



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:59 AM UTC

PDB ID : 8IGV / pdb_00008igv
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

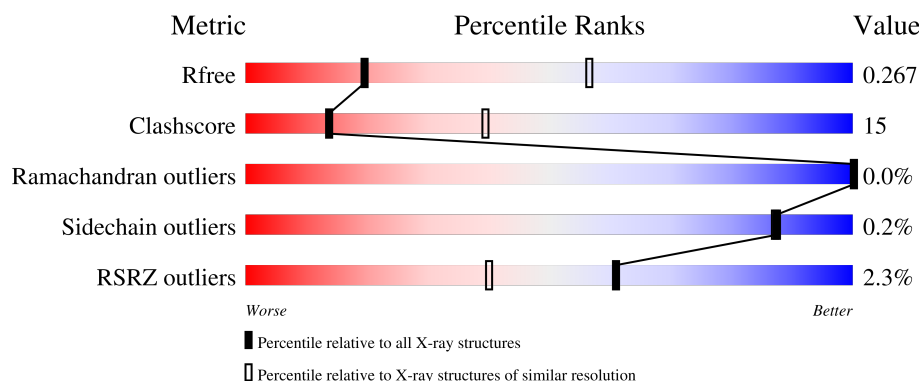
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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	69% 29% .
1	B	596	2% 64% 34% ..
1	C	596	69% 29% .
2	D	458	2% 67% 30% .
2	E	458	4% 67% 28% .

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Mol	Chain	Length	Quality of chain
2	F	458	

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

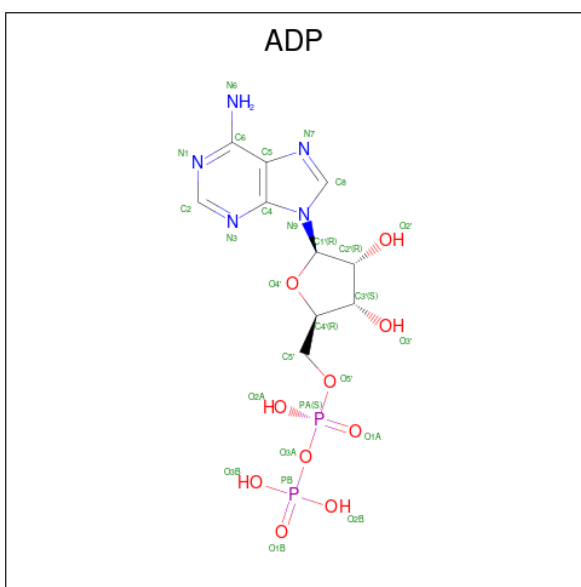
- Molecule 2 is a protein called V-type sodium ATPase subunit B.

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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

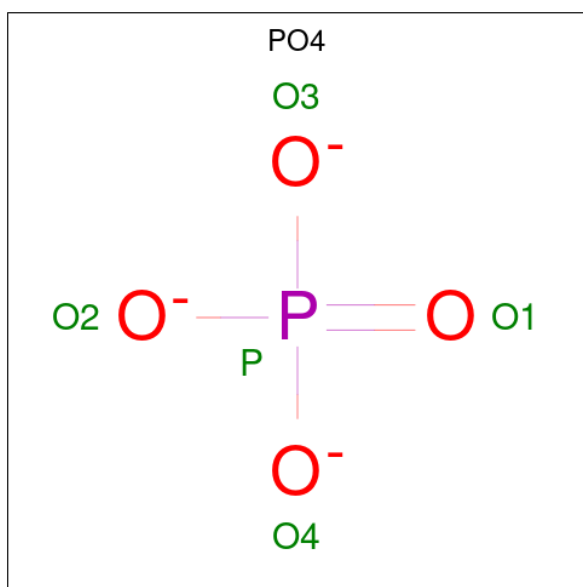


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: 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 (CCD ID: PO4) (formula: O_4P).



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

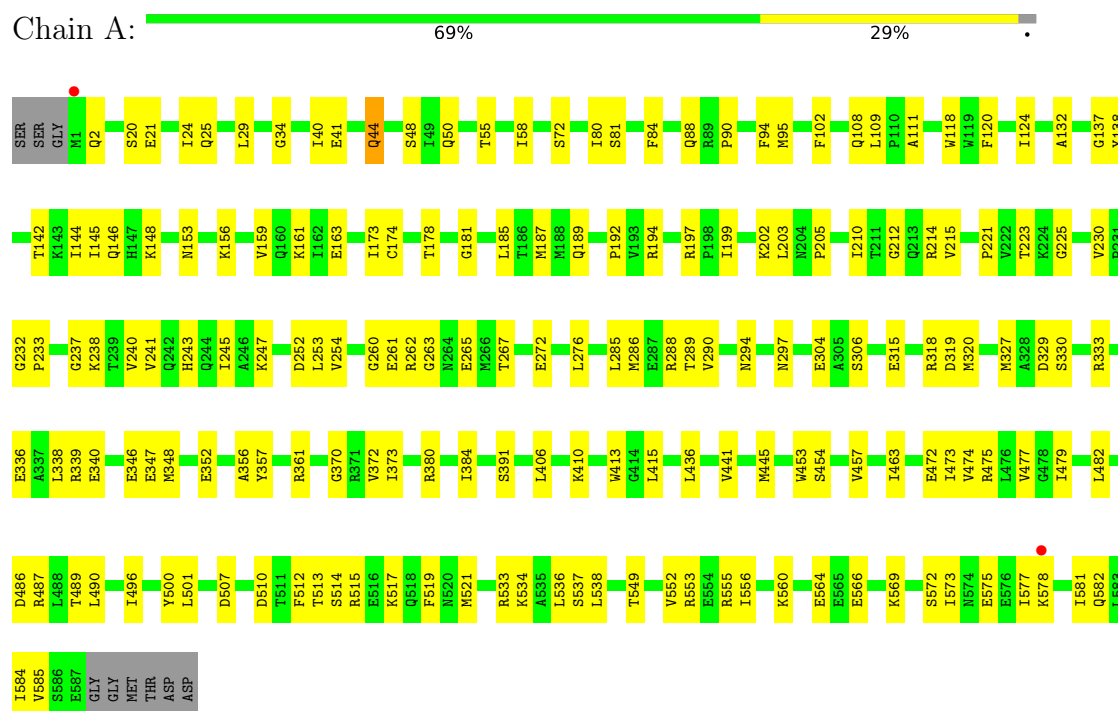
- Molecule 6 is water.

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		

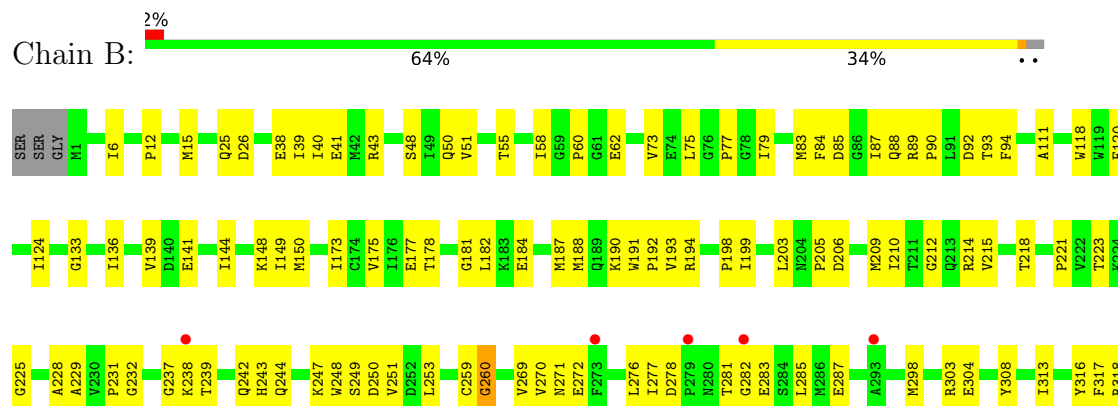
3 Residue-property plots

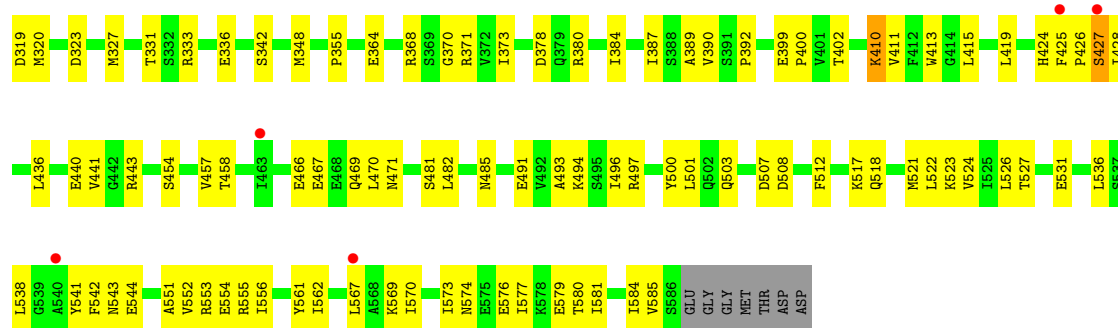
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: V-type sodium ATPase catalytic subunit A



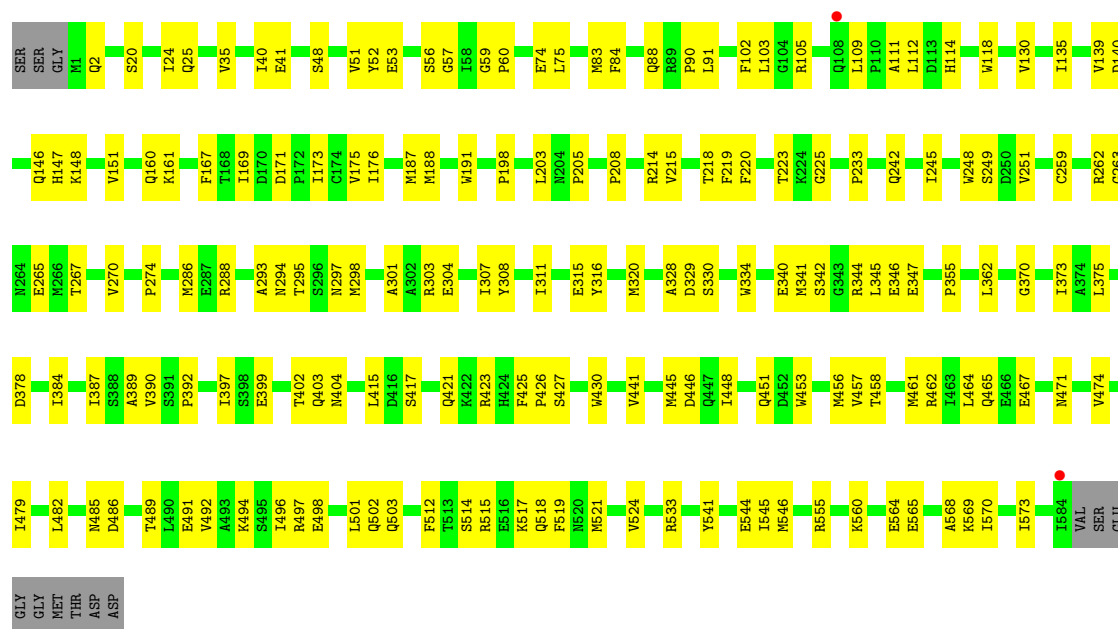
- Molecule 1: V-type sodium ATPase catalytic subunit A





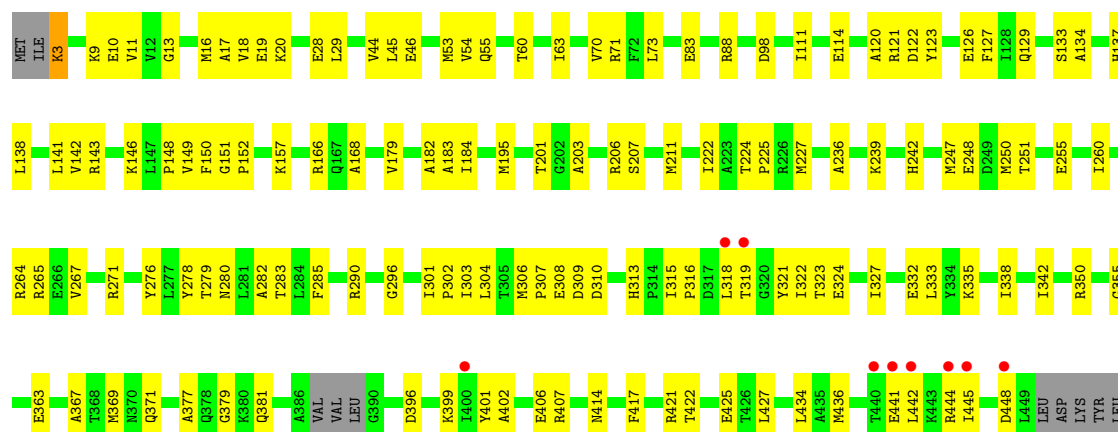
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain C: 69% 29% .



• Molecule 2: V-type sodium ATPase subunit B

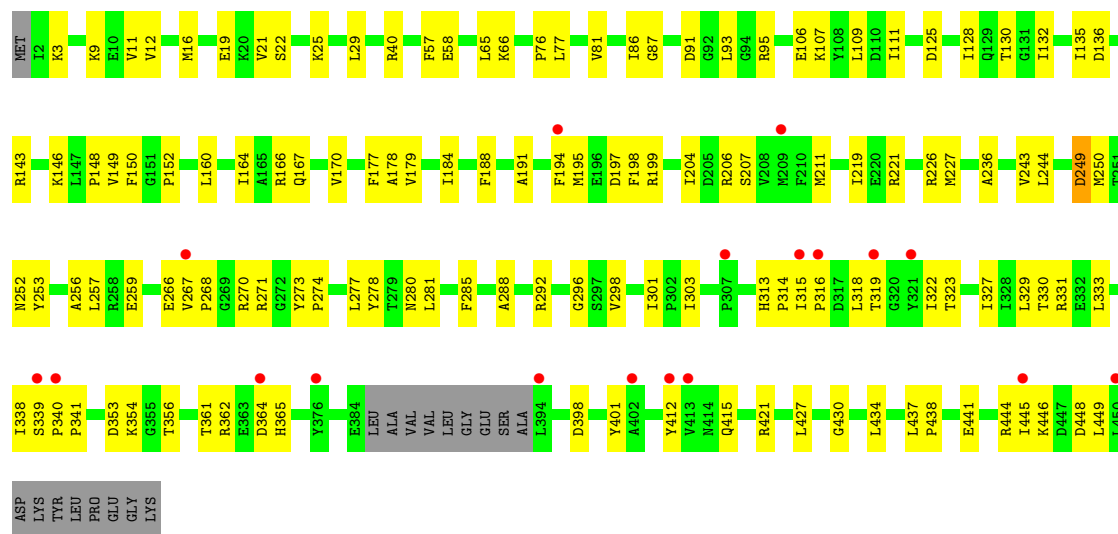
Chain D: 2% 67% 30% .



PRO
GLU
GLY
LYS

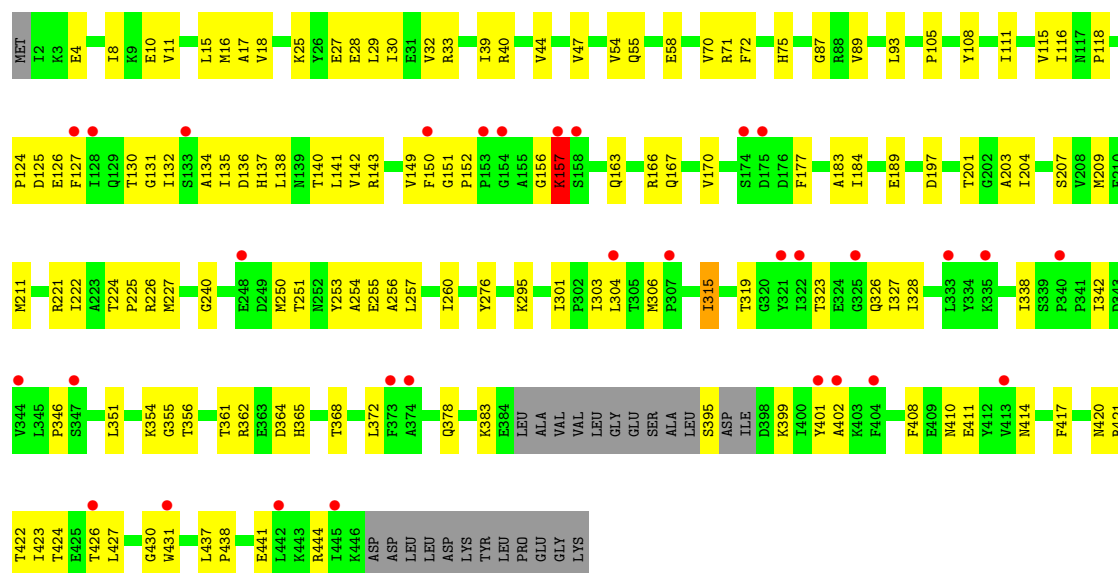
• Molecule 2: V-type sodium ATPase subunit B

Chain E: 4% 67% 28% .



• Molecule 2: V-type sodium ATPase subunit B

Chain F: 7% 65% 29% 5%



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	3152 reflections (3.85%)	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, 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	0.31	0/4647	0.58	0/6287
1	B	0.21	0/4638	0.52	2/6275 (0.0%)
1	C	0.19	0/4625	0.49	0/6257
2	D	0.23	0/3531	0.54	4/4770 (0.1%)
2	E	0.22	0/3510	0.58	1/4742 (0.0%)
2	F	0.24	1/3461 (0.0%)	0.55	2/4673 (0.0%)
All	All	0.24	1/24412 (0.0%)	0.54	9/33004 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	315	ILE	CA-CB	5.16	1.60	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	156	GLY	O-C-N	-9.28	111.48	122.33
2	D	307	PRO	N-CA-C	-8.36	97.38	110.50
2	F	157	LYS	N-CA-C	-7.99	103.33	113.23
2	E	266	GLU	N-CA-C	-7.92	91.78	107.69
1	B	410	LYS	CB-CG-CD	-6.60	96.12	111.30
2	D	444	ARG	CB-CG-CD	-6.49	96.36	111.30
2	D	444	ARG	CA-CB-CG	6.30	126.70	114.10
2	D	309	ASP	CB-CA-C	5.77	121.43	109.95
1	B	427	SER	N-CA-C	-5.39	99.32	110.80

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	135	0
1	B	4562	0	4527	151	0
1	C	4549	0	4511	125	0
2	D	3471	0	3484	105	0
2	E	3450	0	3470	108	0
2	F	3402	0	3418	105	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	2	0
6	C	30	0	0	1	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	700	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 15.

All (700) 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
1:B:244:GLN:HE21	1:B:248:TRP:CD1	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:GLN:OE1	2:D:264:ARG:NH1	2.28	0.67
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:150:MET:HE1	1:B:319:ASP:HB3	1.80	0.64
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:B:77:PRO:HG2	1:B:187:MET:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:118:TRP:HB2	1:B:187:MET:HE1	1.83	0.61
2:D:129:GLN:NE2	2:D:422:THR:HA	2.15	0.61
1:C:342:SER:OG	1:C:347:GLU:OE1	2.13	0.60
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
1:C:445:MET:HE1	6:C:717:HOH:O	2.02	0.60
2:F:150:PHE:HA	2:F:304:LEU:O	2.02	0.60
1:A:178:THR:OG1	1:A:181:GLY:O	2.17	0.59
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:188:MET:HE3	1:B:190:LYS:HG3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:445:MET:HA	1:C:448:ILE:HG22	1.86	0.57
1:C:456:MET:HE1	1:C:519:PHE:CD1	2.39	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:A:521:MET:HE1	1:A:560:LYS:HA	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:PRO:HG3	1:B:402:THR:HG21	1.86	0.55
1:B:425:PHE:C	1:B:427:SER:H	2.14	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:453:TRP:HA	1:C:456:MET:HE2	1.87	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
2:E:3:LYS:NZ	2:E:22:SER:O	2.36	0.55
1:B:144:ILE:HD13	1:B:287:GLU:HB3	1.89	0.55
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:A:44:GLN:CD	2:E:9:LYS:HE3	2.32	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
2:F:93:LEU:HA	2:F:227:MET:HE3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:139:VAL:HG11	1:B:187:MET:HE3	1.89	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
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
2:D:308:GLU:H	2:D:308:GLU:CD	2.09	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:A:514:SER:OG	1:A:564:GLU:OE1	2.22	0.52
1:B:454:SER:O	1:B:458:THR:HG23	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:486:ASP:O	1:C:489:THR:OG1	2.21	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:425:PHE:C	1:B:427:SER:N	2.67	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
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:517:LYS:HG2	1:A:521:MET:HE3	1.92	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: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:15:MET:HE1	6:B:710:HOH:O	2.11	0.50
1:A:348:MET:HE2	2:E:267:VAL:HA	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:456:MET:HE1	1:C:519:PHE:HD1	1.75	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:118:TRP:HB2	1:A:187:MET:HE1	1.93	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:PRO:HG3	2:F:306:MET:HE2	1.95	0.48
2:F:163:GLN:HG3	2:F:417:PHE:O	2.13	0.48
2:E:170:VAL:HG12	2:E:177:PHE:HB2	1.94	0.48
1:B:83:MET:HE1	1:B:270:VAL:HG13	1.96	0.48
1:B:259:CYS:O	1:B:260:GLY:C	2.57	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
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
1:C:245:ILE:O	1:C:249:SER:OG	2.28	0.48
2:D:60:THR:HA	2:D:63:ILE:HD12	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:195:MET:HG3	2:D:211:MET:HE2	1.97	0.47
2:E:77:LEU:O	2:E:111:ILE:HG12	2.15	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
2:E:195:MET:HE3	2:E:211:MET:HE2	1.97	0.47
1:A:315:GLU:O	1:A:318:ARG:HG2	2.15	0.47
1:B:237:GLY:C	1:B:239:THR:H	2.23	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
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
1:C:461:MET:HE3	1:C:465:GLN:HG2	1.97	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:93:LEU:C	2:E:227:MET:HE3	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:83:MET:HE2	1:C:293:ALA:HB2	1.98	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:B:410:LYS:NZ	2:F:189:GLU:OE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:341:MET:HE3	1:C:345:LEU:HG	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:347:GLU:OE2	1:A:357:TYR:OH	2.19	0.44
1:A:473:ILE:HG21	1:A:482:LEU:HD21	1.99	0.44
1:B:85:ASP:HB2	1:B:298:MET:HE1	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:445:MET:HE3	1:A:445:MET:HB3	1.92	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
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:111:ILE:HG21	2:D:227:MET:HE2	1.99	0.43
2:D:332:GLU:O	2:D:335:LYS:HG2	2.17	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
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:A:252:ASP:C	1:A:253:LEU:HD12	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:LYS:HZ3	2:D:71:ARG:HE	1.67	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: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:E:130:THR:HG22	2:E:136:ASP:CG	2.44	0.42
2:F:365:HIS:O	2:F:368:THR:OG1	2.37	0.42
2:D:407:ARG:HD3	2:D:436:MET:HE1	2.01	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
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:C:294:ASN:OD1	1:C:298:MET:HE2	2.19	0.42
2:D:13:GLY:O	2:D:60:THR:OG1	2.33	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:245:ILE:HB	1:A:327:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG12	1:B:308:TYR:HB3	2.01	0.41
1:B:277:ILE:HG13	1:B:283:GLU:C	2.46	0.41
2:E:19:GLU:O	2:E:21:VAL:HG23	2.20	0.41
2:E:364:ASP:CG	2:E:427:LEU:HD22	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:194:PHE:HB3	2:E:195:MET:HE2	2.03	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:81:SER:HA	1:A:286:MET:HE3	2.03	0.40
1:A:247:LYS:HD2	1:A:276:LEU:HD13	2.02	0.40
1:B:348:MET:HE3	1:B:348:MET:HB3	2.00	0.40
1:B:426:PRO:HG2	1:B:503:GLN:N	2.36	0.40
1:C:514:SER:OG	1:C:564:GLU:OE1	2.35	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: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
1:C:57:GLY:C	2:F:25:LYS:HB3	2.45	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:E:29:LEU:HD13	2:E:76:PRO:C	2.47	0.40
2:F:157:LYS:HG3	2:F:303:ILE:HG21	2.02	0.40
2:F:326:GLN:CD	2:F:328:ILE:HD11	2.46	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:491:GLU:CD	1:C:546:MET:HE1	2.46	0.40
2:F:204:ILE:HA	2:F:207:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/596 (98%)	572 (98%)	13 (2%)	0	100	100
1	B	584/596 (98%)	562 (96%)	21 (4%)	1 (0%)	43	71
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

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%)	87	87
1	B	502/509 (99%)	502 (100%)	0	100	100
1	C	500/509 (98%)	500 (100%)	0	100	100
2	D	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	E	366/380 (96%)	365 (100%)	1 (0%)	86	85
2	F	360/380 (95%)	359 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2598/2667 (97%)	2594 (100%)	4 (0%)	87 87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
2	D	3	LYS
2	E	249	ASP
2	F	157	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	114	HIS
1	A	244	GLN
1	A	264	ASN
1	A	404	ASN
1	B	50	GLN
1	B	101	ASN
1	C	99	GLN
1	C	213	GLN
1	C	243	HIS
1	C	244	GLN
2	E	163	GLN
2	E	326	GLN
2	E	415	GLN
2	F	67	ASN
2	F	163	GLN
2	F	167	GLN
2	F	326	GLN
2	F	370	ASN
2	F	371	GLN
2	F	378	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	600	4	28,29,29	1.44	5 (17%)	43,45,45	1.78	7 (16%)
3	ADP	C	600	4	28,29,29	1.42	4 (14%)	43,45,45	1.77	8 (18%)
3	ADP	B	600	4	28,29,29	1.45	5 (17%)	43,45,45	1.83	10 (23%)
3	ADP	D	600	4	28,29,29	1.46	5 (17%)	43,45,45	1.98	9 (20%)
5	PO4	A	602	4	4,4,4	1.00	0	6,6,6	0.51	0
3	ADP	A	600	4	28,29,29	1.41	4 (14%)	43,45,45	1.78	7 (16%)

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	E	600	4	-	3/16/32/32	0/3/3/3
3	ADP	C	600	4	-	1/16/32/32	0/3/3/3
3	ADP	B	600	4	-	5/16/32/32	0/3/3/3
3	ADP	D	600	4	-	4/16/32/32	0/3/3/3
3	ADP	A	600	4	-	3/16/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	ADP	C5-C4	4.99	1.48	1.39
3	A	600	ADP	C5-C4	4.87	1.47	1.39
3	E	600	ADP	C5-C4	4.87	1.47	1.39
3	B	600	ADP	C5-C4	4.80	1.47	1.39
3	C	600	ADP	C5-C4	4.77	1.47	1.39
3	D	600	ADP	C5-C6	2.87	1.49	1.41
3	B	600	ADP	C5-C6	2.77	1.48	1.41
3	C	600	ADP	C5-C6	2.67	1.48	1.41
3	E	600	ADP	C5-C6	2.66	1.48	1.41
3	A	600	ADP	C5-C6	2.64	1.48	1.41
3	A	600	ADP	C8-N7	2.40	1.36	1.31
3	A	600	ADP	C5-N7	-2.39	1.34	1.39
3	B	600	ADP	C8-N7	2.39	1.36	1.31
3	C	600	ADP	C5-N7	-2.37	1.34	1.39
3	E	600	ADP	C5-N7	-2.35	1.34	1.39
3	D	600	ADP	C5-N7	-2.32	1.34	1.39
3	C	600	ADP	C8-N7	2.28	1.36	1.31
3	D	600	ADP	C8-N7	2.28	1.36	1.31
3	B	600	ADP	C5-N7	-2.27	1.34	1.39
3	E	600	ADP	C8-N7	2.23	1.36	1.31
3	E	600	ADP	PA-O3A	2.18	1.61	1.59
3	B	600	ADP	PA-O3A	2.03	1.61	1.59
3	D	600	ADP	PA-O3A	2.01	1.61	1.59

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	ADP	C5-C4-N3	-6.91	117.20	126.72
3	A	600	ADP	C5-C4-N3	-6.01	118.44	126.72
3	E	600	ADP	C5-C4-N3	-5.99	118.47	126.72
3	B	600	ADP	C5-C4-N3	-5.85	118.66	126.72
3	C	600	ADP	C5-C4-N3	-5.64	118.95	126.72
3	D	600	ADP	N3-C4-N9	5.57	136.64	127.17
3	E	600	ADP	N3-C4-N9	4.83	135.39	127.17
3	A	600	ADP	N3-C4-N9	4.66	135.10	127.17
3	B	600	ADP	N3-C4-N9	4.62	135.03	127.17
3	C	600	ADP	N3-C4-N9	4.47	134.77	127.17
3	D	600	ADP	C2-N3-C4	4.12	121.89	111.83
3	B	600	ADP	C2-N3-C4	3.70	120.88	111.83
3	E	600	ADP	C2-N3-C4	3.63	120.70	111.83
3	A	600	ADP	C2-N3-C4	3.63	120.69	111.83
3	C	600	ADP	C2-N3-C4	3.56	120.52	111.83
3	B	600	ADP	C4-C5-N7	-3.51	106.57	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	600	ADP	C4-C5-N7	-3.33	106.78	110.58
3	A	600	ADP	C4-C5-N7	-3.29	106.81	110.58
3	D	600	ADP	C4-C5-N7	-3.27	106.84	110.58
3	B	600	ADP	N3-C2-N1	-3.23	123.69	128.58
3	D	600	ADP	N3-C2-N1	-3.21	123.72	128.58
3	E	600	ADP	C4-C5-N7	-3.21	106.91	110.58
3	C	600	ADP	N3-C2-N1	-3.13	123.85	128.58
3	E	600	ADP	N3-C2-N1	-3.06	123.95	128.58
3	A	600	ADP	N3-C2-N1	-3.00	124.05	128.58
3	C	600	ADP	C2'-C1'-N9	-2.63	106.76	113.30
3	B	600	ADP	C4-N9-C8	2.60	108.47	105.74
3	B	600	ADP	C5-N7-C8	2.56	107.47	103.45
3	D	600	ADP	C5-N7-C8	2.49	107.36	103.45
3	C	600	ADP	C4-N9-C8	2.43	108.29	105.74
3	C	600	ADP	C5-N7-C8	2.37	107.18	103.45
3	D	600	ADP	O4'-C1'-N9	2.37	112.64	108.09
3	E	600	ADP	C5-N7-C8	2.36	107.16	103.45
3	B	600	ADP	C2'-C1'-N9	-2.33	107.51	113.30
3	A	600	ADP	C5-N7-C8	2.31	107.08	103.45
3	E	600	ADP	C4-N9-C8	2.29	108.15	105.74
3	D	600	ADP	C3'-C2'-C1'	2.28	105.77	101.46
3	B	600	ADP	C6-C5-N7	2.10	136.14	132.09
3	A	600	ADP	C4-N9-C8	2.05	107.89	105.74
3	D	600	ADP	C1'-N9-C8	-2.05	122.55	127.09
3	B	600	ADP	C3'-C2'-C1'	2.03	105.30	101.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	ADP	O4'-C1'-N9-C8
3	A	600	ADP	O4'-C1'-N9-C4
3	B	600	ADP	C5'-O5'-PA-O1A
3	B	600	ADP	C5'-O5'-PA-O2A
3	B	600	ADP	C5'-O5'-PA-O3A
3	D	600	ADP	C5'-O5'-PA-O2A
3	D	600	ADP	C5'-O5'-PA-O3A
3	D	600	ADP	C2'-C1'-N9-C4
3	B	600	ADP	O4'-C4'-C5'-O5'
3	D	600	ADP	C2'-C1'-N9-C8
3	E	600	ADP	O4'-C4'-C5'-O5'
3	E	600	ADP	C3'-C4'-C5'-O5'

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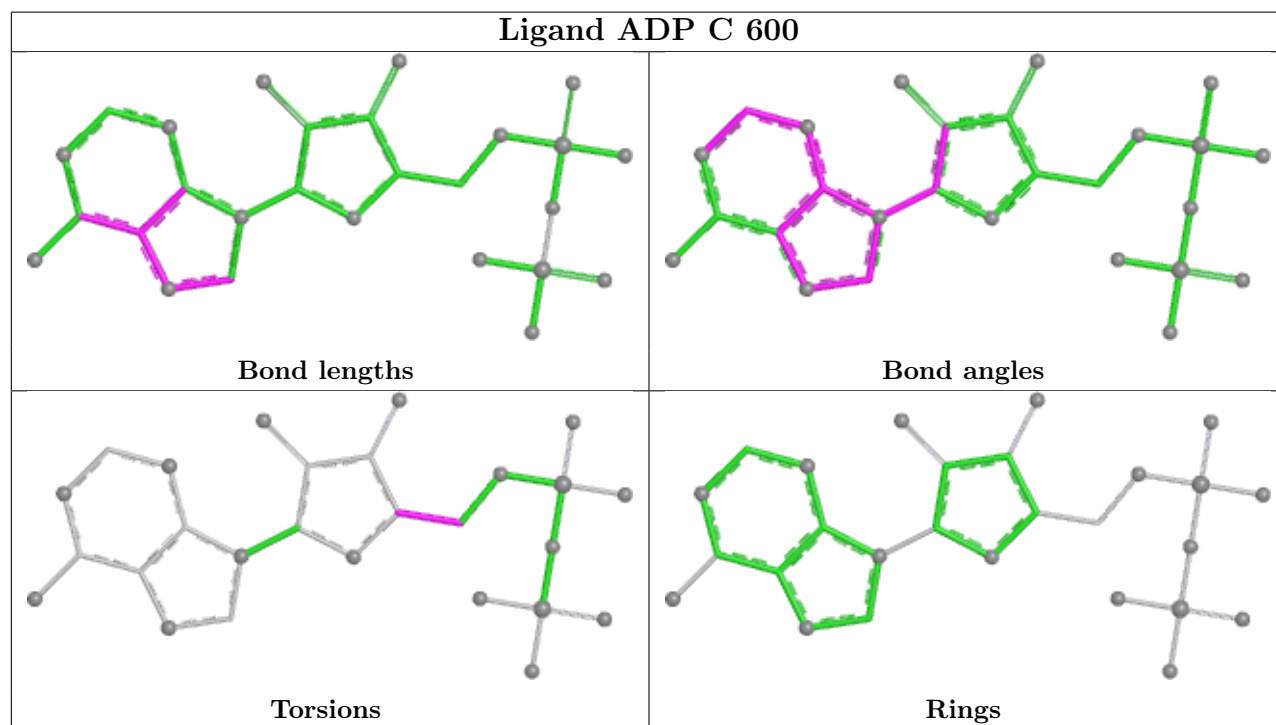
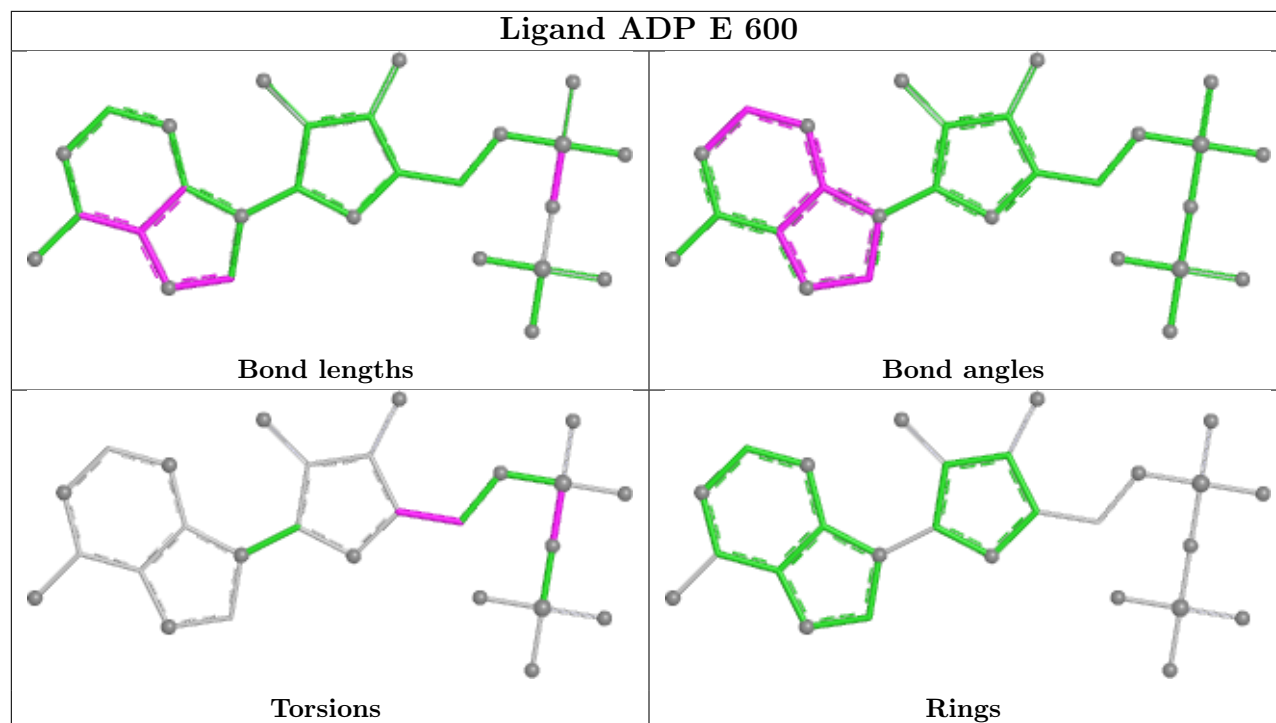
Mol	Chain	Res	Type	Atoms
3	B	600	ADP	C3'-C4'-C5'-O5'
3	E	600	ADP	PB-O3A-PA-O5'
3	A	600	ADP	O4'-C4'-C5'-O5'
3	C	600	ADP	O4'-C4'-C5'-O5'

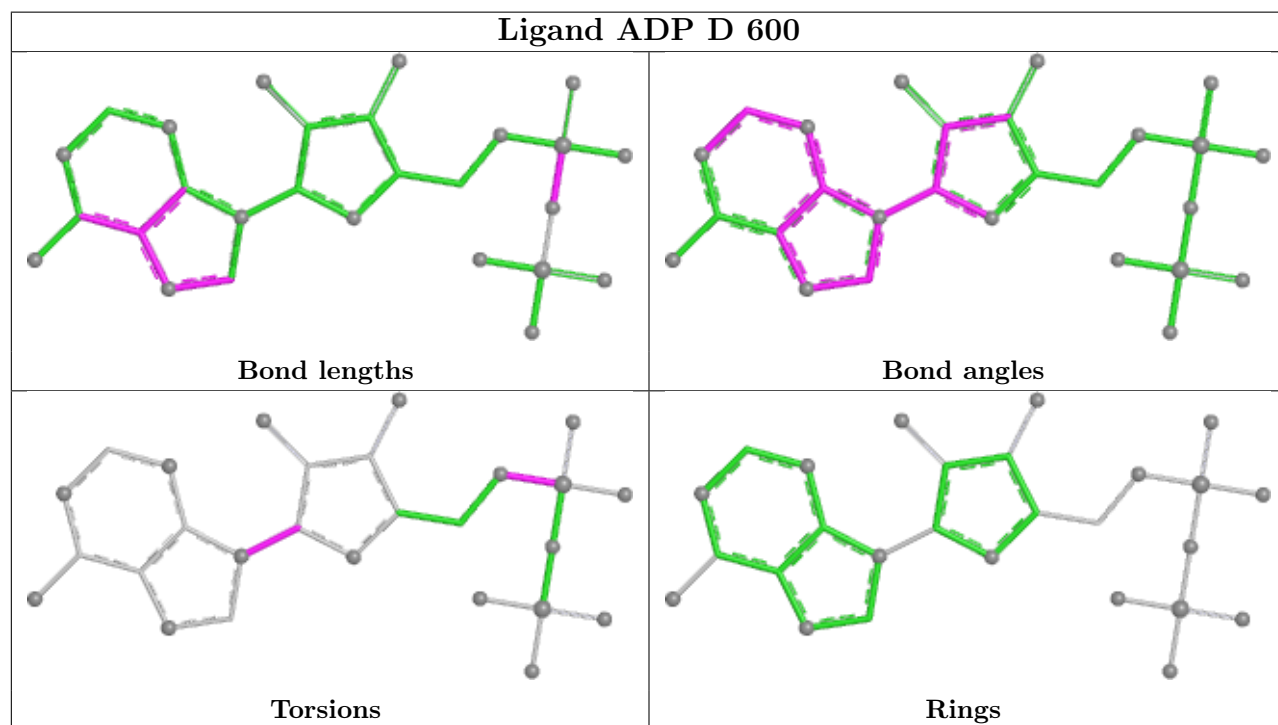
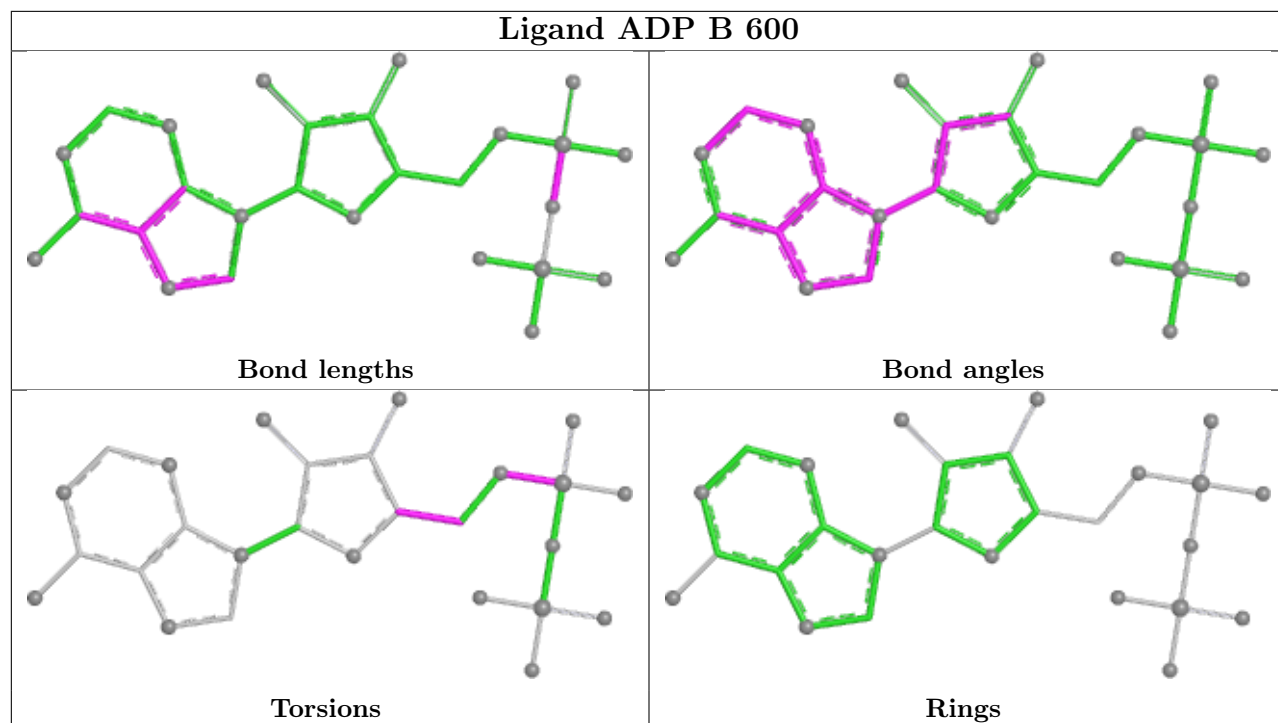
There are no ring outliers.

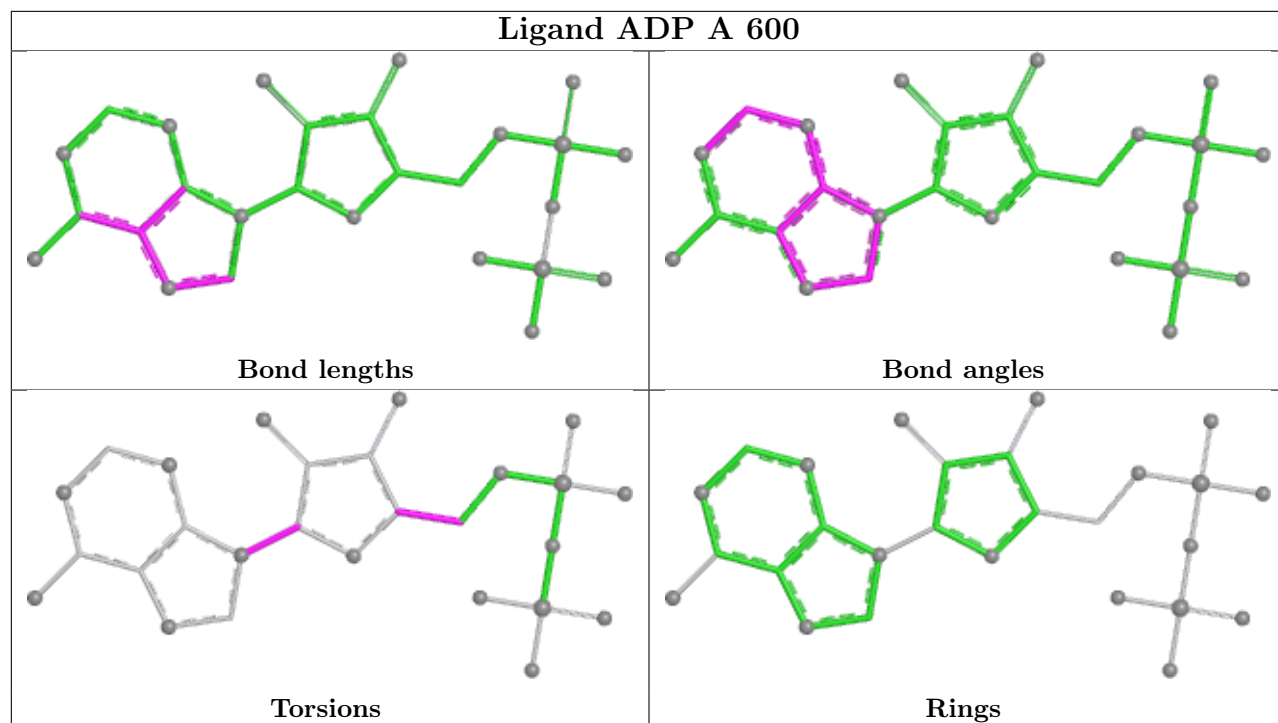
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	600	ADP	1	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	A	600	ADP	4	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%)	-0.17	2 (0%) 90 81	22, 41, 73, 100	0
1	B	586/596 (98%)	0.15	10 (1%) 69 48	28, 61, 103, 128	0
1	C	584/596 (97%)	-0.09	2 (0%) 90 81	19, 39, 99, 123	0
2	D	444/458 (96%)	-0.09	9 (2%) 65 44	20, 36, 84, 109	0
2	E	440/458 (96%)	0.44	18 (4%) 41 24	26, 71, 118, 136	0
2	F	433/458 (94%)	0.42	31 (7%) 21 12	20, 58, 123, 138	1 (0%)
All	All	3074/3162 (97%)	0.09	72 (2%) 61 40	19, 50, 106, 138	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	PHE	3.5
2	E	315	ILE	3.5
2	D	441	GLU	3.4
2	F	153	PRO	3.3
2	F	157	LYS	3.2
1	B	282	GLY	3.2
2	F	347	SER	3.1
2	F	442	LEU	3.1
2	F	128	ILE	3.1
2	F	174	SER	3.0
2	D	442	LEU	3.0
2	F	373	PHE	3.0
2	E	445	ILE	2.9
2	E	450	LEU	2.9
2	F	150	PHE	2.9
2	F	431	TRP	2.9
2	E	412	TYR	2.9
2	E	319	THR	2.8
2	E	364	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	304	LEU	2.7
2	F	426	THR	2.7
1	B	540	ALA	2.7
2	F	248	GLU	2.6
1	B	293	ALA	2.6
2	F	325	GLY	2.6
2	F	321	TYR	2.6
2	E	267	VAL	2.6
1	A	1	MET	2.5
2	F	344	VAL	2.5
1	C	584	ILE	2.5
2	D	440	THR	2.5
2	E	316	PRO	2.5
2	F	340	PRO	2.5
1	C	108	GLN	2.5
1	B	427	SER	2.4
2	F	158	SER	2.4
2	D	444	ARG	2.4
2	F	175	ASP	2.4
2	D	445	ILE	2.4
2	F	402	ALA	2.4
2	E	307	PRO	2.4
2	E	321	TYR	2.4
2	E	402	ALA	2.3
2	F	374	ALA	2.3
1	B	463	ILE	2.3
2	F	404	PHE	2.3
2	E	340	PRO	2.3
1	B	567	LEU	2.3
2	D	318	LEU	2.3
2	F	127	PHE	2.3
2	F	154	GLY	2.3
2	F	401	TYR	2.2
2	F	445	ILE	2.2
2	D	319	THR	2.2
2	E	413	VAL	2.2
2	F	335	LYS	2.2
2	F	333	LEU	2.2
1	B	238	LYS	2.2
2	D	448	ASP	2.2
1	B	273	PHE	2.1
2	E	394	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	209	MET	2.1
2	F	307	PRO	2.1
2	E	194	PHE	2.1
2	D	400	ILE	2.1
1	B	279	PRO	2.1
1	A	578	LYS	2.1
2	E	376	TYR	2.1
2	E	339	SER	2.1
2	F	133	SER	2.0
2	F	413	VAL	2.0
2	F	322	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

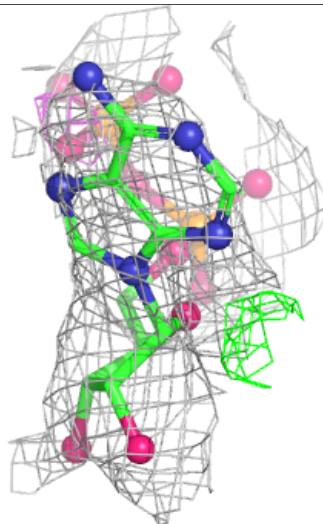
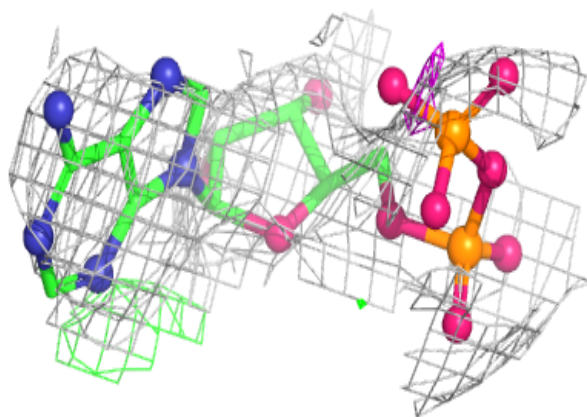
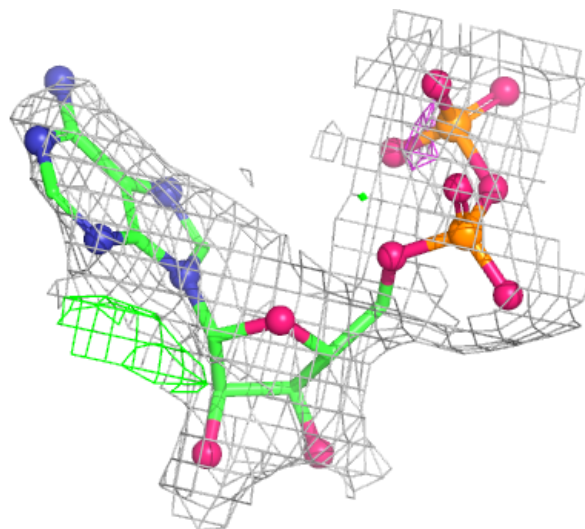
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	E	600	27/27	0.77	0.13	65,86,111,120	0
4	MG	E	601	1/1	0.85	0.08	91,91,91,91	0
3	ADP	D	600	27/27	0.87	0.11	44,52,67,71	0
4	MG	C	601	1/1	0.88	0.26	39,39,39,39	0
4	MG	B	601	1/1	0.88	0.15	58,58,58,58	0
4	MG	A	601	1/1	0.89	0.20	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.

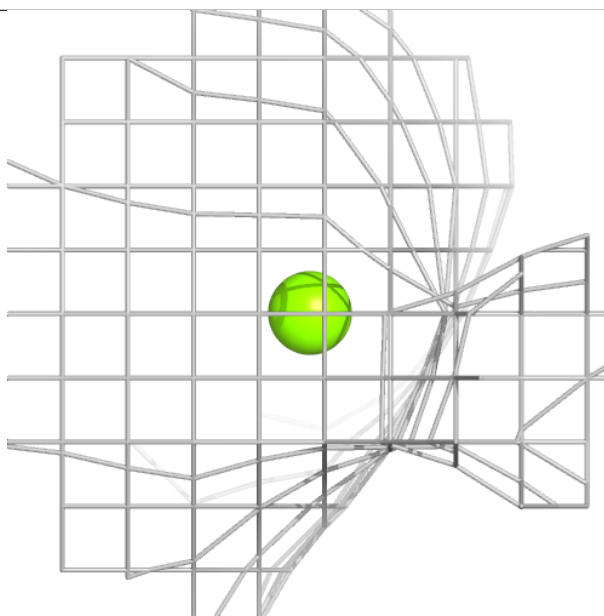
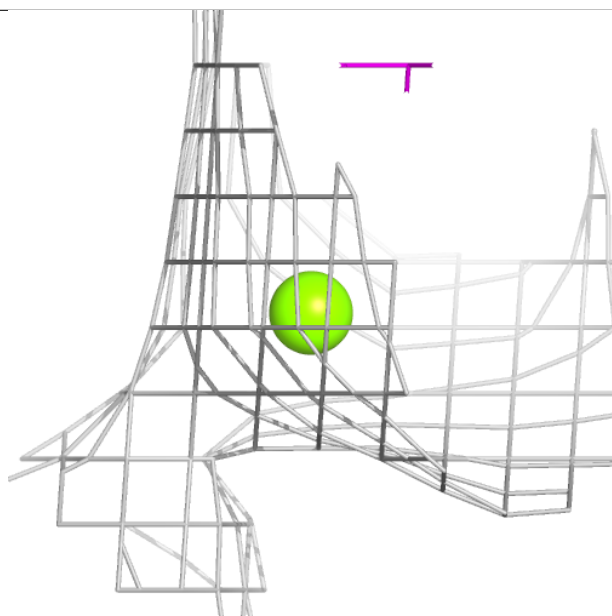
Electron density around ADP E 600:

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



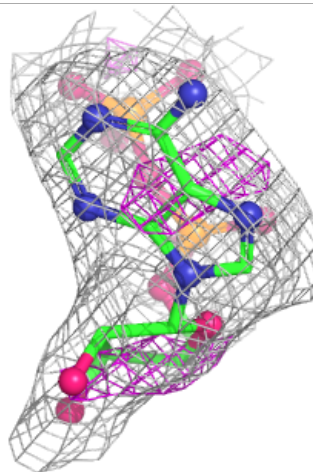
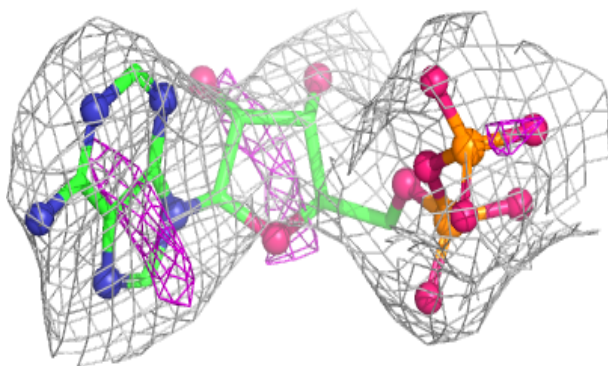
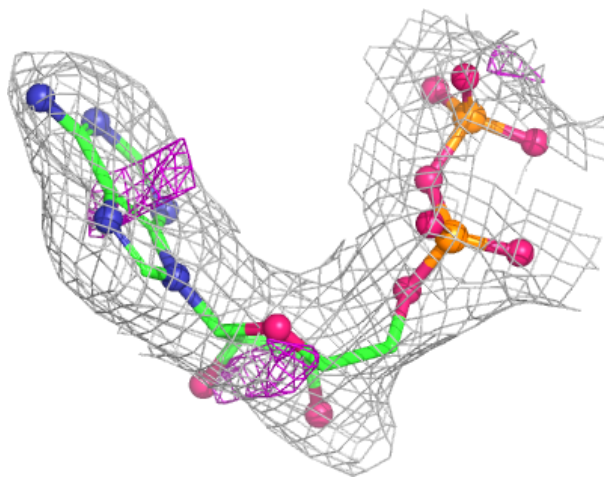
Electron density around MG E 601:

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and green (positive)



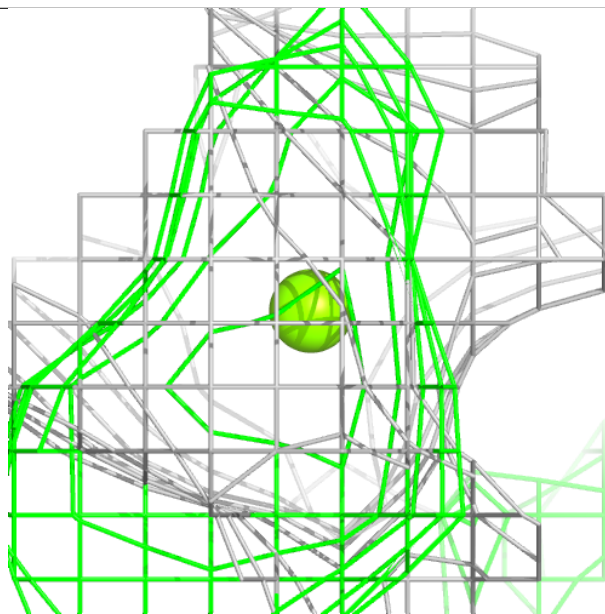
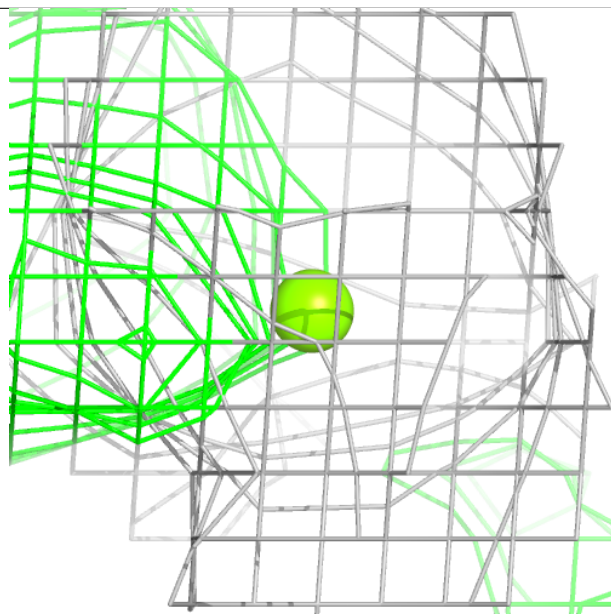
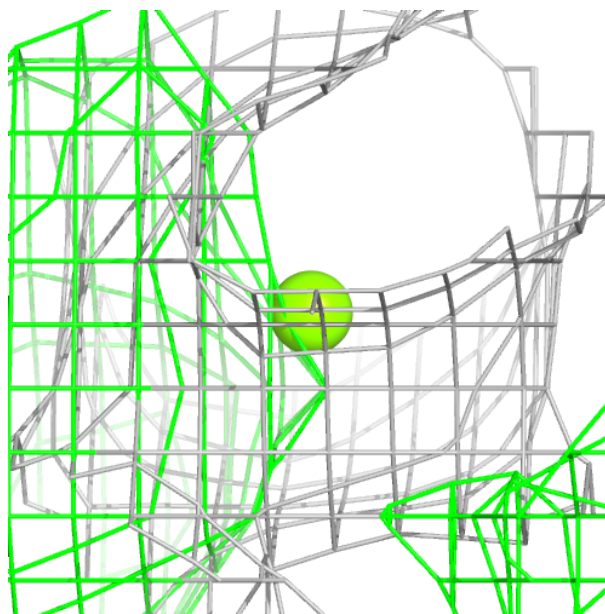
Electron density around ADP D 600:

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and green (positive)



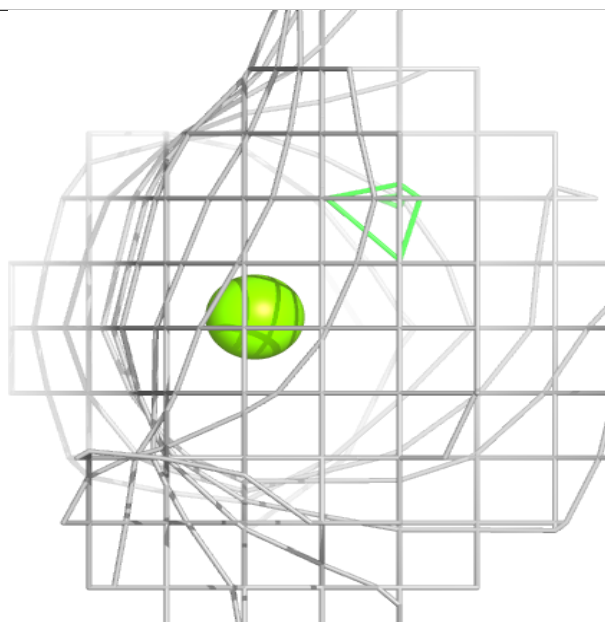
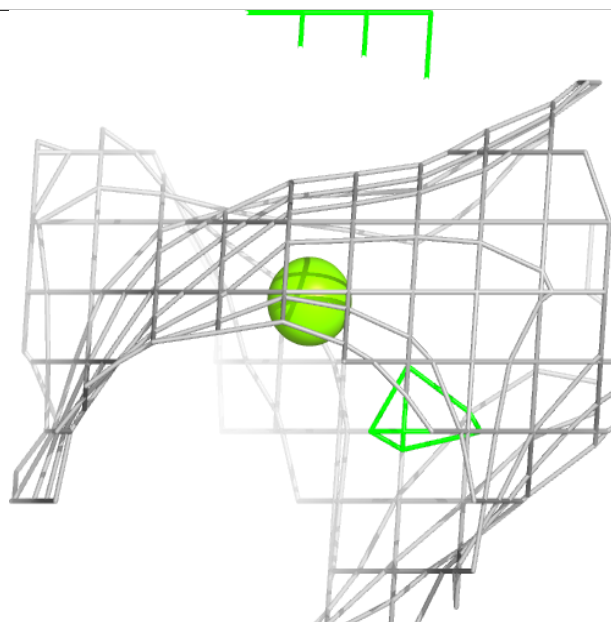
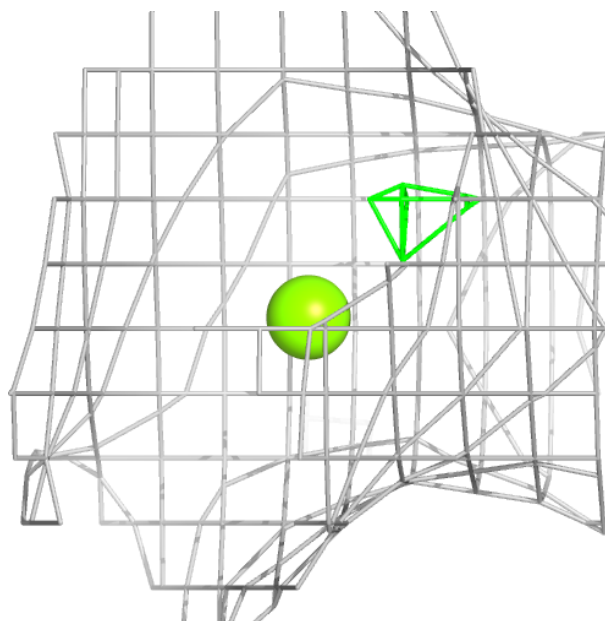
Electron density around MG C 601:

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and green (positive)



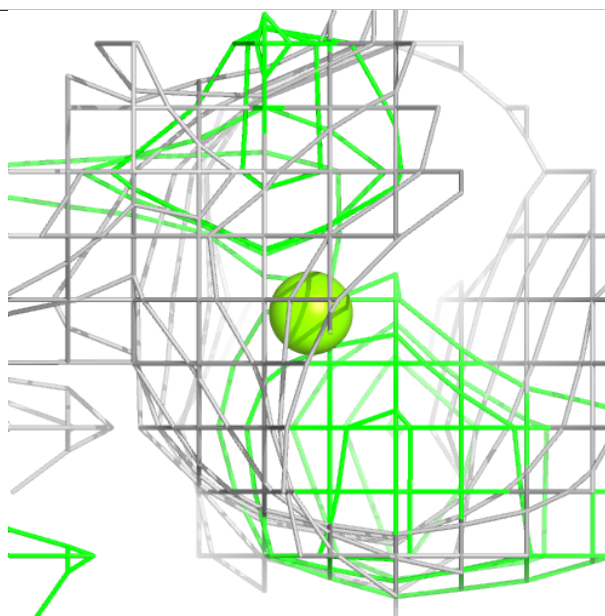
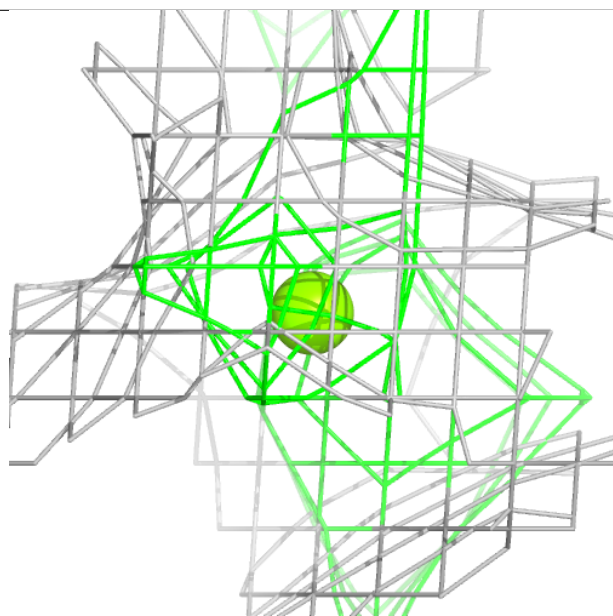
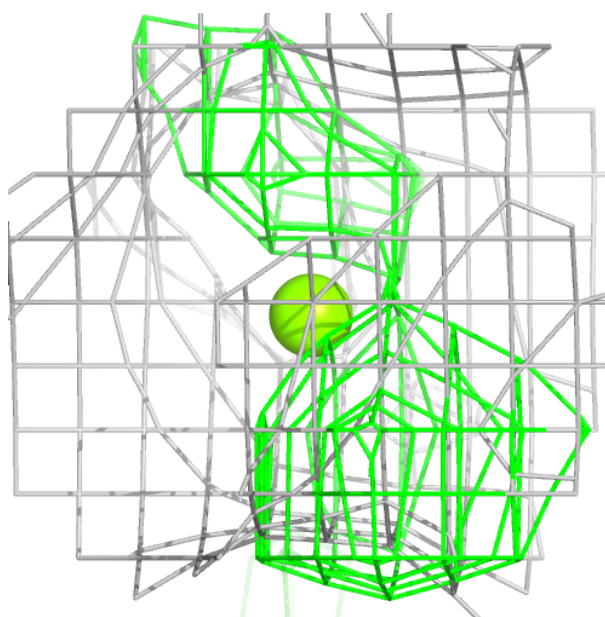
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and green (positive)



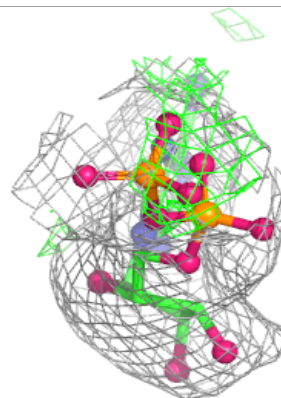
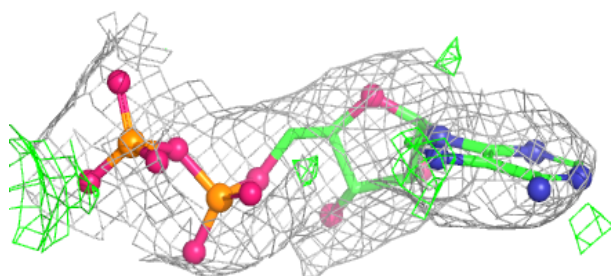
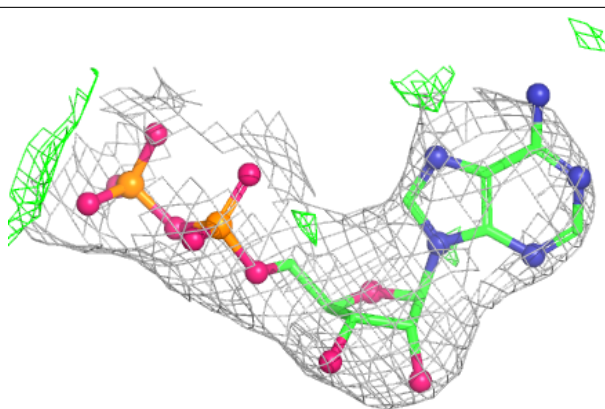
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and green (positive)

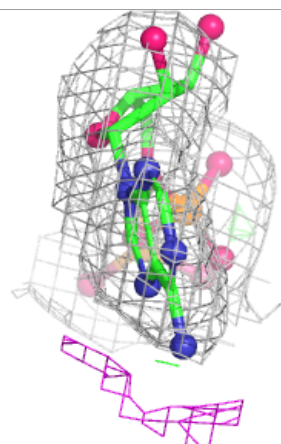
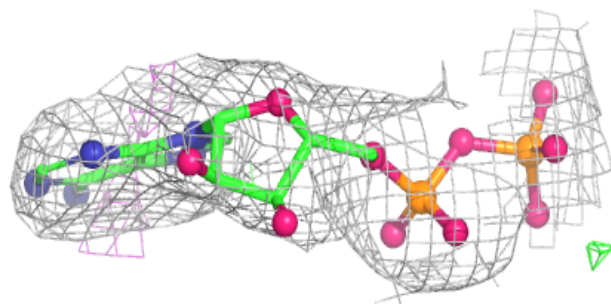


Electron density around ADP C 600:

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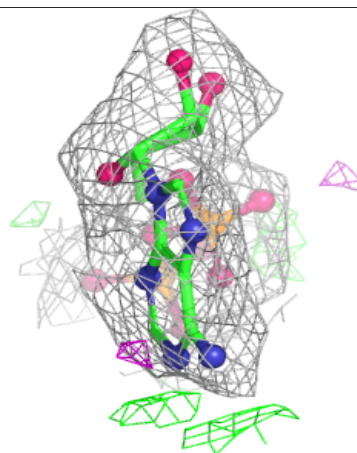
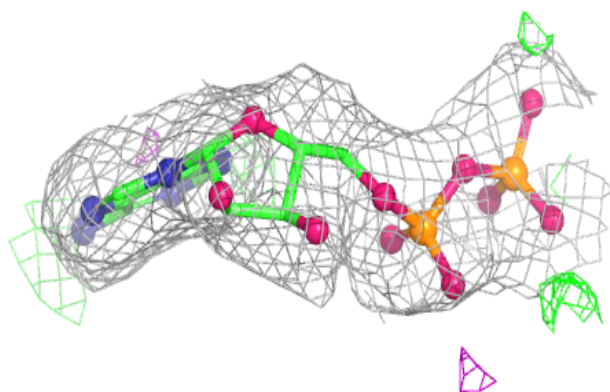
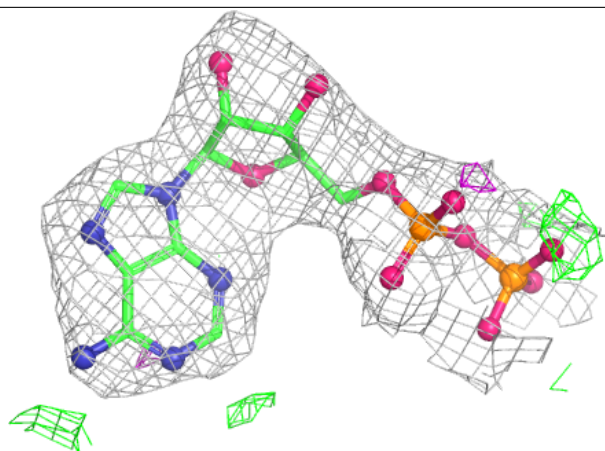
**Electron density around ADP B 600:**

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



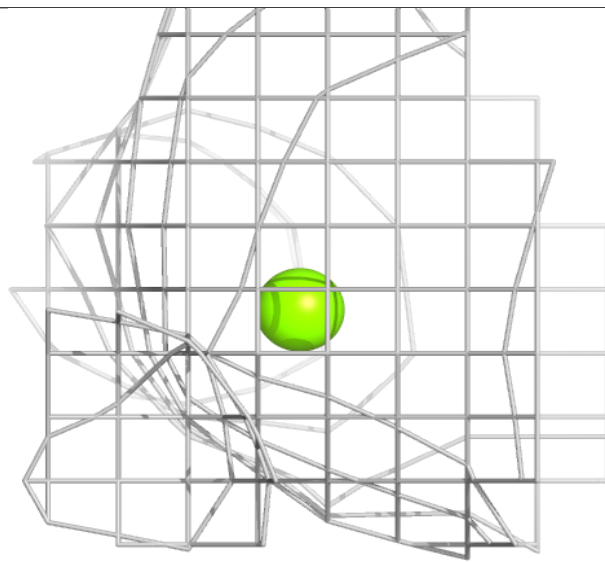
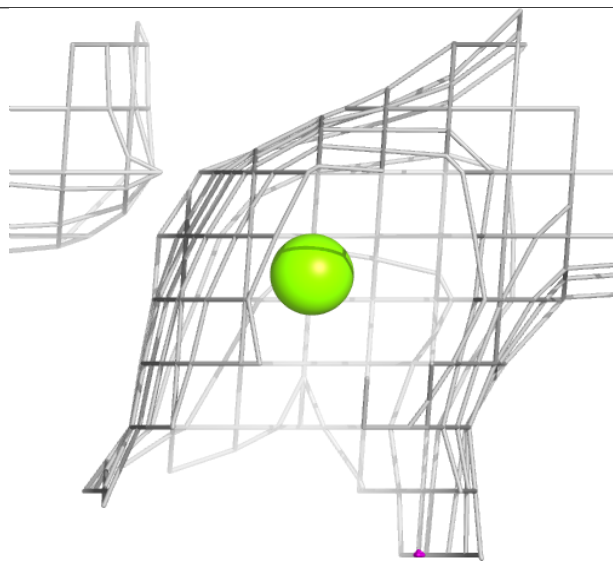
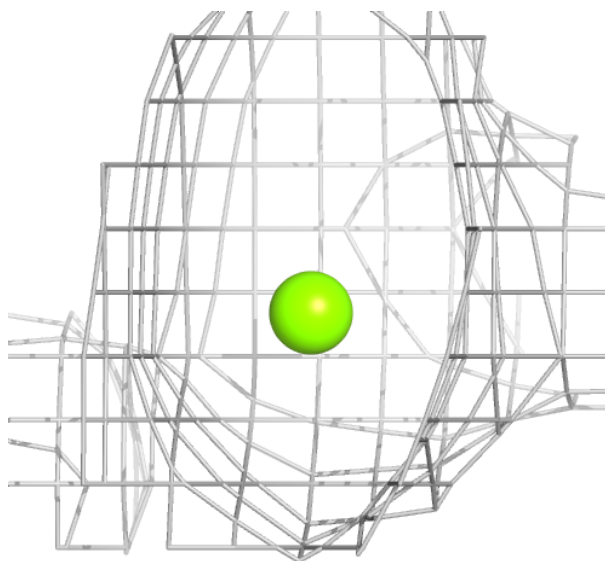
Electron density around ADP A 600:

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and green (positive)



Electron density around MG D 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.