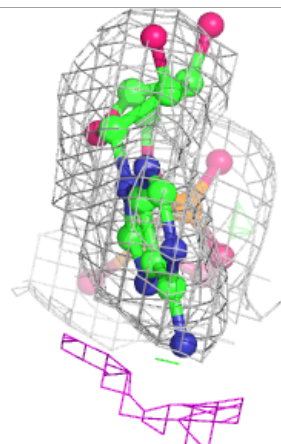
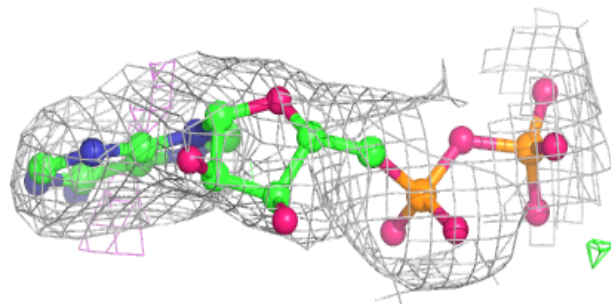
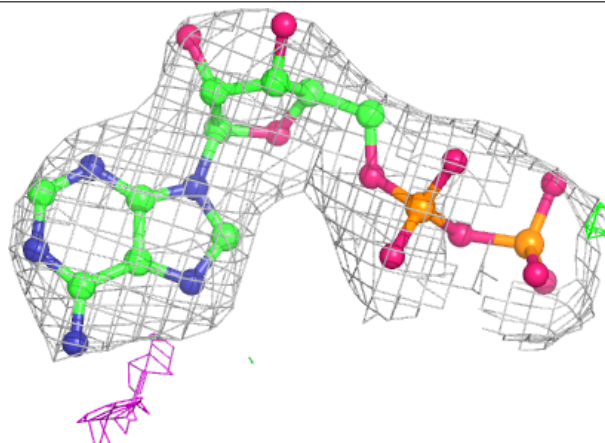


Electron density around ADP C 600:

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

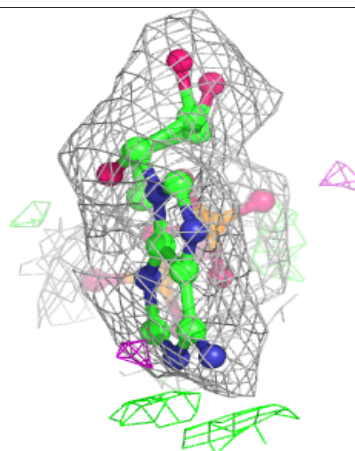
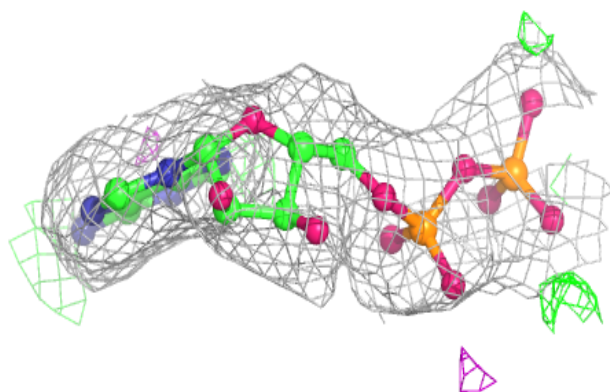
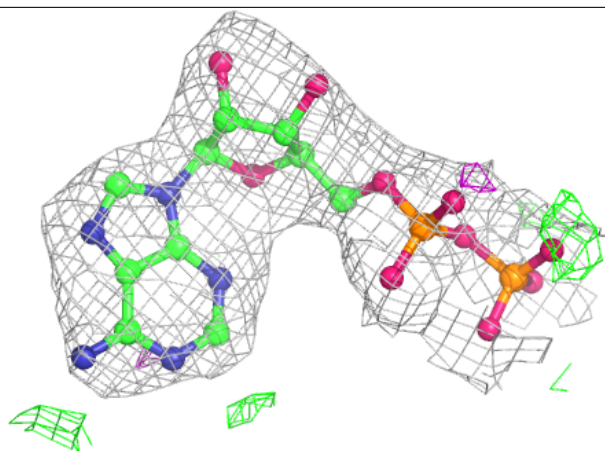
**Electron density around ADP B 600:**

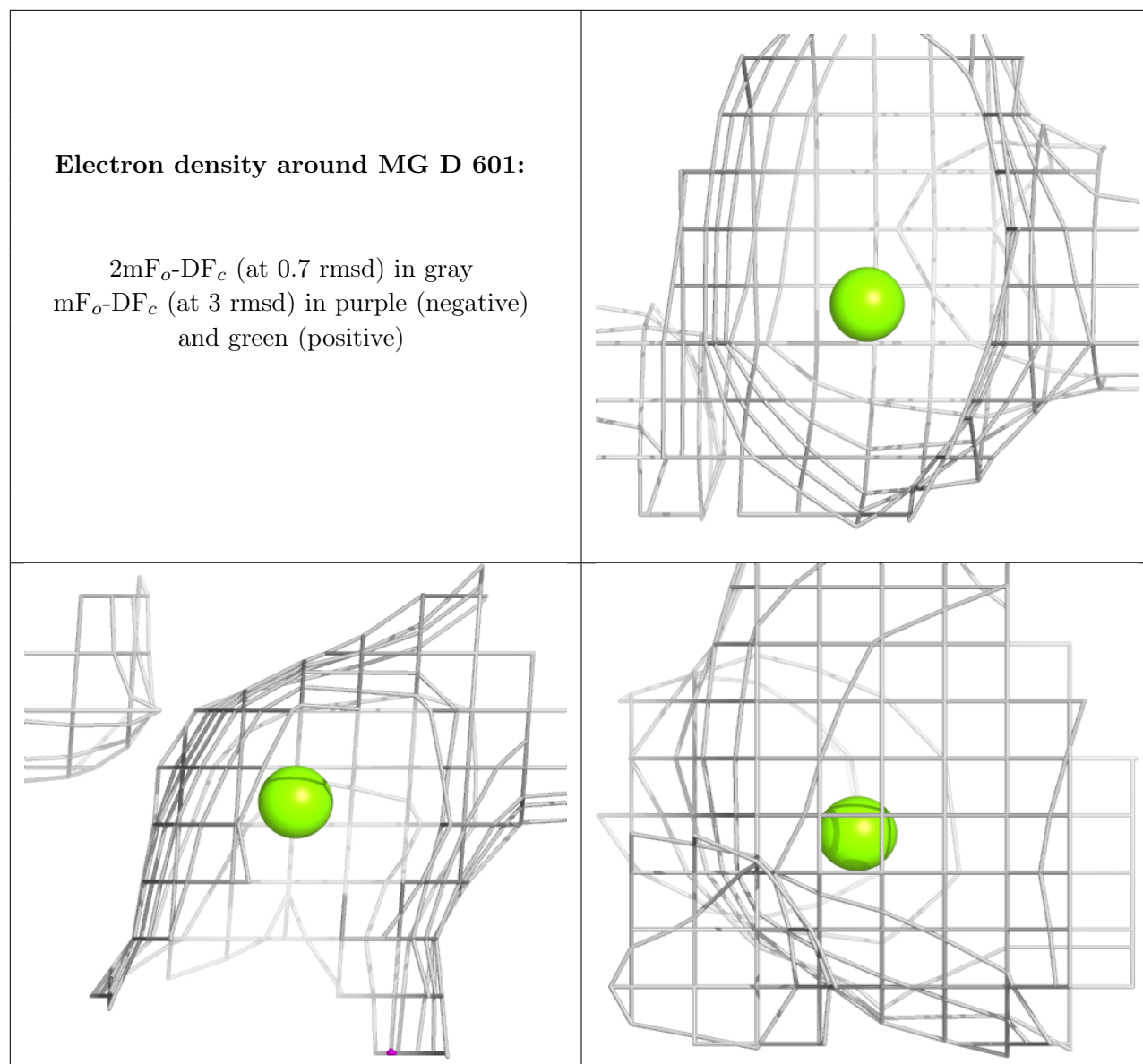
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 600:

$2mF_o-DF_c$ (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.