



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:56 am BST

PDB ID : 6FSA
Title : Beta-Cardiac myosin post-rigor
Authors : Robert-Paganin, J.; Auguin, D.; Houdusse, A.
Deposited on : 2018-02-19
Resolution : 2.33 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	:	2.11
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)	:	2.11

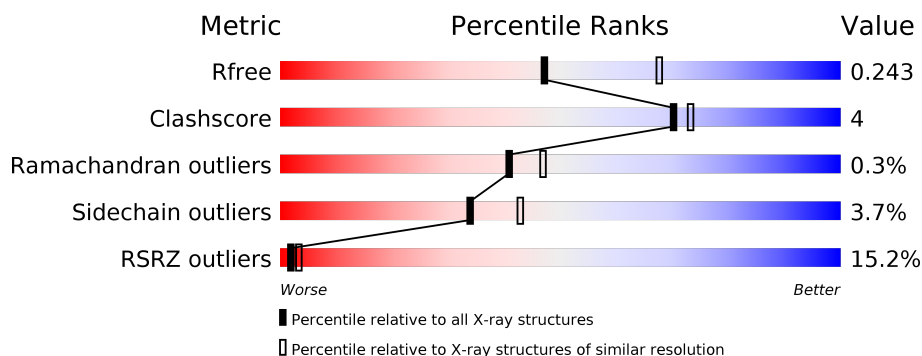
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on 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	1935	<div> <div style="width: 36%; background-color: red;"></div> <div style="width: 36%; background-color: orange;"></div> <div style="width: 36%; background-color: yellow;"></div> <div style="width: 36%; background-color: green;"></div> <div style="width: 60%; background-color: grey;"></div> </div>
1	B	1935	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 35%; background-color: orange;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 61%; background-color: green;"></div> <div style="width: 61%; background-color: grey;"></div> </div>
2	D	199	<div> <div style="width: 41%; background-color: red;"></div> <div style="width: 65%; background-color: orange;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 23%; background-color: green;"></div> <div style="width: 23%; background-color: grey;"></div> </div>
2	H	199	<div> <div style="width: 64%; background-color: red;"></div> <div style="width: 64%; background-color: orange;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 25%; background-color: green;"></div> <div style="width: 25%; background-color: grey;"></div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15508 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 Myosin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	783	Total	C	N	O	S	0	4	0
			6241	3978	1069	1162	32			
1	B	756	Total	C	N	O	S	0	5	0
			6021	3841	1023	1125	32			

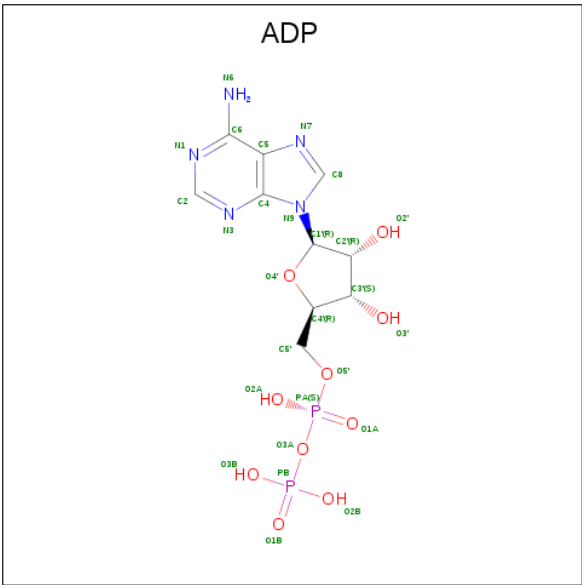
- Molecule 2 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	154	Total	C	N	O	S	0	0	0
			1215	766	201	240	8			
2	H	150	Total	C	N	O	S	0	0	0
			1178	742	196	232	8			

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

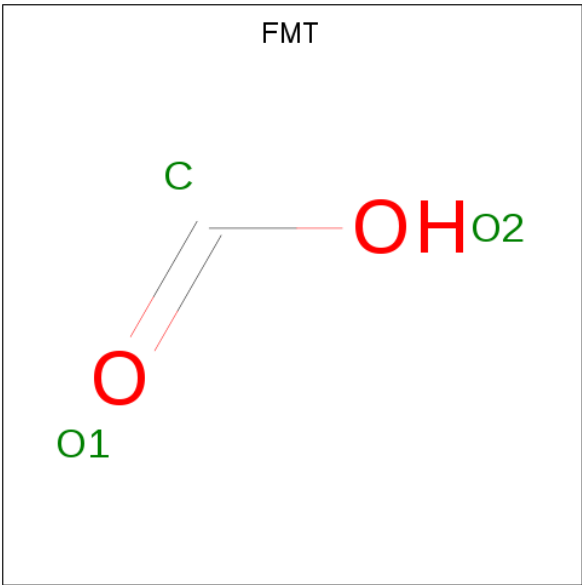
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

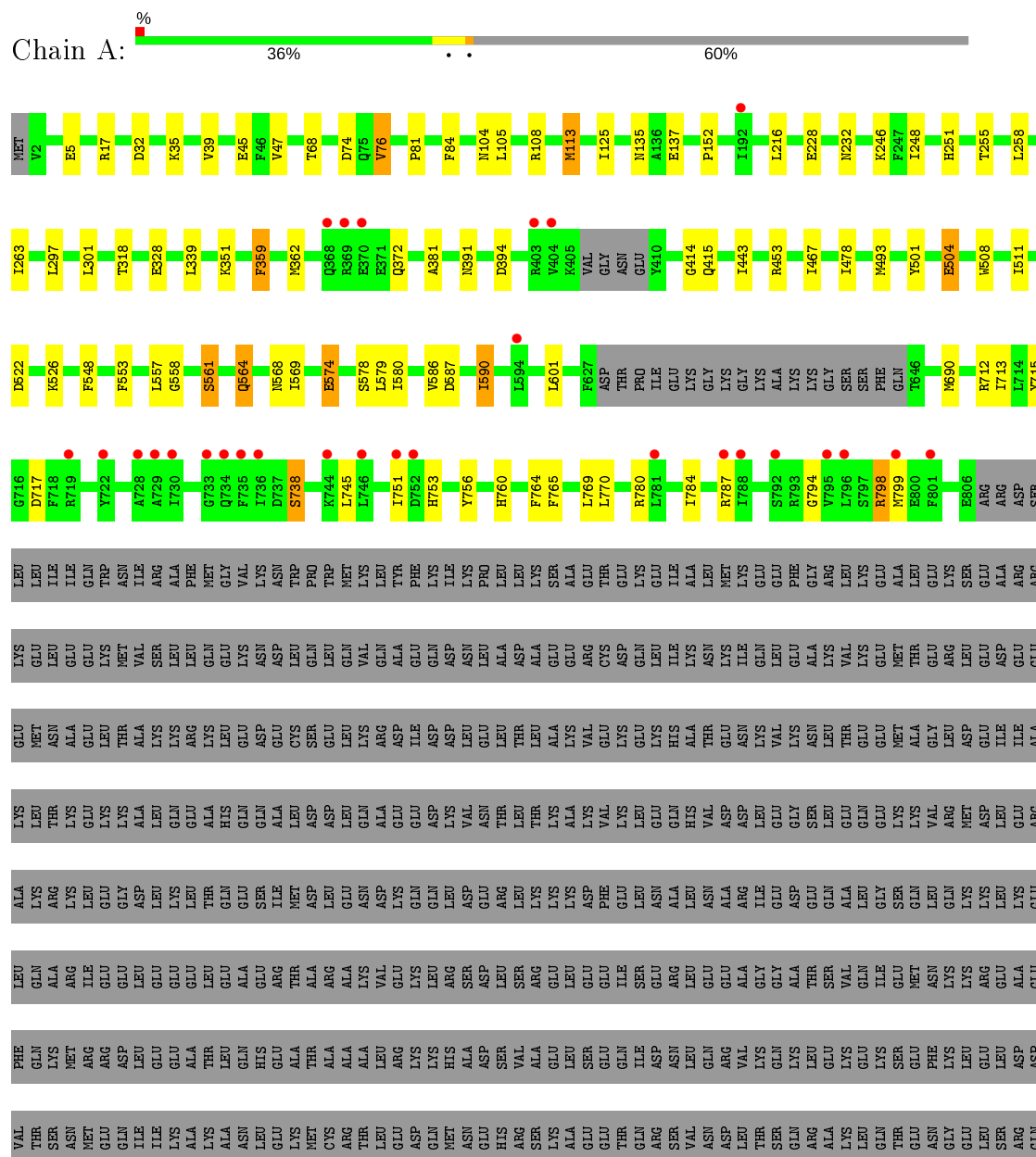
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	458	Total	O	0	0
			458	458		
7	B	314	Total	O	0	0
			314	314		
7	D	2	Total	O	0	0
			2	2		

3 Residue-property plots

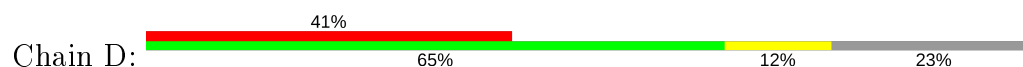
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

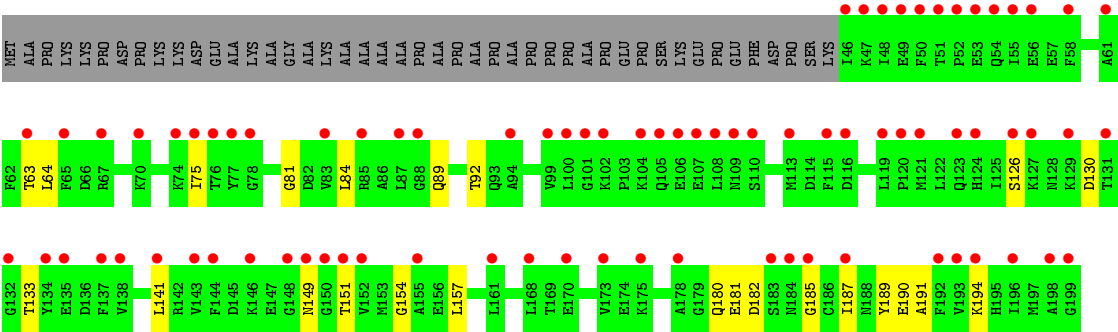
- Molecule 1: Myosin-7



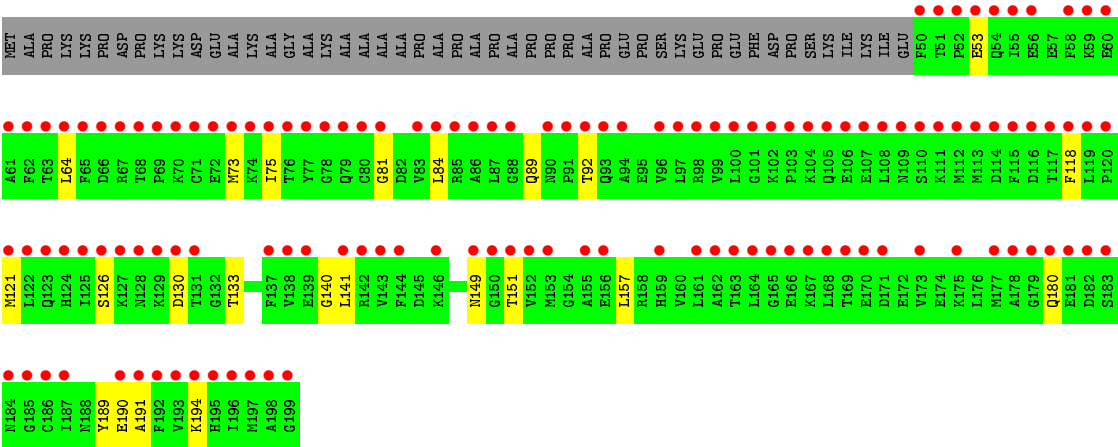


- Molecule 2: Myosin light chain 3





● Molecule 2: Myosin light chain 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.12Å 94.32Å 125.41Å 104.76° 92.34° 100.06°	Depositor
Resolution (Å)	47.97 – 2.33 47.97 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.97-2.33) 98.5 (47.97-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.227 0.204 , 0.243	Depositor DCC
R_{free} test set	4907 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15508	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, MLY, FMT, ADP, EDO

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	0.53	1/6358 (0.0%)	0.70	0/8579
1	B	0.50	0/6130	0.68	0/8273
2	D	0.44	0/1234	0.62	0/1657
2	H	0.43	0/1197	0.59	0/1608
All	All	0.50	1/14919 (0.0%)	0.68	0/20117

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	MET	SD-CE	-5.19	1.48	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	730	ILE	Mainchain

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	6241	0	6128	47	0
1	B	6021	0	5890	44	0
2	D	1215	0	1192	10	0
2	H	1178	0	1149	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	6	0	3	0	0
5	B	9	0	4	0	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
7	A	458	0	0	4	0
7	B	314	0	0	3	0
7	D	2	0	0	0	0
All	All	15508	0	14402	105	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 4.

All (105) 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:784:ILE:HD11	2:H:140:GLY:HA3	1.41	1.02
1:A:152:PRO:HD2	7:A:2143:HOH:O	1.77	0.84
1:A:493:MET:HE1	7:A:2300:HOH:O	1.87	0.75
1:A:493:MET:CE	7:A:2300:HOH:O	2.35	0.74
1:A:45:GLU:HG2	1:A:690:MET:HG3	1.69	0.73
1:B:784:ILE:CD1	2:H:140:GLY:HA3	2.20	0.68
1:A:504:GLU:HG3	1:A:760:HIS:H	1.58	0.68
1:B:301:LEU:HD22	1:B:351:LYS:HA	1.79	0.65
1:B:577:PHE:HE2	1:B:579:LEU:HD13	1.68	0.59
1:B:73:GLU:O	1:B:76:VAL:HG22	2.03	0.59
1:A:765:PHE:HD1	1:A:769:LEU:HD23	1.69	0.57
2:D:154:GLY:HA2	2:D:187:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:HA	1:A:362:MET:HE3	1.87	0.55
1:B:228:GLU:O	1:B:232:ASN:HB2	2.08	0.54
1:A:362:MET:HE2	1:A:381:ALA:HA	1.89	0.54
1:B:787:ARG:HH21	2:H:92:THR:HG23	1.72	0.54
1:A:301:LEU:HD22	1:A:351:LYS:HA	1.90	0.53
1:A:553:PHE:HD2	1:A:557:LEU:HD22	1.72	0.53
1:B:467:ILE:HG12	1:B:586:VAL:HG22	1.91	0.53
2:H:191:ALA:HA	2:H:194:LYS:HE3	1.90	0.53
1:A:557:LEU:O	1:A:557:LEU:HG	2.09	0.52
2:D:191:ALA:HA	2:D:194:LYS:HE3	1.90	0.52
1:A:32:ASP:HB3	1:A:35:LYS:HB2	1.92	0.51
1:A:228:GLU:O	1:A:232:ASN:HB2	2.09	0.51
1:A:216:LEU:HD23	1:A:258:LEU:HG	1.92	0.51
1:A:391:ASN:HD22	1:A:394:ASP:H	1.59	0.50
1:B:484[B]:LYS:HG3	1:B:655:LEU:HD21	1.94	0.50
1:B:391:ASN:HD22	1:B:394:ASP:H	1.58	0.50
1:B:723:ARG:HG3	1:B:730:ILE:HD13	1.93	0.50
1:B:765:PHE:HD2	1:B:769:LEU:HD23	1.75	0.50
1:A:104:ASN:O	1:A:108:ARG:HG3	2.13	0.49
1:B:72:LYS:HB2	1:B:75:GLN:HG3	1.95	0.48
1:B:216:LEU:HD23	1:B:258:LEU:HG	1.94	0.48
2:H:149:ASN:HD22	2:H:151:THR:HG22	1.78	0.48
2:D:189:TYR:O	2:D:190:GLU:HB3	2.14	0.48
2:D:89:GLN:HE22	2:D:126:SER:HA	1.79	0.47
1:A:504:GLU:HG2	1:A:764:PHE:HE1	1.79	0.47
1:B:297:LEU:O	1:B:301:LEU:HG	2.14	0.47
1:A:81:PRO:HG2	1:A:84:PHE:HD2	1.79	0.47
1:B:104:ASN:O	1:B:108:ARG:HG3	2.14	0.47
1:B:576:HIS:CG	1:B:590:ILE:HG13	2.49	0.47
1:A:753:HIS:HD2	1:A:756:TYR:OH	1.98	0.47
1:A:251:HIS:HB3	1:A:453:ARG:HG2	1.96	0.47
1:A:372:GLN:HE22	1:A:414:GLY:HA2	1.80	0.47
2:D:149:ASN:HD22	2:D:151:THR:HG22	1.79	0.47
1:A:246:LYS:HD2	1:A:248[B]:ILE:HD11	1.96	0.46
1:B:713:ILE:HD11	1:B:770:LEU:HD21	1.97	0.46
1:B:282:ASP:OD2	1:B:313:ILE:HG22	2.16	0.46
1:A:255:THR:O	1:A:255:THR:HG22	2.16	0.46
1:B:789:GLN:HA	1:B:792:SER:HB2	1.97	0.46
2:H:89:GLN:HE22	2:H:126:SER:HA	1.80	0.46
1:A:17:ARG:HA	1:A:113:MET:HE3	1.97	0.46
2:H:189:TYR:O	2:H:190:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:OD1	1:A:137:GLU:HB3	2.15	0.45
1:B:484[A]:LYS:HD2	1:B:659:MET:HG3	1.98	0.45
2:D:141:LEU:HD22	2:D:157:LEU:HD11	1.99	0.45
1:B:17:ARG:HA	1:B:113:MET:HE3	1.99	0.45
1:B:81:PRO:HG2	1:B:84:PHE:HD2	1.81	0.45
2:H:141:LEU:HD22	2:H:157:LEU:HD11	1.99	0.45
1:A:713:ILE:HD11	1:A:770:LEU:HD21	1.97	0.45
1:A:81:PRO:HG2	1:A:84:PHE:CD2	2.51	0.45
1:A:372:GLN:HE22	1:A:415:GLN:H	1.63	0.45
1:A:501:TYR:HD2	1:A:508:TRP:CE3	2.35	0.45
1:B:535:GLU:HG2	1:B:646:THR:HG21	1.98	0.45
1:A:339:LEU:HD13	1:A:443:ILE:HG12	1.99	0.45
1:A:548:PHE:CE2	1:A:590:ILE:HG12	2.51	0.45
1:A:39:VAL:HG12	1:A:76:VAL:HG22	1.99	0.45
1:B:186:VAL:O	1:B:190:ARG:HG2	2.17	0.44
2:D:181:GLU:HB3	2:D:187:ILE:HG12	1.98	0.44
1:A:467:ILE:HG12	1:A:586:VAL:HG22	1.99	0.44
2:D:81:GLY:HA2	2:D:84:LEU:HD12	1.99	0.44
1:B:577:PHE:CE2	1:B:579:LEU:HD13	2.51	0.44
1:B:135:ASN:OD1	1:B:137:GLU:HB3	2.17	0.44
1:A:794:GLY:O	1:A:798:ARG:HD3	2.18	0.44
1:B:448:GLU:HG3	7:B:2201:HOH:O	2.17	0.44
1:B:114:ILE:O	1:B:124:THR:HA	2.18	0.44
1:B:616:MET:O	1:B:620:LEU:HG	2.18	0.43
1:A:574:GLU:HG3	1:B:72:LYS:HG3	2.01	0.43
2:H:81:GLY:HA2	2:H:84:LEU:HD12	2.00	0.43
1:A:548:PHE:CE2	1:A:590:ILE:CG1	3.02	0.43
1:B:81:PRO:HG2	1:B:84:PHE:CD2	2.53	0.43
1:A:5:GLU:HG2	7:A:2429:HOH:O	2.18	0.43
1:A:564:GLN:NE2	1:A:580:ILE:HD11	2.34	0.43
1:B:113:MET:CE	7:B:2103:HOH:O	2.67	0.43
1:B:39:VAL:HG12	1:B:76:VAL:HG12	2.00	0.43
1:B:339:LEU:HD13	1:B:443:ILE:HG12	2.00	0.43
1:A:359:PHE:O	1:A:362:MET:HG2	2.19	0.43
1:B:493:MET:CE	7:B:2148:HOH:O	2.66	0.43
1:B:359:PHE:O	1:B:362:MET:HG2	2.19	0.42
1:A:787:ARG:HH21	2:D:92:THR:HG23	1.85	0.42
1:A:715:TYR:HB3	1:A:738:SER:HB3	2.00	0.42
1:A:561:SER:HB2	1:B:561:SER:HB3	2.01	0.42
1:A:105:LEU:HB3	1:A:125:ILE:HD11	2.02	0.42
2:D:154:GLY:HA2	2:D:187:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:H	1:A:511:ILE:HD12	1.83	0.41
1:B:480:PHE:CZ	1:B:525:GLU:HB3	2.55	0.41
1:B:522:ASP:O	1:B:526:LYS:HB2	2.20	0.41
2:H:118:PHE:HA	2:H:121:MET:HE2	2.02	0.41
1:A:522:ASP:O	1:A:526:LYS:HB2	2.21	0.41
1:A:248[B]:ILE:HG12	1:A:263:ILE:HG12	2.02	0.41
1:B:103:TYR:HA	1:B:106:LYS:HG2	2.02	0.41
1:B:29:ARG:HE	1:B:82:PRO:HB3	1.86	0.40
1:A:297:LEU:O	1:A:301:LEU:HG	2.21	0.40
1:B:308:TYR:HA	1:B:314:SER:CB	2.51	0.40
1:B:589:ASN:HD21	1:B:591:ILE:HD12	1.86	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	780/1935 (40%)	757 (97%)	21 (3%)	2 (0%)	41	47
1	B	746/1935 (39%)	730 (98%)	15 (2%)	1 (0%)	51	62
2	D	152/199 (76%)	142 (93%)	8 (5%)	2 (1%)	12	9
2	H	148/199 (74%)	140 (95%)	8 (5%)	0	100	100
All	All	1826/4268 (43%)	1769 (97%)	52 (3%)	5 (0%)	41	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	SER
2	D	185	GLY
2	D	180	GLN
1	B	767	ALA

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Mol	Chain	Res	Type
1	A	558	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	657/1696 (39%)	629 (96%)	28 (4%)	29	36
1	B	634/1696 (37%)	617 (97%)	17 (3%)	44	55
2	D	131/165 (79%)	125 (95%)	6 (5%)	27	33
2	H	126/165 (76%)	119 (94%)	7 (6%)	21	24
All	All	1548/3722 (42%)	1490 (96%)	58 (4%)	34	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	68	THR
1	A	74	ASP
1	A	76	VAL
1	A	318	THR
1	A	328	GLU
1	A	359	PHE
1	A	478	ILE
1	A	504	GLU
1	A	564	GLN
1	A	568	ASN
1	A	569	ILE
1	A	574	GLU
1	A	578[A]	SER
1	A	578[B]	SER
1	A	579	LEU
1	A	587	ASP
1	A	590	ILE
1	A	601	LEU
1	A	712	ARG

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Mol	Chain	Res	Type
1	A	717	ASP
1	A	738	SER
1	A	745	LEU
1	A	751	ILE
1	A	780	ARG
1	A	784	ILE
1	A	798	ARG
1	A	799	MET
1	B	47	VAL
1	B	63	THR
1	B	69	VAL
1	B	106	LYS
1	B	359	PHE
1	B	454	GLN
1	B	455	TYR
1	B	546	MET
1	B	587	ASP
1	B	601	LEU
1	B	646	THR
1	B	712	ARG
1	B	717	ASP
1	B	745	LEU
1	B	761	THR
1	B	780	ARG
1	B	784	ILE
2	D	63	THR
2	D	64	LEU
2	D	75	ILE
2	D	130	ASP
2	D	133	THR
2	D	182	ASP
2	H	53	GLU
2	H	64	LEU
2	H	73	MET
2	H	75	ILE
2	H	130	ASP
2	H	133	THR
2	H	180	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	A	391	ASN
1	A	564	GLN
1	A	753	HIS
1	B	391	ASN
1	B	451	GLN
1	B	564	GLN
2	D	149	ASN
2	H	149	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	MLY	A	129	1	9,10,11	1.01	1 (11%)	6,11,13	2.27	2 (33%)
1	MLY	B	129	1	9,10,11	1.13	1 (11%)	6,11,13	1.98	2 (33%)

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	MLY	A	129	1	-	2/8/9/11	-
1	MLY	B	129	1	-	2/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	MLY	CB-CA	2.89	1.57	1.53
1	A	129	MLY	CB-CA	2.53	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	MLY	CH2-NZ-CH1	-3.91	99.62	109.73
1	B	129	MLY	CH2-NZ-CH1	-3.34	101.09	109.73
1	A	129	MLY	CH2-NZ-CE	-2.68	100.11	110.74
1	B	129	MLY	CH2-NZ-CE	-2.39	101.25	110.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	129	MLY	CD-CE-NZ-CH1
1	A	129	MLY	CD-CE-NZ-CH2
1	B	129	MLY	CD-CE-NZ-CH1
1	B	129	MLY	CD-CE-NZ-CH2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
6	EDO	B	2006	-	3,3,3	0.44	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	2002	3	24,29,29	0.77	0	29,45,45	0.85	2 (6%)
5	FMT	B	2003	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	2005	-	3,3,3	0.12	0	2,2,2	0.38	0
5	FMT	A	2004	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	2003	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	2005	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ADP	B	2002	3	24,29,29	0.59	0	29,45,45	0.73	1 (3%)
5	FMT	B	2004	-	0,2,2	0.00	-	0,1,1	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
6	EDO	B	2006	-	-	0/1/1/1	-
6	EDO	A	2005	-	-	0/1/1/1	-
4	ADP	A	2002	3	-	3/12/32/32	0/3/3/3
4	ADP	B	2002	3	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	ADP	C5-C6-N6	2.35	123.93	120.35
4	A	2002	ADP	C5-C6-N6	2.15	123.62	120.35
4	A	2002	ADP	PA-O3A-PB	2.02	139.77	132.83

There are no chirality outliers.

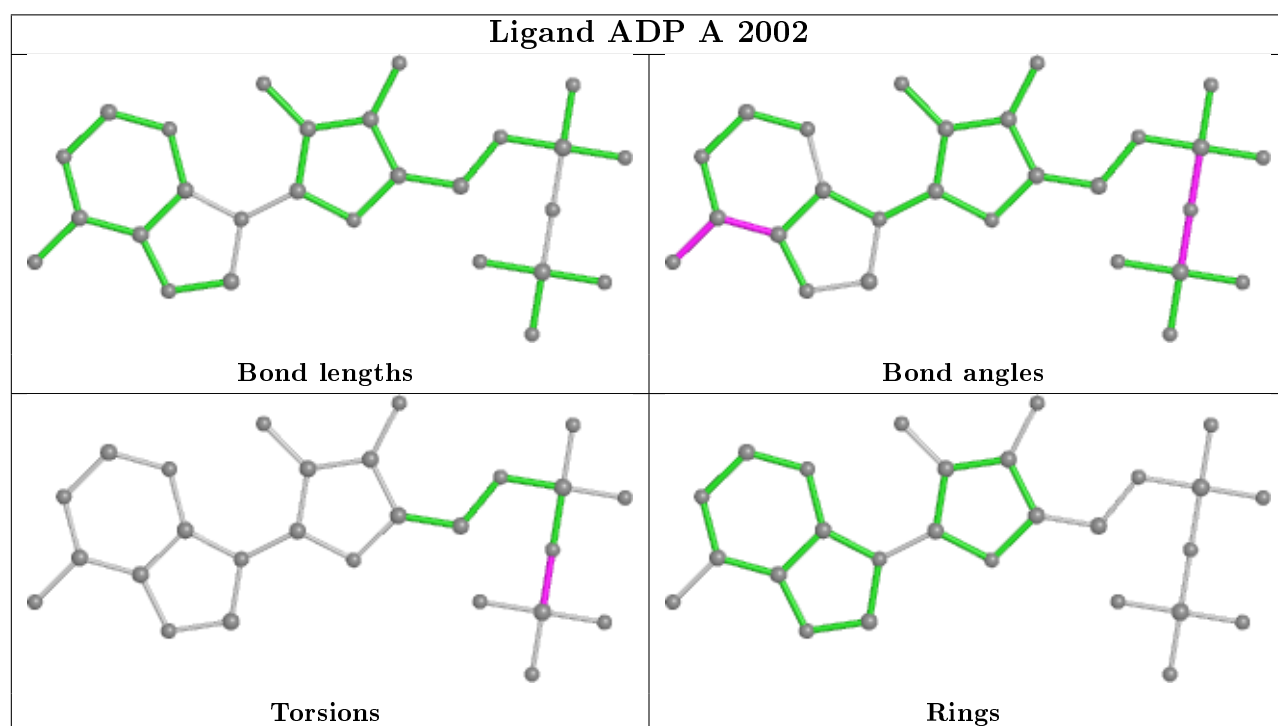
All (6) torsion outliers are listed below:

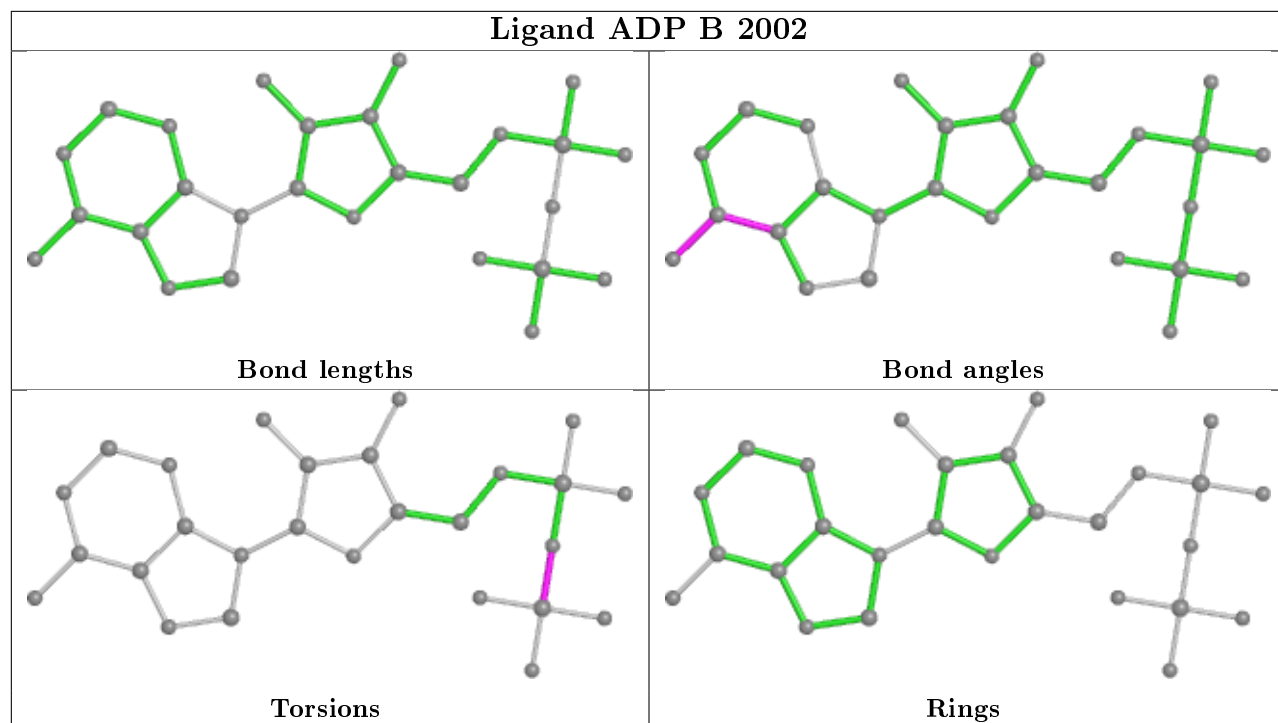
Mol	Chain	Res	Type	Atoms
4	B	2002	ADP	PA-O3A-PB-O3B
4	A	2002	ADP	PA-O3A-PB-O2B
4	A	2002	ADP	PA-O3A-PB-O3B
4	B	2002	ADP	PA-O3A-PB-O2B
4	A	2002	ADP	PA-O3A-PB-O1B
4	B	2002	ADP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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	782/1935 (40%)	0.29	28 (3%) 42 53	22, 42, 94, 129	0
1	B	755/1935 (39%)	0.40	43 (5%) 23 33	25, 55, 103, 135	0
2	D	154/199 (77%)	2.51	81 (52%) 0 0	88, 130, 159, 167	0
2	H	150/199 (75%)	5.14	128 (85%) 0 0	121, 162, 191, 198	0
All	All	1841/4268 (43%)	0.91	280 (15%) 2 3	22, 56, 160, 198	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	65	PHE	20.9
2	H	75	ILE	14.0
2	H	119	LEU	12.5
2	H	50	PHE	12.0
2	H	69	PRO	11.3
2	H	168	LEU	11.1
2	H	67	ARG	10.1
2	H	68	THR	9.9
2	H	105	GLN	9.9
2	H	83	VAL	9.9
2	H	120	PRO	9.8
2	H	106	GLU	9.4
1	B	792	SER	9.3
2	H	112	MET	9.0
2	H	96	VAL	9.0
2	H	77	TYR	8.9
2	H	122	LEU	8.9
2	H	117	THR	8.9
2	H	73	MET	8.6
2	H	124	HIS	8.6
2	H	99	VAL	8.5

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Mol	Chain	Res	Type	RSRZ
2	H	118	PHE	8.4
2	D	123	GLN	8.2
2	H	101	GLY	8.2
2	H	87	LEU	8.2
2	H	74	LYS	8.1
2	H	108	LEU	7.9
2	H	104	LYS	7.8
2	H	123	GLN	7.8
2	H	141	LEU	7.8
2	H	70	LYS	7.6
2	H	198	ALA	7.6
2	H	103	PRO	7.6
2	H	164	LEU	7.5
2	H	171	ASP	7.4
2	H	152	VAL	7.3
2	H	71	CYS	7.3
2	H	128	ASN	7.2
2	H	162	ALA	7.1
2	H	51	THR	7.1
1	A	734	GLN	7.1
2	H	58	PHE	7.1
2	H	187	ILE	7.0
2	H	150	GLY	7.0
2	H	178	ALA	7.0
2	D	65	PHE	7.0
1	B	791	GLN	6.9
2	H	121	MET	6.8
2	D	108	LEU	6.8
2	H	61	ALA	6.8
2	H	113	MET	6.8
2	H	186	CYS	6.7
2	H	115	PHE	6.7
2	D	58	PHE	6.7
1	B	782	SER	6.7
2	H	102	LYS	6.6
1	B	785	ILE	6.5
2	H	52	PRO	6.5
2	H	88	GLY	6.5
2	D	198	ALA	6.5
2	H	76	THR	6.4
2	H	127	LYS	6.4
2	H	183	SER	6.3

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Mol	Chain	Res	Type	RSRZ
2	H	125	ILE	6.3
2	H	92	THR	6.2
2	H	110	SER	6.2
2	H	177	MET	6.2
2	H	100	LEU	6.1
2	H	55	ILE	6.1
2	D	149	ASN	6.0
2	D	121	MET	5.9
1	A	735	PHE	5.8
2	D	56	GLU	5.7
2	D	105	GLN	5.7
2	H	161	LEU	5.6
2	D	196	ILE	5.6
2	D	55	ILE	5.5
2	D	101	GLY	5.5
2	D	178	ALA	5.5
2	H	78	GLY	5.4
2	D	50	PHE	5.4
2	H	116	ASP	5.4
2	H	109	ASN	5.3
2	D	146	LYS	5.3
2	D	78	GLY	5.3
2	H	138	VAL	5.2
2	H	175	LYS	5.2
2	D	74	LYS	5.2
1	B	796	LEU	5.2
2	H	94	ALA	5.2
2	H	165	GLY	5.1
2	H	56	GLU	5.1
2	H	63	THR	5.0
1	A	736	ILE	5.0
2	D	51	THR	5.0
1	A	733	GLY	5.0
2	D	183	SER	5.0
2	H	62	PHE	4.8
1	B	772	LEU	4.8
2	H	173	VAL	4.8
2	H	170	GLU	4.7
1	A	369	ARG	4.7
2	H	197	MET	4.7
2	H	129	LYS	4.7
2	H	146	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	730	ILE	4.6
2	D	102	LYS	4.6
2	H	91	PRO	4.6
2	H	155	ALA	4.6
1	B	789	GLN	4.5
2	H	144	PHE	4.5
1	A	368	GLN	4.5
1	B	795	VAL	4.5
2	H	167	LYS	4.5
2	H	98	ARG	4.4
1	B	371	GLU	4.4
2	D	143	VAL	4.4
2	H	137	PHE	4.4
2	H	199	GLY	4.3
2	D	87	LEU	4.3
2	H	72	GLU	4.3
1	A	795	VAL	4.3
1	A	728	ALA	4.3
1	B	784	ILE	4.2
2	H	80	CYS	4.2
1	B	786	THR	4.2
2	D	52	PRO	4.2
2	H	193	VAL	4.2
2	H	64	LEU	4.1
2	D	127	LYS	4.1
2	D	199	GLY	4.1
1	B	751	ILE	4.1
2	D	94	ALA	4.0
2	H	111	LYS	4.0
2	D	116	ASP	4.0
2	D	150	GLY	4.0
2	H	149	ASN	4.0
1	B	793	ARG	3.9
2	D	88	GLY	3.9
2	D	124	HIS	3.9
1	B	788	ILE	3.9
2	D	104	LYS	3.9
2	D	194	LYS	3.9
2	H	93	GLN	3.9
2	D	49	GLU	3.9
2	H	166	GLU	3.9
2	D	83	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	70	LYS	3.8
2	D	134	TYR	3.8
2	D	187	ILE	3.8
2	H	169	THR	3.8
2	D	141	LEU	3.8
2	D	144	PHE	3.7
2	D	185	GLY	3.7
2	H	194	LYS	3.7
2	D	173	VAL	3.7
1	B	790	ALA	3.7
2	D	175	LYS	3.6
2	D	113	MET	3.6
2	D	184	ASN	3.6
2	H	97	LEU	3.6
2	H	182	ASP	3.6
2	H	60	GLU	3.6
2	D	77	TYR	3.6
2	D	110	SER	3.6
2	H	139	GLU	3.6
1	B	787	ARG	3.6
2	H	184	ASN	3.5
2	D	137	PHE	3.5
2	H	192	PHE	3.5
2	D	120	PRO	3.5
2	H	131	THR	3.5
2	D	47	LYS	3.5
2	H	54	GLN	3.5
1	B	776	MET	3.5
1	B	778	ASP	3.5
2	H	151	THR	3.4
1	B	399	LEU	3.4
2	H	126	SER	3.4
1	B	393	ALA	3.4
2	D	106	GLU	3.4
1	A	729	ALA	3.4
1	B	420	VAL	3.4
2	H	156	GLU	3.4
2	H	86	ALA	3.4
1	B	797	SER	3.3
1	B	781	LEU	3.3
2	D	161	LEU	3.3
2	D	63	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	539	MET	3.3
2	H	66	ASP	3.3
2	D	129	LYS	3.2
2	H	107	GLU	3.2
1	A	751	ILE	3.2
1	B	611	LYS	3.2
2	D	126	SER	3.1
2	H	142	ARG	3.1
2	H	196	ILE	3.1
2	H	81	GLY	3.1
2	D	75	ILE	3.1
2	D	138	VAL	3.1
2	H	85	ARG	3.1
2	H	114	ASP	3.0
2	D	192	PHE	2.9
2	D	76	THR	2.9
2	D	151	THR	2.9
1	A	799	MET	2.9
1	A	404	VAL	2.9
2	D	61	ALA	2.9
2	D	46	ILE	2.8
2	H	185	GLY	2.8
2	D	53	GLU	2.8
2	D	135	GLU	2.8
2	H	130	ASP	2.8
1	B	779	GLU	2.8
1	B	510	PHE	2.7
2	D	107	GLU	2.8
1	B	794	GLY	2.7
2	H	180	GLN	2.7
2	H	90	ASN	2.7
2	H	59	LYS	2.6
1	A	594	LEU	2.6
2	H	159	HIS	2.6
2	D	119	LEU	2.6
1	A	403	ARG	2.6
2	D	48	ILE	2.6
1	B	623	ASN	2.6
2	H	191	ALA	2.6
2	D	54	GLN	2.6
2	H	179	GLY	2.6
1	A	788	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	143	VAL	2.5
2	D	67	ARG	2.5
2	D	152	VAL	2.5
1	B	709	PHE	2.5
2	H	53	GLU	2.5
1	B	368	GLN	2.5
1	B	573	PRO	2.4
2	H	190	GLU	2.4
2	D	170	GLU	2.4
1	B	427	LEU	2.4
2	H	84	LEU	2.4
1	A	719	ARG	2.3
2	H	195	HIS	2.3
2	D	131	THR	2.3
2	D	132	GLY	2.3
1	A	192	ILE	2.3
1	B	211	THR	2.3
1	A	787	ARG	2.3
1	B	391	ASN	2.3
2	D	85	ARG	2.3
1	A	746	LEU	2.3
2	D	100	LEU	2.3
1	A	722	TYR	2.3
2	H	79	GLN	2.3
2	H	153	MET	2.3
2	D	99	VAL	2.3
2	D	168	LEU	2.2
1	A	801	PHE	2.2
1	B	395	LEU	2.2
1	B	373	ALA	2.2
1	A	744	LYS	2.2
1	B	403	ARG	2.2
1	A	370	GLU	2.2
1	A	792	SER	2.2
2	D	115	PHE	2.1
1	A	781	LEU	2.1
1	B	366	LEU	2.1
2	D	148	GLY	2.1
2	H	181	GLU	2.1
1	B	722	TYR	2.1
2	H	163	THR	2.1
2	D	155	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	622	ALA	2.1
1	A	796	LEU	2.1
1	B	415	GLN	2.0
2	D	109	ASN	2.0
2	D	193	VAL	2.0
1	B	590	ILE	2.0
1	A	752	ASP	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	MLY	A	129	11/12	0.97	0.14	35,37,40,41	0
1	MLY	B	129	11/12	0.97	0.13	41,41,47,48	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

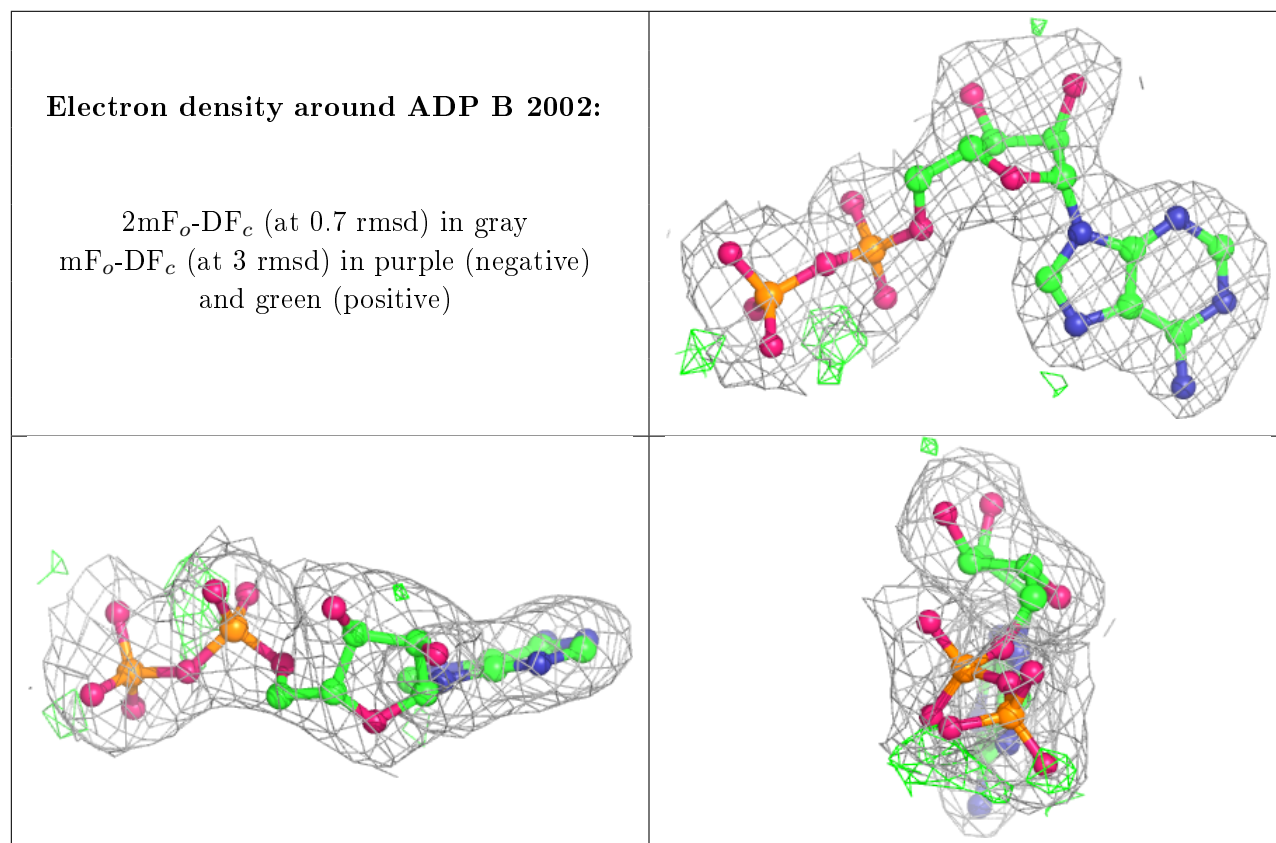
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FMT	B	2003	3/3	0.82	0.17	48,48,49,49	0
3	MG	B	2001	1/1	0.90	0.10	65,65,65,65	0
5	FMT	B	2005	3/3	0.91	0.16	58,58,59,60	0
5	FMT	B	2004	3/3	0.92	0.15	42,42,48,52	0
5	FMT	A	2003	3/3	0.93	0.11	36,36,43,49	0
6	EDO	B	2006	4/4	0.94	0.17	42,44,44,47	0
6	EDO	A	2005	4/4	0.95	0.20	32,33,33,39	0
5	FMT	A	2004	3/3	0.96	0.18	44,44,46,46	0
3	MG	A	2001	1/1	0.97	0.08	39,39,39,39	0

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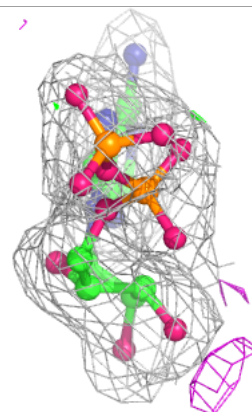
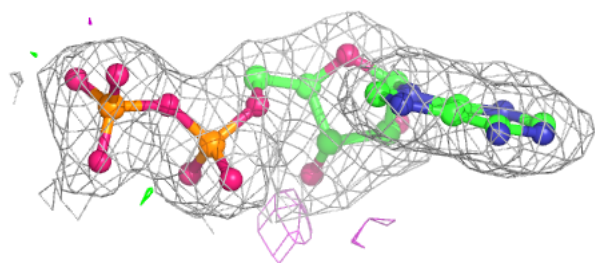
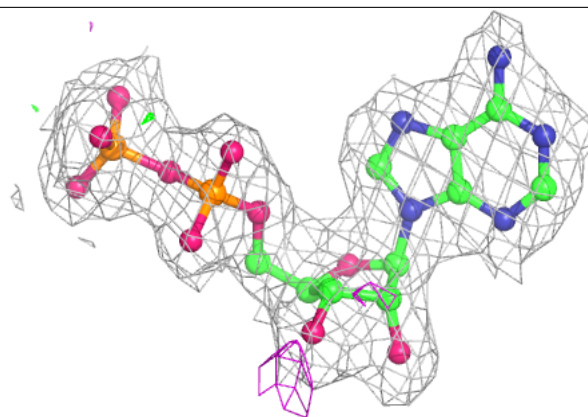
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ADP	B	2002	27/27	0.98	0.14	35,39,47,52	0
4	ADP	A	2002	27/27	0.99	0.14	24,28,35,42	0

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 2002:

$2mF_o-DF_c$ (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.