



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:12 AM UTC

PDB ID : 6FSA / pdb_00006fsa
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 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

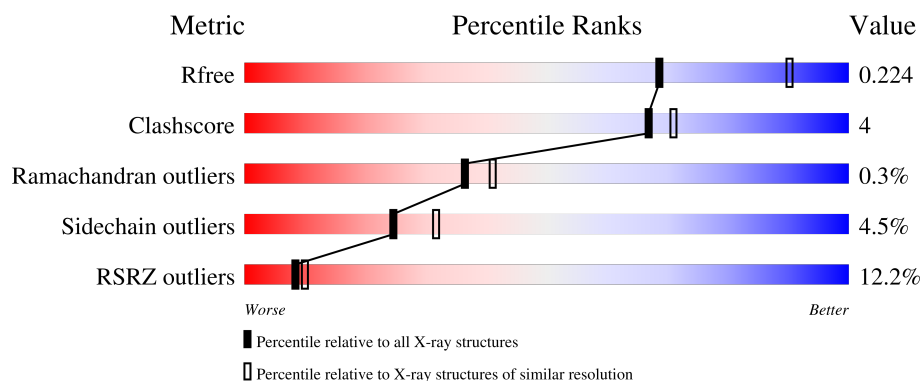
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 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	1935	2% 35% 5% 60%
1	B	1935	3% 34% 5% 61%
2	D	199	33% 62% 14% 23%
2	H	199	31% 62% 13% 25%

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			

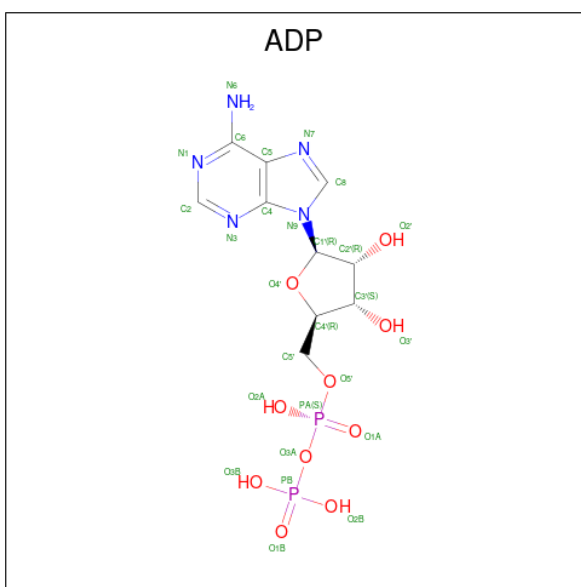
- Molecule 2 is a protein called Myosin light chain 3.

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

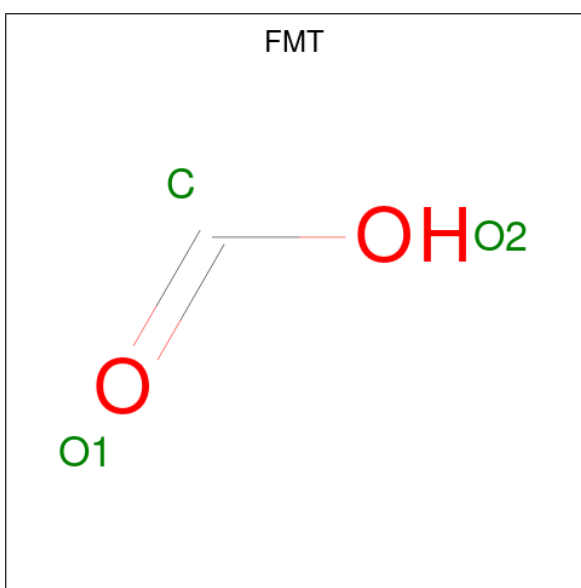
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



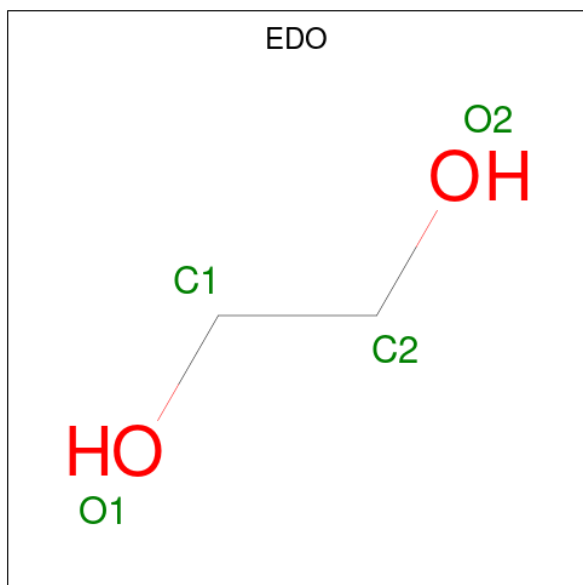
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0

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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 (CCD ID: 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		

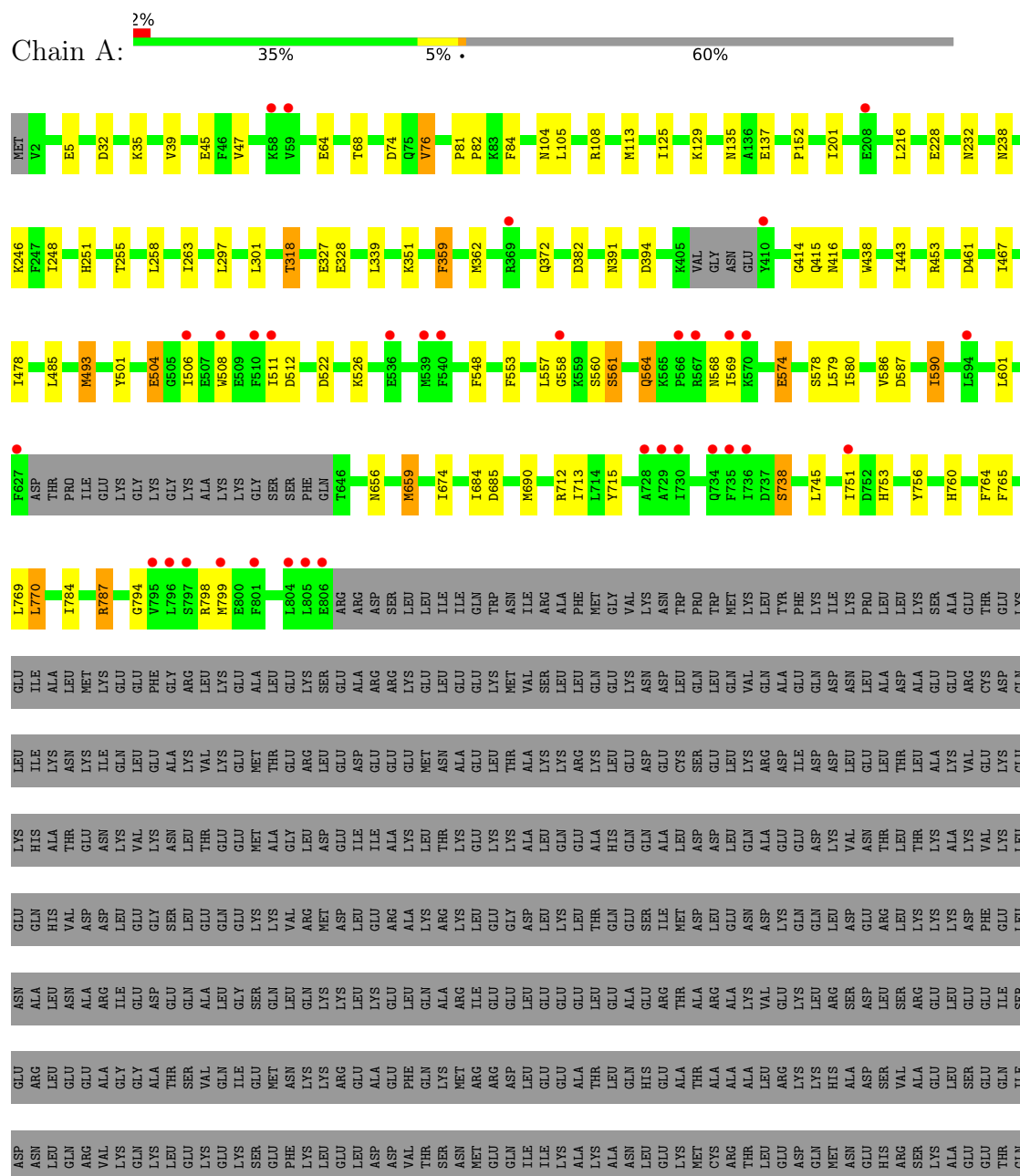
- Molecule 7 is water.

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

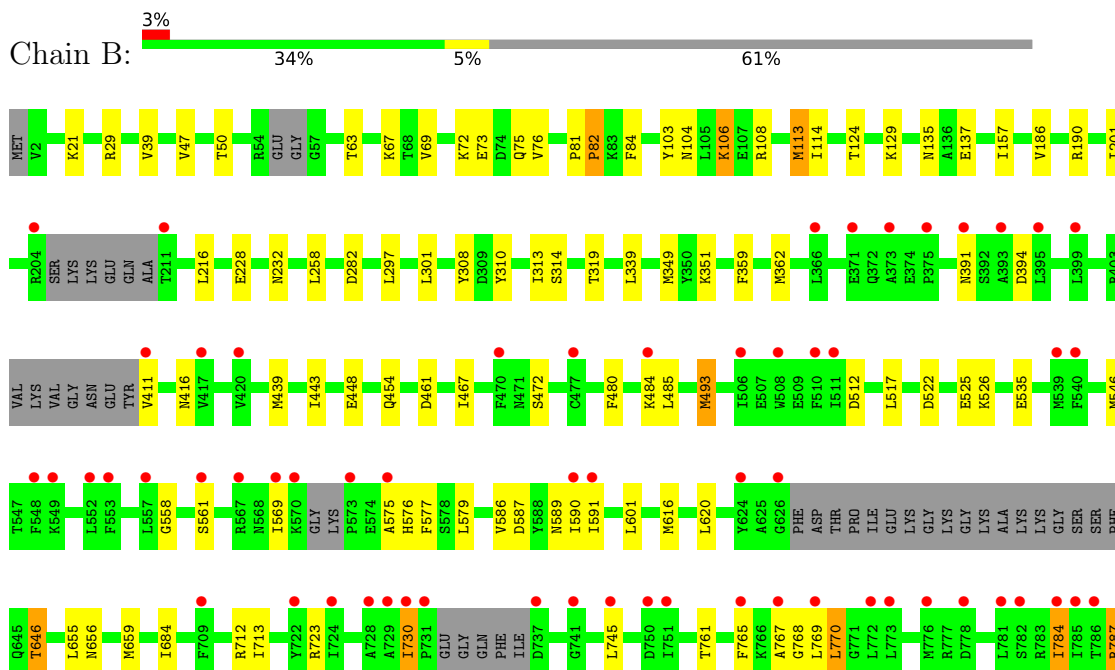
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Myosin-7



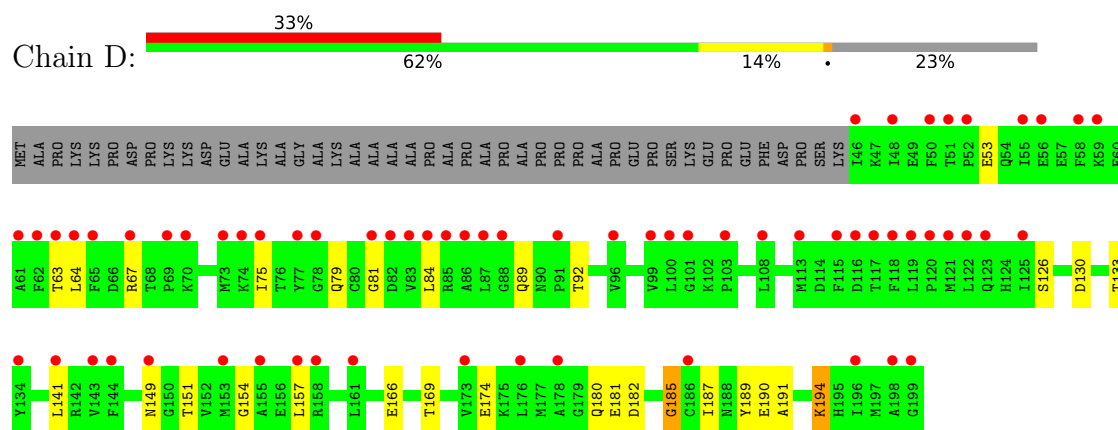
[illegible]

- Molecule 1: Myosin-7

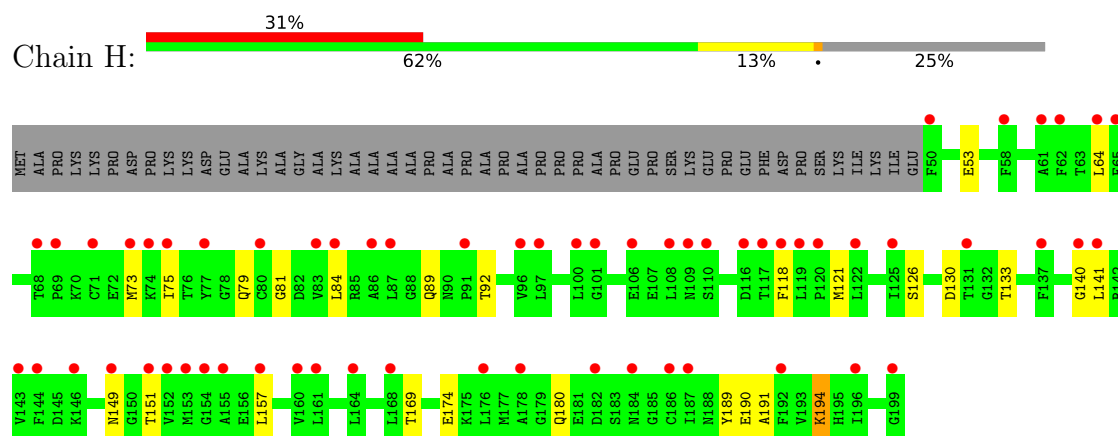




- Molecule 2: Myosin light chain 3



- 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 (Not available) , 0.224	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)	0.32 , 68.8	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

5.1 Standard geometry

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

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	0.92	4/6358 (0.1%)	1.40	20/8579 (0.2%)
1	B	0.88	2/6130 (0.0%)	1.38	21/8273 (0.3%)
2	D	0.81	0/1234	1.42	8/1657 (0.5%)
2	H	0.81	0/1197	1.41	4/1608 (0.2%)
All	All	0.88	6/14919 (0.0%)	1.39	53/20117 (0.3%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	MET	SD-CE	-12.31	1.48	1.79
1	B	113	MET	SD-CE	-11.67	1.50	1.79
1	A	493	MET	SD-CE	-7.71	1.60	1.79
1	B	493	MET	SD-CE	-6.99	1.62	1.79
1	A	674	ILE	CA-C	6.33	1.58	1.53
1	A	659	MET	SD-CE	-5.46	1.66	1.79

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	ASP	CA-CB-CG	9.43	122.03	112.60
1	A	560[A]	SER	CA-C-N	9.28	139.26	121.54
1	A	560[A]	SER	C-N-CA	9.28	139.26	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560[B]	SER	CA-C-N	9.28	139.26	121.54
1	A	560[B]	SER	C-N-CA	9.28	139.26	121.54
1	A	64	GLU	N-CA-C	-8.11	99.83	110.53
1	B	461	ASP	CA-CB-CG	7.21	119.81	112.60
1	B	82	PRO	CA-C-N	6.80	129.69	120.38
1	B	82	PRO	C-N-CA	6.80	129.69	120.38
2	D	185	GLY	CA-C-N	6.72	133.79	121.70
2	D	185	GLY	C-N-CA	6.72	133.79	121.70
1	A	82	PRO	CA-C-N	6.69	129.54	120.38
1	A	82	PRO	C-N-CA	6.69	129.54	120.38
1	A	461	ASP	CA-CB-CG	6.65	119.25	112.60
1	B	512	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	768	GLY	N-CA-C	6.59	121.92	114.67
1	A	238	ASN	CA-CB-CG	6.46	119.06	112.60
1	B	310	TYR	CA-C-N	5.69	127.91	120.28
1	B	310	TYR	C-N-CA	5.69	127.91	120.28
1	B	558	GLY	CA-C-N	5.66	128.18	120.54
1	B	558	GLY	C-N-CA	5.66	128.18	120.54
1	B	517	LEU	CA-C-N	5.61	128.06	120.38
1	B	517	LEU	C-N-CA	5.61	128.06	120.38
1	A	512	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	416	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	318	THR	N-CA-CB	-5.36	103.86	111.00
2	D	194	LYS	CA-C-N	5.31	127.34	120.44
2	D	194	LYS	C-N-CA	5.31	127.34	120.44
1	B	656	ASN	CA-C-N	5.20	127.19	120.44
1	B	656	ASN	C-N-CA	5.20	127.19	120.44
1	B	416	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	472	SER	CA-C-N	5.16	127.19	120.28
1	B	472	SER	C-N-CA	5.16	127.19	120.28
2	D	79	GLN	CA-C-N	5.14	127.43	120.38
2	D	79	GLN	C-N-CA	5.14	127.43	120.38
2	H	79	GLN	CA-C-N	5.14	127.43	120.38
2	H	79	GLN	C-N-CA	5.14	127.43	120.38
1	B	21	LYS	CA-C-N	5.14	127.17	120.28
1	B	21	LYS	C-N-CA	5.14	127.17	120.28
1	A	327	GLU	CA-C-N	5.12	127.57	120.29
1	A	327	GLU	C-N-CA	5.12	127.57	120.29
1	A	438	TRP	CA-C-N	5.09	127.10	120.28
1	A	438	TRP	C-N-CA	5.09	127.10	120.28
2	H	194	LYS	CA-C-N	5.08	127.35	120.44
2	H	194	LYS	C-N-CA	5.08	127.35	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	575	ALA	N-CA-C	5.08	118.34	110.17
1	B	157	ILE	CA-C-N	5.04	127.00	120.44
1	B	157	ILE	C-N-CA	5.04	127.00	120.44
1	A	656	ASN	CA-C-N	5.03	127.02	120.28
1	A	656	ASN	C-N-CA	5.03	127.02	120.28
2	D	166	GLU	CA-C-N	5.02	128.79	121.31
2	D	166	GLU	C-N-CA	5.02	128.79	121.31

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	46	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	107	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 (107) 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: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:A:493:MET:HE1	7:A:2300:HOH:O	1.93	0.68
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:A:359:PHE:HA	1:A:362:MET:HE3	1.77	0.65
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
1:B:228:GLU:O	1:B:232:ASN:HB2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:A:255:THR:O	2.16	0.46
2:H:118:PHE:HA	2:H:121:MET:HE2	1.97	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
2:H:189:TYR:O	2:H:190:GLU:HB3	2.16	0.46
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: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:81:PRO:HG2	1:A:84:PHE:CD2	2.51	0.45
1:A:713:ILE:HD11	1:A:770:LEU:HD21	1.97	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:349:MET:HE1	1:B:439:MET:SD	2.58	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:VAL:HG12	1:B:76:VAL:HG12	2.00	0.43
1:B:113:MET:CE	7:B:2103:HOH:O	2.67	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:485:LEU:HD23	1:A:659:MET:HE1	2.01	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
1:A:485:LEU:CD2	1:A:659:MET:HE1	2.50	0.42
2:D:154:GLY:HA2	2:D:187:ILE:CD1	2.50	0.41
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
1:B:485:LEU:CD2	1:B:659:MET:HE1	2.51	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:B:485:LEU:HD23	1:B:659:MET:HE1	2.03	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%)	36	41
1	B	746/1935 (39%)	730 (98%)	15 (2%)	1 (0%)	48	57
2	D	152/199 (76%)	142 (93%)	8 (5%)	2 (1%)	9	7
2	H	148/199 (74%)	140 (95%)	8 (5%)	0	100	100
All	All	1826/4268 (43%)	1769 (97%)	52 (3%)	5 (0%)	36	41

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
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%)	627 (95%)	30 (5%)	24	31
1	B	634/1696 (37%)	612 (96%)	22 (4%)	32	41
2	D	131/165 (79%)	121 (92%)	10 (8%)	12	13
2	H	126/165 (76%)	117 (93%)	9 (7%)	13	14
All	All	1548/3722 (42%)	1477 (95%)	71 (5%)	24	31

All (71) 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	201	ILE
1	A	318	THR

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Mol	Chain	Res	Type
1	A	328	GLU
1	A	359	PHE
1	A	478	ILE
1	A	504	GLU
1	A	506	ILE
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	684	ILE
1	A	712	ARG
1	A	738	SER
1	A	745	LEU
1	A	751	ILE
1	A	770	LEU
1	A	784	ILE
1	A	787	ARG
1	A	799	MET
1	B	47	VAL
1	B	50	THR
1	B	63	THR
1	B	67	LYS
1	B	69	VAL
1	B	106	LYS
1	B	201	ILE
1	B	319	THR
1	B	411	VAL
1	B	454	GLN
1	B	546	MET
1	B	569	ILE
1	B	587	ASP
1	B	601	LEU
1	B	646	THR
1	B	684	ILE
1	B	712	ARG
1	B	745	LEU

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Mol	Chain	Res	Type
1	B	761	THR
1	B	770	LEU
1	B	784	ILE
1	B	787	ARG
2	D	53	GLU
2	D	63	THR
2	D	64	LEU
2	D	67	ARG
2	D	75	ILE
2	D	130	ASP
2	D	133	THR
2	D	169	THR
2	D	174	GLU
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	169	THR
2	H	174	GLU
2	H	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	276	GLN
1	A	292	ASN
1	A	372	GLN
1	A	391	ASN
1	A	401	HIS
1	A	486	GLN
1	A	487	GLN
1	A	564	GLN
1	A	661	ASN
1	A	686	ASN
1	A	753	HIS
1	B	163	GLN
1	B	187	ASN
1	B	232	ASN

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Mol	Chain	Res	Type
1	B	276	GLN
1	B	292	ASN
1	B	315	GLN
1	B	391	ASN
1	B	401	HIS
1	B	451	GLN
1	B	486	GLN
1	B	490	ASN
1	B	661	ASN
1	B	754	ASN
1	B	789	GLN
1	B	791	GLN
2	D	109	ASN
2	D	128	ASN
2	D	149	ASN
2	D	188	ASN
2	H	109	ASN
2	H	123	GLN
2	H	128	ASN
2	H	149	ASN
2	H	188	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	B	129	1	9,10,11	1.04	1 (11%)	6,11,13	1.98	2 (33%)
1	MLY	A	129	1	9,10,11	0.93	1 (11%)	6,11,13	2.28	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	B	129	1	-	2/8/9/11	-
1	MLY	A	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	2.53	1.57	1.53
1	A	129	MLY	CB-CA	2.22	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	-3.94	99.62	109.72
1	B	129	MLY	CH2-NZ-CH1	-3.37	101.09	109.72
1	A	129	MLY	CH2-NZ-CE	-2.68	100.11	110.75
1	B	129	MLY	CH2-NZ-CE	-2.40	101.25	110.75

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	B	129	MLY	CD-CE-NZ-CH1
1	A	129	MLY	CD-CE-NZ-CH2
1	B	129	MLY	CD-CE-NZ-CH2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
5	FMT	A	2004	-	2,2,2	1.31	0	1,1,1	1.01	0
4	ADP	A	2002	3	28,29,29	0.55	0	43,45,45	0.59	1 (2%)
5	FMT	B	2003	-	2,2,2	1.48	1 (50%)	1,1,1	1.02	0
6	EDO	A	2005	-	3,3,3	0.12	0	2,2,2	0.41	0
5	FMT	A	2003	-	2,2,2	1.20	0	1,1,1	1.13	0
4	ADP	B	2002	3	28,29,29	0.33	0	43,45,45	0.42	0
5	FMT	B	2005	-	2,2,2	1.11	0	1,1,1	1.09	0
5	FMT	B	2004	-	2,2,2	1.15	0	1,1,1	1.06	0
6	EDO	B	2006	-	3,3,3	0.40	0	2,2,2	0.57	0

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	A	2005	-	-	0/1/1/1	-
4	ADP	B	2002	3	-	3/16/32/32	0/3/3/3
6	EDO	B	2006	-	-	0/1/1/1	-
4	ADP	A	2002	3	-	3/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2003	FMT	O2-C	2.07	1.39	1.28

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	ADP	O2A-PA-O3A	2.03	112.75	107.27

There are no chirality outliers.

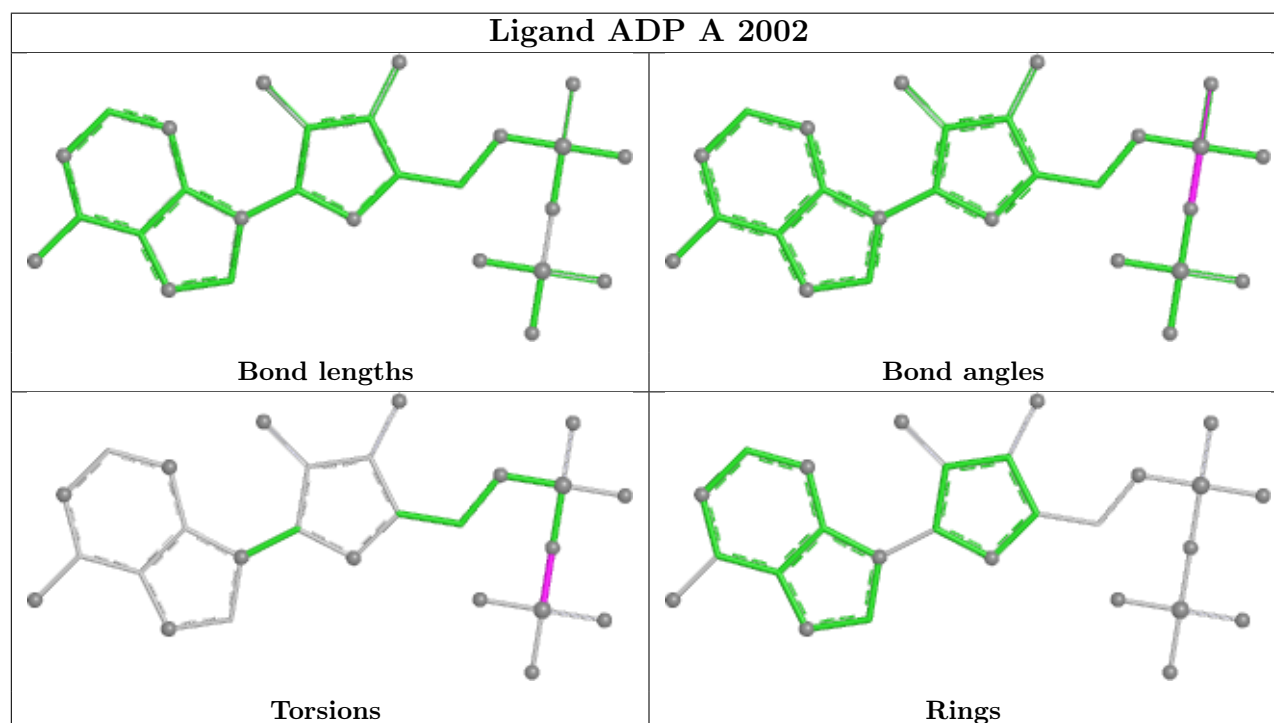
All (6) torsion outliers are listed below:

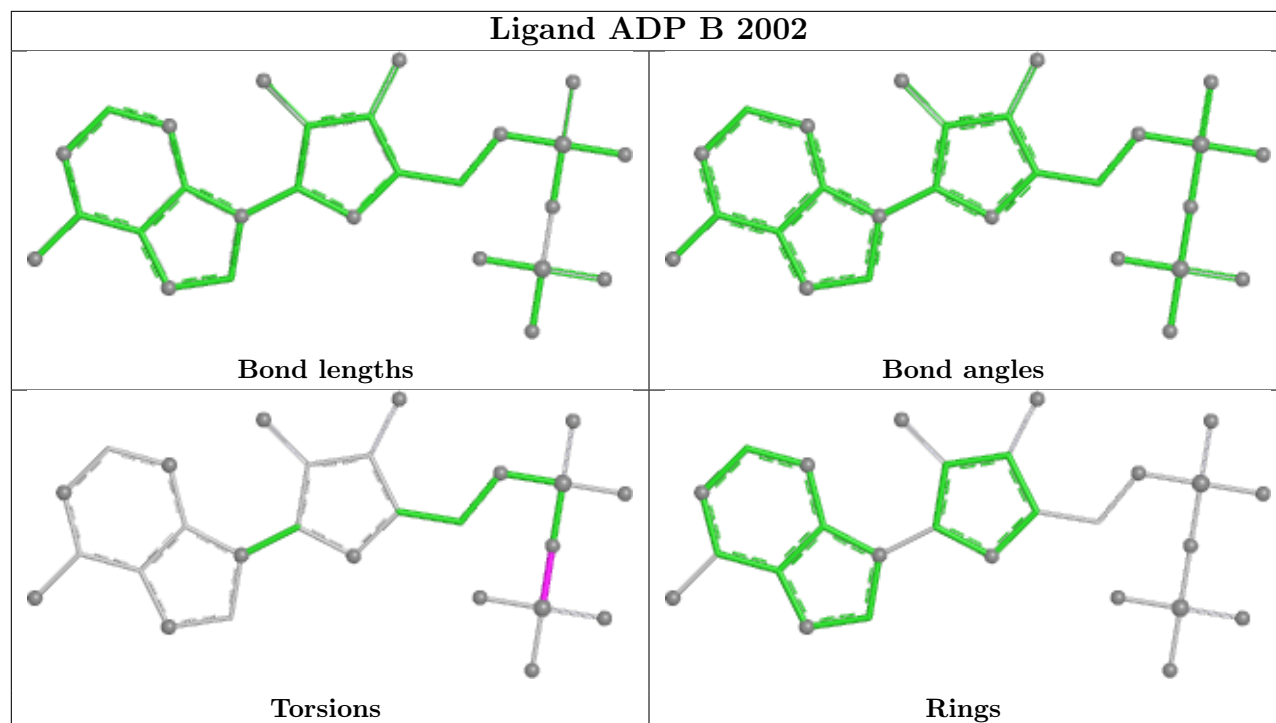
Mol	Chain	Res	Type	Atoms
4	B	2002	ADP	PA-O3A-PB-O3B
4	A	2002	ADP	PA-O3A-PB-O2B
4	A	2002	ADP	PA-O3A-PB-O3B
4	B	2002	ADP	PA-O3A-PB-O2B
4	A	2002	ADP	PA-O3A-PB-O1B
4	B	2002	ADP	PA-O3A-PB-O1B

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%)	0.18	34 (4%)	40 46	12, 42, 94, 129	4 (0%)
1	B	755/1935 (39%)	0.59	64 (8%)	16 20	15, 55, 103, 135	5 (0%)
2	D	154/199 (77%)	1.95	65 (42%)	0 0	88, 130, 159, 167	0
2	H	150/199 (75%)	2.00	61 (40%)	0 0	121, 162, 191, 198	0
All	All	1841/4268 (43%)	0.65	224 (12%)	8 10	12, 55, 160, 198	9 (0%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	65	PHE	6.2
1	B	784	ILE	5.9
1	B	731	PRO	5.3
2	D	58	PHE	5.2
1	A	735	PHE	4.9
2	D	65	PHE	4.9
2	D	78	GLY	4.5
2	H	119	LEU	4.5
2	D	196	ILE	4.4
2	H	141	LEU	4.4
2	H	61	ALA	4.4
2	D	122	LEU	4.4
2	D	61	ALA	4.3
2	H	83	VAL	4.2
2	D	118	PHE	4.2
2	H	151	THR	4.1
1	A	795	VAL	4.1
2	D	143	VAL	4.1
2	H	87	LEU	4.1
1	A	736	ILE	4.0
1	B	785	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	178	ALA	3.9
2	D	70	LYS	3.9
2	D	119	LEU	3.9
1	B	371	GLU	3.8
1	A	751	ILE	3.7
2	D	125	ILE	3.7
2	D	87	LEU	3.7
1	B	373	ALA	3.7
1	B	792	SER	3.6
2	H	64	LEU	3.6
1	B	573	PRO	3.6
1	B	626	GLY	3.5
2	H	143	VAL	3.5
1	B	570	LYS	3.5
1	A	728	ALA	3.5
2	H	176	LEU	3.5
2	D	108	LEU	3.5
2	H	73	MET	3.4
2	H	199	GLY	3.4
2	D	75	ILE	3.4
2	H	84	LEU	3.4
2	H	125	ILE	3.4
2	H	75	ILE	3.4
2	H	120	PRO	3.3
2	H	161	LEU	3.3
1	B	511	ILE	3.3
2	D	83	VAL	3.3
2	H	168	LEU	3.3
2	H	184	ASN	3.2
2	D	55	ILE	3.2
2	H	186	CYS	3.2
2	H	157	LEU	3.2
2	H	144	PHE	3.2
2	D	46	ILE	3.2
2	D	199	GLY	3.1
2	H	86	ALA	3.1
1	A	594	LEU	3.1
2	H	71	CYS	3.1
1	B	575	ALA	3.1
2	D	178	ALA	3.1
1	B	709	PHE	3.1
2	D	86	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	64	LEU	3.1
2	D	141	LEU	3.1
2	H	196	ILE	3.0
1	B	569	ILE	3.0
1	B	730	ILE	3.0
2	D	149	ASN	3.0
2	D	62	PHE	3.0
1	B	411	VAL	3.0
2	D	96	VAL	3.0
1	B	510	PHE	3.0
1	B	781	LEU	3.0
2	D	99	VAL	3.0
1	B	788	ILE	3.0
2	H	69	PRO	3.0
1	B	470	PHE	2.9
2	H	96	VAL	2.9
2	H	58	PHE	2.9
2	D	120	PRO	2.9
2	H	160	VAL	2.9
1	B	751	ILE	2.9
2	D	153	MET	2.9
2	D	74	LYS	2.8
1	A	511	ILE	2.8
1	A	567	ARG	2.8
2	H	68	THR	2.8
2	D	82	ASP	2.8
1	A	510	PHE	2.8
2	H	182	ASP	2.8
2	D	121	MET	2.8
1	A	569	ILE	2.7
2	D	48	ILE	2.7
2	H	149	ASN	2.7
2	H	118	PHE	2.7
1	A	805	LEU	2.7
2	H	122	LEU	2.7
2	D	113	MET	2.7
2	H	108	LEU	2.7
1	B	729	ALA	2.6
2	D	198	ALA	2.6
1	A	570	LYS	2.6
2	H	152	VAL	2.6
2	H	140	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	782	SER	2.6
1	B	366	LEU	2.6
2	D	157	LEU	2.6
2	H	100	LEU	2.6
1	B	508	TRP	2.6
2	H	155	ALA	2.6
1	A	558	GLY	2.6
2	D	88	GLY	2.6
1	A	796	LEU	2.6
1	B	552	LEU	2.6
2	H	146	LYS	2.6
1	B	767	ALA	2.6
1	A	627	PHE	2.6
1	B	553	PHE	2.6
1	B	399	LEU	2.6
1	B	557	LEU	2.6
2	D	100	LEU	2.6
1	B	204	ARG	2.6
2	D	63	THR	2.6
1	B	745	LEU	2.5
1	A	804	LEU	2.5
1	B	539	MET	2.5
2	D	52	PRO	2.5
2	H	91	PRO	2.5
2	D	144	PHE	2.5
1	A	734	GLN	2.5
1	A	506	ILE	2.5
1	B	506	ILE	2.5
1	A	410	TYR	2.5
2	H	74	LYS	2.5
2	D	59	LYS	2.5
1	B	778	ASP	2.5
2	D	103	PRO	2.5
2	H	80	CYS	2.4
1	B	540	PHE	2.4
2	D	173	VAL	2.4
2	H	192	PHE	2.4
2	H	187	ILE	2.4
1	B	484[A]	LYS	2.4
2	H	110	SER	2.4
1	B	776	MET	2.4
1	A	208	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	81	GLY	2.4
1	B	395	LEU	2.4
2	D	176	LEU	2.4
1	A	369	ARG	2.4
1	B	391	ASN	2.4
1	B	786	THR	2.4
2	D	51	THR	2.4
2	H	97	LEU	2.4
2	D	50	PHE	2.3
2	D	158	ARG	2.3
1	B	772	LEU	2.3
1	B	791	GLN	2.3
2	D	77	TYR	2.3
1	A	539	MET	2.3
2	D	117	THR	2.3
1	A	806	GLU	2.3
2	D	115	PHE	2.3
2	D	186	CYS	2.3
1	B	722	TYR	2.3
2	H	153	MET	2.3
1	A	797	SER	2.3
1	B	548	PHE	2.3
1	B	737	ASP	2.3
1	B	567	ARG	2.3
1	B	728	ALA	2.3
2	D	123	GLN	2.3
1	A	540	PHE	2.2
2	D	161	LEU	2.2
1	A	799	MET	2.2
2	D	101	GLY	2.2
2	H	101	GLY	2.2
1	A	536	GLU	2.2
1	B	724	ILE	2.2
1	B	750	ASP	2.2
2	D	134	TYR	2.2
2	H	77	TYR	2.2
1	B	591	ILE	2.2
1	B	773	LEU	2.2
1	B	765	PHE	2.2
2	D	69	PRO	2.2
1	B	393	ALA	2.2
2	H	50	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	137	PHE	2.2
1	B	624	TYR	2.1
2	D	67	ARG	2.1
1	A	59	VAL	2.1
1	B	417	VAL	2.1
1	B	420	VAL	2.1
2	H	116	ASP	2.1
1	A	566	PRO	2.1
2	D	91	PRO	2.1
2	H	62	PHE	2.1
1	B	741	GLY	2.1
1	A	729	ALA	2.1
1	B	561	SER	2.1
2	D	85	ARG	2.1
1	A	58	LYS	2.1
1	B	549	LYS	2.1
1	B	769	LEU	2.1
1	B	375	PRO	2.1
2	D	73	MET	2.1
2	H	106	GLU	2.1
1	A	508	TRP	2.1
1	B	211	THR	2.1
2	H	117	THR	2.1
2	D	155	ALA	2.1
1	A	801	PHE	2.1
1	B	477	CYS	2.0
2	D	84	LEU	2.0
2	H	109	ASN	2.0
2	H	164	LEU	2.0
1	B	590	ILE	2.0
2	H	154	GLY	2.0
2	D	56	GLU	2.0
2	H	131	THR	2.0
2	D	116	ASP	2.0
1	A	730	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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($\text{\AA}^2$)	Q<0.9
1	MLY	A	129	11/12	0.96	0.07	35,37,40,41	0
1	MLY	B	129	11/12	0.96	0.07	41,41,47,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

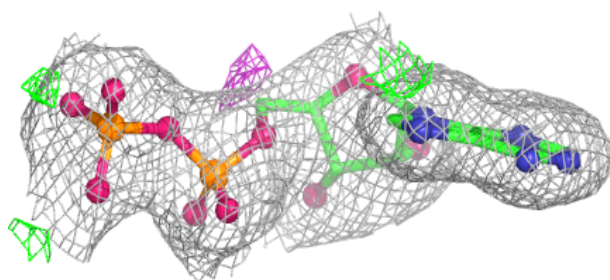
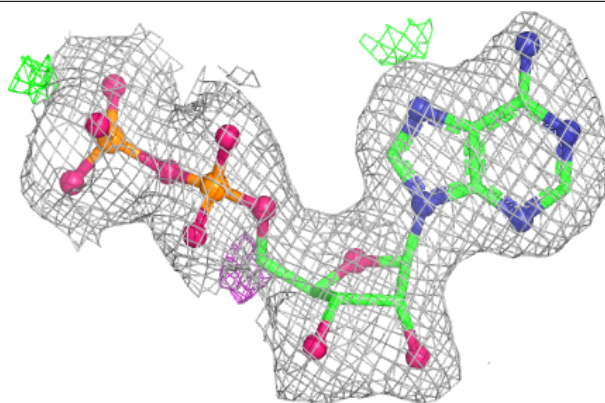
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	B	2005	3/3	0.87	0.16	58,58,59,60	0
5	FMT	B	2003	3/3	0.88	0.15	48,48,49,49	0
3	MG	B	2001	1/1	0.88	0.12	65,65,65,65	0
5	FMT	B	2004	3/3	0.89	0.15	42,42,48,52	0
6	EDO	B	2006	4/4	0.90	0.12	42,44,44,47	0
5	FMT	A	2003	3/3	0.91	0.11	36,36,43,49	0
6	EDO	A	2005	4/4	0.93	0.10	32,33,33,39	0
5	FMT	A	2004	3/3	0.94	0.15	44,44,46,46	0
4	ADP	B	2002	27/27	0.97	0.06	35,39,47,52	0
3	MG	A	2001	1/1	0.97	0.07	39,39,39,39	0
4	ADP	A	2002	27/27	0.99	0.04	24,28,35,42	0

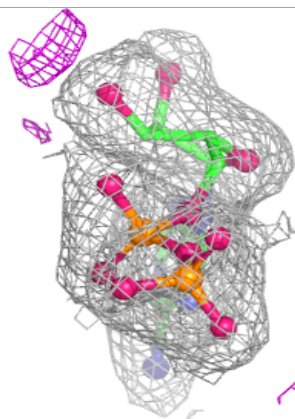
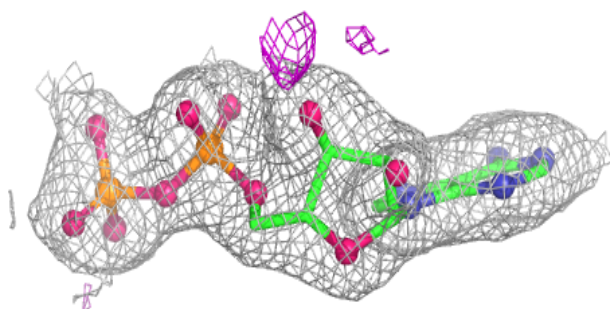
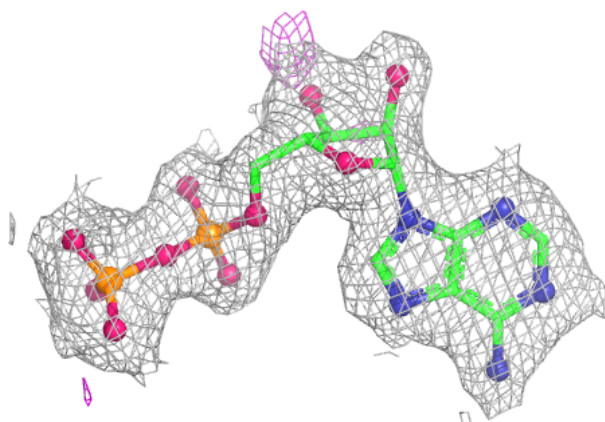
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 2002:

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

**Electron density around ADP 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 ⓘ

There are no such residues in this entry.