



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2021 – 04:10 PM JST

PDB ID : 7DQE  
Title : Crystal structure of the ADP-bound mutant A(S23C)3B(N64C)3 complex from enterococcus hirae V-ATPase  
Authors : Maruyama, S.; Nakamoto, K.; Suzuki, K.; Mizutani, K.; Imai, F.L.; Ishizuka-Katsura, Y.; Shirouzu, M.; Murata, T.  
Deposited on : 2020-12-23  
Resolution : 2.69 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.25
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.25

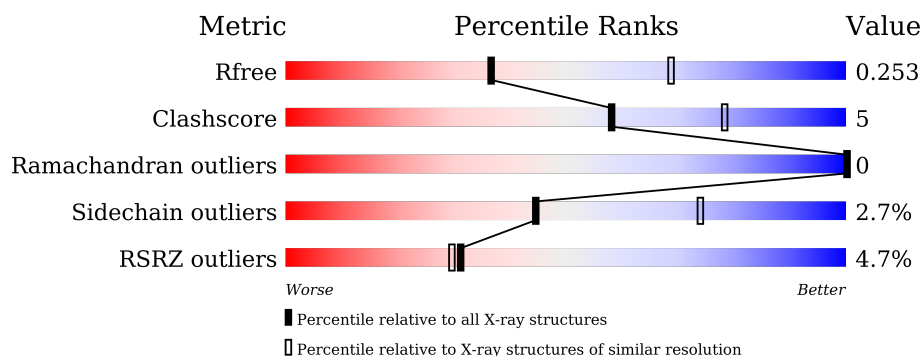
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	600	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	B	600	<div> <div>4%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	C	600	<div> <div>5%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
2	D	465	<div> <div>4%</div> <div>82%</div> <div>13%</div> <div>..</div> </div>
2	E	465	<div> <div>12%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	F	465	<div> <div>%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24093 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	584	Total	C	N	O	S	0	0	0
			4511	2837	756	892	26			
1	B	584	Total	C	N	O	S	0	0	0
			4520	2843	758	892	27			
1	C	584	Total	C	N	O	S	0	0	0
			4450	2793	749	882	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
A	23	CYS	SER	engineered mutation	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	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
B	23	CYS	SER	engineered mutation	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636
C	-3	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	CYS	SER	engineered mutation	UNP Q08636

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	446	Total	C	N	O	S	0	0	0
			3402	2154	589	644	15			
2	E	454	Total	C	N	O	S	0	0	0
			3398	2146	589	648	15			
2	F	454	Total	C	N	O	S	0	0	0
			3532	2241	604	671	16			

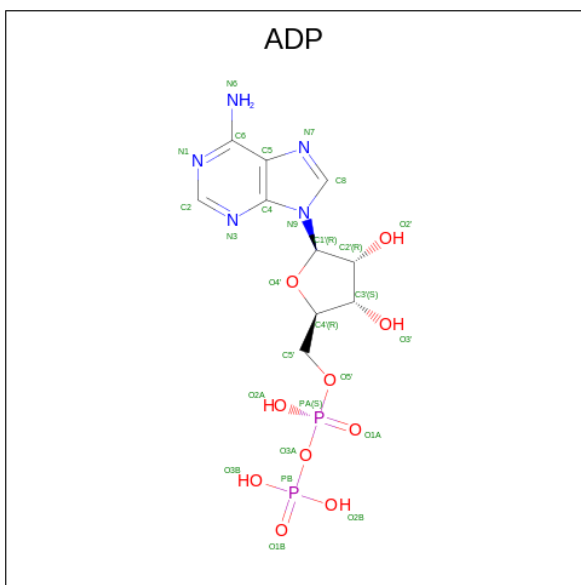
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
D	64	CYS	ASN	engineered mutation	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
E	64	CYS	ASN	engineered mutation	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637
F	64	CYS	ASN	engineered mutation	UNP Q08637

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

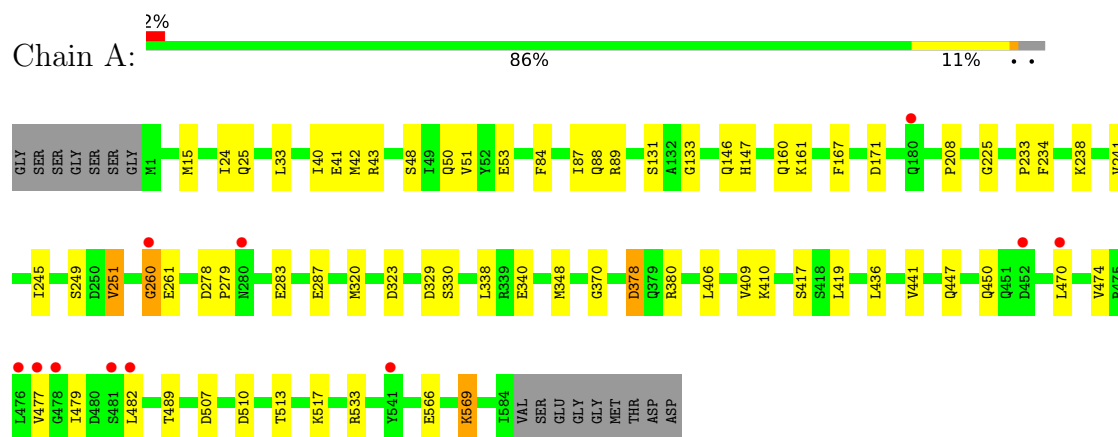
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total	O	0	0
			26	26		
6	B	38	Total	O	0	0
			38	38		
6	C	50	Total	O	0	0
			50	50		
6	D	18	Total	O	0	0
			18	18		
6	E	23	Total	O	0	0
			23	23		
6	F	36	Total	O	0	0
			36	36		

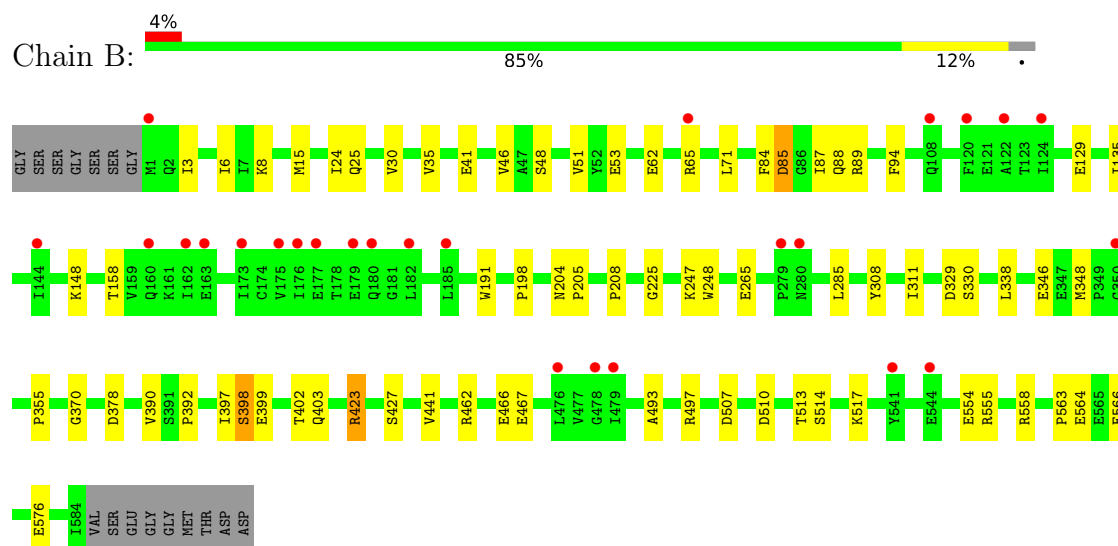
### 3 Residue-property plots [i](#)

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.

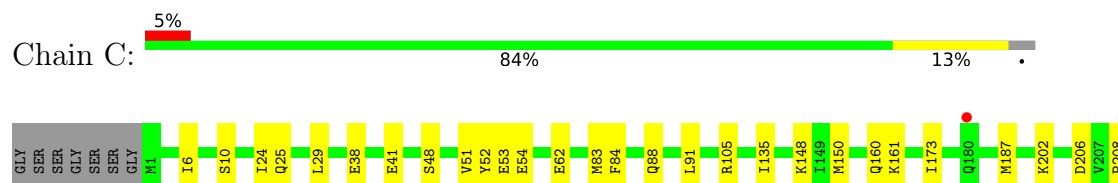
- Molecule 1: V-type sodium ATPase catalytic subunit A

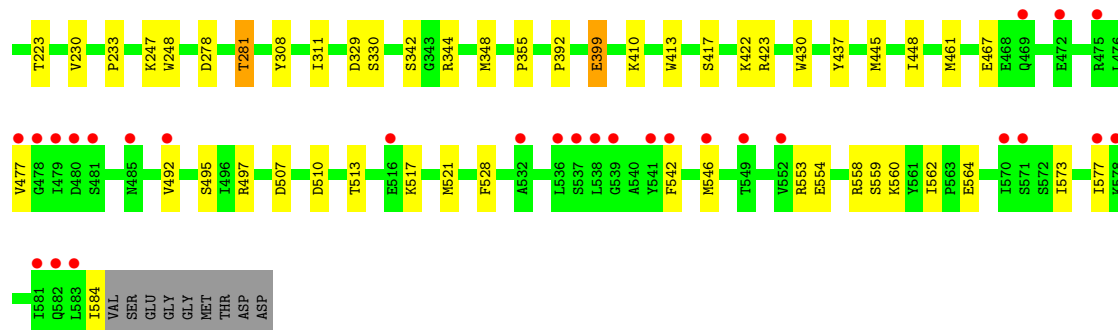


- Molecule 1: V-type sodium ATPase catalytic subunit A

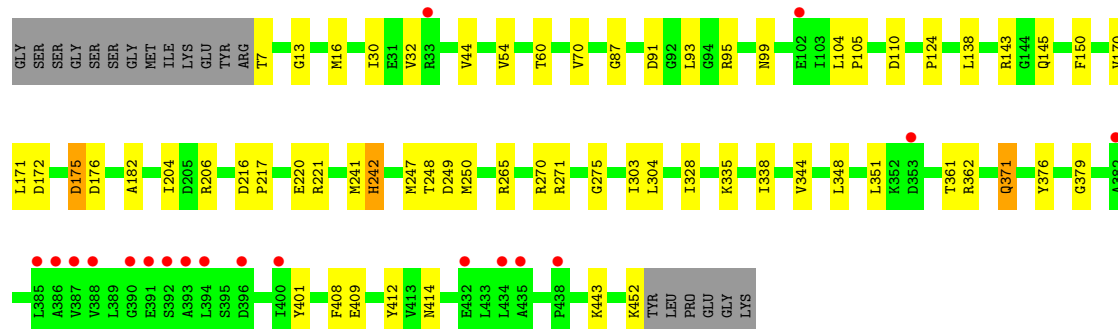
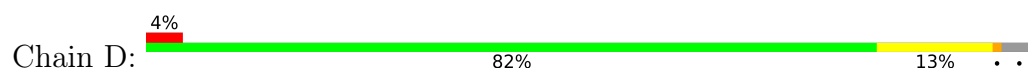


- Molecule 1: V-type sodium ATPase catalytic subunit A

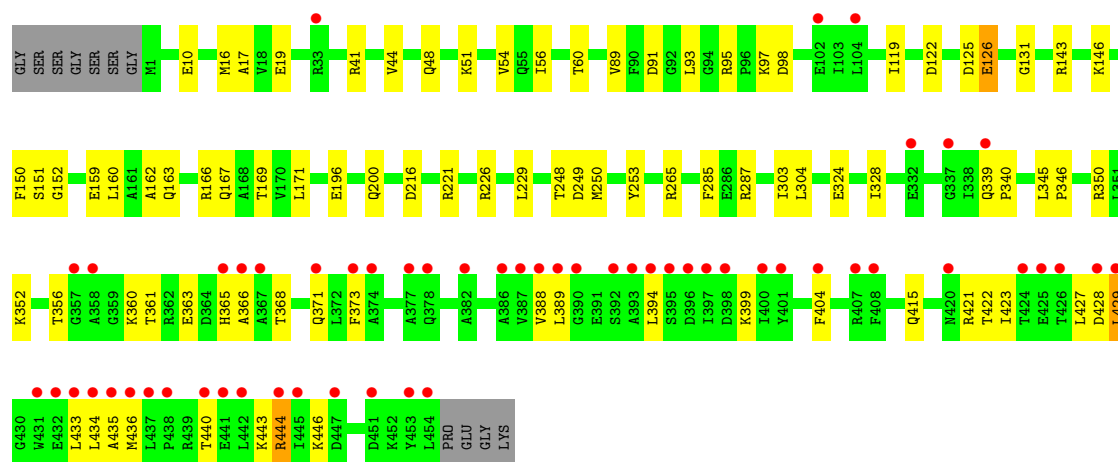
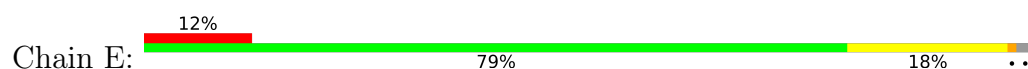




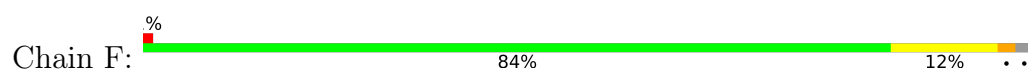
- Molecule 2: V-type sodium ATPase subunit B



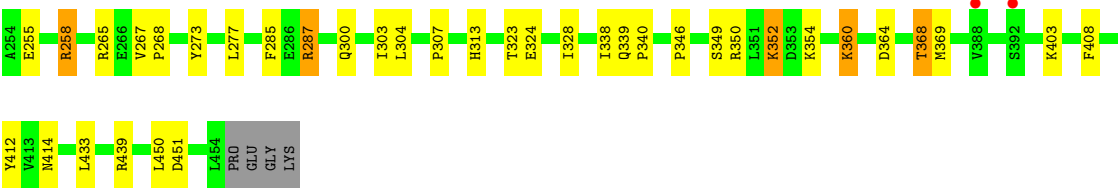
- Molecule 2: V-type sodium ATPase subunit B



- Molecule 2: V-type sodium ATPase subunit B







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.03Å 121.09Å 231.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 2.69 48.77 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.63-2.69) 98.7 (48.77-2.69)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.226 , 0.253 0.228 , 0.253	Depositor DCC
$R_{free}$ test set	4793 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, SO4

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	0.21	0/4587	0.39	1/6210 (0.0%)
1	B	0.21	0/4596	0.37	0/6222
1	C	0.20	0/4525	0.38	0/6136
2	D	0.20	0/3462	0.38	0/4690
2	E	0.22	0/3454	0.41	0/4686
2	F	0.21	0/3594	0.38	0/4862
All	All	0.21	0/24218	0.38	1/32806 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	GLY	N-CA-C	-5.07	100.42	113.10

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	4511	0	4447	39	0
1	B	4520	0	4468	39	0
1	C	4450	0	4321	42	0
2	D	3402	0	3340	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3398	0	3293	45	0
2	F	3532	0	3535	36	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	2	0
4	C	27	0	12	0	0
5	A	5	0	0	1	0
6	A	26	0	0	0	0
6	B	38	0	0	2	0
6	C	50	0	0	0	0
6	D	18	0	0	0	0
6	E	23	0	0	0	0
6	F	36	0	0	0	0
All	All	24093	0	23440	227	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 5.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:MET:HA	1:C:553:ARG:HH22	1.48	0.79
2:E:328:ILE:HG13	2:E:346:PRO:HB2	1.70	0.73
1:C:24:ILE:HG22	1:C:25:GLN:HG2	1.70	0.72
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.73	0.71
2:E:371:GLN:HG3	2:E:444:ARG:HG2	1.72	0.70
1:B:129:GLU:HG2	1:B:158:THR:HG22	1.73	0.70
1:C:467:GLU:OE2	1:C:497:ARG:NH1	2.26	0.69
1:B:24:ILE:HG22	1:B:25:GLN:HG2	1.74	0.69
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.74	0.68
2:E:388:VAL:HG13	2:E:389:LEU:HD12	1.75	0.68
2:E:126:GLU:HG3	2:E:143:ARG:HB2	1.75	0.67
2:F:354:LYS:O	2:F:360:LYS:NZ	2.27	0.67
1:C:54:GLU:HB2	1:C:105:ARG:HD3	1.77	0.66
1:A:260:GLY:HA3	1:A:261:GLU:HG2	1.78	0.65
1:C:51:VAL:HG12	1:C:53:GLU:H	1.62	0.64
1:C:348:MET:HG3	2:D:265:ARG:HA	1.78	0.64
1:A:133:GLY:O	1:A:380:ARG:NH2	2.30	0.64
2:F:250:MET:HB2	2:F:304:LEU:HB3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:HG12	1:B:53:GLU:H	1.63	0.62
1:B:346:GLU:O	2:F:265:ARG:NH1	2.33	0.62
2:D:248:THR:HB	2:D:303:ILE:HB	1.82	0.61
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.83	0.61
1:C:546:MET:SD	1:C:553:ARG:NH2	2.73	0.61
1:B:467:GLU:OE2	1:B:497:ARG:NH1	2.34	0.61
2:D:175:ASP:OD2	2:D:175:ASP:N	2.35	0.60
2:E:423:ILE:O	2:E:427:LEU:HG	2.02	0.59
1:A:283:GLU:HG3	1:A:287:GLU:HG3	1.85	0.59
1:C:233:PRO:HG3	1:C:417:SER:HB2	1.83	0.59
2:F:10:GLU:HG2	2:F:17:ALA:HB3	1.85	0.59
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.83	0.59
1:A:43:ARG:HG2	2:E:10:GLU:HG3	1.85	0.59
2:F:248:THR:HB	2:F:303:ILE:HB	1.84	0.58
1:B:208:PRO:HG3	1:B:441:VAL:HG22	1.86	0.57
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.86	0.57
1:C:513:THR:HG23	1:C:517:LYS:HD3	1.87	0.57
2:F:44:VAL:HA	2:F:54:VAL:HG12	1.86	0.57
2:E:444:ARG:HA	2:E:444:ARG:NE	2.20	0.56
1:A:410:LYS:HB3	1:A:436:LEU:HB2	1.86	0.56
2:D:124:PRO:HG2	2:D:351:LEU:HD13	1.88	0.56
2:F:364:ASP:O	2:F:368:THR:OG1	2.22	0.56
2:E:226:ARG:NH2	2:E:253:TYR:OH	2.38	0.56
2:D:216:ASP:O	2:D:221:ARG:NH1	2.39	0.55
1:C:38:GLU:OE2	1:C:52:TYR:OH	2.24	0.55
2:D:13:GLY:O	2:D:60:THR:OG1	2.21	0.55
2:E:324:GLU:HA	2:E:350:ARG:HD2	1.89	0.54
2:D:32:VAL:HG22	2:D:70:VAL:HG22	1.90	0.54
2:D:143:ARG:HG3	2:D:242:HIS:CE1	2.43	0.54
1:A:474:VAL:HG22	1:A:482:LEU:HD21	1.88	0.54
2:E:10:GLU:HB3	2:E:17:ALA:HB3	1.89	0.54
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.90	0.54
2:E:363:GLU:HA	2:E:366:ALA:HB3	1.90	0.54
1:C:278:ASP:OD1	1:C:281:THR:OG1	2.27	0.53
2:E:19:GLU:HG2	2:E:51:LYS:HG2	1.89	0.53
1:B:247:LYS:HB2	1:B:285:LEU:HD21	1.90	0.53
1:C:6:ILE:HD12	1:C:62:GLU:HB2	1.91	0.53
2:D:376:TYR:OH	2:D:409:GLU:OE2	2.20	0.53
2:F:138:LEU:HD22	2:F:369:MET:HG3	1.91	0.53
2:F:412:TYR:HB2	2:F:433:LEU:HD11	1.92	0.52
1:C:230:VAL:HG22	1:C:413:TRP:HE3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASP:HB2	1:B:89:ARG:HB2	1.91	0.52
2:E:56:ILE:HD13	2:E:60:THR:HG22	1.92	0.52
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.91	0.51
1:B:3:ILE:HD12	1:B:65:ARG:HG2	1.92	0.51
2:E:89:VAL:HB	2:E:98:ASP:HB3	1.91	0.51
1:B:8:LYS:HD3	2:E:48:GLN:HB2	1.92	0.51
1:C:10:SER:OG	1:C:344:ARG:NH1	2.45	0.50
2:E:91:ASP:OD1	2:E:95:ARG:NH2	2.44	0.50
2:F:233:GLU:OE1	2:F:287:ARG:NH2	2.44	0.50
2:E:44:VAL:HA	2:E:54:VAL:HG12	1.92	0.50
1:A:87:ILE:HG13	1:A:89:ARG:HG3	1.94	0.49
1:A:160:GLN:HG2	1:A:161:LYS:HG3	1.94	0.49
2:E:131:GLY:HA3	2:E:167:GLN:HE21	1.77	0.49
1:C:559:SER:HA	1:C:562:ILE:HG13	1.94	0.49
1:B:555:ARG:NH1	1:B:576:GLU:OE2	2.43	0.49
2:E:216:ASP:O	2:E:221:ARG:NH1	2.46	0.49
1:A:208:PRO:HG3	1:A:441:VAL:HG22	1.94	0.48
1:B:87:ILE:HD11	1:B:89:ARG:HH11	1.78	0.48
2:D:170:VAL:HG11	2:D:242:HIS:CD2	2.48	0.48
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.94	0.48
2:F:176:ASP:OD1	2:F:176:ASP:N	2.45	0.48
1:B:8:LYS:HB3	1:B:15:MET:HB2	1.95	0.48
1:B:338:LEU:HB3	1:B:355:PRO:HG3	1.96	0.48
2:E:360:LYS:HA	2:E:361:THR:HA	1.54	0.48
2:E:151:SER:OG	2:E:152:GLY:N	2.47	0.48
2:F:89:VAL:HG22	2:F:209:MET:HG3	1.95	0.48
2:E:352:LYS:O	2:E:356:THR:OG1	2.25	0.48
2:E:394:LEU:O	2:E:399:LYS:N	2.44	0.48
2:F:183:ALA:HB3	2:F:211:MET:HA	1.94	0.48
4:B:602:ADP:O1A	6:B:701:HOH:O	2.20	0.48
2:D:379:GLY:HA2	2:D:401:TYR:HB3	1.94	0.48
1:A:329:ASP:HA	1:A:330:SER:HA	1.56	0.48
1:A:513:THR:HG23	1:A:517:LYS:HD3	1.96	0.48
2:F:338:ILE:HG23	2:F:414:ASN:HB2	1.96	0.48
1:A:147:HIS:HA	1:A:320:MET:HE1	1.95	0.47
2:D:408:PHE:O	2:D:412:TYR:HB3	2.14	0.47
2:E:229:LEU:HD13	2:E:287:ARG:HG3	1.96	0.47
1:A:489:THR:HG23	1:A:533:ARG:HH12	1.79	0.47
1:C:342:SER:HB2	1:C:355:PRO:HG3	1.97	0.47
1:C:135:ILE:HD12	1:C:148:LYS:HB3	1.96	0.47
2:F:1:MET:HB3	2:F:2:ILE:H	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:182:ALA:HB3	2:F:247:MET:HG2	1.97	0.47
2:D:145:GLN:HG3	2:D:351:LEU:HD12	1.96	0.47
1:A:238:LYS:NZ	5:A:603:SO4:O3	2.48	0.47
1:B:225:GLY:O	1:B:370:GLY:HA2	2.15	0.46
1:C:507:ASP:HB3	1:C:510:ASP:HB3	1.98	0.46
1:A:245:ILE:O	1:A:249:SER:OG	2.29	0.46
1:B:513:THR:HG23	1:B:517:LYS:HD3	1.96	0.46
1:A:167:PHE:HB3	1:A:171:ASP:HB2	1.97	0.46
2:D:270:ARG:HG2	2:D:271:ARG:HG2	1.98	0.46
1:A:447:GLN:O	1:A:450:GLN:NE2	2.45	0.46
1:C:445:MET:HA	1:C:448:ILE:HG22	1.97	0.46
2:E:435:ALA:HA	2:E:436:MET:HA	1.51	0.46
1:B:329:ASP:HA	1:B:330:SER:HA	1.59	0.46
1:C:528:PHE:HA	1:C:577:ILE:HD11	1.97	0.46
2:D:30:ILE:HD13	2:D:54:VAL:HG21	1.96	0.46
4:B:602:ADP:O1A	2:E:350:ARG:NH1	2.48	0.46
1:C:517:LYS:HG2	1:C:521:MET:HE2	1.98	0.46
2:E:150:PHE:HB2	2:E:328:ILE:HD13	1.97	0.46
2:E:93:LEU:HD12	2:E:95:ARG:HH12	1.81	0.46
2:F:439:ARG:NH2	2:F:451:ASP:OD1	2.48	0.46
1:B:265:GLU:OE2	6:B:701:HOH:O	2.21	0.46
2:D:176:ASP:HB3	2:D:241:MET:HA	1.98	0.46
2:E:365:HIS:CB	2:E:427:LEU:HD22	2.45	0.46
1:A:348:MET:HG3	2:E:265:ARG:HA	1.98	0.45
1:C:392:PRO:HB3	1:C:399:GLU:HG2	1.98	0.45
2:F:307:PRO:HG2	2:F:313:HIS:CE1	2.51	0.45
1:C:173:ILE:HD13	1:C:187:MET:HG3	1.99	0.45
2:D:217:PRO:HG2	2:D:220:GLU:HG3	1.99	0.45
2:E:345:LEU:HB2	2:E:346:PRO:HD3	1.99	0.45
1:B:423:ARG:HD3	2:E:373:PHE:HB3	1.99	0.45
1:C:461:MET:HE2	2:D:335:LYS:HD2	1.98	0.45
2:E:250:MET:HB2	2:E:304:LEU:HB3	1.99	0.45
2:F:226:ARG:NH2	2:F:253:TYR:OH	2.50	0.44
2:D:44:VAL:HA	2:D:54:VAL:HG12	1.99	0.44
2:F:150:PHE:HB2	2:F:328:ILE:HG12	1.99	0.44
1:B:507:ASP:HB3	1:B:510:ASP:HB3	1.99	0.44
1:C:160:GLN:HG2	1:C:161:LYS:HG3	1.99	0.44
2:D:87:GLY:HA2	2:D:204:ILE:O	2.17	0.44
2:E:163:GLN:O	2:E:167:GLN:HG2	2.18	0.44
2:E:429:LEU:O	2:E:433:LEU:N	2.51	0.44
1:B:247:LYS:HG3	1:B:248:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLU:HB3	1:A:569:LYS:HG3	1.99	0.44
1:A:225:GLY:O	1:A:370:GLY:HA2	2.18	0.44
1:C:247:LYS:HG3	1:C:248:TRP:CD1	2.53	0.44
2:F:146:LYS:HD3	2:F:285:PHE:O	2.18	0.44
1:A:479:ILE:HD12	1:A:482:LEU:HD23	2.00	0.43
1:A:233:PRO:HG2	1:A:417:SER:HB3	1.99	0.43
2:D:250:MET:HB2	2:D:304:LEU:HB3	2.00	0.43
2:E:146:LYS:HD3	2:E:285:PHE:O	2.18	0.43
2:E:196:GLU:OE2	2:E:200:GLN:NE2	2.50	0.43
1:B:204:ASN:HA	1:B:205:PRO:HD3	1.85	0.43
2:E:162:ALA:O	2:E:166:ARG:HG3	2.18	0.43
2:E:91:ASP:N	2:E:95:ARG:O	2.51	0.43
1:B:89:ARG:HH21	1:B:94:PHE:HE1	1.67	0.43
1:B:135:ILE:HD12	1:B:148:LYS:HB3	2.00	0.43
2:F:146:LYS:HD2	2:F:323:THR:HA	2.00	0.43
2:F:273:TYR:HB3	2:F:277:LEU:HD22	2.01	0.43
1:B:398:SER:HA	1:B:403:GLN:HE21	1.84	0.43
1:C:329:ASP:HA	1:C:330:SER:HA	1.70	0.43
1:C:422:LYS:HB3	1:C:422:LYS:HE2	1.61	0.43
1:A:241:VAL:O	1:A:245:ILE:HG12	2.18	0.43
2:F:287:ARG:O	2:F:300:GLN:NE2	2.51	0.43
1:A:40:ILE:HD13	1:A:50:GLN:HG2	2.01	0.43
1:B:462:ARG:NH2	1:B:466:GLU:OE1	2.49	0.43
1:C:202:LYS:HE2	1:C:202:LYS:HB3	1.91	0.43
2:F:324:GLU:HA	2:F:350:ARG:HD2	2.01	0.43
1:A:489:THR:HG22	1:A:533:ARG:HH22	1.83	0.43
2:F:328:ILE:HD12	2:F:346:PRO:HB2	2.01	0.43
1:B:378:ASP:OD1	1:B:378:ASP:N	2.50	0.42
2:F:408:PHE:O	2:F:412:TYR:HB3	2.19	0.42
1:A:51:VAL:HG12	1:A:53:GLU:H	1.83	0.42
1:C:492:VAL:O	1:C:495:SER:OG	2.30	0.42
1:A:569:LYS:HE3	1:A:569:LYS:HB3	1.68	0.42
1:B:6:ILE:HD12	1:B:62:GLU:HB2	2.01	0.42
1:C:135:ILE:HD13	1:C:150:MET:HG2	2.01	0.42
2:D:91:ASP:N	2:D:95:ARG:O	2.52	0.42
2:F:349:SER:O	2:F:352:LYS:HG2	2.19	0.42
2:F:450:LEU:HD12	2:F:450:LEU:HA	1.92	0.42
1:A:470:LEU:O	1:A:474:VAL:HG23	2.19	0.42
1:B:493:ALA:O	1:B:497:ARG:HG3	2.19	0.42
2:D:150:PHE:HB2	2:D:328:ILE:HD13	2.00	0.42
2:F:255:GLU:OE1	2:F:258:ARG:NH1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:403:LYS:HD2	2:F:403:LYS:HA	1.89	0.42
1:A:378:ASP:OD1	1:A:378:ASP:N	2.52	0.42
1:B:191:TRP:CZ2	1:B:198:PRO:HD3	2.54	0.42
1:C:573:ILE:O	1:C:577:ILE:HG22	2.19	0.42
2:F:146:LYS:HE2	2:F:324:GLU:HG3	2.01	0.42
2:D:371:GLN:OE1	2:D:443:LYS:N	2.52	0.42
1:A:161:LYS:HE2	1:A:161:LYS:HB3	1.83	0.42
1:C:542:PHE:O	1:C:546:MET:HG2	2.19	0.42
2:D:338:ILE:HG23	2:D:414:ASN:HB2	2.01	0.42
2:E:248:THR:HB	2:E:303:ILE:HB	2.00	0.42
2:F:126:GLU:OE1	2:F:143:ARG:HD2	2.20	0.42
1:B:397:ILE:HB	1:B:402:THR:HG21	2.01	0.41
1:B:554:GLU:OE2	1:B:558:ARG:NH2	2.53	0.41
1:B:563:PRO:HB2	1:B:566:GLU:HG2	2.02	0.41
2:F:339:GLN:HA	2:F:340:PRO:HA	1.88	0.41
1:B:390:VAL:O	1:B:392:PRO:HD3	2.20	0.41
1:A:251:VAL:HG22	1:A:323:ASP:O	2.19	0.41
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.91	0.41
2:F:267:VAL:HA	2:F:268:PRO:HD3	1.86	0.41
1:C:83:MET:HG2	1:C:91:LEU:HD12	2.01	0.41
1:C:410:LYS:HD3	1:C:437:TYR:OH	2.20	0.41
2:E:415:GLN:HA	2:E:421:ARG:CZ	2.49	0.41
1:A:340:GLU:HG3	2:D:275:GLY:O	2.21	0.41
1:A:507:ASP:HB3	1:A:510:ASP:HB3	2.02	0.41
1:C:208:PRO:HA	1:C:223:THR:HA	2.02	0.41
2:F:29:LEU:HD13	2:F:77:LEU:HD13	2.02	0.41
1:A:406:LEU:HA	1:A:409:VAL:HG22	2.02	0.41
1:B:308:TYR:HA	1:B:311:ILE:HG22	2.02	0.41
2:D:104:LEU:HA	2:D:105:PRO:HD3	1.84	0.41
1:C:308:TYR:HA	1:C:311:ILE:HG22	2.02	0.41
1:A:234:PHE:HD1	2:D:348:LEU:HD22	1.86	0.41
1:B:30:VAL:HB	1:B:35:VAL:HG23	2.03	0.41
1:C:206:ASP:OD1	1:C:206:ASP:N	2.53	0.41
2:D:171:LEU:HA	2:D:172:ASP:HA	1.67	0.41
2:E:446:LYS:HE3	2:E:446:LYS:HB2	1.91	0.41
1:B:514:SER:OG	1:B:564:GLU:OE2	2.26	0.40
1:C:517:LYS:HB2	1:C:564:GLU:OE2	2.22	0.40
2:D:30:ILE:HG21	2:D:54:VAL:HG11	2.03	0.40
2:E:248:THR:HA	2:E:249:ASP:HA	1.80	0.40
2:D:361:THR:OG1	2:D:362:ARG:N	2.54	0.40
2:D:138:LEU:HD12	2:D:344:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:TRP:CH2	1:C:497:ARG:HD2	2.56	0.40
2:D:249:ASP:OD1	2:D:304:LEU:HA	2.21	0.40
2:E:160:LEU:HD13	2:E:340:PRO:HB3	2.03	0.40
2:E:159:GLU:OE1	2:E:159:GLU:N	2.53	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	582/600 (97%)	573 (98%)	9 (2%)	0	100	100
1	B	582/600 (97%)	568 (98%)	14 (2%)	0	100	100
1	C	582/600 (97%)	568 (98%)	14 (2%)	0	100	100
2	D	444/465 (96%)	430 (97%)	14 (3%)	0	100	100
2	E	452/465 (97%)	433 (96%)	19 (4%)	0	100	100
2	F	452/465 (97%)	438 (97%)	14 (3%)	0	100	100
All	All	3094/3195 (97%)	3010 (97%)	84 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	490/511 (96%)	479 (98%)	11 (2%)	52	79
1	B	493/511 (96%)	485 (98%)	8 (2%)	62	85
1	C	474/511 (93%)	465 (98%)	9 (2%)	57	82
2	D	345/387 (89%)	335 (97%)	10 (3%)	42	71
2	E	336/387 (87%)	317 (94%)	19 (6%)	20	44
2	F	371/387 (96%)	361 (97%)	10 (3%)	44	74
All	All	2509/2694 (93%)	2442 (97%)	67 (3%)	44	74

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	33	LEU
1	A	42	MET
1	A	131	SER
1	A	146	GLN
1	A	251	VAL
1	A	338	LEU
1	A	378	ASP
1	A	419	LEU
1	A	477	VAL
1	A	569	LYS
1	B	46	VAL
1	B	71	LEU
1	B	85	ASP
1	B	348	MET
1	B	398	SER
1	B	399	GLU
1	B	423	ARG
1	B	427	SER
1	C	29	LEU
1	C	281	THR
1	C	399	GLU
1	C	423	ARG
1	C	477	VAL
1	C	554	GLU
1	C	558	ARG
1	C	560	LYS
1	C	584	ILE
2	D	7	THR
2	D	16	MET

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Mol	Chain	Res	Type
2	D	93	LEU
2	D	99	ASN
2	D	110	ASP
2	D	175	ASP
2	D	206	ARG
2	D	242	HIS
2	D	371	GLN
2	D	452	LYS
2	E	16	MET
2	E	41	ARG
2	E	97	LYS
2	E	119	ILE
2	E	122	ASP
2	E	125	ASP
2	E	126	GLU
2	E	169	THR
2	E	171	LEU
2	E	339	GLN
2	E	368	THR
2	E	404	PHE
2	E	422	THR
2	E	428	ASP
2	E	429	LEU
2	E	434	LEU
2	E	440	THR
2	E	443	LYS
2	E	444	ARG
2	F	1	MET
2	F	11	VAL
2	F	16	MET
2	F	35	GLN
2	F	138	LEU
2	F	258	ARG
2	F	287	ARG
2	F	352	LYS
2	F	360	LYS
2	F	368	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	242	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ADP	B	602	3	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
5	SO4	A	603	3	4,4,4	0.15	0	6,6,6	0.05	0
4	ADP	C	602	3	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	A	602	3	24,29,29	0.95	1 (4%)	29,45,45	1.45	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
4	ADP	B	602	3	-	8/12/32/32	0/3/3/3
4	ADP	C	602	3	-	8/12/32/32	0/3/3/3
4	ADP	A	602	3	-	7/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ADP	C5-C4	2.51	1.47	1.40
4	B	602	ADP	C5-C4	2.49	1.47	1.40
4	A	602	ADP	C5-C4	2.48	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	ADP	C3'-C2'-C1'	3.51	106.26	100.98
4	B	602	ADP	C3'-C2'-C1'	3.48	106.22	100.98
4	A	602	ADP	C3'-C2'-C1'	3.47	106.21	100.98
4	B	602	ADP	PA-O3A-PB	-3.25	121.66	132.83
4	C	602	ADP	PA-O3A-PB	-3.24	121.71	132.83
4	A	602	ADP	PA-O3A-PB	-3.22	121.79	132.83
4	B	602	ADP	N3-C2-N1	-3.20	123.67	128.68
4	A	602	ADP	N3-C2-N1	-3.17	123.72	128.68
4	C	602	ADP	N3-C2-N1	-3.16	123.74	128.68
4	A	602	ADP	C4-C5-N7	-2.60	106.69	109.40
4	B	602	ADP	C4-C5-N7	-2.55	106.74	109.40
4	C	602	ADP	C4-C5-N7	-2.52	106.77	109.40

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	C5'-O5'-PA-O2A
4	A	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	O4'-C4'-C5'-O5'
4	B	602	ADP	PA-O3A-PB-O3B
4	B	602	ADP	C5'-O5'-PA-O2A
4	B	602	ADP	C5'-O5'-PA-O3A
4	C	602	ADP	C5'-O5'-PA-O1A
4	C	602	ADP	C5'-O5'-PA-O2A
4	C	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	C3'-C4'-C5'-O5'
4	C	602	ADP	O4'-C4'-C5'-O5'
4	C	602	ADP	C3'-C4'-C5'-O5'
4	B	602	ADP	C3'-C4'-C5'-O5'
4	B	602	ADP	O4'-C4'-C5'-O5'
4	C	602	ADP	PA-O3A-PB-O1B
4	B	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	PA-O3A-PB-O1B

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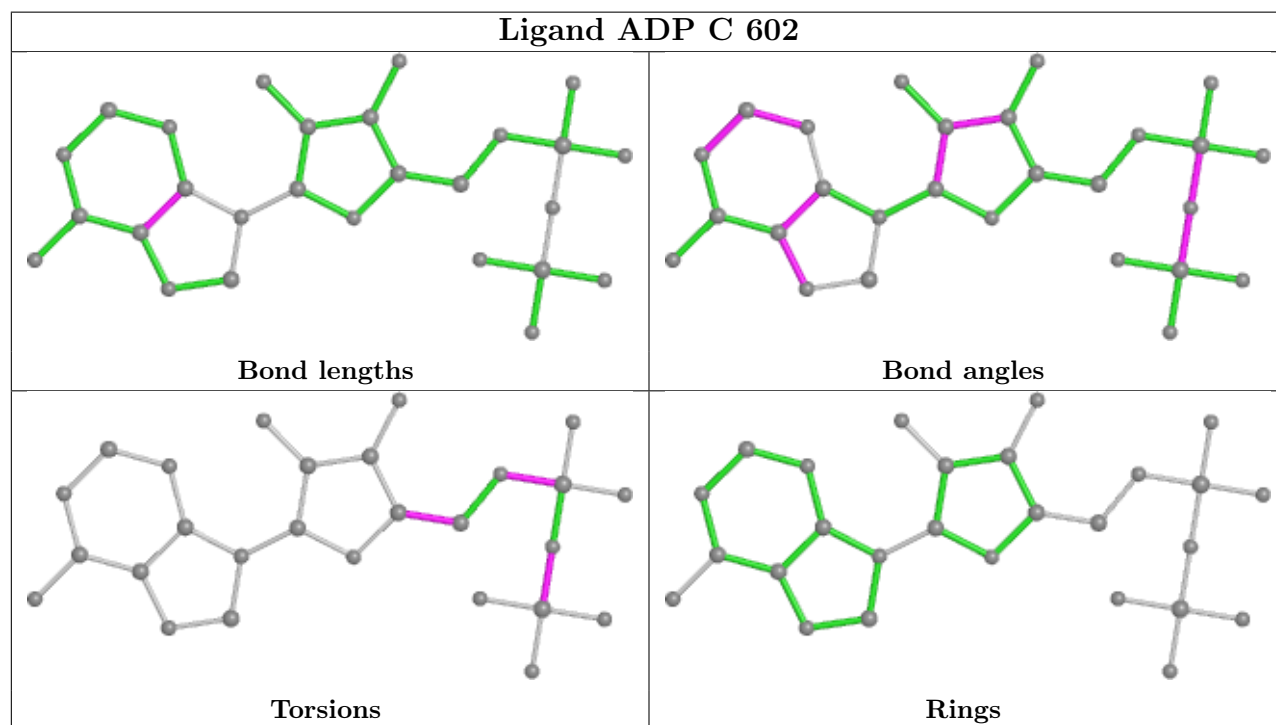
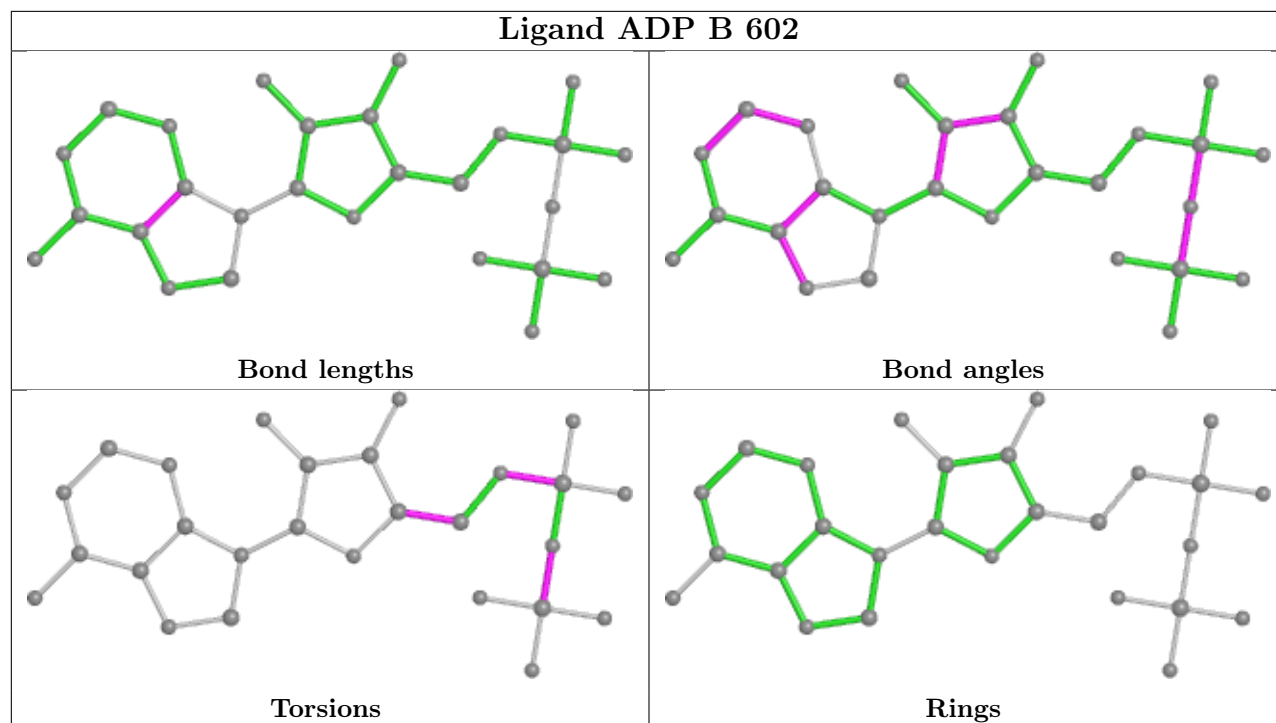
Mol	Chain	Res	Type	Atoms
4	B	602	ADP	PA-O3A-PB-O1B
4	A	602	ADP	PA-O3A-PB-O2B
4	B	602	ADP	PA-O3A-PB-O2B
4	C	602	ADP	PA-O3A-PB-O2B
4	C	602	ADP	PA-O3A-PB-O3B

There are no ring outliers.

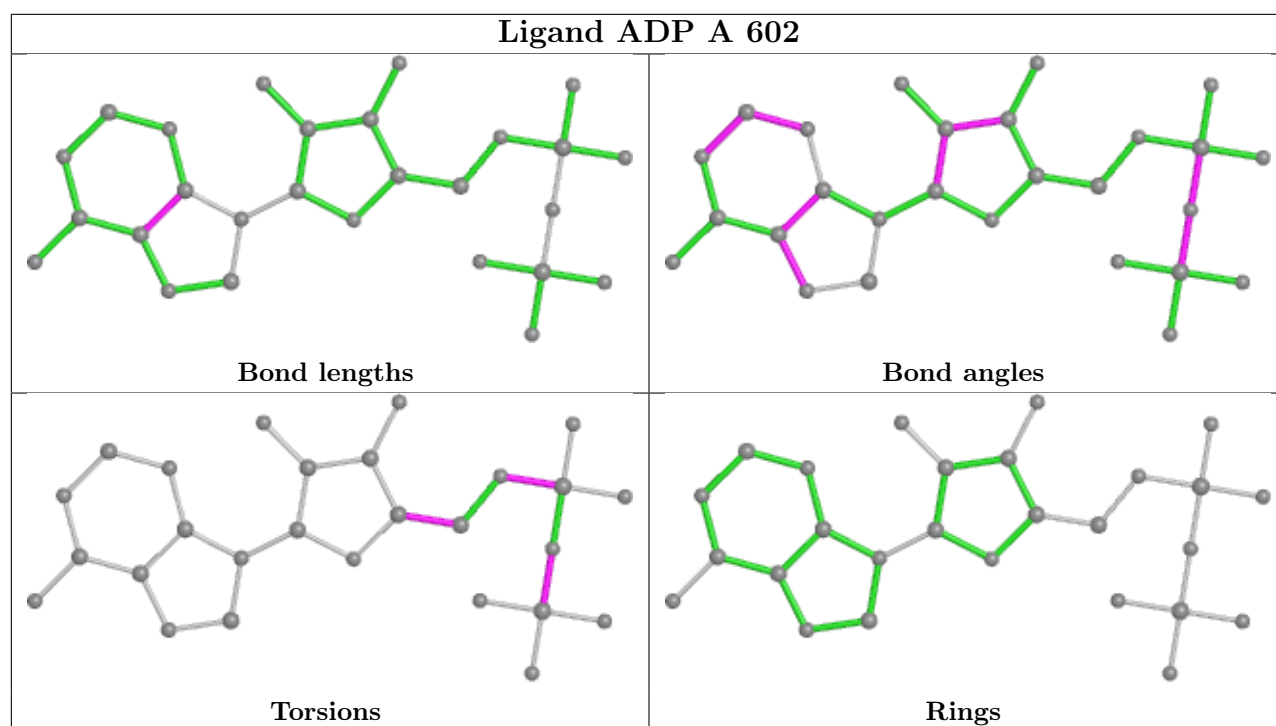
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	ADP	2	0
5	A	603	SO4	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	584/600 (97%)	0.07	11 (1%)	66	69	20, 35, 58, 72	0
1	B	584/600 (97%)	0.22	26 (4%)	33	31	20, 33, 58, 76	0
1	C	584/600 (97%)	0.22	29 (4%)	28	27	18, 35, 89, 116	0
2	D	446/465 (95%)	0.18	19 (4%)	35	33	18, 35, 65, 98	0
2	E	454/465 (97%)	0.57	57 (12%)	3	3	19, 38, 110, 127	0
2	F	454/465 (97%)	-0.02	4 (0%)	84	85	18, 32, 51, 65	0
All	All	3106/3195 (97%)	0.20	146 (4%)	31	30	18, 35, 78, 127	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	396	ASP	13.3
1	C	582	GLN	9.7
2	E	386	ALA	8.9
2	E	387	VAL	8.8
2	E	433	LEU	7.9
2	E	397	ILE	7.6
2	E	436	MET	7.1
2	E	393	ALA	6.8
1	C	478	GLY	5.9
2	E	453	TYR	5.8
2	D	387	VAL	5.7
2	E	367	ALA	5.3
2	E	395	SER	5.3
2	E	438	PRO	5.1
2	D	390	GLY	5.1
1	C	541	TYR	5.0
2	E	390	GLY	5.0
2	E	388	VAL	4.9
1	C	479	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
2	E	435	ALA	4.7
2	D	392	SER	4.4
2	D	385	LEU	4.4
2	F	175	ASP	4.3
1	C	583	LEU	4.3
2	D	386	ALA	4.2
2	D	102	GLU	4.2
2	D	393	ALA	4.1
1	B	279	PRO	4.1
2	E	445	ILE	4.1
2	E	429	LEU	4.1
2	E	444	ARG	4.0
1	C	538	LEU	4.0
2	E	357	GLY	3.9
2	E	428	ASP	3.9
2	E	394	LEU	3.9
1	A	478	GLY	3.9
1	C	480	ASP	3.8
2	E	374	ALA	3.8
2	D	394	LEU	3.8
2	E	358	ALA	3.7
2	E	365	HIS	3.7
1	C	492	VAL	3.7
1	C	549	THR	3.6
2	D	435	ALA	3.6
2	D	388	VAL	3.5
1	B	144	ILE	3.5
2	E	432	GLU	3.4
2	E	424	THR	3.3
2	E	332	GLU	3.3
1	B	182	LEU	3.2
2	E	437	LEU	3.2
1	B	185	LEU	3.2
1	C	577	ILE	3.2
2	D	400	ILE	3.2
2	E	420	ASN	3.2
1	B	175	VAL	3.1
2	E	454	LEU	3.1
1	C	581	ILE	3.1
2	E	431	TRP	3.0
2	E	400	ILE	3.0
1	C	481	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	537	SER	3.0
2	D	33	ARG	3.0
1	B	1	MET	3.0
2	E	377	ALA	2.9
1	A	280	ASN	2.9
2	E	426	THR	2.9
1	B	544	GLU	2.9
2	D	382	ALA	2.8
1	B	179	GLU	2.8
1	C	571	SER	2.8
1	A	452	ASP	2.8
2	E	451	ASP	2.8
2	D	396	ASP	2.8
2	E	104	LEU	2.8
2	E	392	SER	2.8
2	E	33	ARG	2.7
2	D	353	ASP	2.7
2	E	337	GLY	2.7
2	E	371	GLN	2.7
1	C	539	GLY	2.7
2	E	378	GLN	2.7
1	A	476	LEU	2.7
1	C	570	ILE	2.7
1	A	477	VAL	2.7
2	E	389	LEU	2.7
2	D	438	PRO	2.6
2	E	382	ALA	2.6
2	E	434	LEU	2.6
1	A	180	GLN	2.6
1	B	162	ILE	2.6
1	B	108	GLN	2.6
1	A	482	LEU	2.6
1	B	177	GLU	2.6
2	E	404	PHE	2.6
1	B	479	ILE	2.5
2	F	388	VAL	2.5
2	D	391	GLU	2.5
1	C	532	ALA	2.5
2	E	102	GLU	2.5
1	C	552	VAL	2.5
1	B	280	ASN	2.5
1	B	478	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	2.4
1	B	176	ILE	2.4
1	B	476	LEU	2.4
2	E	441	GLU	2.4
1	C	485	ASN	2.4
2	E	447	ASP	2.3
1	B	173	ILE	2.3
2	E	401	TYR	2.3
2	E	408	PHE	2.3
1	B	120	PHE	2.3
2	E	442	LEU	2.3
1	C	546	MET	2.3
2	E	339	GLN	2.2
2	F	173	SER	2.2
1	B	122	ALA	2.2
1	A	541	TYR	2.2
1	A	481	SER	2.2
1	B	163	GLU	2.2
1	C	475	ARG	2.2
2	D	432	GLU	2.2
1	B	541	TYR	2.2
1	A	260	GLY	2.2
1	C	542	PHE	2.2
1	B	180	GLN	2.2
1	C	472	GLU	2.1
1	B	65	ARG	2.1
2	E	398	ASP	2.1
2	E	407	ARG	2.1
1	C	180	GLN	2.1
2	F	392	SER	2.1
1	C	516	GLU	2.1
1	C	477	VAL	2.1
2	E	425	GLU	2.1
2	E	366	ALA	2.1
2	D	434	LEU	2.1
2	E	440	THR	2.1
1	B	350	GLY	2.1
1	C	536	LEU	2.0
1	C	578	LYS	2.0
1	B	160	GLN	2.0
1	C	469	GLN	2.0
2	E	373	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	470	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

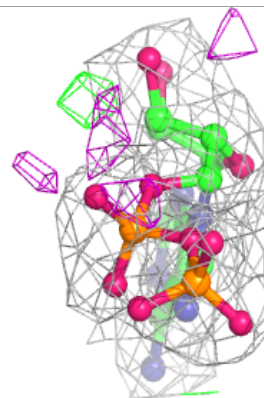
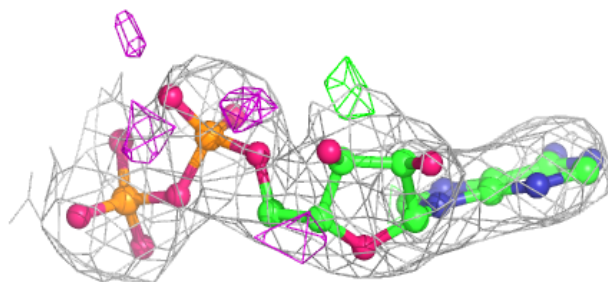
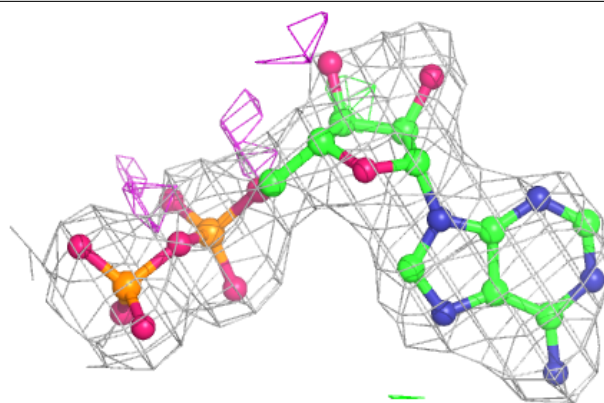
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	C	601	1/1	0.87	0.24	36,36,36,36	0
3	MG	B	601	1/1	0.91	0.25	26,26,26,26	0
4	ADP	A	602	27/27	0.95	0.19	20,44,45,46	0
4	ADP	C	602	27/27	0.96	0.16	19,33,34,35	0
4	ADP	B	602	27/27	0.97	0.18	16,28,30,32	0
3	MG	A	601	1/1	0.98	0.14	21,21,21,21	0
5	SO4	A	603	5/5	0.99	0.17	35,35,36,36	0

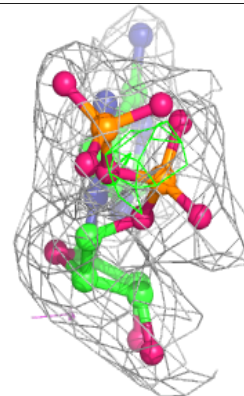
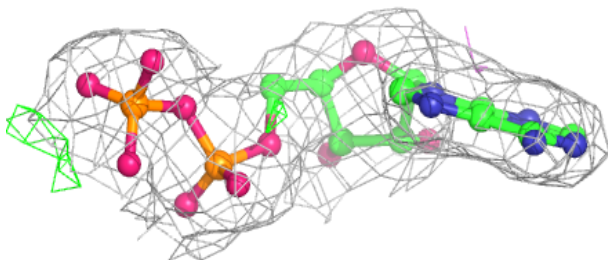
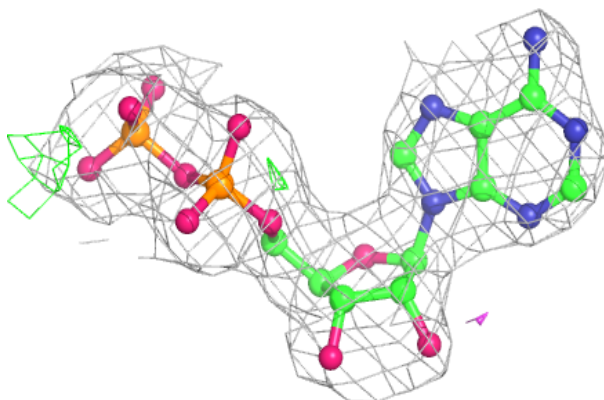
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

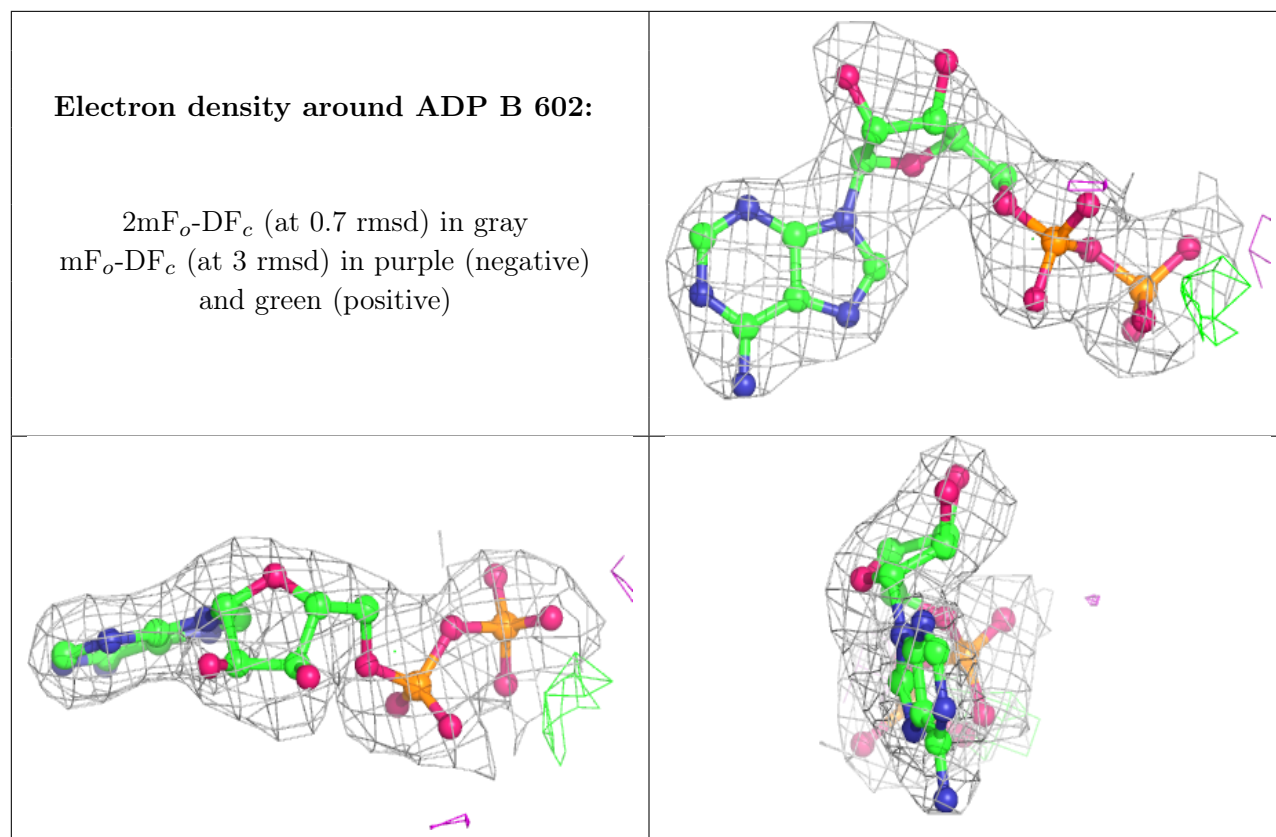
**Electron density around ADP A 602:**

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

**Electron density around ADP C 602:**

$2mF_o-DF_c$  (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.