



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2021 – 12:08 PM JST

PDB ID : 7DHW
Title : Crystal structure of myosin-XI motor domain in complex with ADP-ALF4
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Deposited on : 2020-11-17
Resolution : 2.84 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	:	2.23.2
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)	:	2.23.2

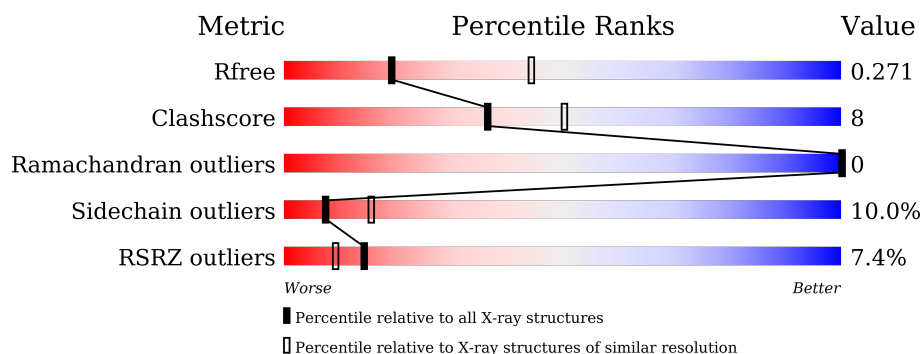
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	771	

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
3	ALF	A	1103	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5778 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 Motor domain of myosin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5709	3615	968	1096	30			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP Q9LKB9
A	-31	ASP	-	expression tag	UNP Q9LKB9
A	-30	TYR	-	expression tag	UNP Q9LKB9
A	-29	LYS	-	expression tag	UNP Q9LKB9
A	-28	ASP	-	expression tag	UNP Q9LKB9
A	-27	ASP	-	expression tag	UNP Q9LKB9
A	-26	ASP	-	expression tag	UNP Q9LKB9
A	-25	ASP	-	expression tag	UNP Q9LKB9
A	-24	LYS	-	expression tag	UNP Q9LKB9
A	-23	ARG	-	expression tag	UNP Q9LKB9
A	-22	SER	-	expression tag	UNP Q9LKB9
A	-21	MET	-	expression tag	UNP Q9LKB9
A	-20	HIS	-	expression tag	UNP Q9LKB9
A	-19	HIS	-	expression tag	UNP Q9LKB9
A	-18	HIS	-	expression tag	UNP Q9LKB9
A	-17	HIS	-	expression tag	UNP Q9LKB9
A	-16	HIS	-	expression tag	UNP Q9LKB9
A	-15	HIS	-	expression tag	UNP Q9LKB9
A	-14	ASP	-	expression tag	UNP Q9LKB9
A	-13	TYR	-	expression tag	UNP Q9LKB9
A	-12	ASP	-	expression tag	UNP Q9LKB9
A	-11	ILE	-	expression tag	UNP Q9LKB9
A	-10	PRO	-	expression tag	UNP Q9LKB9
A	-9	THR	-	expression tag	UNP Q9LKB9
A	-8	THR	-	expression tag	UNP Q9LKB9
A	-7	GLU	-	expression tag	UNP Q9LKB9
A	-6	ASN	-	expression tag	UNP Q9LKB9

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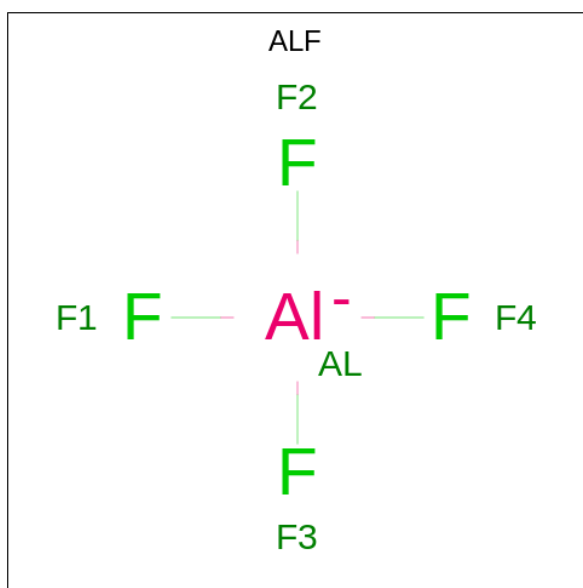
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP Q9LKB9
A	-4	TYR	-	expression tag	UNP Q9LKB9
A	-3	PHE	-	expression tag	UNP Q9LKB9
A	-2	GLN	-	expression tag	UNP Q9LKB9
A	-1	GLY	-	expression tag	UNP Q9LKB9
A	0	ALA	-	expression tag	UNP Q9LKB9

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

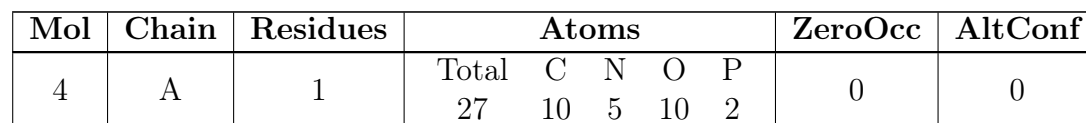
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Al F 5 1 4	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



- GOL
-
- The diagram shows the skeletal structure of 1,2,3-propanetriol (glycerol). The carbon backbone is represented by three vertices labeled C1, C2, and C3 in green. C1 is on the left, C2 is in the middle, and C3 is on the right and slightly higher. Each carbon is bonded to a hydroxyl group (OH) in red. The OH group on C1 is labeled O1 in green below it. The OH group on C2 is labeled O2 in green below it. The OH group on C3 is labeled O3 in green to its right. The bonds between the carbons and between the carbons and the hydroxyl groups are shown as thin grey lines.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

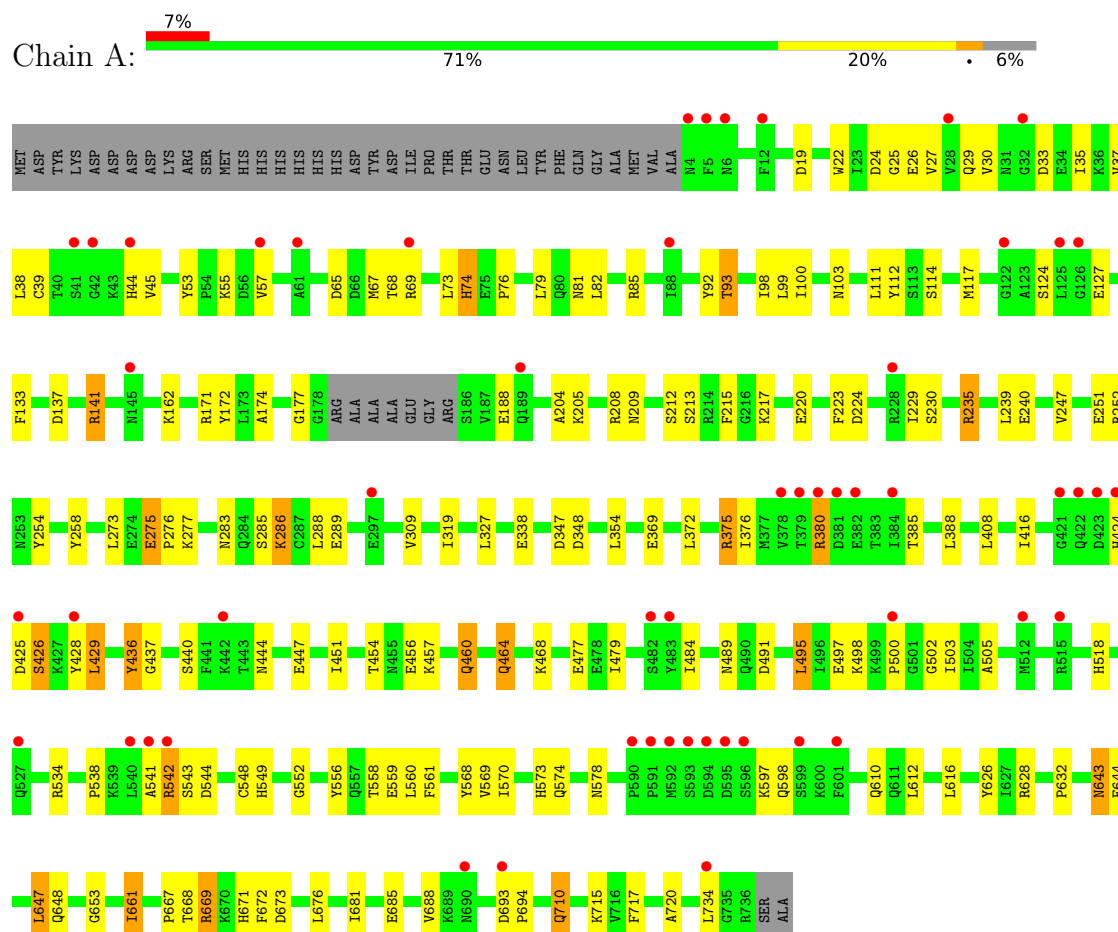
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		

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: Motor domain of myosin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.28Å 73.72Å 187.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.84 19.81 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.81-2.84) 87.4 (19.81-2.84)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.83Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.226 , 0.271 0.227 , 0.271	Depositor DCC
R_{free} test set	1953 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	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	0.93	EDS
Total number of atoms	5778	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: ALF, GOL, MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/5825	0.42	0/7878

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5709	0	5527	90	0
2	A	2	0	0	0	0
3	A	5	0	0	2	0
4	A	27	0	12	2	0
5	A	24	0	32	1	0
6	A	11	0	0	0	0
All	All	5778	0	5571	90	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 8.

All (90) 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:A:177:GLY:HA3	1:A:229:ILE:HG13	1.63	0.81
1:A:112:TYR:O	1:A:171:ARG:NH2	2.16	0.78
1:A:230:SER:HB2	1:A:424:HIS:HB2	1.65	0.77
1:A:502:GLY:H	1:A:505:ALA:HB3	1.54	0.72
1:A:309:VAL:HG11	1:A:416:ILE:HD13	1.72	0.71
1:A:209:ASN:HB3	1:A:212:SER:HB2	1.74	0.69
1:A:518:HIS:HB2	1:A:558:THR:HG23	1.77	0.66
1:A:65:ASP:OD1	1:A:85:ARG:NH2	2.29	0.65
1:A:25:GLY:HA2	1:A:39:CYS:HA	1.79	0.64
1:A:26:GLU:O	1:A:38:LEU:N	2.32	0.63
1:A:230:SER:OG	1:A:426:SER:OG	2.13	0.62
1:A:479:ILE:HG13	1:A:710:GLN:HG2	1.81	0.62
1:A:454:THR:HG23	1:A:612:LEU:HD11	1.83	0.61
1:A:376:ILE:HG22	1:A:385:THR:HG22	1.82	0.60
1:A:456:GLU:OE2	1:A:489:ASN:ND2	2.27	0.59
1:A:79:LEU:HD21	1:A:643:ASN:HB3	1.85	0.59
1:A:27:VAL:HA	1:A:37:VAL:HA	1.85	0.58
1:A:215:PHE:HB3	1:A:239:LEU:HD23	1.86	0.58
1:A:30:VAL:HA	1:A:35:ILE:HG22	1.86	0.56
1:A:460:GLN:OE1	1:A:468:LYS:NZ	2.38	0.56
1:A:162:LYS:NZ	4:A:1104:ADP:O2B	2.37	0.56
1:A:667:PRO:O	1:A:669:ARG:NH2	2.39	0.56
1:A:117:MET:HG2	1:A:172:TYR:HD1	1.71	0.55
1:A:538:PRO:HB2	1:A:541:ALA:HB3	1.88	0.55
1:A:354:LEU:HD21	1:A:369:GLU:HB2	1.88	0.54
1:A:204:ALA:HB2	1:A:254:TYR:HA	1.90	0.54
1:A:137:ASP:OD2	1:A:141[A]:ARG:NH1	2.38	0.54
1:A:205:LYS:HB3	1:A:252:ARG:HB2	1.90	0.53
1:A:252:ARG:HG2	1:A:258:TYR:CZ	2.44	0.53
1:A:209:ASN:ND2	4:A:1104:ADP:O2A	2.42	0.52
1:A:251:GLU:O	1:A:285:SER:OG	2.20	0.52
1:A:498:LYS:HD2	1:A:500:PRO:HD2	1.90	0.52
1:A:286:LYS:O	1:A:286:LYS:HG3	2.08	0.52
1:A:667:PRO:HG2	1:A:720:ALA:HA	1.93	0.52
1:A:643:ASN:N	1:A:643:ASN:OD1	2.43	0.51
1:A:375:ARG:HD2	1:A:388:LEU:HD21	1.93	0.50
1:A:85:ARG:NH1	1:A:92:TYR:O	2.44	0.50
1:A:276:PRO:HB2	1:A:288:LEU:HD22	1.93	0.50
1:A:240:GLU:O	1:A:254:TYR:OH	2.19	0.49
1:A:277:LYS:HB3	1:A:288:LEU:HD11	1.94	0.49
1:A:491:ASP:N	1:A:491:ASP:OD1	2.45	0.48
1:A:220:GLU:HB3	1:A:429:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:H	1:A:380:ARG:HD3	1.79	0.48
1:A:484:ILE:HD12	1:A:661:ILE:HG12	1.96	0.47
1:A:542:ARG:HD3	1:A:542:ARG:HA	1.49	0.47
1:A:534:ARG:HD3	1:A:548:CYS:HB2	1.96	0.47
1:A:538:PRO:HD2	1:A:544:ASP:O	2.14	0.47
1:A:117:MET:HG3	1:A:133:PHE:CE1	2.50	0.47
1:A:644:GLU:H	5:A:1105:GOL:H11	1.79	0.47
1:A:457:LYS:HD2	1:A:612:LEU:HD23	1.98	0.46
1:A:559:GLU:HB2	1:A:560:LEU:HD12	1.97	0.46
1:A:444:ASN:HB2	1:A:556:TYR:HA	1.98	0.46
1:A:319:ILE:HG23	1:A:408:LEU:HD11	1.98	0.45
1:A:628:ARG:NH2	1:A:653:GLY:O	2.49	0.45
1:A:81:ASN:O	1:A:85:ARG:HG3	2.15	0.45
1:A:558:THR:HA	1:A:561:PHE:CD1	2.52	0.45
1:A:479:ILE:CG1	1:A:710:GLN:HG2	2.47	0.45
1:A:477:GLU:HG3	1:A:717:PHE:HZ	1.82	0.45
1:A:22:TRP:CG	1:A:76:PRO:HG3	2.52	0.44
1:A:217:LYS:HA	1:A:235:ARG:O	2.18	0.44
1:A:464:GLN:HA	1:A:468:LYS:HB2	1.99	0.44
1:A:53:TYR:HB3	1:A:74:HIS:CD2	2.52	0.43
1:A:275:GLU:H	1:A:275:GLU:HG3	1.55	0.43
1:A:671:HIS:HA	1:A:715:LYS:HG2	2.00	0.43
1:A:26:GLU:N	1:A:38:LEU:O	2.45	0.43
1:A:124:SER:HB3	1:A:127:GLU:HG3	1.99	0.43
1:A:24:ASP:OD2	1:A:55:LYS:NZ	2.52	0.43
1:A:477:GLU:HG3	1:A:717:PHE:CZ	2.53	0.43
1:A:213:SER:N	3:A:1103:ALF:F2	2.32	0.43
1:A:574:GLN:O	1:A:578:ASN:ND2	2.33	0.43
1:A:543:SER:O	1:A:558:THR:HG22	2.19	0.43
1:A:93:THR:HG23	1:A:100:ILE:HB	2.01	0.42
1:A:98:ILE:HG12	1:A:626:TYR:HB2	2.01	0.42
1:A:223:PHE:O	1:A:426:SER:HB3	2.18	0.42
1:A:239:LEU:HD22	1:A:240:GLU:N	2.35	0.42
1:A:174:ALA:HB1	1:A:188:GLU:HB3	2.02	0.42
1:A:672:PHE:CE2	1:A:694:PRO:HB3	2.55	0.42
1:A:286:LYS:HE3	1:A:286:LYS:HB2	1.67	0.42
1:A:22:TRP:CD2	1:A:76:PRO:HG3	2.55	0.41
1:A:223:PHE:CE2	1:A:229:ILE:HG12	2.55	0.41
1:A:549:HIS:HB2	1:A:552:GLY:O	2.21	0.41
1:A:103:ASN:HB3	1:A:632:PRO:HD3	2.02	0.41
1:A:437:GLY:N	3:A:1103:ALF:F1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:NH1	1:A:440:SER:O	2.54	0.41
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.90	0.41
1:A:643:ASN:O	1:A:647:LEU:HB2	2.21	0.41
1:A:92:TYR:HB3	1:A:99:LEU:HD11	2.03	0.40
1:A:570:ILE:HG22	1:A:573:HIS:H	1.87	0.40
1:A:436:TYR:CD2	1:A:451:ILE:HG12	2.56	0.40
1:A:495:LEU:HD22	1:A:503:ILE:HD11	2.03	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	723/771 (94%)	713 (99%)	10 (1%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	612/674 (91%)	550 (90%)	62 (10%)	7 15

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	29	GLN
1	A	33	ASP
1	A	44	HIS
1	A	45	VAL
1	A	57	VAL
1	A	67	MET
1	A	68	THR
1	A	69	ARG
1	A	73	LEU
1	A	74	HIS
1	A	93	THR
1	A	111	LEU
1	A	114	SER
1	A	141[A]	ARG
1	A	141[B]	ARG
1	A	224	ASP
1	A	235	ARG
1	A	247	VAL
1	A	273	LEU
1	A	275	GLU
1	A	283	ASN
1	A	286	LYS
1	A	289	GLU
1	A	327	LEU
1	A	338	GLU
1	A	347	ASP
1	A	348	ASP
1	A	372	LEU
1	A	375	ARG
1	A	380	ARG
1	A	425	ASP
1	A	426	SER
1	A	428	TYR
1	A	429	LEU
1	A	436	TYR
1	A	447	GLU
1	A	460	GLN
1	A	464	GLN
1	A	495	LEU
1	A	497	GLU
1	A	542	ARG
1	A	568	TYR

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Mol	Chain	Res	Type
1	A	569	VAL
1	A	597	LYS
1	A	598	GLN
1	A	610	GLN
1	A	616	LEU
1	A	643	ASN
1	A	647	LEU
1	A	648	GLN
1	A	661	ILE
1	A	668	THR
1	A	669	ARG
1	A	673	ASP
1	A	676	LEU
1	A	681	ILE
1	A	685	GLU
1	A	688	VAL
1	A	693	ASP
1	A	710	GLN
1	A	734	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	ALF	A	1103	-	0,4,4	-	-	-		
5	GOL	A	1106	-	5,5,5	0.93	0	5,5,5	1.03	0
5	GOL	A	1105	-	5,5,5	0.85	0	5,5,5	1.25	1 (20%)
5	GOL	A	1108	-	5,5,5	0.98	0	5,5,5	1.21	1 (20%)
4	ADP	A	1104	2	24,29,29	0.66	0	29,45,45	0.77	1 (3%)
5	GOL	A	1107	-	5,5,5	0.92	0	5,5,5	0.93	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
5	GOL	A	1106	-	-	0/4/4/4	-
5	GOL	A	1105	-	-	2/4/4/4	-
5	GOL	A	1108	-	-	4/4/4/4	-
4	ADP	A	1104	2	-	0/12/32/32	0/3/3/3
5	GOL	A	1107	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1105	GOL	C3-C2-C1	-2.22	103.07	111.70
4	A	1104	ADP	C5-C6-N6	2.17	123.65	120.35
5	A	1108	GOL	C3-C2-C1	-2.01	103.88	111.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1108	GOL	C1-C2-C3-O3
5	A	1108	GOL	O2-C2-C3-O3
5	A	1108	GOL	O1-C1-C2-O2

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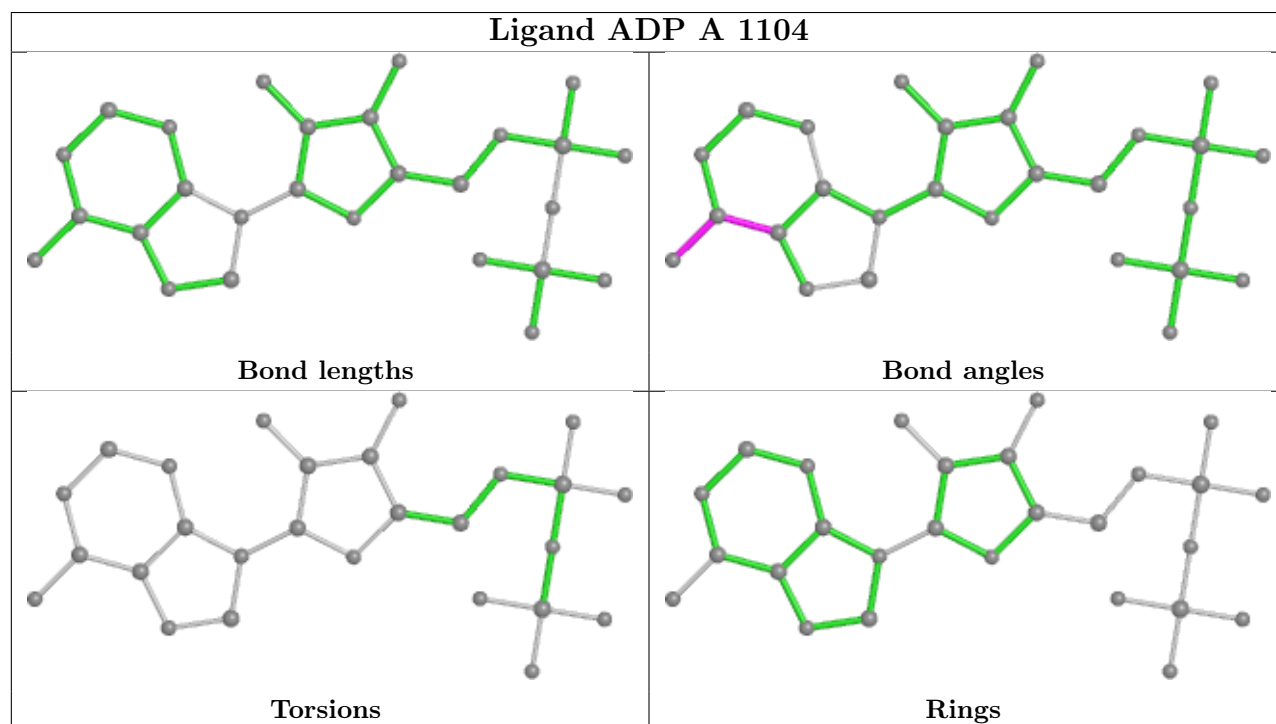
Mol	Chain	Res	Type	Atoms
5	A	1105	GOL	O1-C1-C2-O2
5	A	1108	GOL	O1-C1-C2-C3
5	A	1105	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	ALF	2	0
5	A	1105	GOL	1	0
4	A	1104	ADP	2	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/771 (94%)	0.32	54 (7%) 14 9	40, 77, 132, 202	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	595	ASP	9.6
1	A	594	ASP	8.2
1	A	4	ASN	5.4
1	A	540	LEU	5.3
1	A	542	ARG	4.9
1	A	599	SER	4.7
1	A	601	PHE	4.5
1	A	593	SER	4.4
1	A	541	ALA	4.1
1	A	32	GLY	4.0
1	A	125	LEU	3.9
1	A	591	PRO	3.8
1	A	421	GLY	3.8
1	A	734	LEU	3.7
1	A	423	ASP	3.5
1	A	527	GLN	3.4
1	A	596	SER	3.4
1	A	424	HIS	3.3
1	A	42	GLY	3.2
1	A	693	ASP	3.2
1	A	379	THR	3.1
1	A	61	ALA	3.0
1	A	378	VAL	3.0
1	A	382	GLU	3.0
1	A	126	GLY	2.9
1	A	384	ILE	2.9
1	A	12	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	381	ASP	2.8
1	A	512	MET	2.7
1	A	28	VAL	2.7
1	A	44	HIS	2.7
1	A	189	GLN	2.7
1	A	145	ASN	2.6
1	A	57	VAL	2.5
1	A	422	GLN	2.5
1	A	228	ARG	2.4
1	A	380	ARG	2.4
1	A	297	GLU	2.4
1	A	690	ASN	2.4
1	A	41	SER	2.4
1	A	442	LYS	2.3
1	A	425	ASP	2.2
1	A	428	TYR	2.2
1	A	69	ARG	2.2
1	A	515	ARG	2.2
1	A	5	PHE	2.2
1	A	6	ASN	2.2
1	A	122	GLY	2.2
1	A	592	MET	2.1
1	A	482	SER	2.1
1	A	88	ILE	2.1
1	A	483	TYR	2.0
1	A	590	PRO	2.0
1	A	500	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

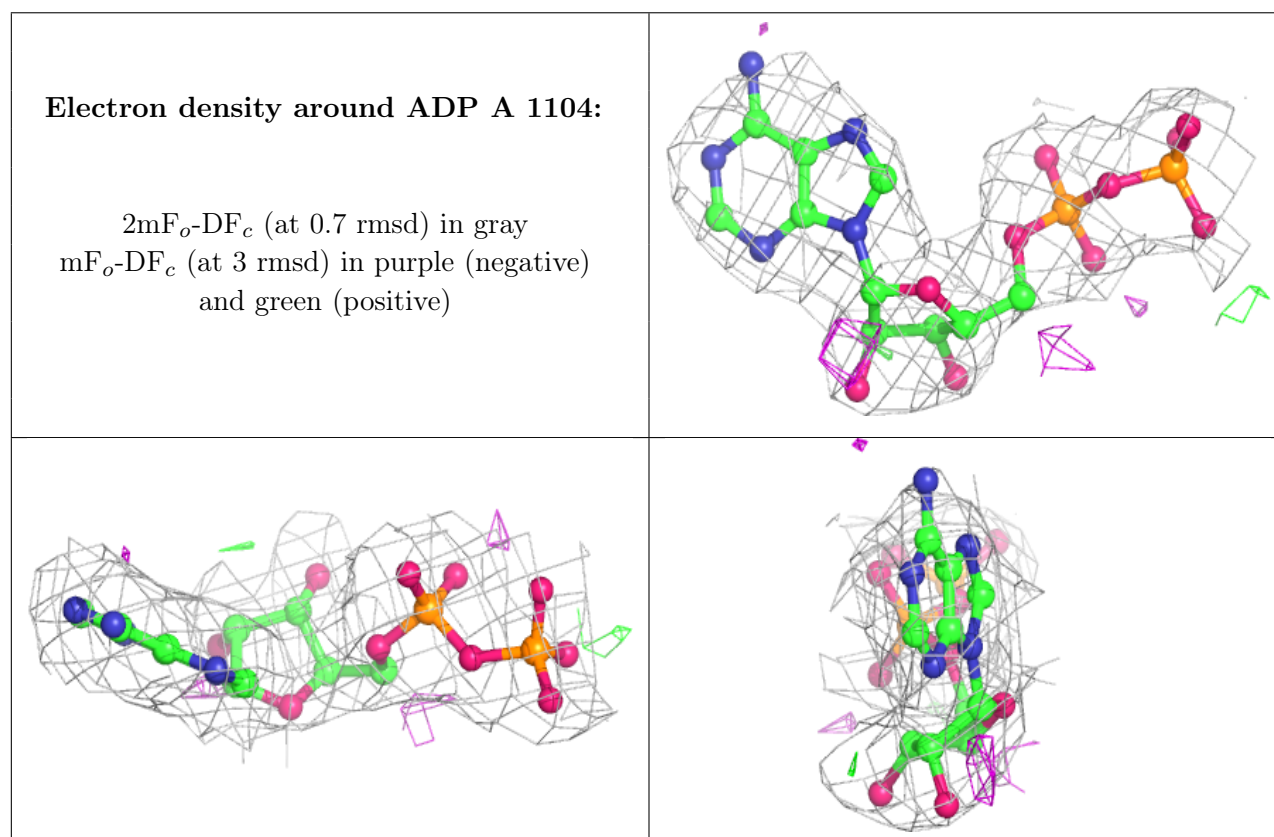
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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(\AA^2)	Q<0.9
5	GOL	A	1105	6/6	0.78	0.30	77,79,85,90	0
5	GOL	A	1107	6/6	0.83	0.27	75,80,83,85	0
2	MG	A	1101	1/1	0.86	0.34	66,66,66,66	0
5	GOL	A	1108	6/6	0.88	0.24	70,76,81,82	0
5	GOL	A	1106	6/6	0.91	0.19	75,78,79,81	0
2	MG	A	1102	1/1	0.92	0.13	48,48,48,48	0
4	ADP	A	1104	27/27	0.95	0.15	41,56,65,73	0
3	ALF	A	1103	5/5	0.97	0.16	54,55,56,57	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.