



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:16 PM UTC

PDB ID : 7DQE / pdb_00007dqe
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

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

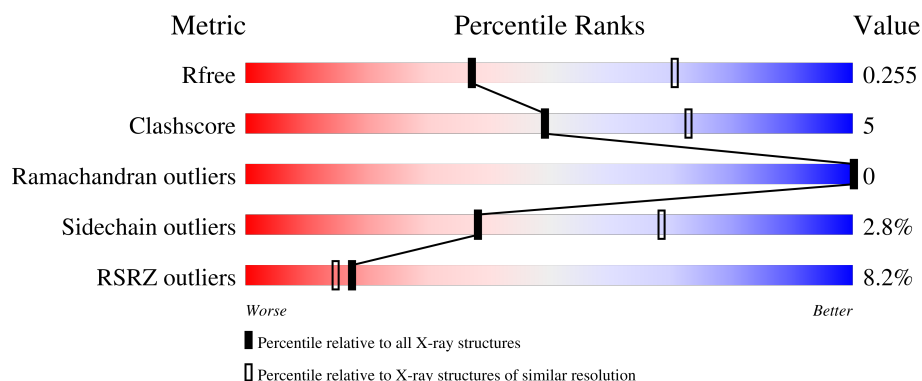
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	3% 84% 13% .
1	B	600	4% 83% 14% .
1	C	600	10% 83% 14% .
2	D	465	7% 81% 14% .

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Mol	Chain	Length	Quality of chain
2	E	465	23% 77% 20% ..
2	F	465	3% 83% 13% ..

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			

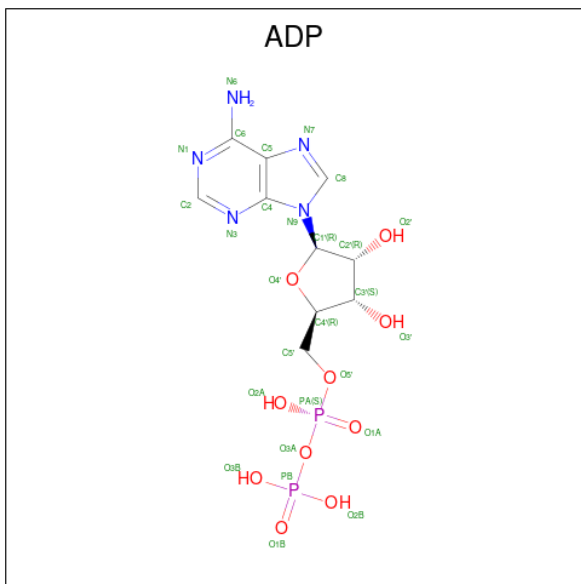
There are 24 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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

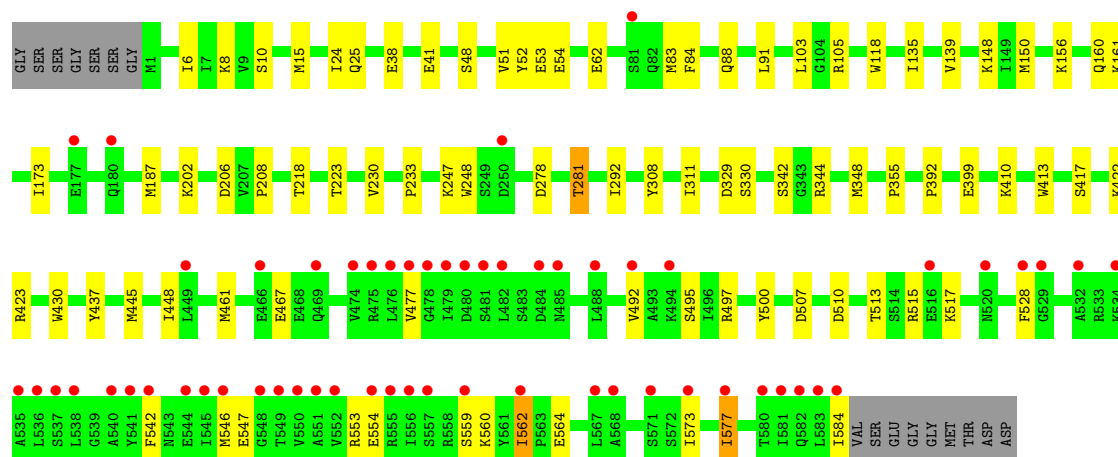
- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



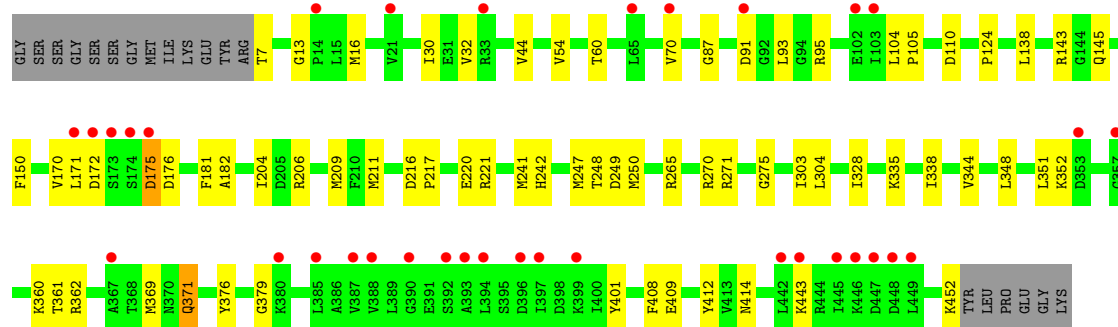
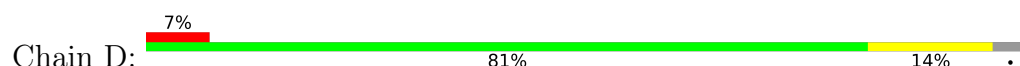
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

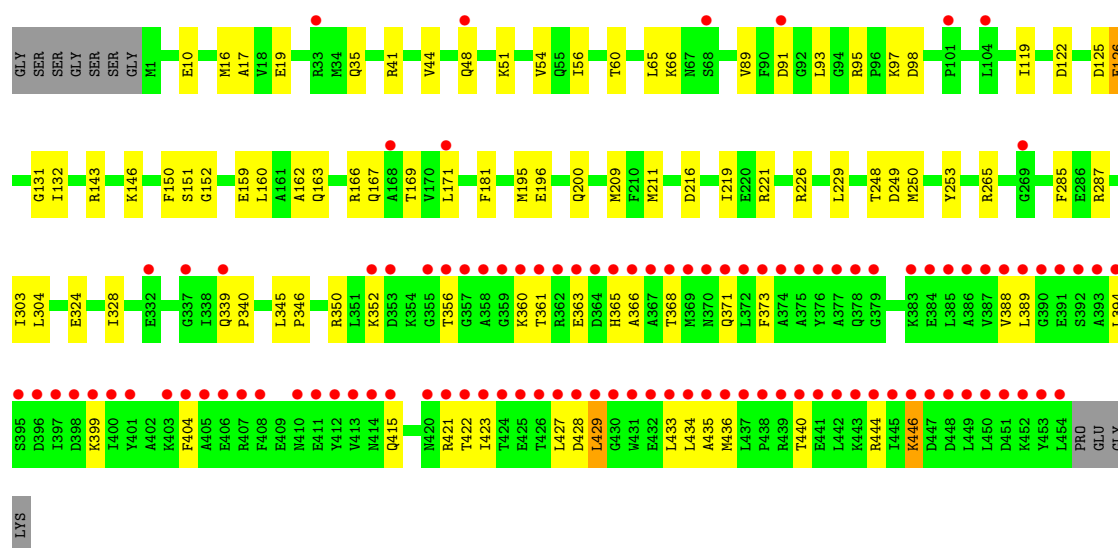
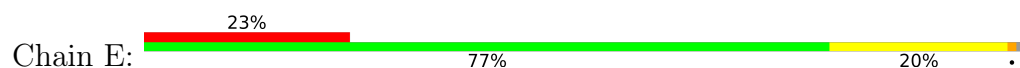
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total	O	0	0
			26	26		
6	B	38	Total	O	0	0
			38	38		
6	C	50	Total	O	0	0
			50	50		
6	D	18	Total	O	0	0
			18	18		
6	E	23	Total	O	0	0
			23	23		
6	F	36	Total	O	0	0
			36	36		



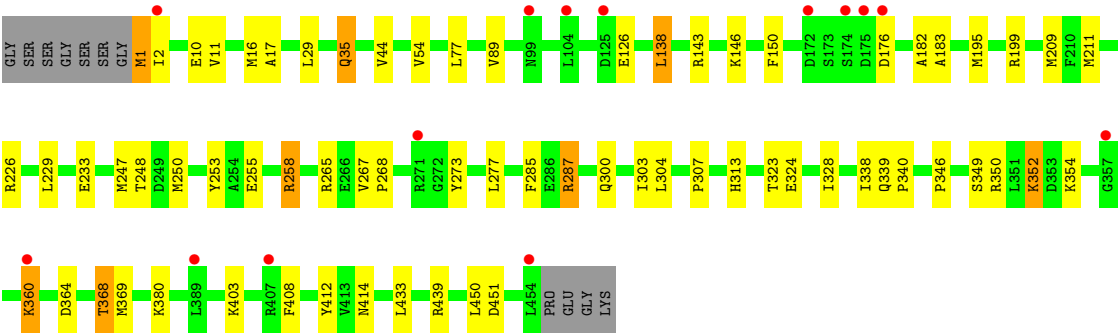
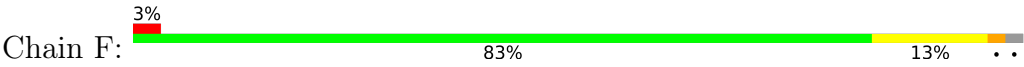
• Molecule 2: V-type sodium ATPase subunit B



• 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, α , β , γ	120.03Å 121.09Å 231.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 2.69 47.63 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.63-2.69) 98.7 (47.63-2.69)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.253 0.230 , 0.255	Depositor DCC
R_{free} test set	4793 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/4587	0.72	1/6210 (0.0%)
1	B	0.27	0/4596	0.69	0/6222
1	C	0.27	0/4525	0.72	0/6136
2	D	0.28	0/3462	0.70	0/4690
2	E	0.31	0/3454	0.76	0/4686
2	F	0.28	0/3594	0.70	0/4862
All	All	0.28	0/24218	0.71	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	259	CYS	N-CA-C	5.97	118.68	111.40

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	43	0
1	B	4520	0	4468	45	0
1	C	4450	0	4321	46	0
2	D	3402	0	3340	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3398	0	3293	50	0
2	F	3532	0	3535	41	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	254	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 (254) 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
1:A:148:LYS:H	1:A:320:MET:HE3	1.51	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:247:MET:HB3	2:F:250:MET:HE3	1.80	0.63
2:F:250:MET:HB2	2:F:304:LEU:HB3	1.79	0.62
2:E:209:MET:HB3	2:E:211:MET:HE3	1.81	0.62
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
1:C:445:MET:HE1	1:C:515:ARG:HG3	1.84	0.60
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:D:209:MET:HB3	2:D:211:MET:HE3	1.85	0.59
2:F:248:THR:HB	2:F:303:ILE:HB	1.84	0.58
1:C:461:MET:HE2	2:D:335:LYS:HD2	1.86	0.58
1:C:8:LYS:HD3	1:C:15:MET:HE2	1.84	0.58
2:E:89:VAL:HG21	2:E:195:MET:HE1	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:118:TRP:HB2	1:C:187:MET:HE1	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ASP:OD1	1:C:281:THR:OG1	2.27	0.53
1:C:139:VAL:HG21	1:C:187:MET:HE3	1.91	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:38:GLU:OE2	1:C:52:TYR:OH	2.24	0.52
1:C:230:VAL:HG22	1:C:413:TRP:HE3	1.74	0.52
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
1:B:416:ASP:OD1	1:B:418:SER:OG	2.27	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
1:B:118:TRP:HB2	1:B:187:MET:HE1	1.95	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:A:298:MET:HE3	1:A:299:PRO:HD2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:218:THR:OG1	1:C:500:TYR:OH	2.26	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
2:F:229:LEU:HG	2:F:247:MET:HE1	1.97	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
2:F:182:ALA:HB3	2:F:247:MET:HG2	1.97	0.47
1:A:514:SER:OG	1:A:564:GLU:OE1	2.26	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
2:E:150:PHE:HB2	2:E:328:ILE:HD13	1.97	0.46
2:D:352:LYS:HD2	2:D:369:MET:HE1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:B:266:MET:HE2	1:B:293:ALA:HB2	2.00	0.44
1:C:247:LYS:HG3	1:C:248:TRP:CD1	2.53	0.44
2:E:181:PHE:HD2	2:E:211:MET:HE1	1.82	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:B:425:PHE:HA	1:B:426:PRO:C	2.44	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:A:320:MET:HE2	1:A:322:TYR:HE2	1.84	0.43
1:B:462:ARG:NH2	1:B:466:GLU:OE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:65:LEU:C	2:E:66:LYS:HD2	2.44	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:E:35:GLN:H	2:E:35:GLN:CD	2.28	0.42
2:F:255:GLU:OE1	2:F:258:ARG:NH1	2.50	0.42
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:35:GLN:CD	2:F:35:GLN:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:246:ALA:HB2	1:B:327:MET:HE3	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:A:491:GLU:HG3	1:A:546:MET:HE3	2.02	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:D:181:PHE:HD2	2:D:211:MET:HE1	1.85	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
1:B:273:PHE:HB2	1:B:286:MET:HE2	2.04	0.40
2:D:138:LEU:HD12	2:D:344:VAL:HG11	2.03	0.40
2:F:195:MET:HE2	2:F:211:MET:HE2	2.04	0.40
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
2:F:369:MET:HE2	2:F:369:MET:HB3	1.96	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	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 ⓘ

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%)	480 (98%)	10 (2%)	48	76
1	B	493/511 (96%)	486 (99%)	7 (1%)	59	82
1	C	474/511 (93%)	462 (98%)	12 (2%)	42	71
2	D	345/387 (89%)	336 (97%)	9 (3%)	40	70
2	E	336/387 (87%)	316 (94%)	20 (6%)	17	41
2	F	371/387 (96%)	359 (97%)	12 (3%)	34	64
All	All	2509/2694 (93%)	2439 (97%)	70 (3%)	38	68

All (70) 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	144	ILE

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Mol	Chain	Res	Type
1	A	251	VAL
1	A	338	LEU
1	A	419	LEU
1	A	477	VAL
1	A	523	LYS
1	A	569	LYS
1	B	46	VAL
1	B	71	LEU
1	B	85	ASP
1	B	142	THR
1	B	398	SER
1	B	399	GLU
1	B	477	VAL
1	C	103	LEU
1	C	156	LYS
1	C	281	THR
1	C	292	ILE
1	C	423	ARG
1	C	477	VAL
1	C	547	GLU
1	C	554	GLU
1	C	560	LYS
1	C	562	ILE
1	C	577	ILE
1	C	584	ILE
2	D	7	THR
2	D	16	MET
2	D	93	LEU
2	D	110	ASP
2	D	175	ASP
2	D	206	ARG
2	D	360	LYS
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	132	ILE

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Mol	Chain	Res	Type
2	E	169	THR
2	E	171	LEU
2	E	219	ILE
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	446	LYS
2	F	1	MET
2	F	11	VAL
2	F	16	MET
2	F	35	GLN
2	F	138	LEU
2	F	199	ARG
2	F	258	ARG
2	F	287	ARG
2	F	352	LYS
2	F	360	LYS
2	F	368	THR
2	F	380	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	379	GLN
1	A	403	GLN
1	B	201	GLN
1	B	403	GLN
1	B	485	ASN
1	B	574	ASN
1	C	153	ASN
1	C	213	GLN
1	C	244	GLN
1	C	465	GLN
1	C	520	ASN
2	D	67	ASN
2	D	242	HIS

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Mol	Chain	Res	Type
2	D	410	ASN
2	E	137	HIS
2	E	139	ASN
2	E	414	ASN
2	F	48	GLN
2	F	139	ASN

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 oligosaccharides 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	28,29,29	1.43	5 (17%)	43,45,45	1.84	9 (20%)
4	ADP	C	602	3	28,29,29	1.43	5 (17%)	43,45,45	1.83	8 (18%)
5	SO4	A	603	3	4,4,4	0.24	0	6,6,6	0.07	0
4	ADP	A	602	3	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)

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	-	8/16/32/32	0/3/3/3
4	ADP	C	602	3	-	8/16/32/32	0/3/3/3
4	ADP	A	602	3	-	7/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ADP	C5-C4	4.75	1.47	1.39
4	B	602	ADP	C5-C4	4.73	1.47	1.39
4	A	602	ADP	C5-C4	4.72	1.47	1.39
4	A	602	ADP	C5-C6	2.75	1.48	1.41
4	B	602	ADP	C5-C6	2.73	1.48	1.41
4	C	602	ADP	C5-C6	2.73	1.48	1.41
4	C	602	ADP	C5-N7	-2.31	1.34	1.39
4	B	602	ADP	C8-N7	2.31	1.36	1.31
4	C	602	ADP	C8-N7	2.29	1.36	1.31
4	A	602	ADP	C8-N7	2.28	1.36	1.31
4	B	602	ADP	C5-N7	-2.27	1.34	1.39
4	A	602	ADP	C5-N7	-2.22	1.35	1.39
4	C	602	ADP	PA-O3A	2.06	1.61	1.59
4	B	602	ADP	PA-O3A	2.04	1.61	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ADP	C5-C4-N3	-5.83	118.69	126.72
4	C	602	ADP	C5-C4-N3	-5.79	118.74	126.72
4	A	602	ADP	C5-C4-N3	-5.76	118.79	126.72
4	B	602	ADP	N3-C4-N9	4.68	135.13	127.17
4	C	602	ADP	N3-C4-N9	4.65	135.07	127.17
4	A	602	ADP	N3-C4-N9	4.59	134.97	127.17
4	B	602	ADP	C2-N3-C4	3.69	120.86	111.83
4	A	602	ADP	C2-N3-C4	3.66	120.76	111.83
4	C	602	ADP	C2-N3-C4	3.65	120.74	111.83
4	A	602	ADP	C4-C5-N7	-3.40	106.69	110.58
4	B	602	ADP	C4-C5-N7	-3.36	106.74	110.58
4	C	602	ADP	C4-C5-N7	-3.34	106.77	110.58
4	B	602	ADP	N3-C2-N1	-3.24	123.67	128.58
4	A	602	ADP	N3-C2-N1	-3.21	123.72	128.58
4	C	602	ADP	N3-C2-N1	-3.20	123.74	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ADP	C4-N9-C8	2.69	108.56	105.74
4	A	602	ADP	C4-N9-C8	2.62	108.48	105.74
4	C	602	ADP	C4-N9-C8	2.56	108.43	105.74
4	C	602	ADP	C3'-C2'-C1'	2.54	106.26	101.46
4	B	602	ADP	C3'-C2'-C1'	2.51	106.22	101.46
4	A	602	ADP	C3'-C2'-C1'	2.51	106.21	101.46
4	A	602	ADP	C5-N7-C8	2.47	107.34	103.45
4	B	602	ADP	C5-N7-C8	2.47	107.33	103.45
4	C	602	ADP	C5-N7-C8	2.46	107.32	103.45
4	A	602	ADP	C6-C5-N7	2.04	136.02	132.09
4	B	602	ADP	C6-C5-N7	2.00	135.96	132.09

There are no chirality outliers.

All (23) torsion outliers are listed below:

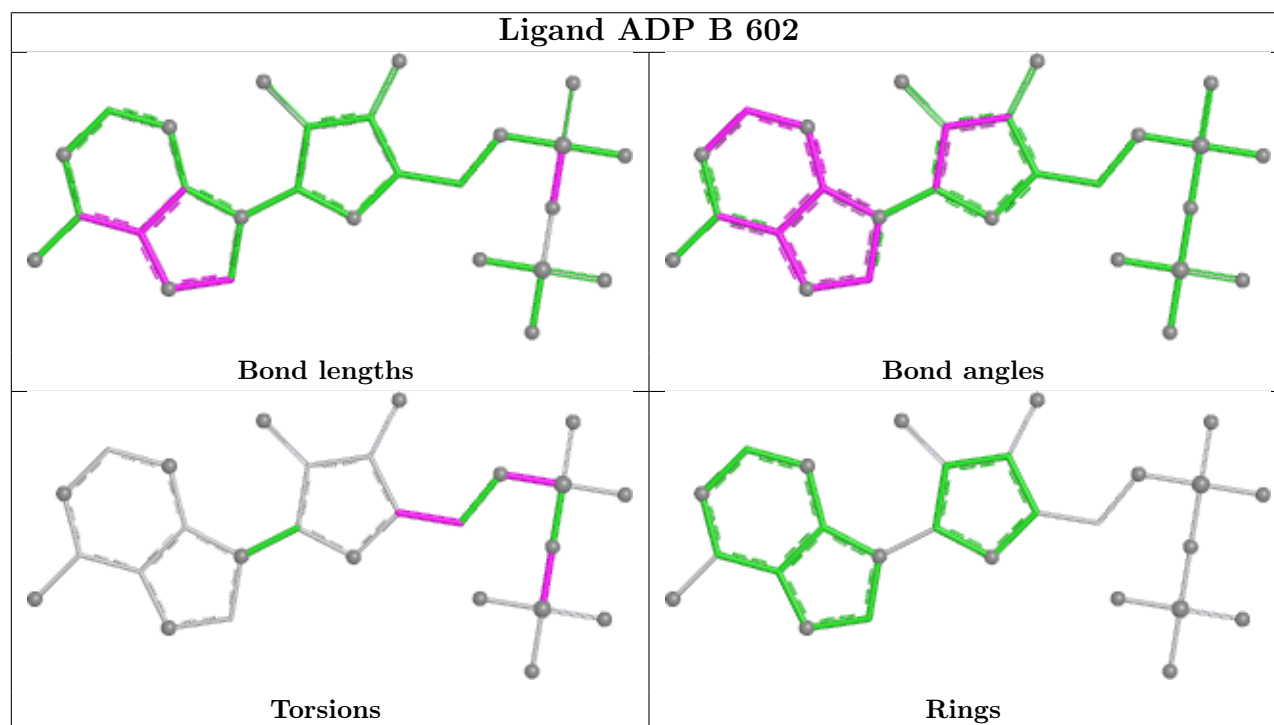
Mol	Chain	Res	Type	Atoms
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	C5'-O5'-PA-O2A
4	A	602	ADP	O4'-C4'-C5'-O5'
4	B	602	ADP	PA-O3A-PB-O3B
4	B	602	ADP	C5'-O5'-PA-O2A
4	C	602	ADP	C5'-O5'-PA-O1A
4	C	602	ADP	C5'-O5'-PA-O2A
4	C	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	C3'-C4'-C5'-O5'
4	C	602	ADP	O4'-C4'-C5'-O5'
4	C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

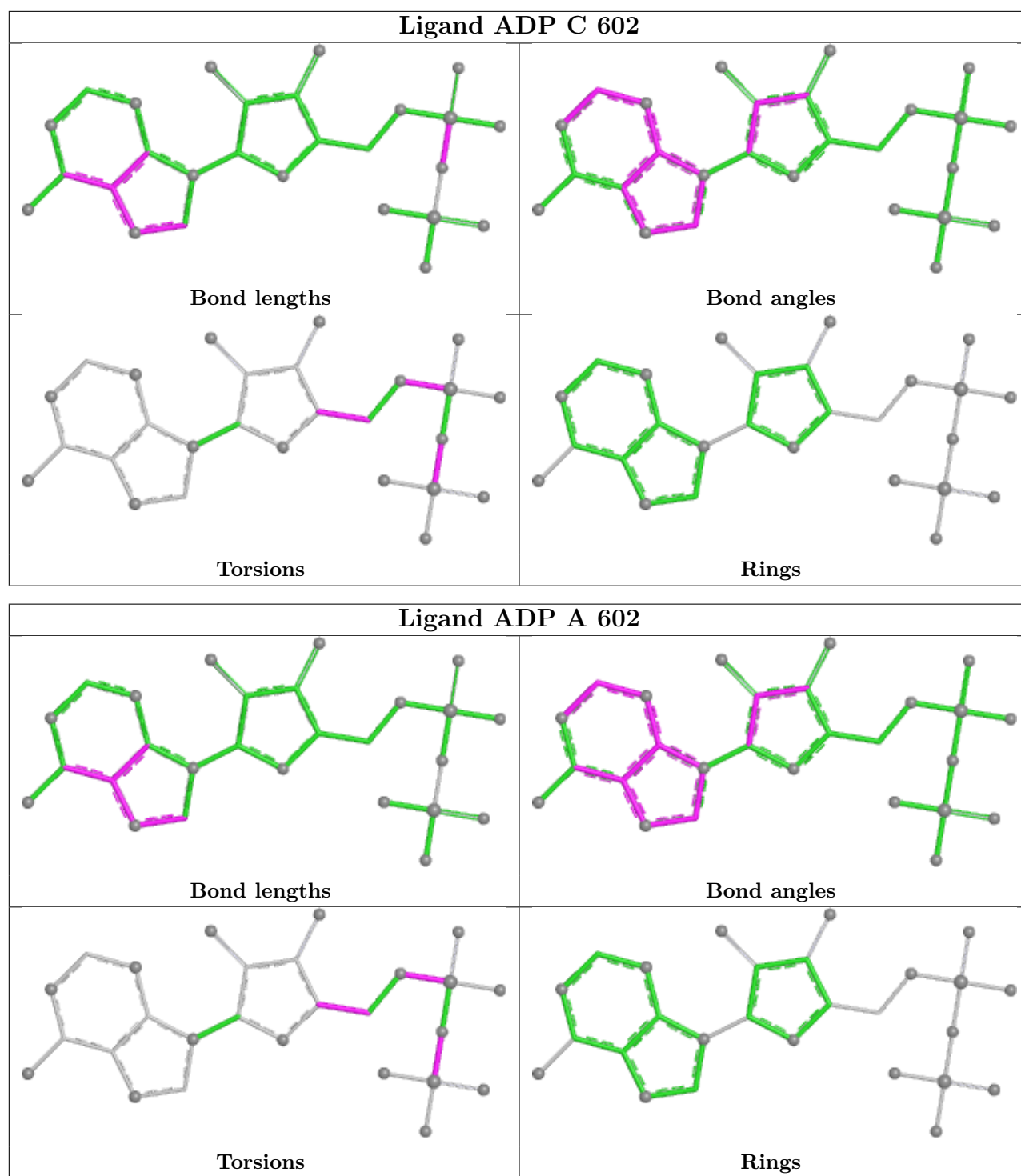
There are no ring outliers.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	584/600 (97%)	0.40	19 (3%)	49	45	20, 35, 58, 72	0
1	B	584/600 (97%)	0.36	26 (4%)	38	34	20, 33, 58, 76	0
1	C	584/600 (97%)	0.55	58 (9%)	13	10	18, 35, 89, 116	0
2	D	446/465 (95%)	0.44	34 (7%)	20	17	18, 35, 65, 98	0
2	E	454/465 (97%)	1.09	105 (23%)	2	2	19, 38, 110, 127	0
2	F	454/465 (97%)	0.28	14 (3%)	51	48	18, 32, 51, 65	0
All	All	3106/3195 (97%)	0.51	256 (8%)	17	15	18, 35, 78, 127	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	396	ASP	8.7
2	E	357	GLY	6.8
2	E	433	LEU	6.6
2	E	435	ALA	6.4
2	E	358	ALA	6.1
2	E	395	SER	6.0
1	C	582	GLN	5.9
2	E	367	ALA	5.9
2	E	444	ARG	5.8
2	E	364	ASP	5.8
2	E	441	GLU	5.7
2	E	445	ILE	5.7
1	C	480	ASP	5.7
2	E	386	ALA	5.7
2	E	454	LEU	5.5
1	C	584	ILE	5.4
2	D	102	GLU	5.3
2	E	400	ILE	5.1
2	E	426	THR	5.1

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Mol	Chain	Res	Type	RSRZ
2	E	429	LEU	5.0
1	C	479	ILE	5.0
2	E	434	LEU	4.9
2	E	432	GLU	4.9
2	E	366	ALA	4.8
2	E	449	LEU	4.8
2	E	387	VAL	4.8
2	E	397	ILE	4.6
2	E	392	SER	4.6
1	B	280	ASN	4.6
2	E	431	TRP	4.5
2	E	440	THR	4.5
2	E	393	ALA	4.5
2	E	446	LYS	4.4
2	E	389	LEU	4.4
2	E	424	THR	4.4
2	E	368	THR	4.3
1	C	571	SER	4.3
2	E	362	ARG	4.2
1	C	541	TYR	4.2
2	E	442	LEU	4.1
2	E	359	GLY	4.1
2	E	453	TYR	4.1
2	E	365	HIS	4.1
2	E	413	VAL	4.1
2	E	376	TYR	4.1
2	E	420	ASN	4.0
2	E	410	ASN	4.0
1	A	584	ILE	4.0
2	E	447	ASP	4.0
2	E	391	GLU	3.9
2	D	174	SER	3.9
1	C	544	GLU	3.9
2	E	373	PHE	3.9
2	E	361	THR	3.8
2	E	360	LYS	3.8
1	A	260	GLY	3.8
1	C	577	ILE	3.8
2	D	394	LEU	3.8
2	F	174	SER	3.8
1	C	552	VAL	3.7
2	E	371	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	438	PRO	3.7
2	E	394	LEU	3.7
2	E	427	LEU	3.6
1	C	581	ILE	3.6
2	E	356	THR	3.6
1	C	580	THR	3.6
2	E	412	TYR	3.6
2	E	436	MET	3.6
2	E	398	ASP	3.5
2	F	175	ASP	3.5
2	E	372	LEU	3.5
2	E	33	ARG	3.5
2	E	374	ALA	3.5
2	E	388	VAL	3.5
2	D	353	ASP	3.5
1	C	538	LEU	3.5
2	E	404	PHE	3.5
2	D	396	ASP	3.4
2	E	448	ASP	3.4
2	E	408	PHE	3.4
1	C	492	VAL	3.4
1	B	144	ILE	3.4
1	B	162	ILE	3.4
2	E	415	GLN	3.4
2	E	430	GLY	3.4
1	C	477	VAL	3.3
2	D	390	GLY	3.3
1	C	532	ALA	3.3
2	D	443	LYS	3.3
1	A	81	SER	3.3
2	E	378	GLN	3.3
1	C	542	PHE	3.3
2	E	414	ASN	3.3
2	D	392	SER	3.2
1	C	583	LEU	3.2
2	E	68	SER	3.1
1	C	534	LYS	3.1
1	A	280	ASN	3.1
2	D	172	ASP	3.1
2	D	449	LEU	3.1
2	E	450	LEU	3.1
2	E	406	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	556	ILE	3.1
1	A	1	MET	3.0
1	C	478	GLY	3.0
2	D	385	LEU	3.0
1	B	279	PRO	3.0
1	C	250	ASP	3.0
2	D	447	ASP	3.0
2	E	439	ARG	3.0
2	E	422	THR	3.0
2	D	387	VAL	3.0
2	E	352	LYS	2.9
1	C	535	ALA	2.9
2	E	369	MET	2.9
1	B	158	THR	2.9
2	E	425	GLU	2.9
1	B	65	ARG	2.9
2	E	428	ASP	2.9
2	E	375	ALA	2.9
1	C	573	ILE	2.9
2	D	91	ASP	2.9
2	D	357	GLY	2.9
1	A	479	ILE	2.8
1	C	551	ALA	2.8
1	C	568	ALA	2.8
2	E	411	GLU	2.8
2	D	399	LYS	2.8
2	E	451	ASP	2.8
1	C	516	GLU	2.8
2	E	407	ARG	2.8
2	E	403	LYS	2.8
2	E	437	LEU	2.8
2	E	91	ASP	2.8
1	C	549	THR	2.8
2	E	405	ALA	2.8
1	A	297	ASN	2.7
2	D	173	SER	2.7
2	F	99	ASN	2.7
1	A	272	GLU	2.7
1	B	125	GLU	2.7
2	E	377	ALA	2.7
2	E	399	LYS	2.7
2	E	423	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	421	ARG	2.6
2	E	443	LYS	2.6
1	A	489	THR	2.6
1	C	481	SER	2.6
1	B	85	ASP	2.6
1	C	476	LEU	2.6
2	D	446	LYS	2.6
1	C	469	GLN	2.6
1	C	555	ARG	2.5
2	F	360	LYS	2.5
1	C	559	SER	2.5
2	D	445	ILE	2.5
2	E	383	LYS	2.5
2	D	397	ILE	2.5
2	D	448	ASP	2.5
2	F	176	ASP	2.5
2	F	454	LEU	2.5
1	B	177	GLU	2.5
1	A	418	SER	2.5
1	C	548	GLY	2.5
2	E	385	LEU	2.4
1	C	567	LEU	2.4
1	B	179	GLU	2.4
2	E	48	GLN	2.4
1	A	154	GLY	2.4
1	C	540	ALA	2.4
1	C	545	ILE	2.4
1	A	278	ASP	2.4
1	A	143	LYS	2.4
2	E	337	GLY	2.4
2	E	339	GLN	2.4
1	B	195	ARG	2.4
1	C	550	VAL	2.4
1	B	541	TYR	2.3
2	E	353	ASP	2.3
1	C	180	GLN	2.3
1	B	175	VAL	2.3
1	C	485	ASN	2.3
2	D	14	PRO	2.3
1	B	350	GLY	2.3
2	D	21	VAL	2.3
1	C	488	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	541	TYR	2.3
2	F	172	ASP	2.3
1	C	474	VAL	2.3
2	D	442	LEU	2.3
2	F	125	ASP	2.3
1	B	107	VAL	2.3
2	D	103	ILE	2.2
2	E	384	GLU	2.2
2	E	401	TYR	2.2
2	F	271	ARG	2.2
1	B	106	GLY	2.2
2	E	390	GLY	2.2
1	B	538	LEU	2.2
1	C	536	LEU	2.2
2	E	101	PRO	2.2
1	B	476	LEU	2.2
1	C	482	LEU	2.2
1	C	562	ILE	2.2
2	D	393	ALA	2.2
2	D	33	ARG	2.2
1	C	494	LYS	2.2
2	D	65	LEU	2.2
2	F	104	LEU	2.2
1	C	546	MET	2.2
1	B	124	ILE	2.2
2	D	380	LYS	2.2
2	E	269	GLY	2.2
2	F	357	GLY	2.2
2	D	367	ALA	2.1
2	E	363	GLU	2.1
1	C	475	ARG	2.1
2	E	452	LYS	2.1
1	C	449	LEU	2.1
2	D	388	VAL	2.1
2	F	2	ILE	2.1
2	E	168	ALA	2.1
1	A	180	GLN	2.1
1	A	259	CYS	2.1
2	E	370	ASN	2.1
1	B	278	ASP	2.1
1	C	537	SER	2.1
1	C	466	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	554	GLU	2.1
1	B	281	THR	2.1
1	B	180	GLN	2.1
2	E	104	LEU	2.1
2	E	171	LEU	2.1
1	C	529	GLY	2.1
1	A	452	ASP	2.1
1	C	484	ASP	2.1
2	E	332	GLU	2.1
1	B	173	ILE	2.1
1	C	528	PHE	2.1
2	F	407	ARG	2.0
1	B	131	SER	2.0
1	C	81	SER	2.0
1	B	1	MET	2.0
1	C	520	ASN	2.0
1	B	127	GLY	2.0
2	E	355	GLY	2.0
2	E	379	GLY	2.0
2	D	70	VAL	2.0
1	C	177	GLU	2.0
2	D	175	ASP	2.0
1	C	557	SER	2.0
1	A	482	LEU	2.0
2	D	171	LEU	2.0
2	F	389	LEU	2.0
1	A	558	ARG	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.

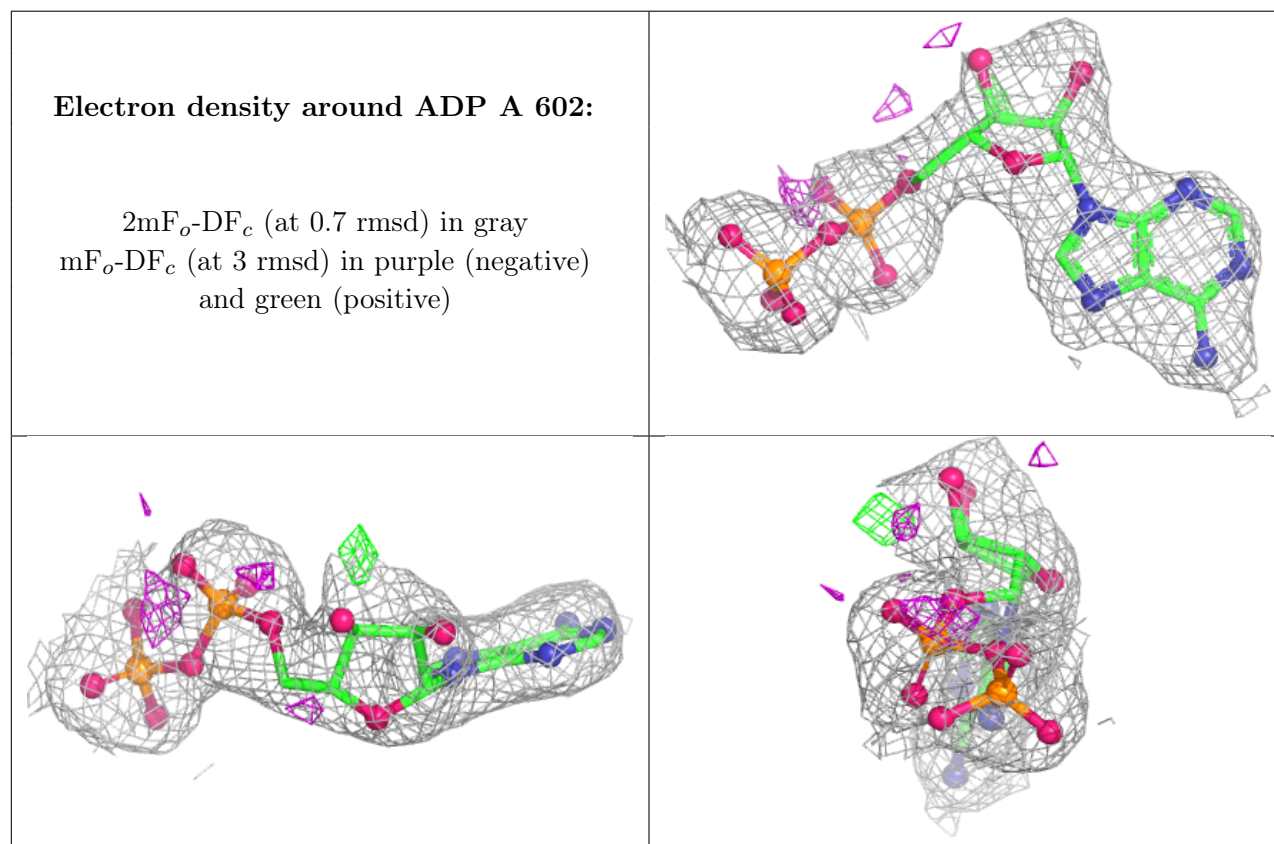
6.4 Ligands [i](#)

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.

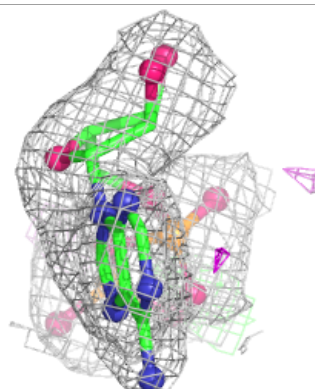
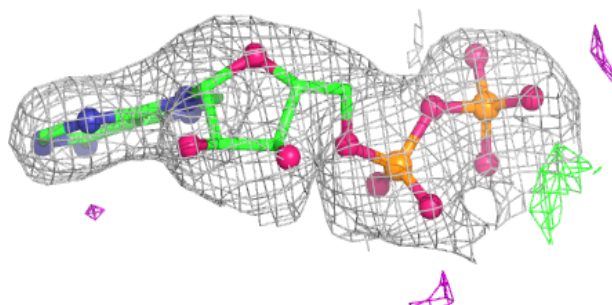
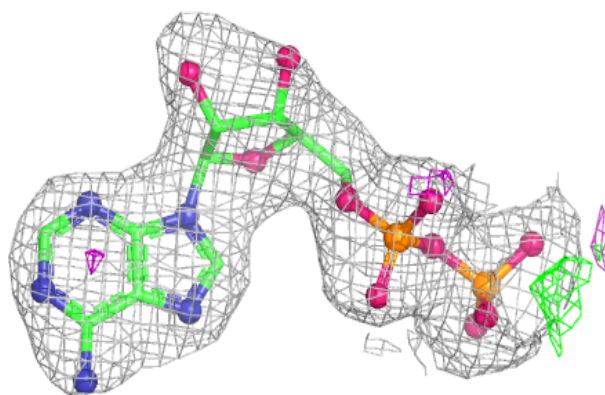
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	601	1/1	0.88	0.12	26,26,26,26	0
3	MG	C	601	1/1	0.88	0.12	36,36,36,36	0
4	ADP	A	602	27/27	0.95	0.10	20,44,45,46	0
4	ADP	B	602	27/27	0.96	0.09	16,28,30,32	0
4	ADP	C	602	27/27	0.96	0.09	19,33,34,35	0
5	SO4	A	603	5/5	0.97	0.07	35,35,36,36	0
3	MG	A	601	1/1	0.98	0.03	21,21,21,21	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.

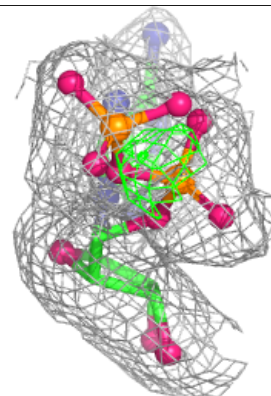
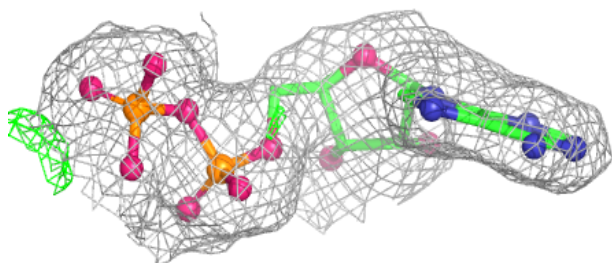
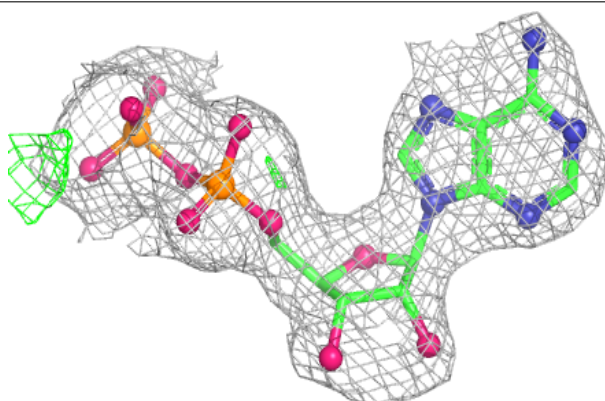


Electron density around ADP B 602:

$2mF_o-DF_c$ (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.