



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 03:08 PM EST

PDB ID : 1R0Z
Title : Phosphorylated Cystic fibrosis transmembrane conductance regulator (CFTR) nucleotide-binding domain one (NBD1) with ATP
Authors : Lewis, H.A.; Buchanan, S.G.; Burley, S.K.; Conners, K.; Dickey, M.; Dorwart, M.; Fowler, R.; Gao, X.; Guggino, W.B.; Hendrickson, W.A.
Deposited on : 2003-09-23
Resolution : 2.35 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 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 : 2.16
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) : 2.16

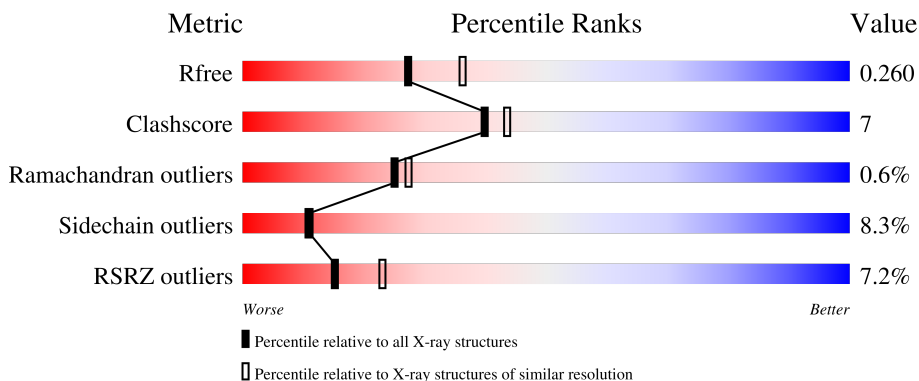
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	286	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 72% 23% • •</p>
1	B	286	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 72% 21% • •</p>
1	C	286	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 81% 15% • •</p>
1	D	286	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 74% 14% • 9%</p>

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
1	SEP	A	422	-	-	-	X
1	SEP	C	422	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9044 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	275	2185	1376	361	432	4	12	0	0	0
1	B	275	2175	1375	360	426	2	12	0	0	0
1	C	277	2190	1383	363	430	2	12	0	0	0
1	D	259	2050	1300	338	398	2	12	0	0	0

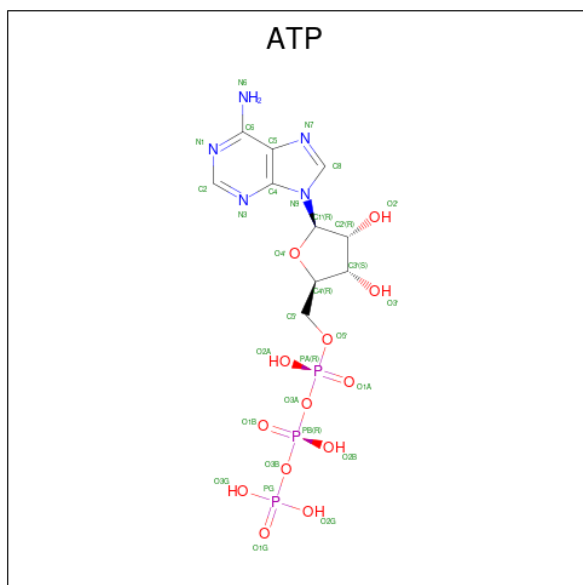
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	SER	-	cloning artifact	UNP P26361
A	422	SEP	SER	modified residue	UNP P26361
A	659	SEP	SER	modified residue	UNP P26361
A	660	SEP	SER	modified residue	UNP P26361
A	670	SEP	SER	modified residue	UNP P26361
B	388	SER	-	cloning artifact	UNP P26361
B	422	SEP	SER	modified residue	UNP P26361
B	659	SEP	SER	modified residue	UNP P26361
B	660	SEP	SER	modified residue	UNP P26361
B	670	SEP	SER	modified residue	UNP P26361
C	388	SER	-	cloning artifact	UNP P26361
C	422	SEP	SER	modified residue	UNP P26361
C	659	SEP	SER	modified residue	UNP P26361
C	660	SEP	SER	modified residue	UNP P26361
C	670	SEP	SER	modified residue	UNP P26361
D	388	SER	-	cloning artifact	UNP P26361
D	422	SEP	SER	modified residue	UNP P26361
D	659	SEP	SER	modified residue	UNP P26361
D	660	SEP	SER	modified residue	UNP P26361
D	670	SEP	SER	modified residue	UNP P26361

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

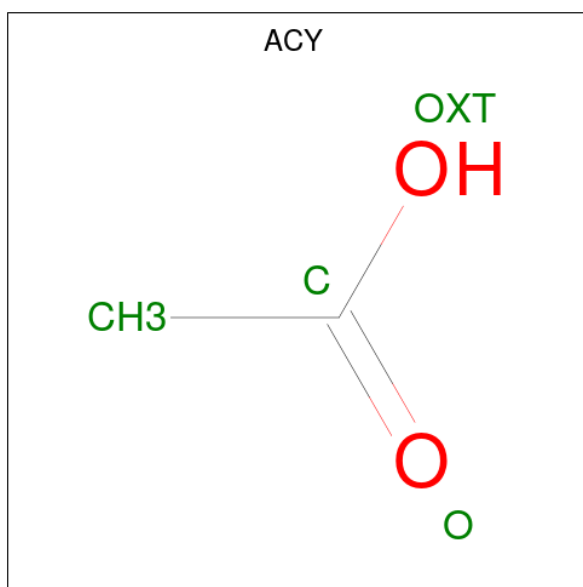
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

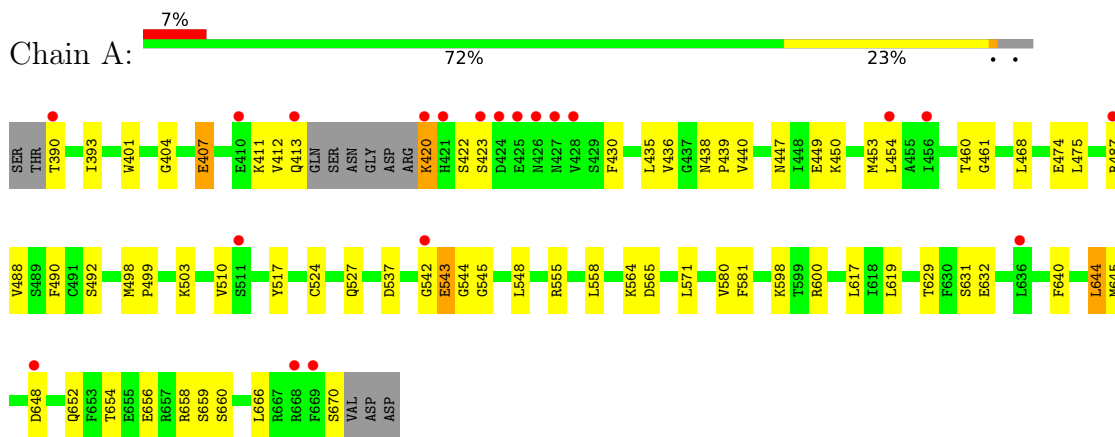
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	74	Total O 74 74	0	0
5	B	88	Total O 88 88	0	0
5	C	79	Total O 79 79	0	0
5	D	59	Total O 59 59	0	0

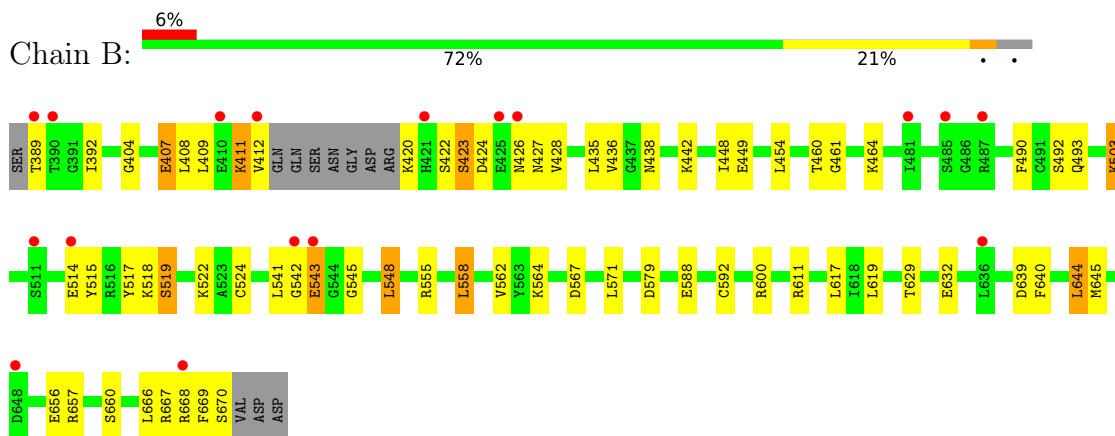
3 Residue-property plots [i](#)

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.

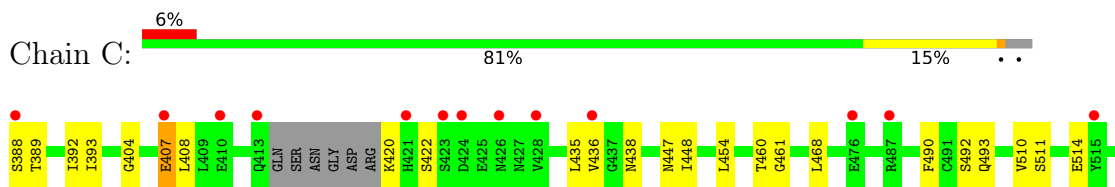
- Molecule 1: Cystic fibrosis transmembrane conductance regulator

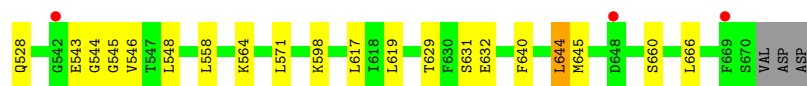


- Molecule 1: Cystic fibrosis transmembrane conductance regulator

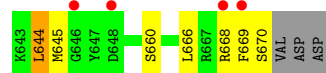
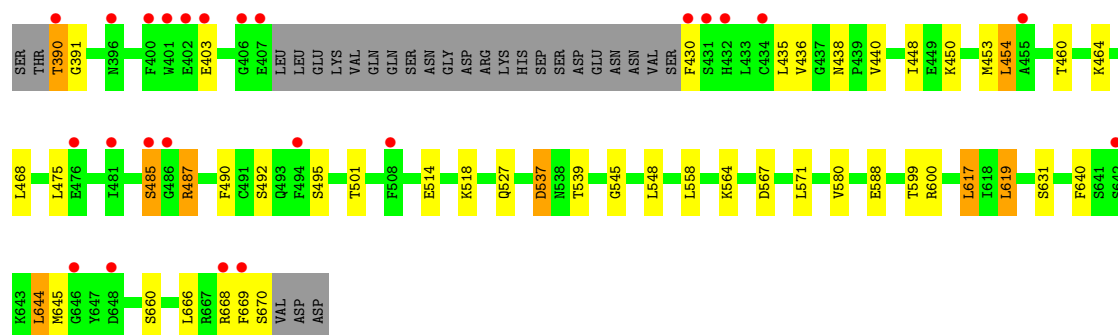
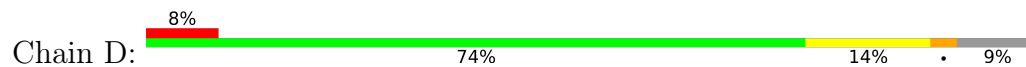


- Molecule 1: Cystic fibrosis transmembrane conductance regulator





- Molecule 1: Cystic fibrosis transmembrane conductance regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.33Å 171.33Å 109.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 2.35 24.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.00-2.35) 97.7 (24.02-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.36Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.258 0.229 , 0.260	Depositor DCC
R_{free} test set	3406 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtrriage
Anisotropy	0.002	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9044	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: MG, ACY, ATP, SEP

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	0.72	0/2179	0.73	0/2927
1	B	0.76	0/2177	0.75	1/2925 (0.0%)
1	C	0.73	0/2192	0.72	0/2945
1	D	0.75	0/2058	0.75	1/2766 (0.0%)
All	All	0.74	0/8606	0.74	2/11563 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	667	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	D	537	ASP	CB-CG-OD1	-5.69	113.18	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	411	LYS	Peptide
1	B	579	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	611	ARG	Sidechain
1	D	390	THR	Peptide
1	D	485	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2185	0	2151	42	0
1	B	2175	0	2152	46	0
1	C	2190	0	2164	20	0
1	D	2050	0	2029	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	5	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	1	0
5	A	74	0	0	11	0
5	B	88	0	0	13	0
5	C	79	0	0	2	0
5	D	59	0	0	2	0
All	All	9044	0	8556	126	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 7.

All (126) 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:B:411:LYS:O	1:B:412:VAL:HG13	1.68	0.92
1:D:588:GLU:HG2	5:D:234:HOH:O	1.70	0.90
1:A:436:VAL:HB	1:A:438:ASN:HD21	1.46	0.80
1:A:390:THR:HA	1:A:450:LYS:HE2	1.64	0.79
1:C:436:VAL:HB	1:C:438:ASN:HD21	1.51	0.74
1:D:487:ARG:HG3	1:D:567:ASP:OD2	1.88	0.74
1:A:565:ASP:OD2	5:A:125:HOH:O	2.06	0.73
1:D:390:THR:N	1:D:450:LYS:HZ3	1.87	0.73
1:C:389:THR:HG21	1:C:598:LYS:HA	1.68	0.72
3:B:675:ATP:O1A	5:B:9:HOH:O	2.10	0.69
1:A:629:THR:OG1	1:A:632:GLU:HG3	1.92	0.69
1:C:629:THR:OG1	1:C:632:GLU:HG3	1.94	0.68
1:B:409:LEU:HD13	5:B:9:HOH:O	1.94	0.67
1:A:543:GLU:HA	1:B:423:SER:O	1.95	0.67
1:D:490:PHE:CE2	1:D:492:SER:HB3	2.30	0.66
1:A:544:GLY:O	1:B:427:ASN:OD1	2.12	0.66
1:B:639:ASP:HB3	1:B:669:PHE:CE2	2.31	0.66
1:B:461:GLY:O	3:B:675:ATP:H3'	1.96	0.65
1:B:420:LYS:N	5:B:284:HOH:O	2.30	0.65
1:A:390:THR:HA	1:A:450:LYS:CE	2.29	0.63
1:C:543:GLU:C	1:C:545:GLY:H	2.02	0.62
1:D:436:VAL:HB	1:D:438:ASN:HD21	1.65	0.61
1:B:514:GLU:OE2	1:B:518:LYS:HE2	2.01	0.61
1:A:420:LYS:N	1:A:656:GLU:OE1	2.36	0.59
1:C:543:GLU:HB2	1:C:546:VAL:H	1.66	0.58
1:B:442:LYS:HE3	5:B:266:HOH:O	2.02	0.58
1:B:668:ARG:HB3	1:B:669:PHE:CE1	2.39	0.57
1:B:515:TYR:O	1:B:519:SER:HB2	2.05	0.57
1:B:436:VAL:HB	1:B:438:ASN:HD21	1.69	0.57
1:A:527:GLN:HG2	5:A:212:HOH:O	2.05	0.56
1:B:411:LYS:C	1:B:412:VAL:HG22	2.26	0.56
1:A:390:THR:HG23	1:A:450:LYS:HE2	1.87	0.56
1:A:430:PHE:HE1	5:A:293:HOH:O	1.89	0.56
1:B:522:LYS:HE2	5:B:301:HOH:O	2.05	0.56
1:A:503:LYS:HG3	1:A:517:TYR:CZ	2.40	0.56
1:B:657:ARG:HD3	5:B:59:HOH:O	2.06	0.56
1:C:404:GLY:O	1:C:407:GLU:HG2	2.06	0.55
1:B:524:CYS:O	1:B:555:ARG:HD2	2.06	0.55
1:C:436:VAL:CB	1:C:438:ASN:HD21	2.18	0.55
1:A:598:LYS:NZ	5:A:125:HOH:O	2.39	0.55
1:D:440:VAL:HG11	1:D:475:LEU:HD21	1.88	0.54
1:B:389:THR:N	1:B:567:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:HG22	1:A:450:LYS:HG3	1.90	0.54
1:A:401:TRP:HH2	5:A:293:HOH:O	1.91	0.53
1:C:543:GLU:C	1:C:545:GLY:N	2.60	0.53
1:C:490:PHE:CE2	1:C:492:SER:HB3	2.44	0.53
1:A:390:THR:HB	5:A:4:HOH:O	2.08	0.53
1:D:514:GLU:OE2	1:D:518:LYS:HE2	2.08	0.53
1:B:409:LEU:CD1	5:B:9:HOH:O	2.54	0.53
1:B:404:GLY:O	1:B:407:GLU:HG2	2.09	0.52
1:A:436:VAL:CB	1:A:438:ASN:HD21	2.19	0.51
1:B:420:LYS:N	1:B:656:GLU:OE1	2.44	0.51
1:A:461:GLY:O	3:A:675:ATP:H3'	2.10	0.51
1:A:390:THR:HA	1:A:450:LYS:NZ	2.26	0.51
1:B:409:LEU:HD22	5:B:9:HOH:O	2.11	0.50
1:B:464:LYS:HZ3	3:B:675:ATP:PB	2.35	0.50
1:D:391:GLY:HA2	1:D:448:ILE:O	2.10	0.50
1:D:390:THR:HG21	1:D:599:THR:HB	1.92	0.50
1:A:490:PHE:CE2	1:A:492:SER:HB3	2.46	0.50
1:A:527:GLN:CG	5:A:112:HOH:O	2.59	0.50
1:A:390:THR:HG22	1:A:450:LYS:H	1.77	0.49
1:C:392:ILE:CG2	1:C:448:ILE:HB	2.43	0.49
1:C:436:VAL:HB	1:C:438:ASN:ND2	2.25	0.49
1:B:392:ILE:HG22	1:B:448:ILE:HB	1.95	0.49
3:B:675:ATP:PA	5:B:9:HOH:O	2.71	0.49
1:D:640:PHE:CZ	1:D:644:LEU:HD13	2.48	0.49
1:C:493:GLN:HG2	5:C:149:HOH:O	2.11	0.49
1:A:453:MET:HG2	1:A:600:ARG:HG3	1.94	0.48
1:A:581:PHE:HE2	1:A:652:GLN:HE22	1.60	0.48
1:A:404:GLY:O	1:A:407:GLU:HG2	2.14	0.48
1:C:528:GLN:HB2	5:C:222:HOH:O	2.13	0.48
1:A:654:THR:O	1:A:658:ARG:HG3	2.14	0.48
1:D:390:THR:HG21	1:D:599:THR:CB	2.43	0.47
1:A:524:CYS:O	1:A:555:ARG:HD2	2.14	0.47
1:D:464:LYS:N	3:D:675:ATP:O1B	2.48	0.47
1:A:440:VAL:HG11	1:A:475:LEU:HD21	1.96	0.47
1:B:490:PHE:CE2	1:B:492:SER:HB3	2.50	0.46
1:C:461:GLY:O	3:C:675:ATP:H3'	2.15	0.46
1:B:392:ILE:CG2	1:B:448:ILE:HB	2.46	0.46
1:A:474:GLU:HG3	1:B:435:LEU:HD11	1.98	0.45
1:B:543:GLU:C	1:B:545:GLY:H	2.18	0.45
1:D:490:PHE:CZ	1:D:492:SER:HB3	2.52	0.45
1:B:503:LYS:HD3	1:B:517:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:LEU:HD12	1:C:435:LEU:HA	1.85	0.45
1:B:669:PHE:N	1:B:669:PHE:CD1	2.83	0.45
1:A:543:GLU:C	1:A:545:GLY:H	2.21	0.45
1:B:640:PHE:CZ	1:B:644:LEU:HD13	2.51	0.45
1:D:545:GLY:HA2	4:D:676:ACY:O	2.17	0.45
1:A:527:GLN:HB2	5:A:112:HOH:O	2.16	0.44
1:A:487:ARG:HA	5:A:148:HOH:O	2.17	0.44
1:B:545:GLY:O	1:B:548:LEU:HB2	2.18	0.44
1:B:558:LEU:HD22	1:B:562:VAL:HG23	2.00	0.44
1:A:510:VAL:HG13	5:A:5:HOH:O	2.18	0.44
1:D:495:SER:HA	5:D:181:HOH:O	2.18	0.43
1:D:448:ILE:HD11	1:D:454:LEU:HG	2.01	0.43
1:A:537:ASP:OD1	1:A:537:ASP:N	2.51	0.43
1:C:510:VAL:HG12	1:C:511:SER:N	2.33	0.43
1:D:435:LEU:HA	1:D:435:LEU:HD12	1.93	0.43
1:A:527:GLN:HG2	5:A:112:HOH:O	2.19	0.43
1:B:435:LEU:HA	1:B:435:LEU:HD12	1.84	0.43
1:A:412:VAL:O	1:A:413:GLN:CB	2.67	0.43
1:C:392:ILE:HG23	1:C:448:ILE:HB	2.01	0.43
1:B:668:ARG:HG3	5:B:109:HOH:O	2.19	0.42
1:C:393:ILE:HG12	1:C:447:ASN:OD1	2.18	0.42
1:D:390:THR:HG22	1:D:391:GLY:N	2.33	0.42
1:B:436:VAL:HA	5:B:166:HOH:O	2.18	0.42
1:B:600:ARG:HG2	1:B:600:ARG:HH11	1.85	0.42
1:B:464:LYS:NZ	3:B:675:ATP:PB	2.92	0.42
1:B:541:LEU:C	1:B:543:GLU:H	2.23	0.42
1:C:543:GLU:O	1:C:545:GLY:N	2.46	0.42
1:D:617:LEU:HD22	1:D:619:LEU:HD13	2.02	0.42
1:B:409:LEU:CD2	5:B:9:HOH:O	2.69	0.41
1:B:426:ASN:HA	1:B:426:ASN:HD22	1.72	0.41
1:C:640:PHE:CZ	1:C:644:LEU:HD13	2.55	0.41
1:A:499:PRO:HG3	1:B:424:ASP:O	2.20	0.41
1:B:493:GLN:HB2	5:B:276:HOH:O	2.20	0.41
1:D:501:THR:HA	1:D:539:THR:O	2.21	0.41
1:A:438:ASN:HA	1:A:439:PRO:HD3	2.00	0.41
1:A:640:PHE:CZ	1:A:644:LEU:HD13	2.56	0.41
1:B:629:THR:OG1	1:B:632:GLU:HG3	2.21	0.41
1:D:453:MET:CG	1:D:600:ARG:HG3	2.51	0.40
1:B:409:LEU:O	1:B:412:VAL:CG2	2.69	0.40
1:B:588:GLU:O	1:B:592:CYS:HB2	2.21	0.40
1:A:393:ILE:HG12	1:A:447:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:MET:SD	1:B:428:VAL:HG22	2.62	0.40
1:A:543:GLU:C	1:A:545:GLY:N	2.75	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	268/286 (94%)	260 (97%)	7 (3%)	1 (0%)	34 38
1	B	268/286 (94%)	254 (95%)	13 (5%)	1 (0%)	34 38
1	C	270/286 (94%)	257 (95%)	12 (4%)	1 (0%)	34 38
1	D	253/286 (88%)	235 (93%)	15 (6%)	3 (1%)	13 11
All	All	1059/1144 (93%)	1006 (95%)	47 (4%)	6 (1%)	25 27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	668	ARG
1	D	669	PHE
1	A	542	GLY
1	D	537	ASP
1	C	544	GLY
1	B	542	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/248 (96%)	215 (90%)	23 (10%)	8	7
1	B	238/248 (96%)	220 (92%)	18 (8%)	13	13
1	C	240/248 (97%)	222 (92%)	18 (8%)	13	13
1	D	223/248 (90%)	204 (92%)	19 (8%)	10	10
All	All	939/992 (95%)	861 (92%)	78 (8%)	11	11

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	GLU
1	A	411	LYS
1	A	420	LYS
1	A	423	SER
1	A	435	LEU
1	A	449	GLU
1	A	454	LEU
1	A	460	THR
1	A	468	LEU
1	A	488	VAL
1	A	543	GLU
1	A	548	LEU
1	A	558	LEU
1	A	564	LYS
1	A	571	LEU
1	A	580	VAL
1	A	617	LEU
1	A	619	LEU
1	A	631	SER
1	A	644	LEU
1	A	645	MET
1	A	648	ASP
1	A	666	LEU
1	B	407	GLU
1	B	408	LEU
1	B	423	SER
1	B	449	GLU
1	B	454	LEU
1	B	460	THR
1	B	503	LYS

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Mol	Chain	Res	Type
1	B	519	SER
1	B	543	GLU
1	B	548	LEU
1	B	558	LEU
1	B	564	LYS
1	B	571	LEU
1	B	617	LEU
1	B	619	LEU
1	B	644	LEU
1	B	645	MET
1	B	666	LEU
1	C	388	SER
1	C	407	GLU
1	C	408	LEU
1	C	420	LYS
1	C	454	LEU
1	C	460	THR
1	C	468	LEU
1	C	514	GLU
1	C	548	LEU
1	C	558	LEU
1	C	564	LYS
1	C	571	LEU
1	C	617	LEU
1	C	619	LEU
1	C	631	SER
1	C	644	LEU
1	C	645	MET
1	C	666	LEU
1	D	403	GLU
1	D	430	PHE
1	D	454	LEU
1	D	460	THR
1	D	468	LEU
1	D	485	SER
1	D	487	ARG
1	D	527	GLN
1	D	548	LEU
1	D	558	LEU
1	D	564	LYS
1	D	571	LEU
1	D	580	VAL

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Mol	Chain	Res	Type
1	D	617	LEU
1	D	619	LEU
1	D	631	SER
1	D	644	LEU
1	D	645	MET
1	D	666	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	ASN
1	A	438	ASN
1	A	652	GLN
1	B	426	ASN
1	B	427	ASN
1	B	438	ASN
1	B	597	ASN
1	C	426	ASN
1	C	438	ASN
1	C	538	ASN
1	C	585	GLN
1	D	438	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	SEP	D	660	1	8,9,10	0.70	0	8,12,14	1.55	2 (25%)
1	SEP	A	670	1	8,9,10	1.78	3 (37%)	8,12,14	1.30	1 (12%)
1	SEP	C	670	1	4,5,10	0.90	0	0,5,14	0.00	-
1	SEP	C	660	1	8,9,10	1.05	1 (12%)	8,12,14	1.64	2 (25%)
1	SEP	B	659	1	4,5,10	0.75	0	0,5,14	0.00	-
1	SEP	A	659	1	8,9,10	2.10	4 (50%)	8,12,14	1.16	1 (12%)
1	SEP	C	422	1	8,9,10	2.02	3 (37%)	8,12,14	1.16	1 (12%)
1	SEP	B	422	1	8,9,10	1.90	3 (37%)	8,12,14	1.41	1 (12%)
1	SEP	A	422	1	8,9,10	1.96	3 (37%)	8,12,14	1.32	1 (12%)
1	SEP	D	659	1	4,5,10	0.56	0	0,5,14	0.00	-
1	SEP	B	670	1	4,5,10	1.59	1 (25%)	0,5,14	0.00	-
1	SEP	D	670	1	8,9,10	1.68	2 (25%)	8,12,14	1.34	1 (12%)
1	SEP	C	659	1	4,5,10	0.81	0	0,5,14	0.00	-
1	SEP	B	660	1	8,9,10	1.05	0	8,12,14	2.92	4 (50%)
1	SEP	A	660	1	8,9,10	1.05	1 (12%)	8,12,14	2.08	4 (50%)

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
1	SEP	D	660	1	-	2/5/8/10	-
1	SEP	A	670	1	-	0/5/8/10	-
1	SEP	C	670	1	-	1/2/4/10	-
1	SEP	C	660	1	-	4/5/8/10	-
1	SEP	B	659	1	-	0/2/4/10	-
1	SEP	A	659	1	-	2/5/8/10	-
1	SEP	C	422	1	-	3/5/8/10	-
1	SEP	B	422	1	-	3/5/8/10	-
1	SEP	A	422	1	-	3/5/8/10	-
1	SEP	D	659	1	-	2/2/4/10	-
1	SEP	B	670	1	-	2/2/4/10	-
1	SEP	D	670	1	-	2/5/8/10	-
1	SEP	C	659	1	-	2/2/4/10	-
1	SEP	B	660	1	-	3/5/8/10	-
1	SEP	A	660	1	-	3/5/8/10	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	422	SEP	P-O1P	3.87	1.63	1.50
1	B	422	SEP	P-O1P	3.76	1.62	1.50
1	A	422	SEP	P-O1P	3.75	1.62	1.50
1	A	659	SEP	P-O1P	3.74	1.62	1.50
1	A	670	SEP	P-O1P	3.35	1.61	1.50
1	D	670	SEP	P-O1P	3.17	1.60	1.50
1	A	659	SEP	P-O2P	2.77	1.65	1.54
1	B	670	SEP	CB-CA	2.76	1.59	1.53
1	A	659	SEP	P-O3P	2.65	1.65	1.54
1	C	660	SEP	P-O1P	2.55	1.58	1.50
1	A	422	SEP	P-O3P	2.55	1.64	1.54
1	C	422	SEP	P-O2P	2.48	1.64	1.54
1	C	422	SEP	P-O3P	2.48	1.64	1.54
1	A	660	SEP	P-O1P	2.46	1.58	1.50
1	B	422	SEP	P-O3P	2.36	1.64	1.54
1	A	422	SEP	P-O2P	2.35	1.63	1.54
1	D	670	SEP	P-O2P	2.30	1.63	1.54
1	A	670	SEP	P-O2P	2.26	1.63	1.54
1	B	422	SEP	P-O2P	2.20	1.63	1.54
1	A	670	SEP	P-O3P	2.06	1.62	1.54
1	A	659	SEP	P-OG	2.05	1.66	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	660	SEP	OG-CB-CA	-5.98	102.33	108.14
1	B	660	SEP	O3P-P-OG	-3.42	97.63	106.73
1	A	660	SEP	OG-CB-CA	-3.27	104.97	108.14
1	B	660	SEP	O3P-P-O1P	3.14	122.98	110.68
1	B	660	SEP	O2P-P-OG	3.10	114.97	106.73
1	A	660	SEP	O3P-P-O1P	3.04	122.57	110.68
1	B	422	SEP	O3P-P-O1P	2.77	121.53	110.68
1	D	660	SEP	O2P-P-OG	2.76	114.09	106.73
1	A	422	SEP	O3P-P-O1P	2.75	121.44	110.68
1	C	660	SEP	O3P-P-O1P	2.74	121.41	110.68
1	C	660	SEP	O3P-P-OG	-2.72	99.48	106.73
1	A	660	SEP	O2P-P-OG	2.72	113.97	106.73
1	C	422	SEP	O3P-P-O1P	2.72	121.32	110.68
1	A	670	SEP	O3P-P-O1P	2.59	120.81	110.68
1	D	670	SEP	O3P-P-O1P	2.40	120.09	110.68
1	A	660	SEP	O3P-P-OG	-2.39	100.37	106.73
1	A	659	SEP	O3P-P-O1P	2.39	120.02	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	660	SEP	O3P-P-O1P	2.30	119.70	110.68

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	660	SEP	N-CA-CB-OG
1	C	660	SEP	CB-OG-P-O1P
1	C	660	SEP	CB-OG-P-O2P
1	C	660	SEP	CB-OG-P-O3P
1	A	659	SEP	N-CA-CB-OG
1	C	422	SEP	CB-OG-P-O1P
1	C	422	SEP	CB-OG-P-O2P
1	C	422	SEP	CB-OG-P-O3P
1	B	422	SEP	CB-OG-P-O1P
1	B	422	SEP	CB-OG-P-O2P
1	B	422	SEP	CB-OG-P-O3P
1	A	422	SEP	CB-OG-P-O1P
1	A	422	SEP	CB-OG-P-O2P
1	A	422	SEP	CB-OG-P-O3P
1	D	659	SEP	C-CA-CB-OG
1	B	670	SEP	C-CA-CB-OG
1	D	670	SEP	N-CA-CB-OG
1	C	659	SEP	N-CA-CB-OG
1	C	659	SEP	C-CA-CB-OG
1	B	660	SEP	N-CA-CB-OG
1	B	660	SEP	CB-OG-P-O3P
1	A	660	SEP	N-CA-CB-OG
1	A	660	SEP	CB-OG-P-O1P
1	A	660	SEP	CB-OG-P-O3P
1	D	670	SEP	CB-OG-P-O1P
1	D	659	SEP	N-CA-CB-OG
1	B	670	SEP	N-CA-CB-OG
1	D	660	SEP	CB-OG-P-O3P
1	A	659	SEP	CA-CB-OG-P
1	B	660	SEP	CB-OG-P-O1P
1	C	670	SEP	N-CA-CB-OG
1	C	660	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	ATP	D	675	2	26,33,33	2.64	11 (42%)	31,52,52	3.37	9 (29%)
4	ACY	A	676	-	1,3,3	2.35	1 (100%)	0,3,3	0.00	-
4	ACY	C	676	-	1,3,3	3.05	1 (100%)	0,3,3	0.00	-
3	ATP	B	675	2	26,33,33	2.59	9 (34%)	31,52,52	3.52	9 (29%)
3	ATP	A	675	2	26,33,33	2.49	10 (38%)	31,52,52	3.42	8 (25%)
3	ATP	C	675	2	26,33,33	2.56	8 (30%)	31,52,52	3.44	8 (25%)
4	ACY	B	676	-	1,3,3	3.94	1 (100%)	0,3,3	0.00	-
4	ACY	D	676	-	1,3,3	3.32	1 (100%)	0,3,3	0.00	-

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	ATP	A	675	2	-	4/18/38/38	0/3/3/3
3	ATP	C	675	2	-	4/18/38/38	0/3/3/3
3	ATP	B	675	2	-	5/18/38/38	0/3/3/3
3	ATP	D	675	2	-	5/18/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	675	ATP	O4'-C1'	6.87	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	675	ATP	O4'-C1'	6.80	1.50	1.41
3	A	675	ATP	O4'-C1'	6.79	1.50	1.41
3	B	675	ATP	O4'-C1'	6.72	1.50	1.41
3	C	675	ATP	C4-N3	6.28	1.44	1.35
3	B	675	ATP	C4-N3	6.13	1.44	1.35
3	A	675	ATP	C4-N3	5.78	1.43	1.35
3	D	675	ATP	O5'-C5'	-5.52	1.23	1.44
3	D	675	ATP	C4-N3	5.50	1.43	1.35
3	B	675	ATP	O5'-C5'	-5.15	1.25	1.44
3	A	675	ATP	O5'-C5'	-4.88	1.26	1.44
3	C	675	ATP	O5'-C5'	-4.79	1.26	1.44
3	C	675	ATP	PA-O5'	-4.13	1.42	1.59
4	B	676	ACY	CH3-C	3.94	1.53	1.48
3	D	675	ATP	PA-O5'	-3.76	1.44	1.59
3	B	675	ATP	C2'-C1'	3.72	1.59	1.53
3	B	675	ATP	PA-O5'	-3.68	1.44	1.59
4	D	676	ACY	CH3-C	3.32	1.53	1.48
3	D	675	ATP	C2-N3	3.32	1.37	1.32
4	C	676	ACY	CH3-C	3.05	1.52	1.48
3	A	675	ATP	PA-O5'	-3.00	1.47	1.59
3	D	675	ATP	PB-O1B	-2.98	1.40	1.50
3	D	675	ATP	C2'-C1'	2.88	1.58	1.53
3	A	675	ATP	C8-N7	-2.77	1.29	1.34
3	A	675	ATP	PB-O1B	-2.72	1.41	1.50
3	C	675	ATP	PB-O1B	-2.68	1.41	1.50
3	B	675	ATP	PB-O1B	-2.56	1.41	1.50
3	B	675	ATP	C2-N3	2.47	1.36	1.32
3	A	675	ATP	C2'-C1'	2.43	1.57	1.53
3	A	675	ATP	C2-N3	2.42	1.36	1.32
3	C	675	ATP	C2-N3	2.41	1.36	1.32
4	A	676	ACY	CH3-C	2.35	1.51	1.48
3	B	675	ATP	C8-N7	-2.20	1.30	1.34
3	D	675	ATP	C3'-C4'	-2.14	1.47	1.53
3	B	675	ATP	PB-O2B	-2.11	1.45	1.55
3	C	675	ATP	PB-O2B	-2.11	1.45	1.55
3	A	675	ATP	PG-O2G	-2.07	1.46	1.54
3	C	675	ATP	C2'-C1'	2.06	1.56	1.53
3	A	675	ATP	PB-O2B	-2.06	1.45	1.55
3	D	675	ATP	PA-O2A	-2.02	1.45	1.55
3	D	675	ATP	PB-O2B	-2.02	1.45	1.55
3	D	675	ATP	PG-O2G	-2.01	1.47	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	675	ATP	O5'-C5'-C4'	14.00	157.18	108.99
3	A	675	ATP	O5'-C5'-C4'	13.69	156.12	108.99
3	C	675	ATP	O5'-C5'-C4'	13.46	155.33	108.99
3	D	675	ATP	O5'-C5'-C4'	12.87	153.30	108.99
3	C	675	ATP	O5'-PA-O1A	-7.68	79.05	109.07
3	A	675	ATP	O5'-PA-O1A	-7.33	80.43	109.07
3	D	675	ATP	O5'-PA-O1A	-7.26	80.69	109.07
3	B	675	ATP	O5'-PA-O1A	-7.22	80.85	109.07
3	C	675	ATP	PA-O5'-C5'	6.98	162.62	121.68
3	B	675	ATP	PA-O5'-C5'	6.63	160.55	121.68
3	A	675	ATP	PA-O5'-C5'	6.56	160.12	121.68
3	D	675	ATP	C5'-C4'-C3'	-5.96	92.85	115.18
3	B	675	ATP	C5'-C4'-C3'	-5.60	94.21	115.18
3	D	675	ATP	PA-O5'-C5'	5.33	152.95	121.68
3	A	675	ATP	C5'-C4'-C3'	-5.13	95.96	115.18
3	C	675	ATP	C5'-C4'-C3'	-4.72	97.49	115.18
3	D	675	ATP	O4'-C4'-C3'	4.14	113.31	105.11
3	D	675	ATP	C3'-C2'-C1'	3.60	106.39	100.98
3	B	675	ATP	C4-C5-N7	3.06	112.58	109.40
3	A	675	ATP	C4-C5-N7	2.95	112.47	109.40
3	C	675	ATP	C4-C5-N7	2.86	112.38	109.40
3	D	675	ATP	C4-C5-N7	2.76	112.28	109.40
3	B	675	ATP	O2A-PA-O5'	-2.54	95.93	107.75
3	A	675	ATP	C3'-C2'-C1'	2.49	104.73	100.98
3	C	675	ATP	O4'-C4'-C3'	2.38	109.83	105.11
3	D	675	ATP	O2A-PA-O1A	2.38	124.01	112.24
3	B	675	ATP	O4'-C4'-C3'	2.35	109.77	105.11
3	C	675	ATP	C1'-N9-C4	-2.31	122.59	126.64
3	B	675	ATP	O2B-PB-O1B	2.27	123.45	112.24
3	A	675	ATP	O4'-C4'-C3'	2.22	109.51	105.11
3	C	675	ATP	O4'-C4'-C5'	-2.19	102.18	109.37
3	D	675	ATP	O2A-PA-O5'	-2.17	97.66	107.75
3	B	675	ATP	C3'-C2'-C1'	2.03	104.03	100.98
3	A	675	ATP	O2B-PB-O1B	2.00	122.14	112.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	675	ATP	PB-O3B-PG-O2G
3	B	675	ATP	PB-O3B-PG-O2G
3	C	675	ATP	PB-O3B-PG-O2G
3	A	675	ATP	PB-O3B-PG-O1G

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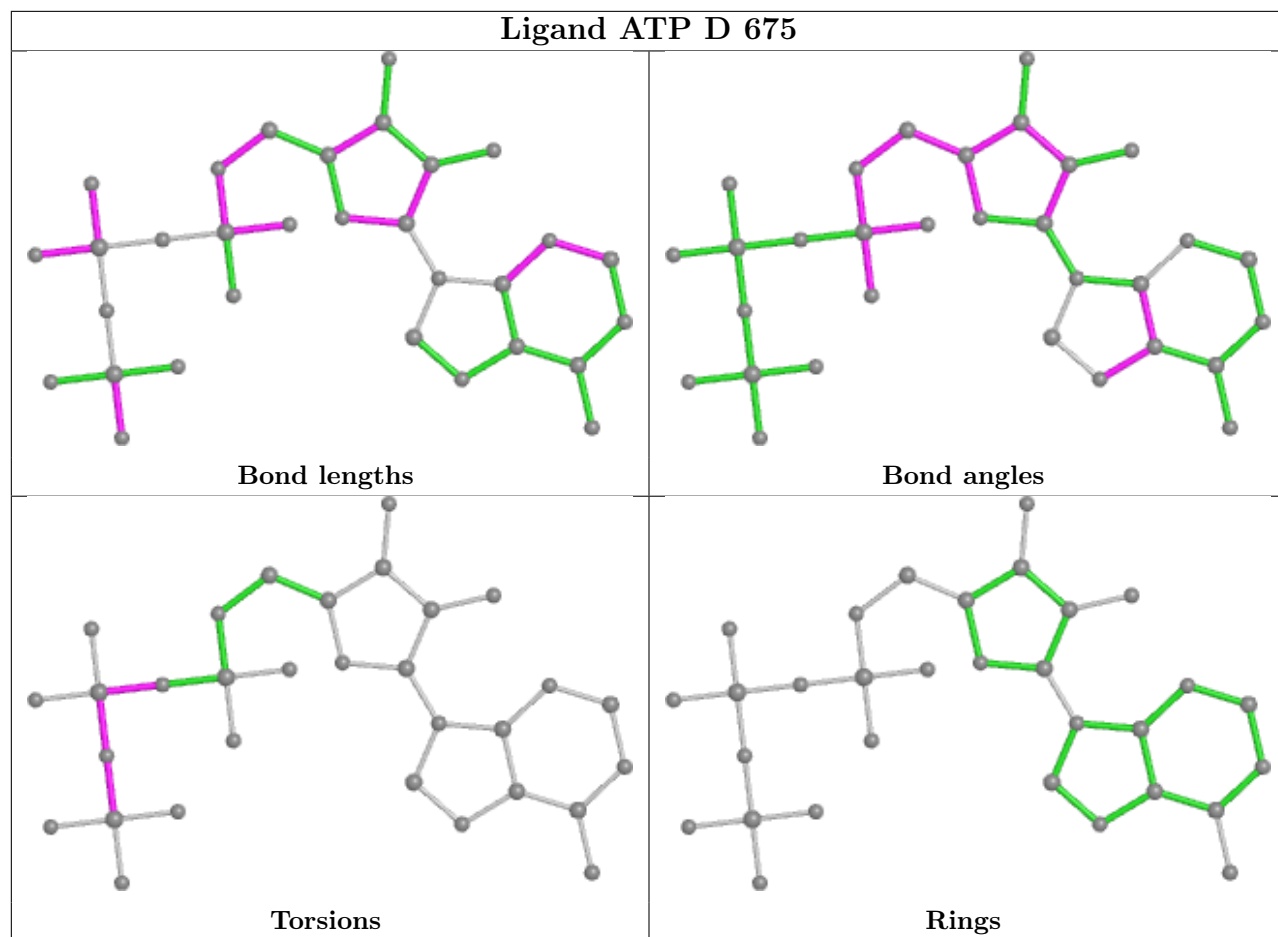
Mol	Chain	Res	Type	Atoms
3	D	675	ATP	PG-O3B-PB-O2B
3	B	675	ATP	PG-O3B-PB-O2B
3	A	675	ATP	PG-O3B-PB-O2B
3	B	675	ATP	C4'-C5'-O5'-PA
3	D	675	ATP	PA-O3A-PB-O2B
3	B	675	ATP	PA-O3A-PB-O2B
3	C	675	ATP	PG-O3B-PB-O2B
3	A	675	ATP	C4'-C5'-O5'-PA
3	C	675	ATP	C4'-C5'-O5'-PA
3	D	675	ATP	PB-O3B-PG-O1G
3	B	675	ATP	PB-O3B-PG-O1G
3	A	675	ATP	PA-O3A-PB-O2B
3	D	675	ATP	PA-O3A-PB-O1B
3	C	675	ATP	PA-O3A-PB-O2B

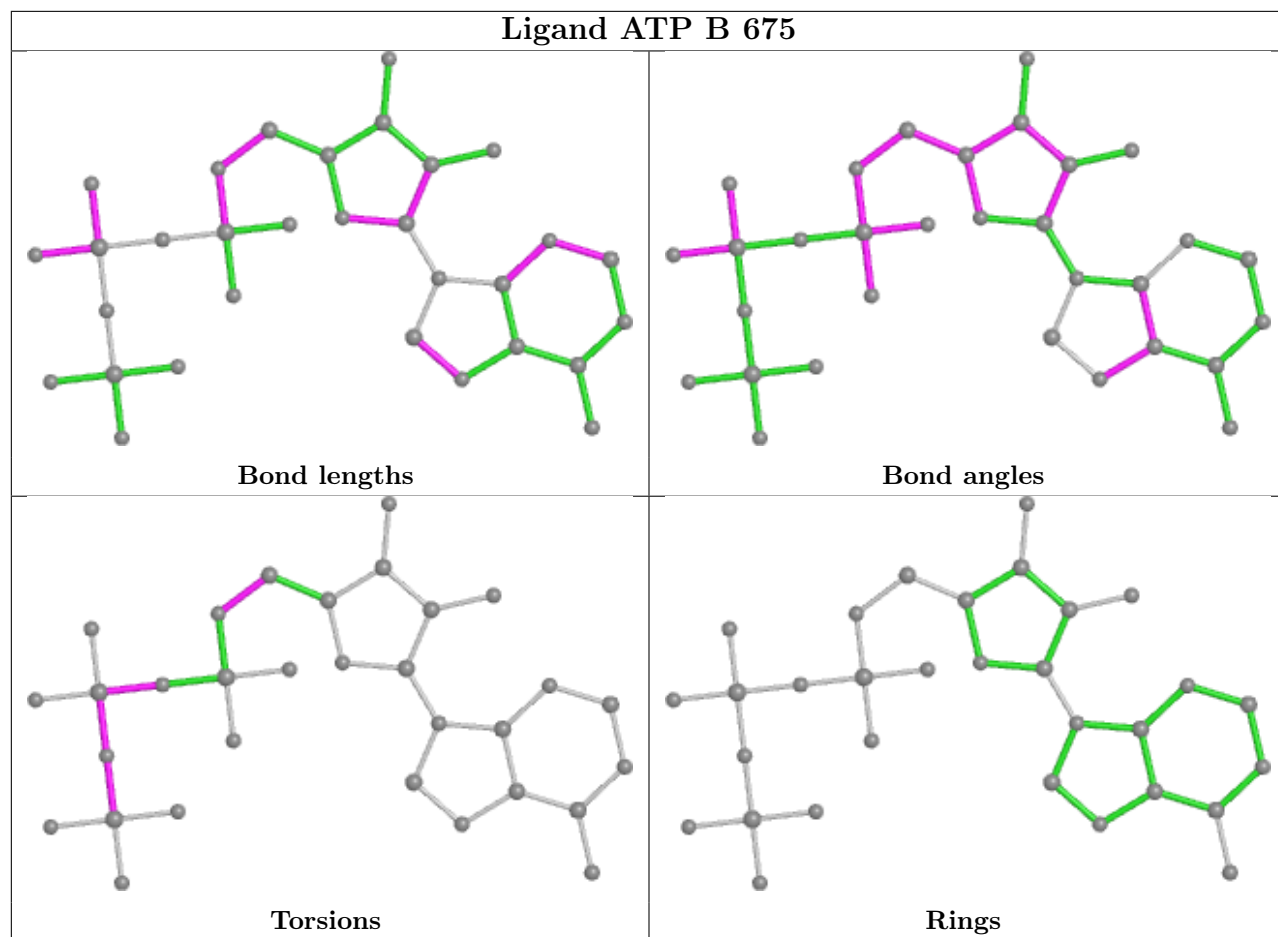
There are no ring outliers.

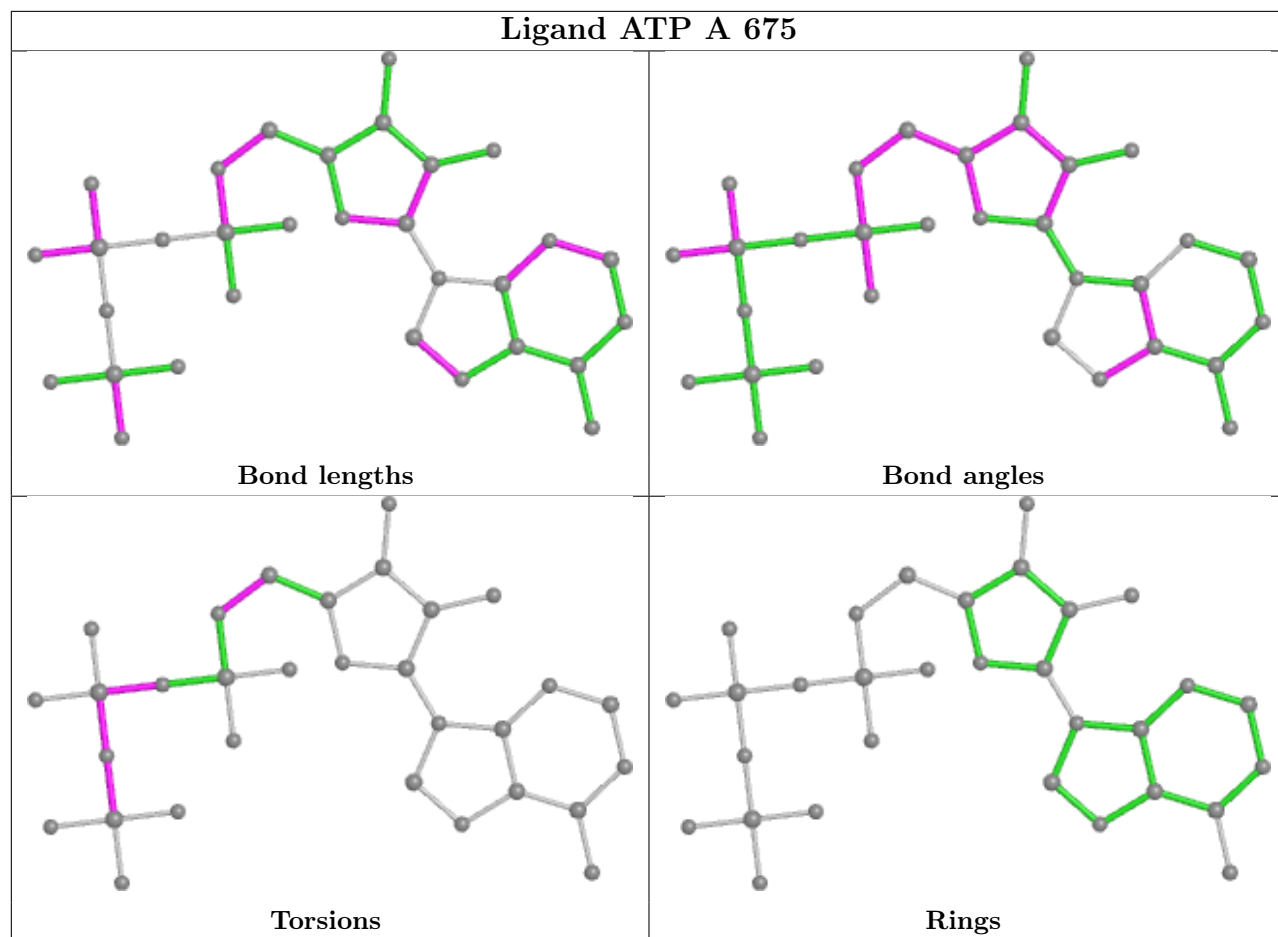
5 monomers are involved in 9 short contacts:

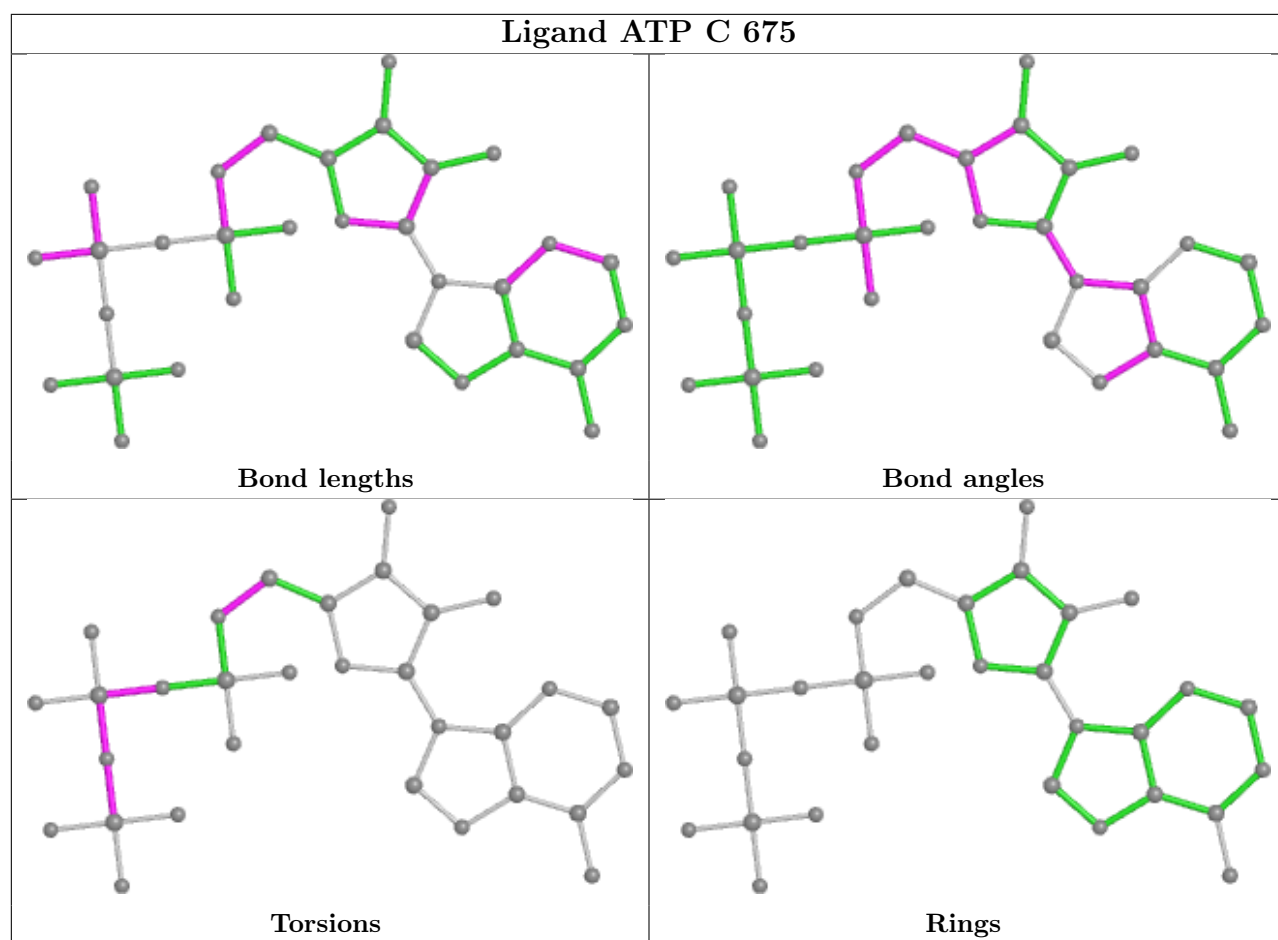
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	675	ATP	1	0
3	B	675	ATP	5	0
3	A	675	ATP	1	0
3	C	675	ATP	1	0
4	D	676	ACY	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	271/286 (94%)	0.31	20 (7%) 14 22	27, 46, 68, 73	0
1	B	271/286 (94%)	0.23	17 (6%) 20 29	29, 46, 68, 73	0
1	C	273/286 (95%)	0.25	16 (5%) 22 33	26, 44, 68, 81	0
1	D	256/286 (89%)	0.34	24 (9%) 8 13	28, 47, 70, 86	0
All	All	1071/1144 (93%)	0.28	77 (7%) 15 23	26, 45, 69, 86	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	ASN	6.3
1	B	426	ASN	5.5
1	C	423	SER	5.3
1	D	407	GLU	5.3
1	B	390	THR	5.2
1	B	542	GLY	5.0
1	C	421	HIS	4.6
1	C	426	ASN	4.6
1	A	428	VAL	4.6
1	D	434	CYS	4.4
1	D	430	PHE	4.4
1	A	425	GLU	4.3
1	A	424	ASP	4.3
1	D	401	TRP	4.2
1	B	648	ASP	4.1
1	A	390	THR	4.1
1	A	427	ASN	4.0
1	A	423	SER	4.0
1	D	648	ASP	3.9
1	D	390	THR	3.8
1	A	487	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	669	PHE	3.6
1	D	431	SER	3.5
1	C	424	ASP	3.5
1	A	413	GLN	3.4
1	C	542	GLY	3.4
1	D	669	PHE	3.3
1	C	669	PHE	3.2
1	C	648	ASP	3.2
1	B	389	THR	3.1
1	D	402	GLU	3.1
1	D	403	GLU	3.1
1	C	413	GLN	3.0
1	A	421	HIS	3.0
1	D	668	ARG	3.0
1	A	636	LEU	2.8
1	D	494	PHE	2.8
1	A	648	ASP	2.8
1	B	481	ILE	2.7
1	D	646	GLY	2.7
1	D	455	ALA	2.7
1	D	406	GLY	2.7
1	C	388	SER	2.6
1	B	511	SER	2.6
1	A	454	LEU	2.6
1	D	508	PHE	2.6
1	B	487	ARG	2.6
1	D	432	HIS	2.5
1	A	511	SER	2.5
1	C	436	VAL	2.5
1	D	481	ILE	2.5
1	A	410	GLU	2.4
1	B	485	SER	2.4
1	B	421	HIS	2.4
1	A	668	ARG	2.4
1	B	543	GLU	2.4
1	D	476	GLU	2.4
1	C	407	GLU	2.3
1	B	412	VAL	2.3
1	D	400	PHE	2.3
1	B	410	GLU	2.3
1	B	425	GLU	2.3
1	C	476	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	420	LYS	2.2
1	C	410	GLU	2.2
1	C	515	TYR	2.2
1	B	668	ARG	2.2
1	D	396	ASN	2.1
1	B	514	GLU	2.1
1	C	428	VAL	2.1
1	A	542	GLY	2.1
1	C	487	ARG	2.1
1	D	485	SER	2.1
1	B	636	LEU	2.1
1	D	642	SER	2.1
1	A	456	ILE	2.0
1	D	486	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	B	670	6/11	0.32	0.27	60,67,68,69	0
1	SEP	C	670	6/11	0.65	0.30	73,76,78,79	0
1	SEP	C	422	10/11	0.72	0.50	69,76,87,87	0
1	SEP	A	659	10/11	0.74	0.28	49,59,80,80	0
1	SEP	A	422	10/11	0.77	0.47	71,78,87,88	0
1	SEP	B	422	10/11	0.77	0.35	67,75,86,86	0
1	SEP	D	670	10/11	0.80	0.19	75,79,83,84	0
1	SEP	A	670	10/11	0.87	0.24	77,81,84,85	0
1	SEP	D	659	6/11	0.91	0.09	45,47,48,49	0
1	SEP	D	660	10/11	0.93	0.14	49,53,64,64	0
1	SEP	B	659	6/11	0.94	0.15	41,43,45,47	0
1	SEP	C	660	10/11	0.96	0.12	43,48,58,59	0
1	SEP	B	660	10/11	0.96	0.14	45,47,55,55	0
1	SEP	C	659	6/11	0.97	0.11	40,42,42,45	0
1	SEP	A	660	10/11	0.97	0.08	48,52,61,63	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

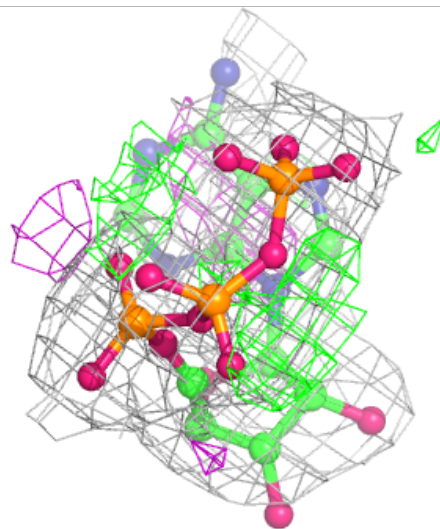
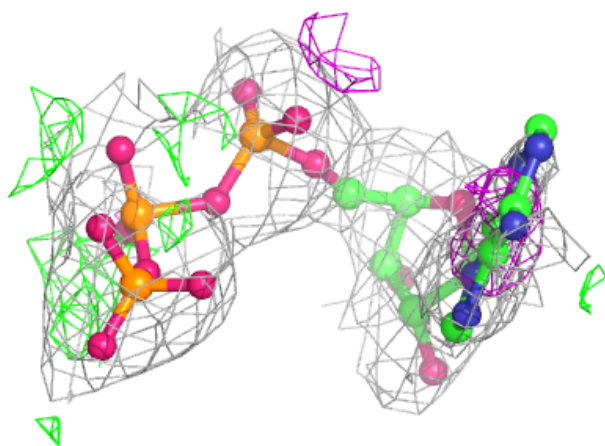
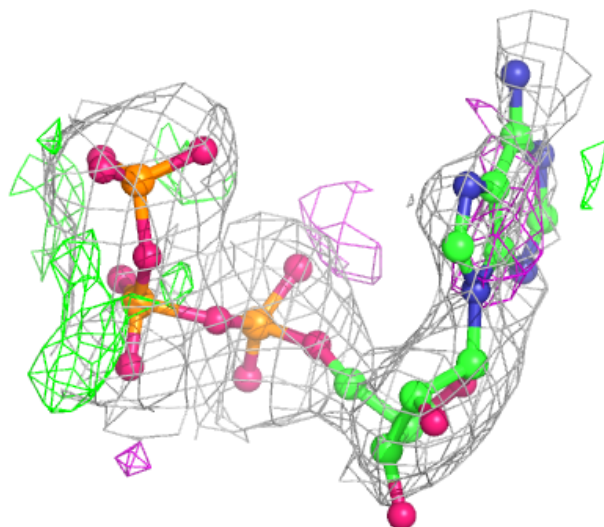
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	D	674	1/1	0.74	0.12	52,52,52,52	0
2	MG	A	674	1/1	0.89	0.16	39,39,39,39	0
3	ATP	D	675	31/31	0.89	0.20	54,71,81,81	0
2	MG	B	674	1/1	0.91	0.16	46,46,46,46	0
2	MG	C	674	1/1	0.94	0.19	41,41,41,41	0
3	ATP	A	675	31/31	0.94	0.16	43,58,64,65	0
3	ATP	B	675	31/31	0.94	0.15	44,55,68,69	0
3	ATP	C	675	31/31	0.95	0.15	37,49,59,60	0
4	ACY	C	676	4/4	0.96	0.11	37,37,39,40	0
4	ACY	A	676	4/4	0.97	0.13	34,35,37,37	0
4	ACY	B	676	4/4	0.97	0.14	38,38,39,39	0
4	ACY	D	676	4/4	0.97	0.12	46,46,46,47	0

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

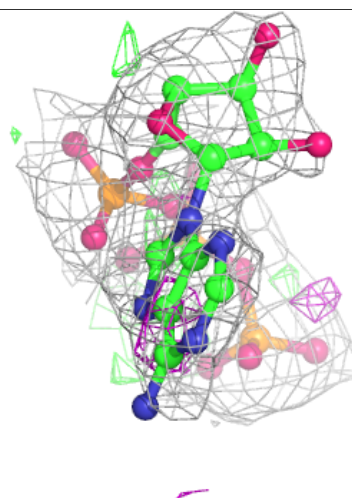
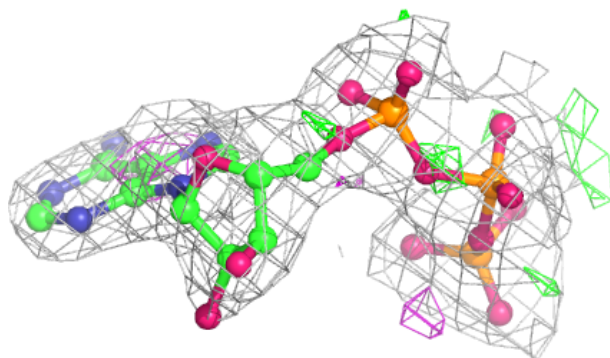
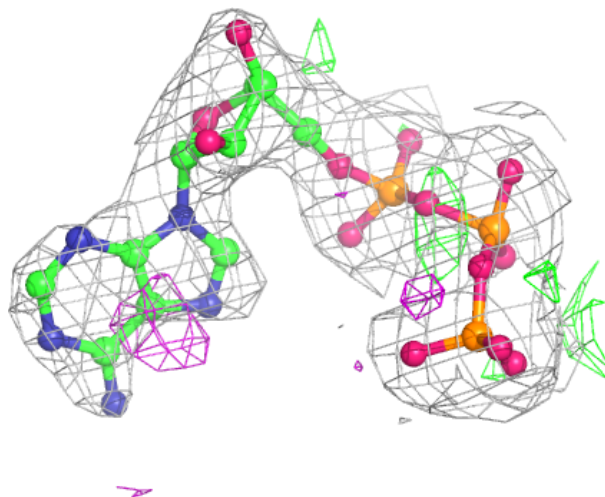
Electron density around ATP D 675:

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



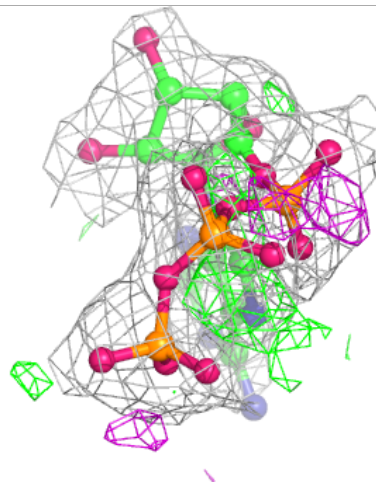
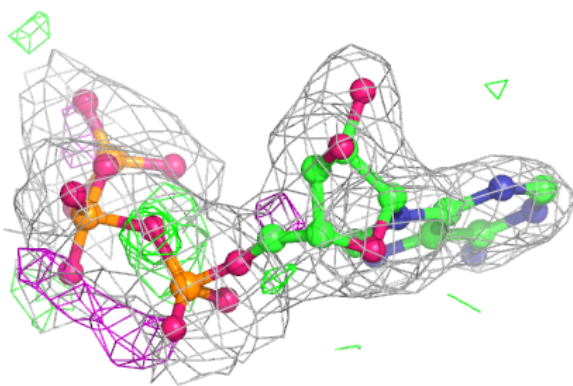
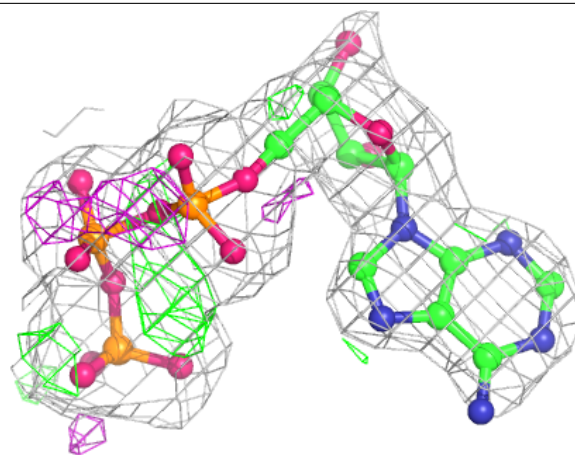
Electron density around ATP A 675:

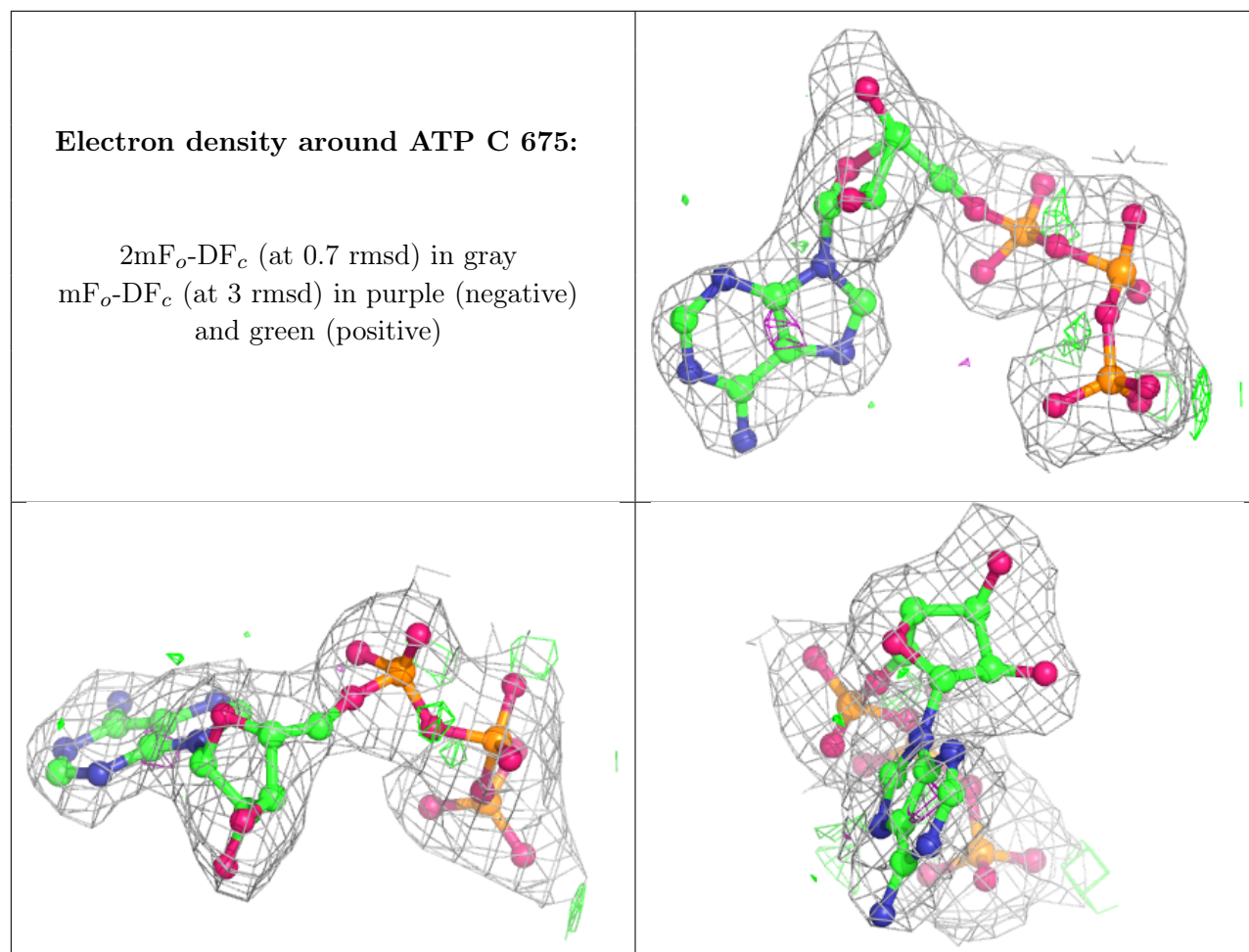
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP B 675:

$2mF_o-DF_c$ (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.