Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2024 – 07:22 pm BST

PDB ID	:	4ANJ
Title	:	MYOSIN VI (MDinsert2-GFP fusion) PRE-POWERSTROKE STATE (MG.ADP.AlF4)
Authors	:	Menetrey, J.; Isabet, T.; Ropars, V.; Mukherjea, M.; Pylypenko, O.; Liu, X.; Perez, J.; Vachette, P.; Sweeney, H.L.; Houdusse, A.M.
Deposited on	:	2012-03-19
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

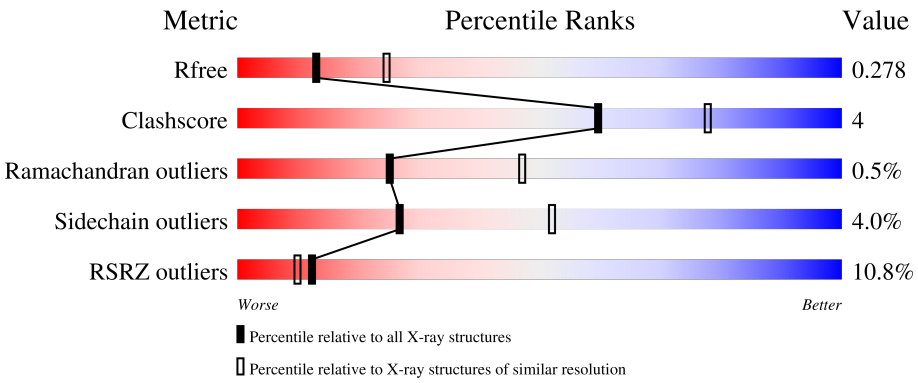
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 <=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	1052	2%, 84%, 10%, • 5%
2	B	149	66%, 74%, 11%, • 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CR2	A	1065	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8845 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 UNCONVENTIONAL MYOSIN-VI, GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	996	7864	5020	1349	1460	35	0	0	0

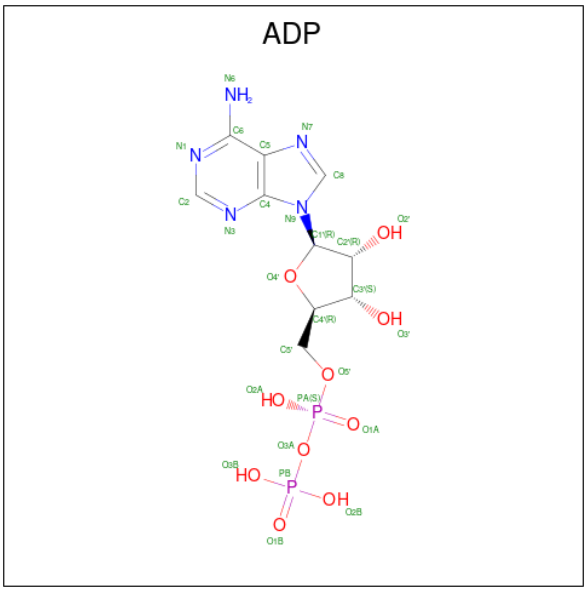
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q29122
A	547	VAL	GLY	SEE REMARK 999	UNP Q29122
A	572	ARG	ALA	SEE REMARK 999	UNP Q29122
A	573	ASP	TYR	SEE REMARK 999	UNP Q29122
A	714	LEU	VAL	SEE REMARK 999	UNP Q29122
A	721	TYR	SER	SEE REMARK 999	UNP Q29122
A	722	MET	LEU	SEE REMARK 999	UNP Q29122
A	1065	CR2	SER	engineered mutation	UNP Q29122
A	1065	CR2	SER	chromophore	UNP P42212
A	1065	CR2	TYR	chromophore	UNP P42212
A	1065	CR2	GLY	chromophore	UNP P42212

- Molecule 2 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	128	854	523	143	180	8	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

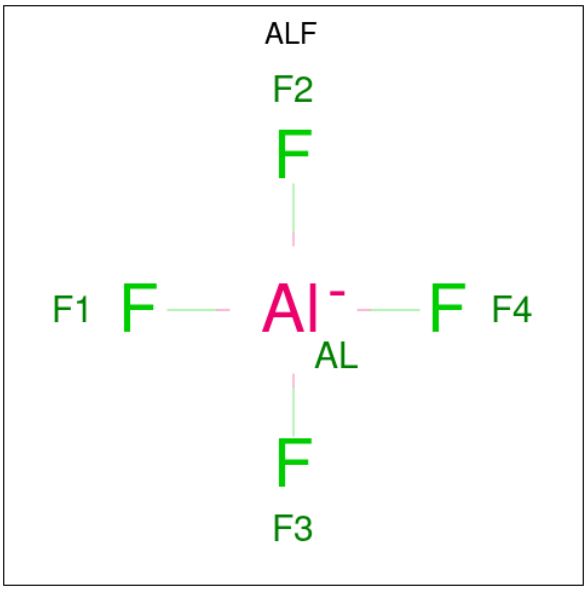


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	B	3	3	3	0	0

- Molecule 7 is water.

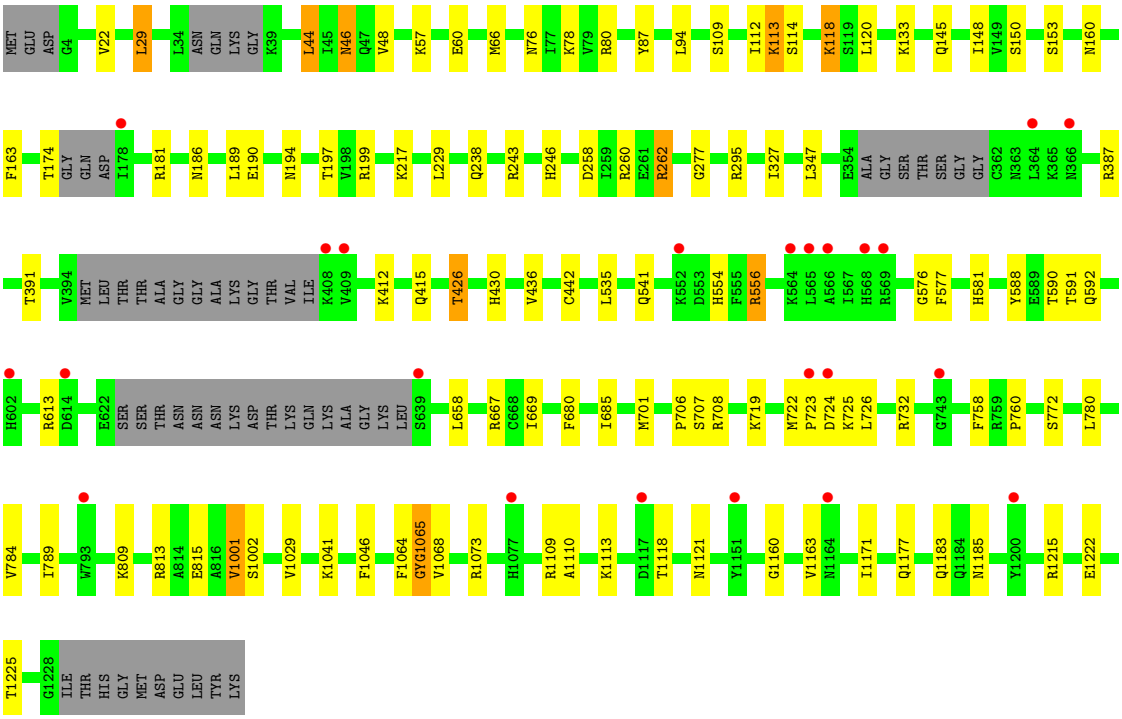
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	91	91	91	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

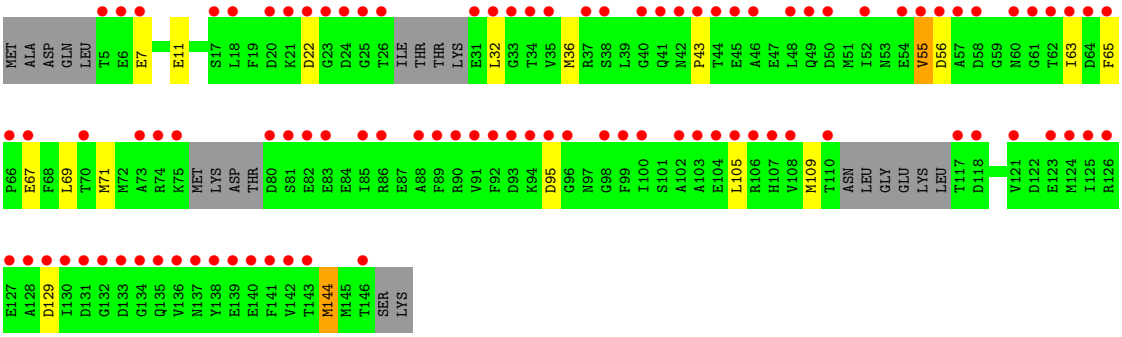
• Molecule 1: UNCONVENTIONAL MYOSIN-VI, GREEN FLUORESCENT PROTEIN

Chain A: 2% 84% 10% • 5%



• Molecule 2: CALMODULIN

Chain B: 66% 74% 11% • 14%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	193.09Å 62.66Å 156.04Å 90.00° 117.96° 90.00°	Depositor
Resolution (Å)	137.36 – 2.60 137.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (137.36-2.60) 100.0 (137.36-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.239 , 0.288 0.233 , 0.278	Depositor DCC
R_{free} test set	2595 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8845	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ALF, CR2, MG, ADP, CA

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	0.41	1/8015 (0.0%)	0.52	0/10835
2	B	0.36	0/860	0.51	0/1161
All	All	0.40	1/8875 (0.0%)	0.52	0/11996

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1001	VAL	CB-CG1	-7.71	1.36	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7864	0	7595	62	0
2	B	854	0	664	7	0
3	A	27	0	12	0	0
4	A	1	0	0	0	0
5	A	5	0	0	1	0
6	B	3	0	0	0	0
7	A	91	0	0	1	0
All	All	8845	0	8271	69	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 (69) 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:197:THR:HG22	1:A:199:ARG:H	1.42	0.83
1:A:1171:ILE:HD11	1:A:1177:GLN:HB2	1.62	0.81
2:B:144:MET:HE3	2:B:144:MET:HA	1.64	0.79
1:A:1064:PHE:C	1:A:1065:CR2:HN11	1.84	0.78
1:A:1065:CR2:HA11	1:A:1222:GLU:OE1	1.86	0.76
1:A:412:LYS:H	1:A:415:GLN:HE21	1.34	0.75
1:A:44:LEU:H	1:A:44:LEU:HD23	1.60	0.66
1:A:554:HIS:HD2	1:A:556:ARG:H	1.44	0.66
2:B:105:LEU:O	2:B:109:MET:HG2	1.96	0.65
1:A:114:SER:O	1:A:118:LYS:HE3	1.96	0.65
1:A:76:ASN:O	1:A:80:ARG:HG3	1.98	0.63
1:A:153:SER:HA	5:A:2232:ALF:F4	1.88	0.62
1:A:1065:CR2:HD2	1:A:1065:CR2:N2	2.16	0.61
1:A:46:ASN:C	1:A:46:ASN:HD22	2.06	0.59
1:A:258:ASP:O	1:A:262:ARG:HG2	2.03	0.59
1:A:29:LEU:HD21	1:A:48:VAL:HG21	1.85	0.59
1:A:1064:PHE:C	1:A:1065:CR2:HN12	2.04	0.58
2:B:32:LEU:O	2:B:36:MET:HB2	2.03	0.58
2:B:55:VAL:HG11	2:B:67:GLU:HA	1.86	0.57
1:A:813:ARG:O	1:A:1001:VAL:HG13	2.05	0.56
1:A:1171:ILE:HD11	1:A:1177:GLN:CB	2.35	0.56
1:A:412:LYS:H	1:A:415:GLN:NE2	2.04	0.54
1:A:109:SER:O	1:A:113:LYS:HG2	2.07	0.54
1:A:581:HIS:HE1	1:A:588:TYR:OH	1.92	0.53
2:B:55:VAL:HG21	2:B:71:MET:HB2	1.92	0.52
1:A:1065:CR2:HA12	1:A:1065:CR2:C3	2.41	0.51
1:A:1046:PHE:CZ	1:A:1064:PHE:HB3	2.46	0.51
1:A:554:HIS:CD2	1:A:556:ARG:H	2.27	0.50
1:A:243:ARG:HH21	1:A:246:HIS:HD2	1.60	0.49
1:A:1064:PHE:O	1:A:1065:CR2:N1	2.47	0.48
1:A:707:SER:HB2	1:A:758:PHE:HB2	1.95	0.48
1:A:1160:GLY:HA3	1:A:1185:ASN:O	2.14	0.48
1:A:87:TYR:HB3	1:A:94:LEU:HD11	1.96	0.47
1:A:1163:VAL:HB	1:A:1183:GLN:HB3	1.96	0.47
1:A:701:MET:CE	1:A:760:PRO:HG3	2.44	0.47
1:A:190:GLU:O	1:A:194:ASN:HB2	2.15	0.47
1:A:426:THR:O	1:A:430:HIS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:O	1:A:391:THR:HB	2.15	0.46
1:A:181:ARG:HD3	1:A:442:CYS:HB3	1.98	0.46
1:A:591:THR:O	1:A:592:GLN:HB2	2.14	0.46
1:A:44:LEU:HD23	1:A:44:LEU:N	2.30	0.46
1:A:723:PRO:O	1:A:724:ASP:HB3	2.15	0.46
1:A:78:LYS:HG3	1:A:680:PHE:CD1	2.52	0.45
2:B:65:PHE:CZ	2:B:69:LEU:HD11	2.51	0.45
1:A:327:ILE:HD12	1:A:442:CYS:SG	2.57	0.45
1:A:813:ARG:O	1:A:1001:VAL:CG1	2.64	0.45
1:A:1110:ALA:HB1	1:A:1121:ASN:HD21	1.81	0.44
1:A:148:ILE:HD11	1:A:658:LEU:HD22	1.97	0.44
1:A:120:LEU:HD11	1:A:133:LYS:HG3	1.99	0.44
1:A:112:ILE:HG22	1:A:113:LYS:HE3	1.99	0.44
1:A:809:LYS:O	1:A:813:ARG:HG2	2.18	0.43
2:B:7:GLU:O	2:B:11:GLU:HG2	2.18	0.43
1:A:669:ILE:HG21	1:A:685:ILE:HG23	2.00	0.43
1:A:701:MET:CE	1:A:706:PRO:HD3	2.48	0.43
1:A:576:GLY:HA2	1:A:590:THR:HG23	2.01	0.43
1:A:150:SER:OG	1:A:667:ARG:NH1	2.52	0.43
1:A:238:GLN:HG2	1:A:277:GLY:HA3	2.01	0.42
1:A:780:LEU:O	1:A:784:VAL:HG13	2.19	0.42
1:A:1041:LYS:NZ	7:A:2074:HOH:O	2.52	0.42
1:A:189:LEU:HD22	1:A:436:VAL:HG12	2.02	0.42
1:A:1065:CR2:C3	1:A:1068:VAL:HG22	2.50	0.41
1:A:60:GLU:HG2	1:A:80:ARG:NH2	2.35	0.41
1:A:701:MET:HE2	1:A:760:PRO:HG3	2.03	0.41
1:A:66:MET:HB3	1:A:66:MET:HE2	1.99	0.41
1:A:701:MET:HE1	1:A:706:PRO:HD3	2.03	0.41
1:A:1073:ARG:HG2	1:A:1225:THR:HG23	2.03	0.41
1:A:260:ARG:HD3	1:A:295:ARG:NE	2.35	0.40
1:A:719:LYS:HA	1:A:722:MET:SD	2.61	0.40
1:A:160:ASN:HA	1:A:163:PHE:CD2	2.57	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	981/1052 (93%)	954 (97%)	25 (2%)	2 (0%)	44	66
2	B	120/149 (80%)	114 (95%)	3 (2%)	3 (2%)	4	8
All	All	1101/1201 (92%)	1068 (97%)	28 (2%)	5 (0%)	25	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	A	725	LYS
2	B	56	ASP
2	B	43	PRO
2	B	129	ASP

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	836/927 (90%)	805 (96%)	31 (4%)	29	55
2	B	66/128 (52%)	61 (92%)	5 (8%)	11	23
All	All	902/1055 (86%)	866 (96%)	36 (4%)	27	52

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	29	LEU
1	A	44	LEU
1	A	46	ASN
1	A	57	LYS
1	A	113	LYS
1	A	118	LYS

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Mol	Chain	Res	Type
1	A	145	GLN
1	A	174	THR
1	A	186	ASN
1	A	217	LYS
1	A	262	ARG
1	A	347	LEU
1	A	426	THR
1	A	535	LEU
1	A	541	GLN
1	A	556	ARG
1	A	577	PHE
1	A	613	ARG
1	A	708	ARG
1	A	726	LEU
1	A	732	ARG
1	A	772	SER
1	A	789	ILE
1	A	815	GLU
1	A	1002	SER
1	A	1029	VAL
1	A	1109	ARG
1	A	1113	LYS
1	A	1118	THR
1	A	1215	ARG
2	B	22	ASP
2	B	55	VAL
2	B	63	ILE
2	B	95	ASP
2	B	144	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	116	GLN
1	A	145	GLN
1	A	194	ASN
1	A	213	HIS
1	A	246	HIS
1	A	290	GLN
1	A	370	GLN
1	A	415	GLN

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Mol	Chain	Res	Type
1	A	430	HIS
1	A	434	HIS
1	A	537	GLN
1	A	554	HIS
1	A	581	HIS
1	A	679	HIS
1	A	684	GLN
1	A	768	GLN
1	A	776	HIS
1	A	1121	ASN
1	A	1135	ASN
1	A	1149	ASN
1	A	1177	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CR2	A	1065	1	20,20,21	5.25	6 (30%)	25,27,29	6.03	8 (32%)

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	CR2	A	1065	1	-	2/6/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1065	CR2	CB2-CA2	20.15	1.52	1.35
1	A	1065	CR2	CA2-C2	-10.33	1.38	1.48
1	A	1065	CR2	C2-N3	-3.46	1.31	1.39
1	A	1065	CR2	CG2-CB2	2.72	1.52	1.46
1	A	1065	CR2	O2-C2	2.42	1.28	1.23
1	A	1065	CR2	C1-N2	2.28	1.36	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1065	CR2	CA2-C2-N3	22.34	113.93	103.37
1	A	1065	CR2	CG2-CB2-CA2	-11.08	116.37	129.94
1	A	1065	CR2	O2-C2-CA2	-10.74	124.93	130.96
1	A	1065	CR2	C2-CA2-N2	-8.51	102.97	108.93
1	A	1065	CR2	C2-N3-C1	-7.43	104.36	107.99
1	A	1065	CR2	CB2-CA2-C2	4.14	127.22	122.28
1	A	1065	CR2	C1-CA1-N1	-2.65	106.99	112.85
1	A	1065	CR2	CA1-C1-N3	2.05	125.27	122.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1065	CR2	C3-CA3-N3-C1
1	A	1065	CR2	C3-CA3-N3-C2

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1065	CR2	7	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	ADP	A	2230	4	24,29,29	0.99	1 (4%)	29,45,45	1.35	4 (13%)
5	ALF	A	2232	-	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	2230	4	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2230	ADP	C5-C4	2.50	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2230	ADP	N3-C2-N1	-3.34	123.46	128.68
3	A	2230	ADP	C4-C5-N7	-2.80	106.48	109.40
3	A	2230	ADP	C3'-C2'-C1'	2.59	104.88	100.98
3	A	2230	ADP	PA-O3A-PB	-2.40	124.58	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2230	ADP	PA-O3A-PB-O3B
3	A	2230	ADP	PA-O3A-PB-O1B

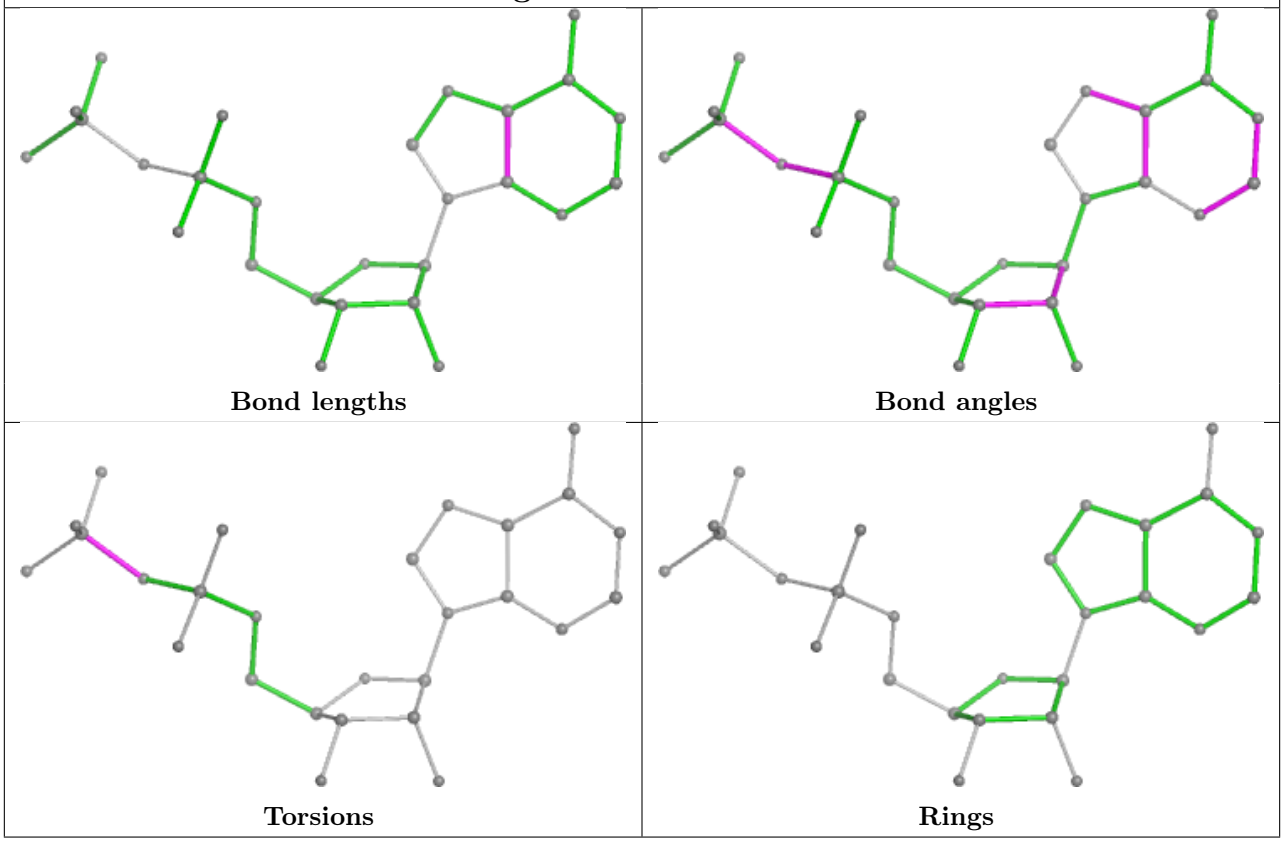
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2232	ALF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ADP A 2230



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1065:CR2	C3	1068:VAL	N	2.28
1	A	1064:PHE	C	1065:CR2	N1	2.12

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	995/1052 (94%)	-0.08	23 (2%) 61 55	9, 20, 35, 46	0
2	B	128/149 (85%)	2.91	98 (76%) 0 0	46, 59, 65, 66	0
All	All	1123/1201 (93%)	0.26	121 (10%) 12 10	9, 22, 59, 66	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	46	ALA	6.1
2	B	63	ILE	5.9
2	B	42	ASN	5.9
2	B	34	THR	5.5
2	B	146	THR	5.5
2	B	136	VAL	5.4
2	B	43	PRO	5.3
2	B	26	THR	5.2
2	B	80	ASP	5.0
2	B	45	GLU	5.0
2	B	94	LYS	4.9
2	B	92	PHE	4.9
2	B	135	GLN	4.7
2	B	103	ALA	4.6
2	B	100	ILE	4.5
2	B	95	ASP	4.4
2	B	64	ASP	4.3
2	B	6	GLU	4.3
2	B	40	GLY	4.2
2	B	66	PRO	4.2
2	B	110	THR	4.1
2	B	58	ASP	4.1
2	B	125	ILE	4.0
2	B	55	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	133	ASP	3.9
2	B	99	PHE	3.9
1	A	1164	ASN	3.9
2	B	57	ALA	3.8
2	B	143	THR	3.8
2	B	32	LEU	3.8
1	A	724	ASP	3.8
1	A	723	PRO	3.8
2	B	31	GLU	3.7
2	B	138	TYR	3.7
2	B	91	VAL	3.7
2	B	49	GLN	3.7
2	B	25	GLY	3.7
2	B	37	ARG	3.6
2	B	86	ARG	3.6
2	B	141	PHE	3.6
2	B	48	LEU	3.5
2	B	52	ILE	3.5
2	B	44	THR	3.5
2	B	22	ASP	3.5
2	B	70	THR	3.4
2	B	117	THR	3.4
1	A	408	LYS	3.4
2	B	35	VAL	3.4
2	B	62	THR	3.4
2	B	130	ILE	3.4
2	B	38	SER	3.4
2	B	21	LYS	3.3
2	B	89	PHE	3.3
2	B	20	ASP	3.3
1	A	178	ILE	3.2
2	B	142	VAL	3.2
2	B	50	ASP	3.2
2	B	98	GLY	3.2
2	B	123	GLU	3.2
1	A	793	TRP	3.2
2	B	108	VAL	3.2
2	B	96	GLY	3.1
2	B	93	ASP	3.1
2	B	139	GLU	3.1
2	B	83	GLU	3.0
1	A	564	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	75	LYS	3.0
1	A	602	HIS	2.9
2	B	61	GLY	2.9
2	B	88	ALA	2.8
2	B	7	GLU	2.8
1	A	1151	TYR	2.8
2	B	24	ASP	2.8
2	B	134	GLY	2.8
2	B	127	GLU	2.7
2	B	41	GLN	2.7
2	B	82	GLU	2.7
2	B	126	ARG	2.7
1	A	409	VAL	2.6
2	B	23	GLY	2.6
2	B	129	ASP	2.6
1	A	565	LEU	2.6
2	B	60	ASN	2.5
2	B	107	HIS	2.5
2	B	90	ARG	2.5
2	B	121	VAL	2.5
1	A	366	ASN	2.4
2	B	56	ASP	2.4
1	A	566	ALA	2.4
2	B	54	GLU	2.4
2	B	73	ALA	2.4
1	A	1200	TYR	2.4
1	A	552	LYS	2.4
2	B	85	ILE	2.4
2	B	102	ALA	2.4
1	A	743	GLY	2.4
2	B	104	GLU	2.3
1	A	569	ARG	2.3
2	B	65	PHE	2.3
1	A	639	SER	2.3
2	B	33	GLY	2.3
2	B	140	GLU	2.3
1	A	1117	ASP	2.3
2	B	74	ARG	2.3
2	B	67	GLU	2.3
2	B	137	ASN	2.2
2	B	17	SER	2.2
2	B	81	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	131	ASP	2.2
2	B	124	MET	2.2
2	B	132	GLY	2.2
2	B	118	ASP	2.2
1	A	1077	HIS	2.1
2	B	105	LEU	2.1
2	B	128	ALA	2.1
1	A	568	HIS	2.1
2	B	5	THR	2.1
1	A	364	LEU	2.0
2	B	18	LEU	2.0
2	B	106	ARG	2.0
1	A	614	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	CR2	A	1065	19/20	0.93	0.09	12,13,14,14	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	B	1147	1/1	0.87	0.11	65,65,65,65	0
6	CA	B	1149	1/1	0.91	0.07	56,56,56,56	0
6	CA	B	1148	1/1	0.95	0.07	63,63,63,63	0
5	ALF	A	2232	5/5	0.98	0.06	13,13,13,13	0

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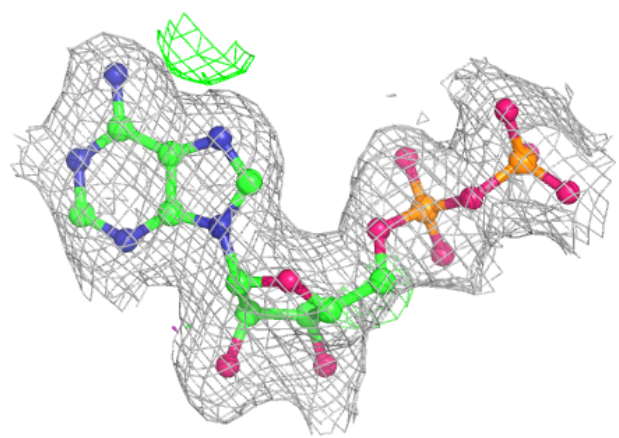
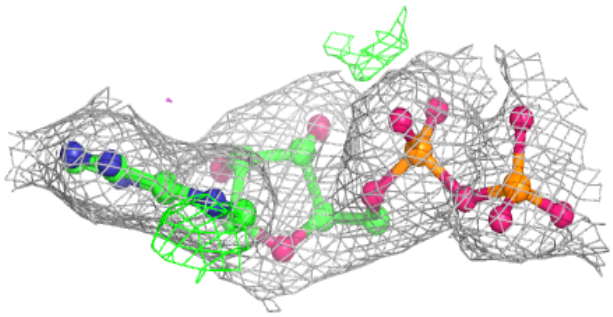
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	2230	27/27	0.98	0.06	2,8,9,10	0
4	MG	A	2231	1/1	0.99	0.02	3,3,3,3	0

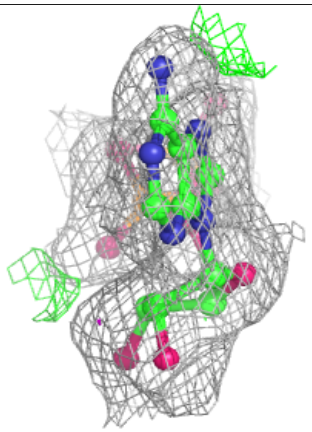
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 2230:

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.