Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 02:18 AM EDT

PDB ID	:	1JWY
Title	:	CRYSTAL STRUCTURE OF THE DYNAMIN A GTPASE DOMAIN COMPLEXED WITH GDP, DETERMINED AS MYOSIN FUSION
Authors	:	Niemann, H.H.; Knetsch, M.L.W.; Scherer, A.; Manstein, D.J.; Kull, F.J.
Deposited on	:	2001-09-05
Resolution	:	2.30 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:

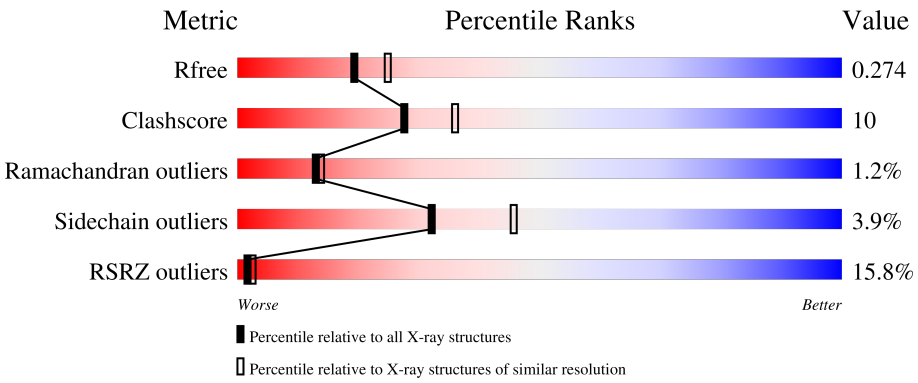
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

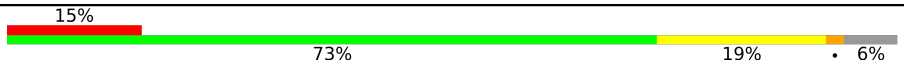
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	1100	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8735 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.

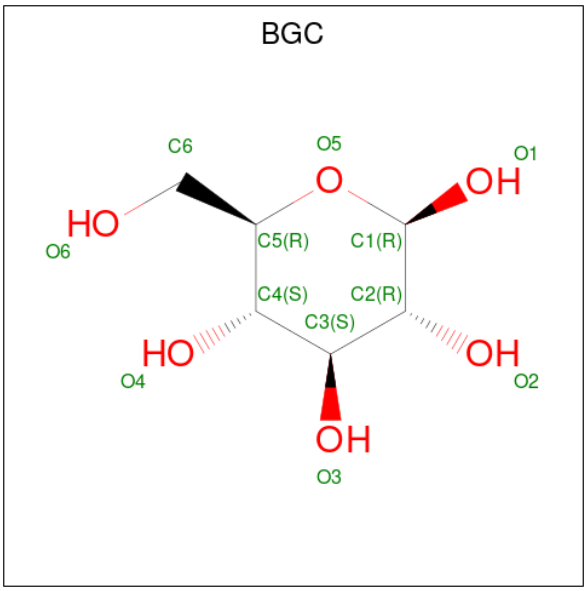
- Molecule 1 is a protein called Myosin-2 heavy chain,Dynamin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1039	8297	5281	1425	1568	23	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P08799
A	2	HIS	-	expression tag	UNP P08799
A	3	HIS	-	expression tag	UNP P08799
A	4	HIS	-	expression tag	UNP P08799
A	5	HIS	-	expression tag	UNP P08799
A	6	HIS	-	expression tag	UNP P08799
A	7	HIS	-	expression tag	UNP P08799
A	8	HIS	-	expression tag	UNP P08799
A	9	ASP	-	expression tag	UNP P08799
A	10	GLY	-	expression tag	UNP P08799
A	11	THR	-	expression tag	UNP P08799
A	12	GLU	-	expression tag	UNP P08799
A	13	ASP	-	expression tag	UNP P08799
A	777	THR	-	linker	UNP P08799
A	778	ARG	-	linker	UNP P08799
A	779	GLY	-	linker	UNP P08799
A	780	LEU	-	linker	UNP P08799
A	781	VAL	-	linker	UNP P08799
A	782	PRO	-	linker	UNP P08799
A	783	ARG	-	linker	UNP P08799
A	784	GLY	-	linker	UNP P08799
A	785	SER	-	linker	UNP P08799

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).

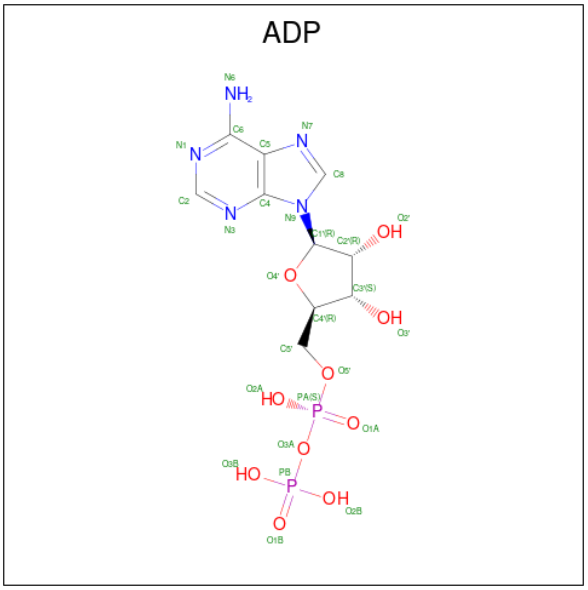


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

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

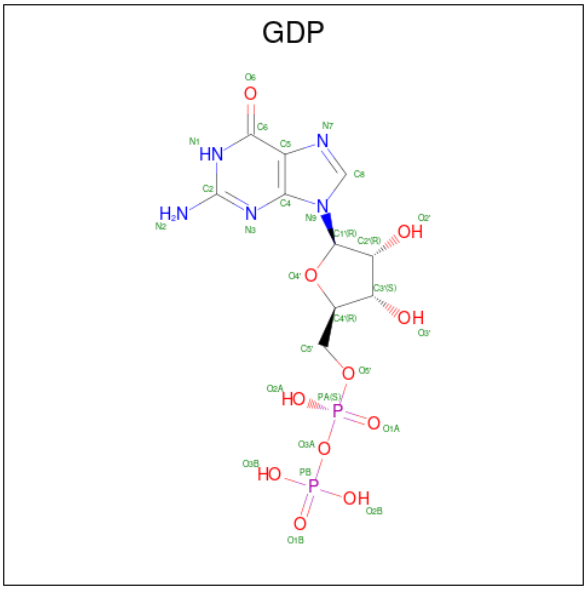
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0

- Molecule 4 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		
4	A	1	27	10	5	10	2	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	28	10	5	11	2	0	0

- Molecule 6 is water.

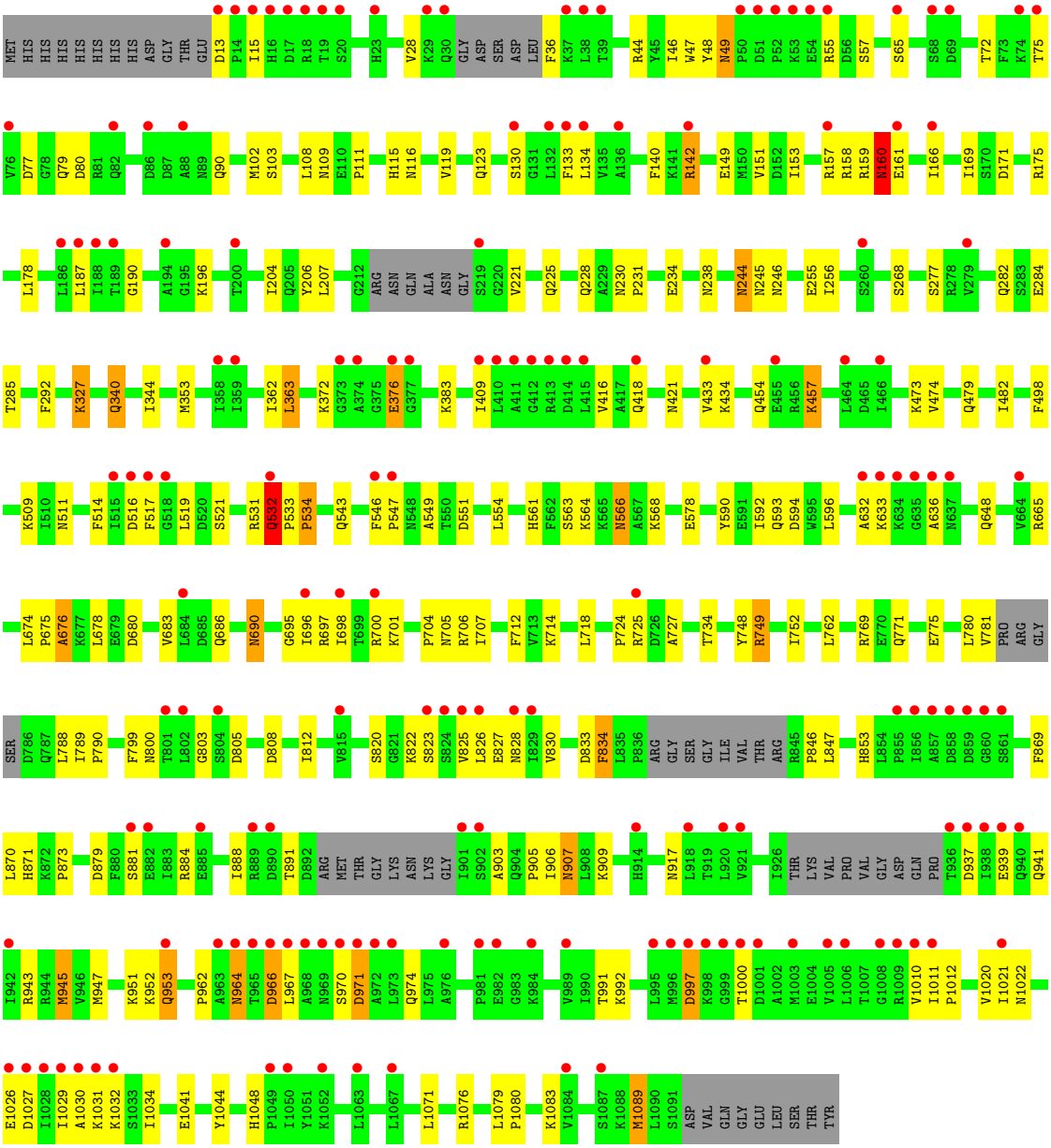
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	369	369	369	0	0

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: Myosin-2 heavy chain,Dynamin-A

Chain A: 15% 73% 19% • 6%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.55Å 61.95Å 181.07Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	29.40 – 2.30 29.44 – 2.32	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.40-2.30) 95.4 (29.44-2.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.02 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.257 0.231 , 0.274	Depositor DCC
R_{free} test set	3470 reflections (6.87%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.0	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	0.92	EDS
Total number of atoms	8735	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: MG, BGC, ADP, GDP

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	0.42	0/8447	0.56	0/11405

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 (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	8297	0	8344	167	0
2	A	12	0	12	0	0
3	A	2	0	0	0	0
4	A	27	0	12	0	0
5	A	28	0	12	1	0
6	A	369	0	0	6	0
All	All	8735	0	8380	167	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 10.

All (167) 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:532:GLN:HB3	1:A:533:PRO:HD3	1.38	1.03
1:A:566:ASN:HD22	1:A:568:LYS:H	1.20	0.90
1:A:244:ASN:ND2	1:A:246:ASN:H	1.76	0.82
1:A:566:ASN:ND2	1:A:568:LYS:H	1.82	0.77
1:A:962:PRO:HB3	1:A:992:LYS:HD2	1.66	0.76
1:A:532:GLN:HB3	1:A:533:PRO:CD	2.15	0.73
1:A:13:ASP:OD1	1:A:15:ILE:HG22	1.89	0.73
1:A:812:ILE:HD11	1:A:1071:LEU:HB2	1.71	0.73
1:A:665:ARG:HD2	1:A:690:ASN:ND2	2.04	0.72
1:A:65:SER:HB3	1:A:72:THR:HB	1.70	0.72
1:A:748:TYR:O	1:A:749:ARG:HD3	1.91	0.69
1:A:788:LEU:HD11	1:A:1076:ARG:HE	1.57	0.69
1:A:853:HIS:H	1:A:917:ASN:ND2	1.90	0.68
1:A:514:PHE:HE1	1:A:701:LYS:HB2	1.58	0.67
1:A:665:ARG:HD2	1:A:690:ASN:HD21	1.59	0.67
1:A:533:PRO:HD2	6:A:1629:HOH:O	1.94	0.66
1:A:632:ALA:HB1	1:A:636:ALA:HB3	1.79	0.65
1:A:166:ILE:HD12	1:A:169:ILE:HD11	1.77	0.64
1:A:532:GLN:CB	1:A:533:PRO:HD3	2.22	0.64
1:A:551:ASP:HB3	1:A:592:ILE:HG23	1.80	0.64
1:A:812:ILE:HG13	1:A:1071:LEU:HD13	1.80	0.64
1:A:803:GLY:HA2	1:A:905:PRO:HD3	1.80	0.63
1:A:1021:ILE:HD11	1:A:1041:GLU:HA	1.81	0.63
1:A:870:LEU:HB2	1:A:907:ASN:HB3	1.82	0.62
1:A:532:GLN:O	1:A:534:PRO:HD3	1.99	0.62
1:A:284:GLU:HG2	1:A:285:THR:HG23	1.82	0.62
1:A:13:ASP:CG	1:A:15:ILE:HG22	2.20	0.61
1:A:140:PHE:O	1:A:675:PRO:HG3	2.00	0.61
1:A:991:THR:HA	1:A:1020:VAL:O	2.01	0.60
1:A:454:GLN:HB3	6:A:1403:HOH:O	2.01	0.60
1:A:700:ARG:HA	1:A:704:PRO:HG3	1.83	0.60
1:A:44:ARG:HH21	1:A:90:GLN:HE22	1.47	0.60
1:A:376:GLU:H	1:A:376:GLU:CD	2.05	0.60
1:A:49:ASN:ND2	1:A:55:ARG:HD2	2.17	0.59
1:A:509:LYS:HE2	1:A:752:ILE:HD11	1.85	0.59
1:A:997:ASP:HB2	1:A:1000:THR:OG1	2.03	0.58
1:A:244:ASN:HD22	1:A:245:ASN:N	2.02	0.58
1:A:695:GLY:O	1:A:698:ILE:HG12	2.04	0.57
1:A:830:VAL:HG21	1:A:834:PHE:CE2	2.39	0.57
1:A:546:PHE:HB3	1:A:549:ALA:HB2	1.85	0.57
1:A:939:GLU:O	1:A:943:ARG:HG2	2.05	0.57
1:A:566:ASN:HD22	1:A:568:LYS:N	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:LYS:NZ	5:A:1205:GDP:C8	2.73	0.56
1:A:991:THR:HG22	1:A:1020:VAL:HG23	1.87	0.56
1:A:700:ARG:HD3	1:A:704:PRO:HG2	1.88	0.55
1:A:805:ASP:HB3	1:A:952:LYS:HE3	1.89	0.55
1:A:879:ASP:OD1	1:A:881:SER:HB2	2.07	0.55
1:A:1044:TYR:O	1:A:1048:HIS:HB2	2.07	0.55
1:A:1021:ILE:O	1:A:1021:ILE:HG13	2.06	0.55
1:A:102:MET:HG2	1:A:116:ASN:ND2	2.22	0.54
1:A:516:ASP:HB3	1:A:519:LEU:HD13	1.88	0.54
1:A:149:GLU:O	1:A:153:ILE:HG13	2.07	0.54
1:A:204:ILE:HD12	1:A:256:ILE:HD11	1.90	0.54
1:A:823:SER:O	1:A:827:GLU:HG3	2.08	0.53
1:A:789:ILE:HB	1:A:790:PRO:HD3	1.91	0.52
1:A:822:LYS:O	1:A:825:VAL:HG12	2.09	0.52
1:A:724:PRO:HG2	1:A:727:ALA:HB2	1.91	0.52
1:A:36:PHE:CZ	1:A:1083:LYS:HD2	2.45	0.52
1:A:1079:LEU:HB3	1:A:1080:PRO:HD3	1.91	0.52
1:A:498:PHE:HB2	1:A:517:PHE:CD1	2.45	0.51
1:A:1026:GLU:HA	1:A:1029:ILE:HD12	1.93	0.51
1:A:941:GLN:HE21	1:A:941:GLN:HA	1.76	0.51
1:A:255:GLU:HB2	1:A:268:SER:OG	2.11	0.51
1:A:340:GLN:HE22	1:A:344:ILE:HG12	1.76	0.51
1:A:228:GLN:O	1:A:231:PRO:HD2	2.11	0.50
1:A:648:GLN:NE2	6:A:1308:HOH:O	2.43	0.50
1:A:151:VAL:HG13	1:A:206:TYR:CD1	2.47	0.50
1:A:102:MET:O	1:A:108:LEU:HD21	2.11	0.50
1:A:686:GLN:O	1:A:690:ASN:HB2	2.12	0.50
1:A:781:VAL:O	1:A:1079:LEU:HD21	2.11	0.50
1:A:953:GLN:HE21	1:A:953:GLN:H	1.59	0.50
1:A:947:MET:O	1:A:951:LYS:HB2	2.11	0.50
1:A:700:ARG:HA	1:A:704:PRO:CG	2.41	0.49
1:A:340:GLN:HE22	1:A:344:ILE:CG1	2.26	0.49
1:A:416:VAL:HG13	1:A:418:GLN:NE2	2.28	0.49
1:A:953:GLN:H	1:A:953:GLN:NE2	2.09	0.49
1:A:521:SER:HA	6:A:1302:HOH:O	2.13	0.49
1:A:362:ILE:HG23	1:A:433:VAL:HG13	1.94	0.49
1:A:820:SER:HB2	1:A:962:PRO:HD3	1.95	0.48
1:A:28:VAL:HG13	1:A:123:GLN:HE22	1.79	0.48
1:A:102:MET:HG2	1:A:116:ASN:HD22	1.77	0.48
1:A:327:LYS:HE2	1:A:327:LYS:H	1.78	0.48
1:A:409:ILE:HG12	1:A:418:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLN:O	1:A:594:ASP:HB2	2.13	0.48
1:A:805:ASP:OD2	1:A:808:ASP:HA	2.14	0.48
1:A:234:GLU:O	1:A:238:ASN:HB2	2.14	0.47
1:A:49:ASN:HB3	1:A:57:SER:O	2.15	0.47
1:A:514:PHE:CE1	1:A:701:LYS:HB2	2.45	0.47
1:A:1079:LEU:O	1:A:1083:LYS:HG3	2.14	0.47
1:A:871:HIS:C	1:A:873:PRO:HD3	2.35	0.47
1:A:158:ARG:H	1:A:161:GLU:CD	2.18	0.47
1:A:884:ARG:O	1:A:888:ILE:HG13	2.15	0.47
1:A:632:ALA:HB1	1:A:636:ALA:CB	2.46	0.46
1:A:825:VAL:HG13	1:A:826:LEU:N	2.31	0.46
1:A:1029:ILE:O	1:A:1030:ALA:HB3	2.15	0.46
1:A:49:ASN:HD21	1:A:55:ARG:HD2	1.81	0.45
1:A:964:ASN:HD22	1:A:964:ASN:C	2.19	0.45
1:A:870:LEU:CB	1:A:907:ASN:HB3	2.44	0.45
1:A:115:HIS:O	1:A:119:VAL:HG23	2.17	0.45
1:A:171:ASP:O	1:A:175:ARG:HG2	2.17	0.45
1:A:327:LYS:HE2	1:A:327:LYS:N	2.32	0.45
1:A:1021:ILE:HG12	1:A:1041:GLU:HG3	1.99	0.45
1:A:888:ILE:O	1:A:891:THR:HG22	2.17	0.45
1:A:964:ASN:OD1	1:A:992:LYS:HD3	2.17	0.44
1:A:277:SER:HA	1:A:434:LYS:HD3	2.00	0.44
1:A:695:GLY:C	1:A:697:ARG:H	2.20	0.44
1:A:75:THR:HG22	1:A:77:ASP:H	1.83	0.44
1:A:244:ASN:HD22	1:A:244:ASN:C	2.20	0.44
1:A:531:ARG:O	1:A:532:GLN:C	2.55	0.44
1:A:292:PHE:CD1	1:A:363:LEU:HD13	2.53	0.44
1:A:1010:VAL:C	1:A:1012:PRO:HD3	2.38	0.43
1:A:158:ARG:H	1:A:161:GLU:CG	2.31	0.43
1:A:158:ARG:HB2	1:A:158:ARG:NH1	2.33	0.43
1:A:833:ASP:HB2	1:A:884:ARG:NH2	2.33	0.43
1:A:44:ARG:HH21	1:A:90:GLN:NE2	2.14	0.43
1:A:820:SER:HA	1:A:962:PRO:CG	2.49	0.43
1:A:714:LYS:HG2	1:A:725:ARG:HE	1.84	0.43
1:A:554:LEU:HD23	1:A:592:ILE:HG13	2.00	0.43
1:A:1027:ASP:O	1:A:1032:LYS:HB3	2.19	0.43
1:A:230:ASN:HB3	1:A:231:PRO:HD3	2.01	0.43
1:A:479:GLN:HA	1:A:482:ILE:HG22	1.99	0.43
1:A:700:ARG:HH12	1:A:705:ASN:HD21	1.67	0.43
1:A:846:PRO:O	1:A:906:ILE:HG22	2.19	0.43
1:A:706:ARG:HD2	6:A:1534:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:NZ	1:A:421:ASN:HB2	2.33	0.42
1:A:907:ASN:ND2	1:A:909:LYS:NZ	2.67	0.42
1:A:48:TYR:OH	1:A:75:THR:HG23	2.18	0.42
1:A:159:ARG:O	1:A:159:ARG:HG2	2.19	0.42
1:A:563:SER:O	1:A:564:LYS:HB2	2.19	0.42
1:A:674:LEU:HA	1:A:675:PRO:HD3	1.86	0.42
1:A:675:PRO:O	1:A:676:ALA:C	2.57	0.42
1:A:826:LEU:O	1:A:830:VAL:HG23	2.18	0.42
1:A:888:ILE:C	1:A:891:THR:HG22	2.40	0.42
1:A:130:SER:O	1:A:133:PHE:HB2	2.18	0.42
1:A:707:ILE:HD11	1:A:762:LEU:HD21	2.00	0.42
1:A:157:ARG:HA	1:A:161:GLU:OE2	2.19	0.42
1:A:678:LEU:HD11	1:A:683:VAL:HG21	2.01	0.42
1:A:714:LYS:HA	1:A:725:ARG:HG3	2.02	0.42
1:A:102:MET:CG	1:A:116:ASN:HD22	2.32	0.42
1:A:803:GLY:HA2	1:A:905:PRO:CD	2.49	0.42
1:A:46:ILE:HG12	1:A:47:TRP:N	2.35	0.42
1:A:187:LEU:HD12	1:A:187:LEU:N	2.35	0.42
1:A:190:GLY:N	1:A:196:LYS:HD3	2.35	0.42
1:A:820:SER:HA	1:A:962:PRO:HG3	2.01	0.42
1:A:828:ASN:HD22	1:A:1034:ILE:HD12	1.85	0.42
1:A:109:ASN:OD1	1:A:111:PRO:HG2	2.20	0.42
1:A:142:ARG:HH11	1:A:142:ARG:HG2	1.85	0.42
1:A:158:ARG:H	1:A:161:GLU:HG2	1.85	0.41
1:A:869:PHE:HE2	1:A:906:ILE:HD11	1.84	0.41
1:A:718:LEU:HD12	1:A:769:ARG:NH1	2.35	0.41
1:A:966:ASP:C	1:A:967:LEU:HD22	2.40	0.41
1:A:712:PHE:CD2	1:A:734:THR:HG23	2.55	0.41
1:A:79:GLN:HG2	1:A:80:ASP:N	2.34	0.41
1:A:578:GLU:HA	1:A:590:TYR:O	2.21	0.41
1:A:771:GLN:O	1:A:775:GLU:HG3	2.21	0.41
1:A:160:ASN:HD22	1:A:160:ASN:HA	1.57	0.41
1:A:1010:VAL:O	1:A:1011:ILE:HD13	2.20	0.41
1:A:1089:MET:O	1:A:1089:MET:HG3	2.20	0.41
1:A:409:ILE:CG1	1:A:418:GLN:HG3	2.51	0.41
1:A:221:VAL:O	1:A:225:GLN:HG3	2.21	0.40
1:A:457:LYS:HD3	1:A:457:LYS:H	1.86	0.40
1:A:473:LYS:HG3	1:A:474:VAL:N	2.37	0.40
1:A:964:ASN:H	1:A:964:ASN:ND2	2.19	0.40
1:A:718:LEU:HD21	1:A:799:PHE:CE2	2.57	0.40
1:A:780:LEU:O	1:A:1083:LYS:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ALA:HA	1:A:945:MET:HE1	2.03	0.40
1:A:561:HIS:HE1	6:A:1516:HOH:O	2.05	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	1025/1100 (93%)	953 (93%)	60 (6%)	12 (1%)	13 14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	970	SER
1	A	1031	LYS
1	A	160	ASN
1	A	966	ASP
1	A	971	ASP
1	A	547	PRO
1	A	834	PHE
1	A	676	ALA
1	A	696	ILE
1	A	800	ASN
1	A	534	PRO
1	A	532	GLN

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	916/968 (95%)	880 (96%)	36 (4%)	32 46

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

Mol	Chain	Res	Type
1	A	49	ASN
1	A	103	SER
1	A	134	LEU
1	A	142	ARG
1	A	160	ASN
1	A	178	LEU
1	A	207	LEU
1	A	244	ASN
1	A	282	GLN
1	A	327	LYS
1	A	340	GLN
1	A	353	MET
1	A	363	LEU
1	A	376	GLU
1	A	383	LYS
1	A	457	LYS
1	A	511	ASN
1	A	532	GLN
1	A	543	GLN
1	A	566	ASN
1	A	596	LEU
1	A	633	LYS
1	A	680	ASP
1	A	690	ASN
1	A	749	ARG
1	A	847	LEU
1	A	907	ASN
1	A	937	ASP
1	A	945	MET
1	A	953	GLN
1	A	964	ASN
1	A	971	ASP
1	A	974	GLN
1	A	997	ASP
1	A	1022	ASN

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Mol	Chain	Res	Type
1	A	1089	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	90	GLN
1	A	160	ASN
1	A	199	ASN
1	A	244	ASN
1	A	245	ASN
1	A	282	GLN
1	A	294	GLN
1	A	308	HIS
1	A	316	ASN
1	A	320	GLN
1	A	340	GLN
1	A	418	GLN
1	A	450	ASN
1	A	511	ASN
1	A	566	ASN
1	A	605	GLN
1	A	627	ASN
1	A	644	GLN
1	A	648	GLN
1	A	690	ASN
1	A	705	ASN
1	A	793	ASN
1	A	811	GLN
1	A	818	GLN
1	A	864	GLN
1	A	904	GLN
1	A	907	ASN
1	A	917	ASN
1	A	941	GLN
1	A	953	GLN
1	A	964	ASN
1	A	1056	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	ADP	A	1203	3	24,29,29	1.70	7 (29%)	29,45,45	1.13	3 (10%)
5	GDP	A	1205	-	24,30,30	1.85	5 (20%)	30,47,47	0.77	1 (3%)
2	BGC	A	1201	-	12,12,12	0.72	0	17,17,17	0.65	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
4	ADP	A	1203	3	-	2/12/32/32	0/3/3/3
5	GDP	A	1205	-	-	1/12/32/32	0/3/3/3
2	BGC	A	1201	-	-	0/2/22/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1205	GDP	C5-C6	-6.08	1.35	1.47
4	A	1203	ADP	C2-N1	3.55	1.40	1.33
4	A	1203	ADP	C8-N7	-3.51	1.28	1.34
4	A	1203	ADP	C4-N3	2.96	1.39	1.35
4	A	1203	ADP	PB-O2B	-2.81	1.44	1.54
5	A	1205	GDP	C6-N1	2.46	1.41	1.37
5	A	1205	GDP	C2-N3	2.31	1.38	1.33
5	A	1205	GDP	PA-O5'	-2.30	1.50	1.59
4	A	1203	ADP	C2'-C1'	-2.18	1.50	1.53
5	A	1205	GDP	PB-O2B	-2.17	1.46	1.54
4	A	1203	ADP	C2-N3	2.03	1.35	1.32
4	A	1203	ADP	PA-O2A	-2.01	1.45	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1203	ADP	O3'-C3'-C4'	2.82	119.21	111.05
5	A	1205	GDP	O6-C6-N1	-2.18	118.07	120.65
4	A	1203	ADP	O3'-C3'-C2'	2.09	118.59	111.82
4	A	1203	ADP	O4'-C4'-C5'	-2.04	102.65	109.37

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1203	ADP	PA-O3A-PB-O2B
5	A	1205	GDP	PA-O3A-PB-O3B
4	A	1203	ADP	PA-O3A-PB-O1B

There are no ring outliers.

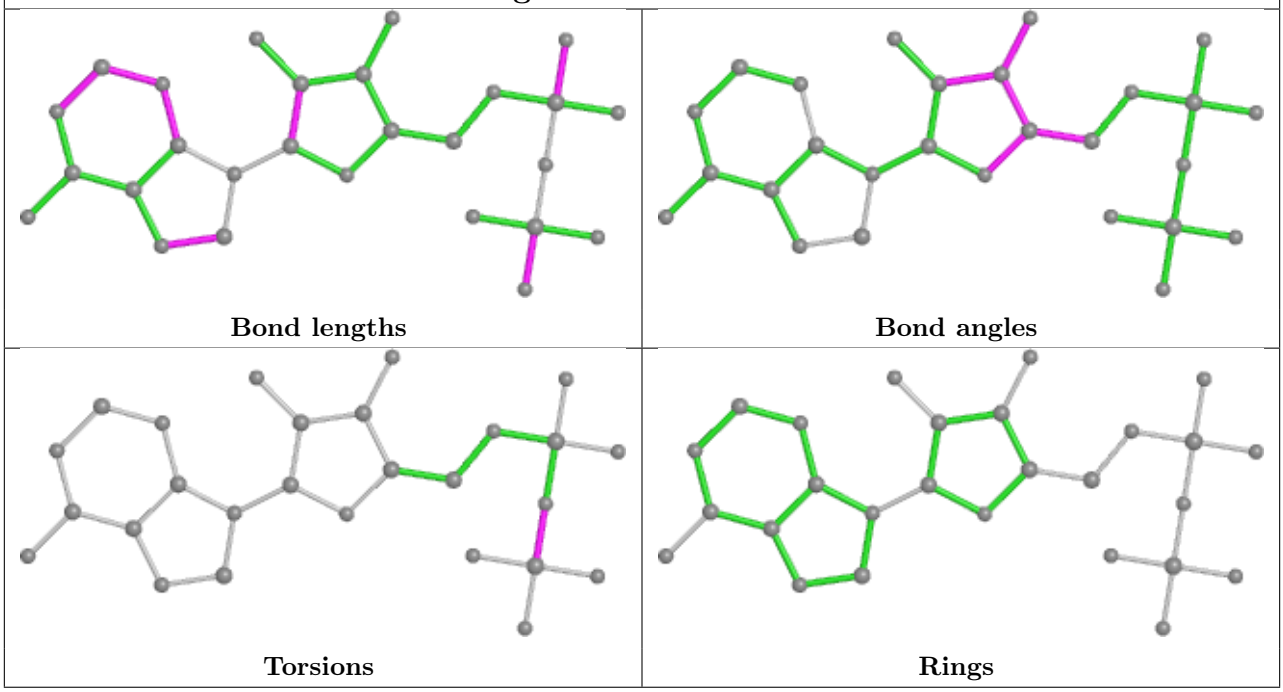
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1205	GDP	1	0

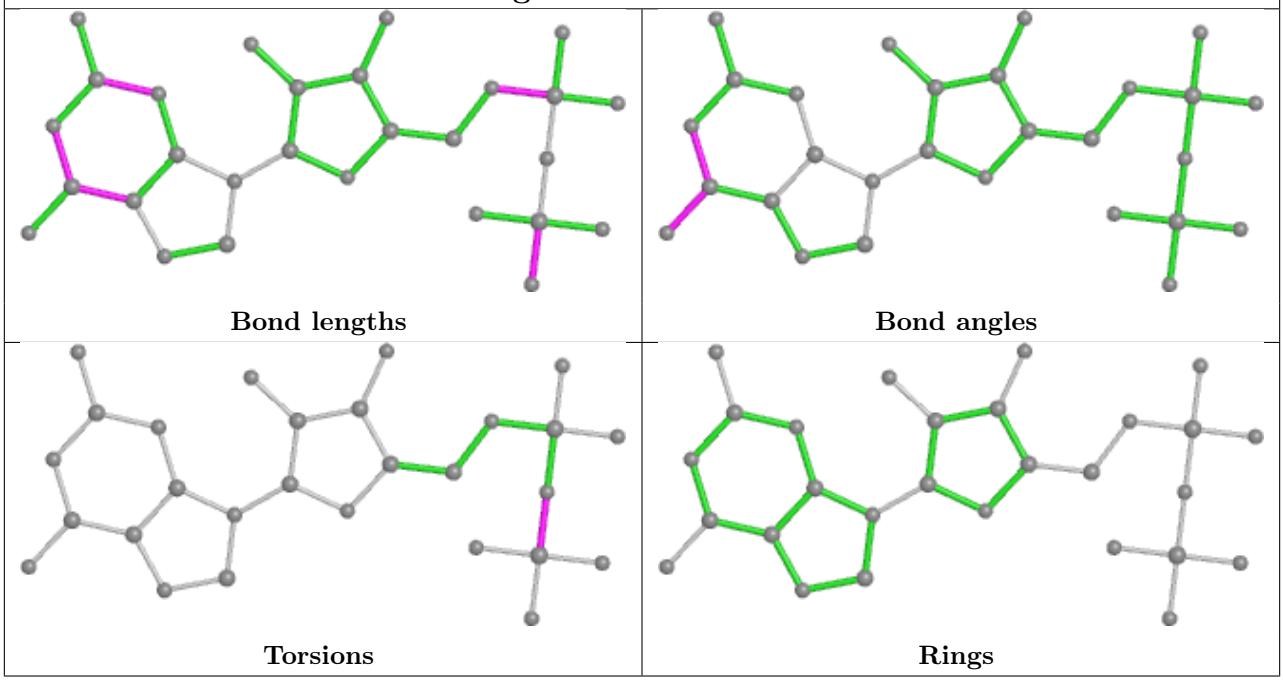
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1203



Ligand GDP A 1205



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 (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	1039/1100 (94%)	0.94	164 (15%) 2 2	11, 41, 91, 123	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	901	ILE	7.9
1	A	413	ARG	7.3
1	A	38	LEU	7.2
1	A	635	GLY	6.9
1	A	968	ALA	6.9
1	A	634	LYS	6.8
1	A	1000	THR	6.4
1	A	53	LYS	6.0
1	A	999	GLY	5.9
1	A	52	PRO	5.6
1	A	976	ALA	5.5
1	A	857	ALA	5.3
1	A	936	THR	5.3
1	A	636	ALA	5.2
1	A	802	LEU	5.1
1	A	1008	GLY	5.0
1	A	970	SER	4.9
1	A	938	ILE	4.8
1	A	969	ASN	4.8
1	A	1030	ALA	4.8
1	A	29	LYS	4.7
1	A	1029	ILE	4.7
1	A	1010	VAL	4.7
1	A	414	ASP	4.7
1	A	856	ILE	4.5
1	A	515	ILE	4.4
1	A	826	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	966	ASP	4.1
1	A	825	VAL	4.0
1	A	982	GLU	4.0
1	A	858	ASP	4.0
1	A	1049	PRO	3.9
1	A	633	LYS	3.9
1	A	19	THR	3.9
1	A	940	GLN	3.8
1	A	219	SER	3.8
1	A	963	ALA	3.8
1	A	75	THR	3.7
1	A	1087	SER	3.7
1	A	939	GLU	3.7
1	A	998	LYS	3.7
1	A	54	GLU	3.6
1	A	1003	MET	3.6
1	A	23	HIS	3.6
1	A	920	LEU	3.6
1	A	17	ASP	3.6
1	A	55	ARG	3.6
1	A	664	VAL	3.6
1	A	972	ALA	3.5
1	A	455	GLU	3.5
1	A	1026	GLU	3.5
1	A	186	LEU	3.5
1	A	69	ASP	3.4
1	A	547	PRO	3.4
1	A	37	LYS	3.4
1	A	861	SER	3.4
1	A	902	SER	3.4
1	A	15	ILE	3.4
1	A	984	LYS	3.3
1	A	374	ALA	3.3
1	A	1050	ILE	3.3
1	A	859	ASP	3.3
1	A	411	ALA	3.3
1	A	412	GLY	3.3
1	A	415	LEU	3.2
1	A	1009	ARG	3.2
1	A	981	PRO	3.2
1	A	188	ILE	3.2
1	A	14	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	882	GLU	3.1
1	A	1084	VAL	3.1
1	A	1031	LYS	3.1
1	A	824	SER	3.1
1	A	942	ILE	3.1
1	A	546	PHE	3.0
1	A	889	ARG	3.0
1	A	30	GLN	3.0
1	A	532	GLN	2.9
1	A	855	PRO	2.9
1	A	953	GLN	2.9
1	A	1028	ILE	2.9
1	A	1063	LEU	2.9
1	A	823	SER	2.8
1	A	696	ILE	2.8
1	A	133	PHE	2.8
1	A	279	VAL	2.8
1	A	632	ALA	2.8
1	A	18	ARG	2.8
1	A	698	ILE	2.8
1	A	157	ARG	2.8
1	A	409	ILE	2.7
1	A	74	LYS	2.7
1	A	358	ILE	2.7
1	A	881	SER	2.7
1	A	997	ASP	2.7
1	A	684	LEU	2.6
1	A	1052	LYS	2.6
1	A	518	GLY	2.6
1	A	965	THR	2.6
1	A	433	VAL	2.6
1	A	82	GLN	2.6
1	A	88	ALA	2.6
1	A	725	ARG	2.6
1	A	39	THR	2.6
1	A	136	ALA	2.6
1	A	1001	ASP	2.6
1	A	76	VAL	2.6
1	A	1032	LYS	2.6
1	A	418	GLN	2.6
1	A	189	THR	2.6
1	A	134	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	51	ASP	2.5
1	A	65	SER	2.5
1	A	860	GLY	2.5
1	A	1011	ILE	2.5
1	A	13	ASP	2.5
1	A	967	LEU	2.5
1	A	359	ILE	2.5
1	A	1021	ILE	2.5
1	A	1067	LEU	2.5
1	A	376	GLU	2.4
1	A	885	GLU	2.4
1	A	1006	LEU	2.4
1	A	260	SER	2.4
1	A	466	ILE	2.4
1	A	161	GLU	2.4
1	A	410	LEU	2.4
1	A	130	SER	2.4
1	A	373	GLY	2.4
1	A	20	SER	2.4
1	A	637	ASN	2.4
1	A	50	PRO	2.3
1	A	86	ASP	2.3
1	A	937	ASP	2.3
1	A	68	SER	2.3
1	A	971	ASP	2.3
1	A	973	LEU	2.3
1	A	996	MET	2.3
1	A	995	LEU	2.3
1	A	187	LEU	2.2
1	A	377	GLY	2.2
1	A	464	LEU	2.2
1	A	804	SER	2.2
1	A	700	ARG	2.2
1	A	890	ASP	2.2
1	A	166	ILE	2.2
1	A	918	LEU	2.2
1	A	1027	ASP	2.2
1	A	829	ILE	2.2
1	A	132	LEU	2.2
1	A	921	VAL	2.1
1	A	914	HIS	2.1
1	A	964	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	516	ASP	2.1
1	A	815	VAL	2.1
1	A	200	THR	2.1
1	A	828	ASN	2.1
1	A	1005	VAL	2.0
1	A	16	HIS	2.0
1	A	801	THR	2.0
1	A	194	ALA	2.0
1	A	142	ARG	2.0
1	A	989	VAL	2.0
1	A	517	PHE	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)

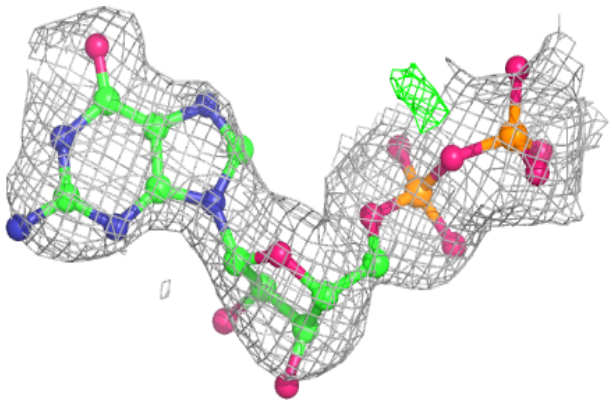
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

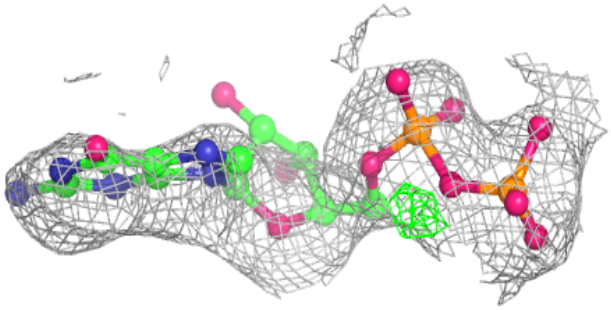
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1204	1/1	0.79	0.28	77,77,77,77	0
5	GDP	A	1205	28/28	0.79	0.23	78,88,92,93	0
3	MG	A	1202	1/1	0.90	0.19	15,15,15,15	0
2	BGC	A	1201	12/12	0.91	0.14	32,41,49,51	0
4	ADP	A	1203	27/27	0.95	0.17	14,20,26,28	0

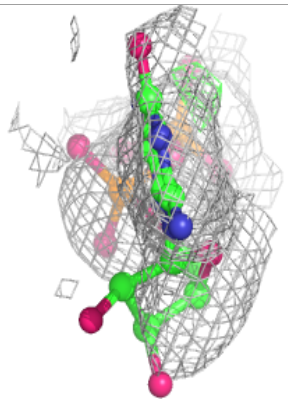
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP A 1205:

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

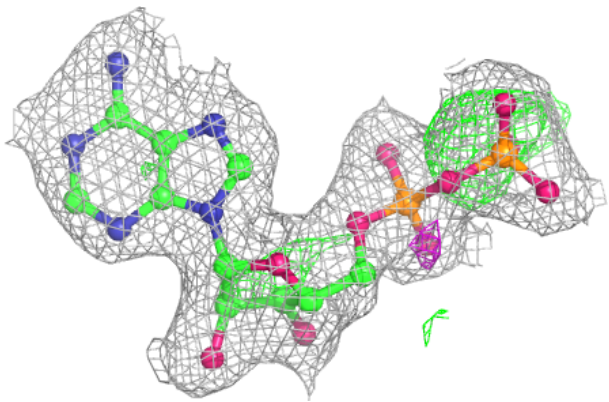


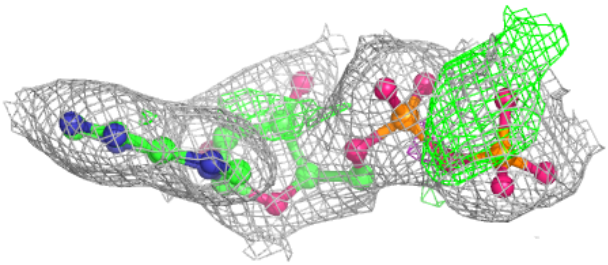


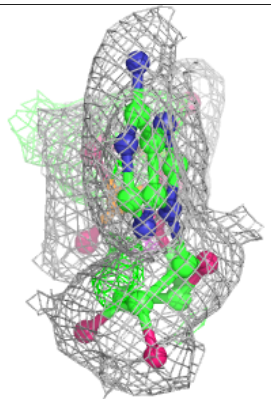


Electron density around ADP A 1203:

$2mF_o$-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.