Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2023 – 08:19 am GMT

PDB ID	:	2JJ9
Title	:	Crystal structure of myosin-2 in complex with ADP-metavanadate
Authors	:	Fedorov, R.; Boehl, M.; Tsiavaliaris, G.; Hartmann, F.K.; Baruch, P.; Brenner, B.; Martin, R.; Knoelker, H.J.; Gutzeit, H.O.; Manstein, D.J.
Deposited on	:	2008-03-25
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:

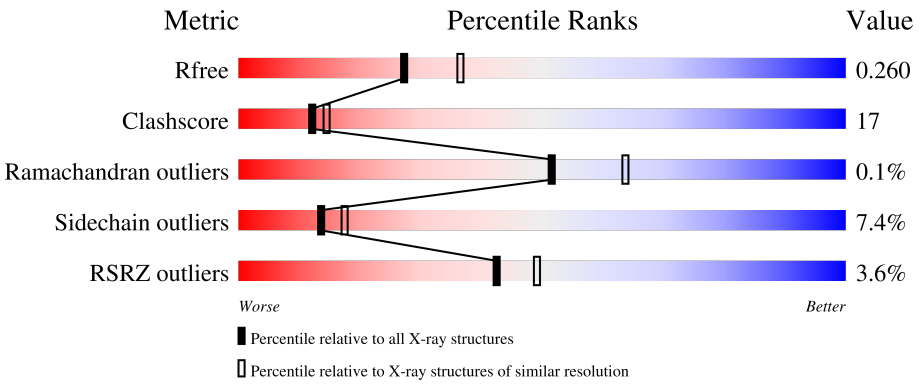
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	788	3% 59% 25% • 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6079 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	692	5539	3516	954	1053	16	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P08799
A	-9	HIS	-	expression tag	UNP P08799
A	-8	HIS	-	expression tag	UNP P08799
A	-7	HIS	-	expression tag	UNP P08799
A	-6	HIS	-	expression tag	UNP P08799
A	-5	HIS	-	expression tag	UNP P08799
A	-4	HIS	-	expression tag	UNP P08799
A	-3	HIS	-	expression tag	UNP P08799
A	-2	ASP	-	expression tag	UNP P08799
A	-1	GLY	-	expression tag	UNP P08799
A	0	THR	-	expression tag	UNP P08799
A	1	GLU	-	expression tag	UNP P08799
A	762	LEU	-	expression tag	UNP P08799
A	763	GLU	-	expression tag	UNP P08799
A	764	SER	-	expression tag	UNP P08799
A	765	ASN	-	expression tag	UNP P08799
A	766	GLU	-	expression tag	UNP P08799
A	767	PRO	-	expression tag	UNP P08799
A	768	PRO	-	expression tag	UNP P08799
A	769	MET	-	expression tag	UNP P08799
A	770	ASP	-	expression tag	UNP P08799
A	771	PHE	-	expression tag	UNP P08799
A	772	ASP	-	expression tag	UNP P08799
A	773	ASP	-	expression tag	UNP P08799
A	774	ASP	-	expression tag	UNP P08799
A	775	ILE	-	expression tag	UNP P08799
A	776	PRO	-	expression tag	UNP P08799

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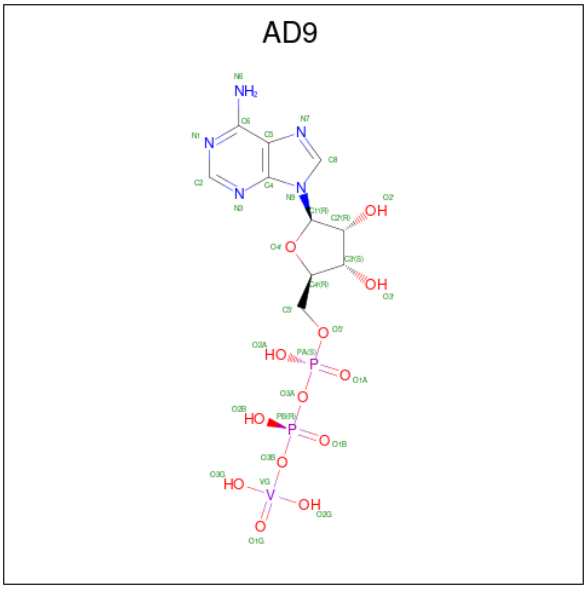
Chain	Residue	Modelled	Actual	Comment	Reference
A	777	PHE	-	expression tag	UNP P08799

- Molecule 2 is ADP METAVANADATE (three-letter code: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	V		
2	A	1	31	10	5	13	2	1	0	0

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

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

- Molecule 4 is water.

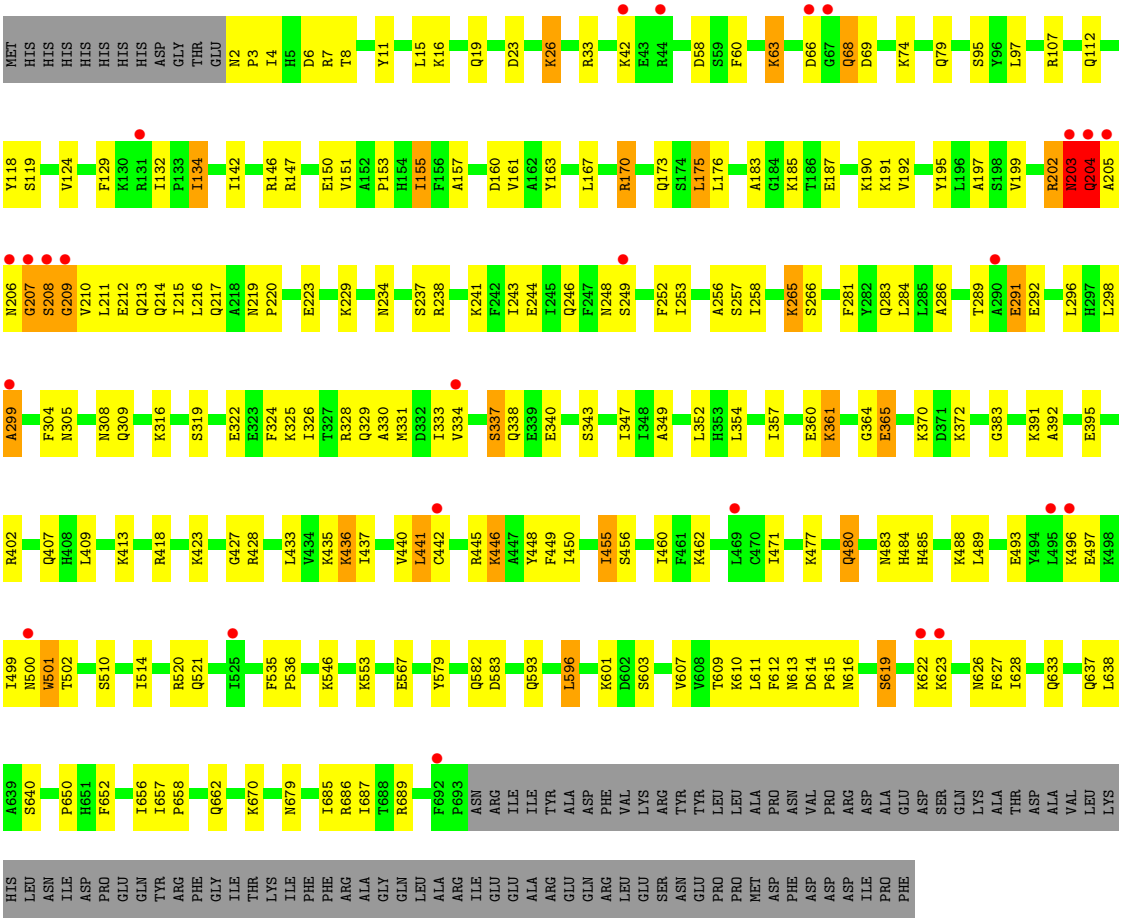
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	508	508	508	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.42Å 147.22Å 153.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 24.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.30) 100.0 (24.55-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.18 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.275 0.206 , 0.260	Depositor DCC
R_{free} test set	2969 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6079	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, AD9

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	0.50	3/5647 (0.1%)	0.85	9/7619 (0.1%)

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	A	1	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLN	C-O	17.35	1.56	1.23
1	A	204	GLN	C-N	-12.35	1.05	1.34
1	A	203	ASN	C-N	-10.80	1.09	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	501	TRP	N-CA-C	11.37	141.71	111.00
1	A	204	GLN	CA-C-N	10.27	139.80	117.20
1	A	203	ASN	C-N-CA	9.63	145.78	121.70
1	A	299	ALA	CB-CA-C	-9.34	96.08	110.10
1	A	204	GLN	CA-C-O	-8.51	102.23	120.10
1	A	418	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	A	203	ASN	O-C-N	-6.62	112.10	122.70
1	A	204	GLN	C-N-CA	6.35	137.58	121.70
1	A	238	ARG	CD-NE-CZ	5.32	131.05	123.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	501	TRP	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ASN	Peptide
1	A	204	GLN	Peptide
1	A	205	ALA	Peptide
1	A	206	ASN	Peptide
1	A	207	GLY	Peptide
1	A	209	GLY	Peptide
1	A	500	ASN	Peptide,Mainchain

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	5539	0	5494	189	1
2	A	31	0	14	1	0
3	A	1	0	0	0	0
4	A	508	0	0	20	0
All	All	6079	0	5508	189	1

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 17.

All (189) 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:142:ILE:O	1:A:146:ARG:HD2	1.39	1.18
1:A:209:GLY:HA2	1:A:212:GLU:HB2	1.30	1.10
1:A:299:ALA:O	1:A:304:PHE:HE2	1.48	0.94
1:A:241:LYS:HD2	1:A:243:ILE:HD11	1.51	0.92
1:A:657:ILE:HD12	1:A:658:PRO:HD2	1.50	0.91
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:HE21	1:A:69:ASP:H	1.22	0.86
1:A:142:ILE:O	1:A:146:ARG:CD	2.26	0.80
1:A:68:GLN:NE2	1:A:69:ASP:H	1.79	0.79
1:A:107:ARG:HD3	4:A:2111:HOH:O	1.82	0.79
1:A:499:ILE:O	1:A:499:ILE:CG2	2.30	0.78
1:A:203:ASN:O	1:A:204:GLN:HG3	1.84	0.77
1:A:16:LYS:HE3	4:A:2096:HOH:O	1.85	0.77
1:A:623:LYS:HD2	4:A:2469:HOH:O	1.84	0.77
1:A:324:PHE:O	1:A:328:ARG:HG3	1.85	0.76
1:A:207:GLY:O	1:A:210:VAL:HG23	1.86	0.74
1:A:299:ALA:O	1:A:304:PHE:CE2	2.36	0.74
1:A:155:ILE:HD11	1:A:192:VAL:HG23	1.67	0.74
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.88	0.74
1:A:6:ASP:OD1	1:A:8:THR:HG22	1.88	0.73
1:A:305:ASN:HB3	4:A:2242:HOH:O	1.87	0.73
1:A:391:LYS:HE2	4:A:2287:HOH:O	1.87	0.73
1:A:623:LYS:HG3	1:A:628:ILE:HA	1.70	0.72
1:A:615:PRO:O	1:A:619:SER:HB2	1.89	0.71
1:A:330:ALA:O	1:A:334:VAL:HG23	1.91	0.70
1:A:409:LEU:HB3	1:A:413:LYS:HB2	1.75	0.69
1:A:499:ILE:O	1:A:499:ILE:HG22	1.92	0.69
1:A:155:ILE:HD12	1:A:191:LYS:HB2	1.73	0.69
1:A:68:GLN:HE21	1:A:69:ASP:N	1.91	0.69
1:A:462:LYS:HE3	4:A:2350:HOH:O	1.93	0.69
1:A:623:LYS:HE2	1:A:628:ILE:HG13	1.75	0.69
1:A:392:ALA:HB1	1:A:596:LEU:HD13	1.75	0.68
1:A:190:LYS:HE2	1:A:223:GLU:OE2	1.93	0.68
1:A:209:GLY:N	1:A:212:GLU:OE1	2.25	0.67
1:A:97:LEU:HD23	1:A:686:ARG:HG3	1.75	0.66
1:A:265:LYS:HE2	1:A:427:GLY:HA3	1.76	0.66
1:A:480:GLN:HE21	1:A:480:GLN:HA	1.61	0.66
1:A:685:ILE:HG22	1:A:689:ARG:HD3	1.77	0.66
1:A:456:SER:HB2	1:A:471:ILE:HD12	1.76	0.65
1:A:197:ALA:HA	1:A:253:ILE:HD11	1.79	0.65
1:A:173:GLN:HB2	1:A:450:ILE:HG12	1.78	0.64
1:A:520:ARG:NH1	1:A:521:GLN:OE1	2.31	0.64
1:A:170:ARG:HG2	1:A:448:TYR:OH	1.98	0.63
1:A:340:GLU:OE2	1:A:436:LYS:CE	2.48	0.61
1:A:33:ARG:HH21	1:A:79:GLN:HE22	1.47	0.61
1:A:146:ARG:HD3	1:A:151:VAL:HG11	1.82	0.61
1:A:132:ILE:HG22	1:A:134:ILE:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLY:CA	1:A:212:GLU:HB2	2.19	0.61
1:A:383:GLY:O	1:A:603:SER:HA	2.01	0.60
1:A:433:LEU:O	1:A:437:ILE:HG12	2.00	0.60
1:A:4:ILE:HD12	1:A:142:ILE:HD12	1.84	0.60
1:A:4:ILE:CD1	1:A:146:ARG:NH1	2.64	0.60
1:A:243:ILE:HD12	1:A:258:ILE:HG13	1.83	0.59
1:A:361:LYS:HE2	1:A:365:GLU:HA	1.84	0.59
1:A:334:VAL:HG11	1:A:437:ILE:HD13	1.85	0.59
1:A:97:LEU:HD23	1:A:686:ARG:CG	2.34	0.58
1:A:328:ARG:HA	1:A:331:MET:HE2	1.85	0.58
1:A:329:GLN:O	1:A:333:ILE:HG12	2.03	0.58
1:A:325:LYS:O	1:A:329:GLN:HG3	2.03	0.58
1:A:146:ARG:HD3	1:A:151:VAL:CG1	2.34	0.58
1:A:147:ARG:O	1:A:150:GLU:HB2	2.05	0.57
1:A:361:LYS:HE2	1:A:364:GLY:O	2.04	0.57
1:A:354:LEU:O	1:A:357:ILE:HD13	2.04	0.57
1:A:4:ILE:HD13	1:A:146:ARG:NH1	2.19	0.57
1:A:197:ALA:HA	1:A:253:ILE:CD1	2.34	0.57
1:A:296:LEU:HD23	4:A:2238:HOH:O	2.05	0.56
1:A:319:SER:OG	1:A:322:GLU:HG3	2.05	0.56
1:A:147:ARG:NE	1:A:147:ARG:HA	2.20	0.56
1:A:409:LEU:HB3	1:A:413:LYS:CB	2.34	0.56
1:A:229:LYS:HG3	1:A:234:ASN:HD22	1.70	0.56
1:A:455:ILE:HD12	4:A:2338:HOH:O	2.06	0.56
1:A:97:LEU:CD2	1:A:686:ARG:HG3	2.36	0.55
1:A:183:ALA:HA	1:A:657:ILE:HD13	1.87	0.55
1:A:286:ALA:HB2	4:A:2237:HOH:O	2.05	0.55
1:A:319:SER:CB	1:A:322:GLU:HG3	2.36	0.55
1:A:217:GLN:HG3	1:A:333:ILE:HG13	1.89	0.55
1:A:129:PHE:CZ	1:A:662:GLN:HA	2.42	0.55
1:A:175:LEU:HD22	1:A:192:VAL:HG21	1.88	0.54
1:A:477:LYS:CD	1:A:514:ILE:HD12	2.37	0.54
1:A:68:GLN:HE21	1:A:68:GLN:HA	1.72	0.54
1:A:241:LYS:CD	1:A:243:ILE:HD11	2.32	0.54
1:A:334:VAL:HG11	1:A:437:ILE:CD1	2.38	0.54
1:A:195:TYR:CZ	1:A:199:VAL:HG11	2.42	0.54
1:A:609:THR:HG23	1:A:613:ASN:OD1	2.08	0.53
1:A:499:ILE:O	1:A:499:ILE:HG23	2.09	0.53
1:A:207:GLY:C	1:A:210:VAL:HG23	2.30	0.52
1:A:319:SER:HB3	1:A:322:GLU:HG3	1.90	0.52
1:A:3:PRO:HB2	1:A:142:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLU:O	1:A:499:ILE:HD12	2.10	0.52
1:A:155:ILE:HD11	1:A:192:VAL:CG2	2.39	0.52
1:A:340:GLU:OE2	1:A:436:LYS:HE2	2.09	0.52
1:A:343:SER:HB3	1:A:607:VAL:HB	1.90	0.52
1:A:234:ASN:H	1:A:662:GLN:HE22	1.58	0.52
1:A:326:ILE:HD13	4:A:2258:HOH:O	2.11	0.51
1:A:623:LYS:HG3	1:A:628:ILE:CA	2.40	0.51
1:A:129:PHE:CZ	1:A:657:ILE:HD11	2.46	0.51
1:A:395:GLU:HA	1:A:407:GLN:O	2.10	0.51
1:A:157:ALA:O	1:A:161:VAL:HG23	2.11	0.51
1:A:354:LEU:HA	1:A:357:ILE:HD13	1.93	0.51
1:A:361:LYS:HG3	4:A:2143:HOH:O	2.11	0.51
1:A:244:GLU:O	1:A:256:ALA:HA	2.12	0.50
1:A:289:THR:HG1	1:A:292:GLU:HG3	1.77	0.50
1:A:365:GLU:HG2	4:A:2315:HOH:O	2.10	0.50
1:A:58:ASP:C	1:A:74:LYS:HG3	2.32	0.49
1:A:155:ILE:HD12	1:A:191:LYS:CB	2.41	0.49
1:A:6:ASP:CG	1:A:8:THR:HG22	2.33	0.49
1:A:42:LYS:HD2	4:A:2042:HOH:O	2.13	0.49
1:A:202:ARG:C	1:A:208:SER:HB2	2.33	0.49
1:A:163:TYR:CE2	1:A:167:LEU:HD11	2.48	0.49
1:A:347:ILE:HD11	1:A:607:VAL:HG12	1.94	0.49
1:A:248:ASN:HD21	1:A:252:PHE:HB2	1.78	0.48
1:A:623:LYS:HE2	1:A:628:ILE:CD1	2.43	0.48
1:A:623:LYS:HE2	1:A:628:ILE:CG1	2.41	0.48
1:A:63:LYS:HE2	1:A:69:ASP:OD1	2.13	0.48
1:A:601:LYS:HG3	1:A:612:PHE:HB3	1.95	0.48
1:A:2:ASN:OD1	1:A:4:ILE:HD13	2.14	0.48
1:A:456:SER:CB	1:A:471:ILE:HD12	2.42	0.48
1:A:68:GLN:HE21	1:A:68:GLN:CA	2.27	0.48
1:A:175:LEU:HD22	1:A:192:VAL:CG2	2.44	0.48
1:A:291:GLU:HG2	1:A:292:GLU:N	2.28	0.48
1:A:582:GLN:O	1:A:583:ASP:HB2	2.14	0.48
1:A:281:PHE:CD1	1:A:352:LEU:HD21	2.49	0.48
1:A:510:SER:O	1:A:514:ILE:HG12	2.14	0.47
1:A:493:GLU:O	1:A:496:LYS:HB3	2.14	0.47
1:A:614:ASP:OD1	1:A:616:ASN:HB2	2.15	0.47
1:A:209:GLY:O	1:A:213:GLN:HB2	2.15	0.47
1:A:60:PHE:CE1	1:A:74:LYS:HE2	2.50	0.47
1:A:480:GLN:NE2	1:A:483:ASN:HD22	2.13	0.47
1:A:614:ASP:HA	1:A:615:PRO:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:HB3	1:A:324:PHE:HD1	1.80	0.47
1:A:308:ASN:HA	4:A:2243:HOH:O	2.14	0.47
1:A:187:GLU:O	1:A:191:LYS:HG2	2.15	0.47
1:A:203:ASN:ND2	1:A:203:ASN:N	2.64	0.46
1:A:244:GLU:HG2	1:A:449:PHE:CD2	2.50	0.46
1:A:202:ARG:HB3	1:A:208:SER:HB2	1.98	0.46
1:A:428:ARG:HD3	1:A:611:LEU:O	2.14	0.46
1:A:442:CYS:HB2	4:A:2209:HOH:O	2.15	0.45
1:A:208:SER:O	1:A:208:SER:OG	2.34	0.45
1:A:107:ARG:NH2	4:A:2112:HOH:O	2.49	0.45
1:A:246:GLN:HB3	1:A:446:LYS:HB3	1.97	0.45
1:A:283:GLN:HB3	1:A:324:PHE:CD1	2.52	0.45
1:A:347:ILE:HD11	1:A:607:VAL:CG1	2.46	0.45
1:A:370:LYS:NZ	4:A:2277:HOH:O	2.50	0.45
1:A:402:ARG:NH2	4:A:2302:HOH:O	2.50	0.45
1:A:308:ASN:OD1	1:A:309:GLN:NE2	2.48	0.45
1:A:284:LEU:HA	1:A:324:PHE:CE1	2.52	0.45
1:A:203:ASN:N	1:A:203:ASN:HD22	2.15	0.45
1:A:4:ILE:HD11	1:A:146:ARG:NH1	2.31	0.44
1:A:266:SER:HA	1:A:423:LYS:HD3	1.99	0.44
1:A:593:GLN:HB2	1:A:596:LEU:HD22	1.99	0.44
1:A:7:ARG:NH2	1:A:19:GLN:OE1	2.49	0.44
1:A:211:LEU:O	1:A:214:GLN:N	2.50	0.44
1:A:11:TYR:O	1:A:15:LEU:HB2	2.18	0.44
1:A:622:LYS:HE3	1:A:627:PHE:CE1	2.53	0.44
1:A:493:GLU:O	1:A:496:LYS:N	2.50	0.44
1:A:462:LYS:HE2	4:A:2351:HOH:O	2.18	0.43
1:A:480:GLN:NE2	1:A:510:SER:H	2.16	0.43
1:A:160:ASP:OD2	1:A:195:TYR:OH	2.29	0.43
1:A:485:HIS:CE1	1:A:650:PRO:HG3	2.52	0.43
1:A:593:GLN:O	1:A:596:LEU:HB2	2.18	0.43
1:A:211:LEU:O	1:A:215:ILE:HG12	2.18	0.43
1:A:68:GLN:NE2	1:A:68:GLN:HA	2.34	0.42
1:A:258:ILE:HD12	1:A:258:ILE:N	2.33	0.42
1:A:284:LEU:HA	1:A:324:PHE:CZ	2.55	0.42
1:A:304:PHE:CD1	1:A:352:LEU:HB3	2.54	0.42
1:A:124:VAL:HG13	1:A:656:ILE:HD12	2.02	0.42
1:A:338:GLN:HB2	4:A:2261:HOH:O	2.19	0.42
1:A:26:LYS:HB3	1:A:26:LYS:HE2	1.78	0.42
1:A:237:SER:HB2	2:A:1694:AD9:O2G	2.20	0.41
1:A:176:LEU:HD12	1:A:652:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:HB3	1:A:220:PRO:HD3	2.02	0.41
1:A:185:LYS:HB2	1:A:185:LYS:HE2	1.64	0.41
1:A:440:VAL:HG12	1:A:441:LEU:HD23	2.02	0.41
1:A:657:ILE:CD1	1:A:658:PRO:HD2	2.37	0.41
1:A:484:HIS:O	1:A:488:LYS:HB3	2.21	0.41
1:A:4:ILE:CD1	1:A:142:ILE:HD12	2.49	0.41
1:A:129:PHE:CE2	1:A:662:GLN:HA	2.55	0.41
1:A:298:LEU:HD21	1:A:349:ALA:HB2	2.03	0.41
1:A:484:HIS:CE1	1:A:489:LEU:HG	2.56	0.41
1:A:124:VAL:CG1	1:A:656:ILE:HD12	2.50	0.41
1:A:329:GLN:HE21	1:A:329:GLN:HB3	1.64	0.41
1:A:460:ILE:HD13	1:A:460:ILE:HG21	1.81	0.41
1:A:477:LYS:HD2	1:A:514:ILE:HD12	2.03	0.41
1:A:657:ILE:HD12	1:A:657:ILE:HA	1.86	0.41
1:A:118:TYR:CE2	1:A:153:PRO:HA	2.55	0.40
1:A:354:LEU:CA	1:A:357:ILE:HD13	2.51	0.40
1:A:535:PHE:CD1	1:A:536:PRO:HD2	2.57	0.40
1:A:567:GLU:HA	1:A:579:TYR:O	2.22	0.40
1:A:633:GLN:O	1:A:637:GLN:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:OD2	1:A:204:GLN:NE2[8_455]	2.18	0.02

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	690/788 (88%)	666 (96%)	23 (3%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	SER

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	606/691 (88%)	561 (93%)	45 (7%)	13 17

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	63	LYS
1	A	66	ASP
1	A	68	GLN
1	A	95	SER
1	A	112	GLN
1	A	119	SER
1	A	134	ILE
1	A	155	ILE
1	A	170	ARG
1	A	175	LEU
1	A	202	ARG
1	A	203	ASN
1	A	208	SER
1	A	216	LEU
1	A	249	SER
1	A	257	SER
1	A	265	LYS
1	A	291	GLU
1	A	316	LYS
1	A	337	SER
1	A	360	GLU
1	A	361	LYS
1	A	365	GLU

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Mol	Chain	Res	Type
1	A	372	LYS
1	A	435	LYS
1	A	436	LYS
1	A	441	LEU
1	A	445	ARG
1	A	446	LYS
1	A	455	ILE
1	A	480	GLN
1	A	501	TRP
1	A	502	THR
1	A	546	LYS
1	A	553	LYS
1	A	596	LEU
1	A	610	LYS
1	A	619	SER
1	A	626	ASN
1	A	638	LEU
1	A	640	SER
1	A	670	LYS
1	A	679	ASN
1	A	687	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	79	GLN
1	A	171	GLN
1	A	203	ASN
1	A	214	GLN
1	A	219	ASN
1	A	234	ASN
1	A	283	GLN
1	A	329	GLN
1	A	443	GLN
1	A	480	GLN
1	A	532	GLN
1	A	541	ASN
1	A	613	ASN
1	A	626	ASN
1	A	662	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)

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	AD9	A	1694	4,3	24,33,33	1.93	5 (20%)	26,52,52	1.19	2 (7%)

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
2	AD9	A	1694	4,3	-	1/12/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1694	AD9	PA-O1A	5.72	1.71	1.50
2	A	1694	AD9	O4'-C1'	4.44	1.47	1.41
2	A	1694	AD9	PB-O2B	2.79	1.68	1.55
2	A	1694	AD9	C2-N3	2.65	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1694	AD9	PB-O1B	2.11	1.58	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1694	AD9	O2B-PB-O3B	-2.63	98.34	107.52
2	A	1694	AD9	O2A-PA-O5'	2.26	118.22	107.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1694	AD9	PA-O3A-PB-O2B

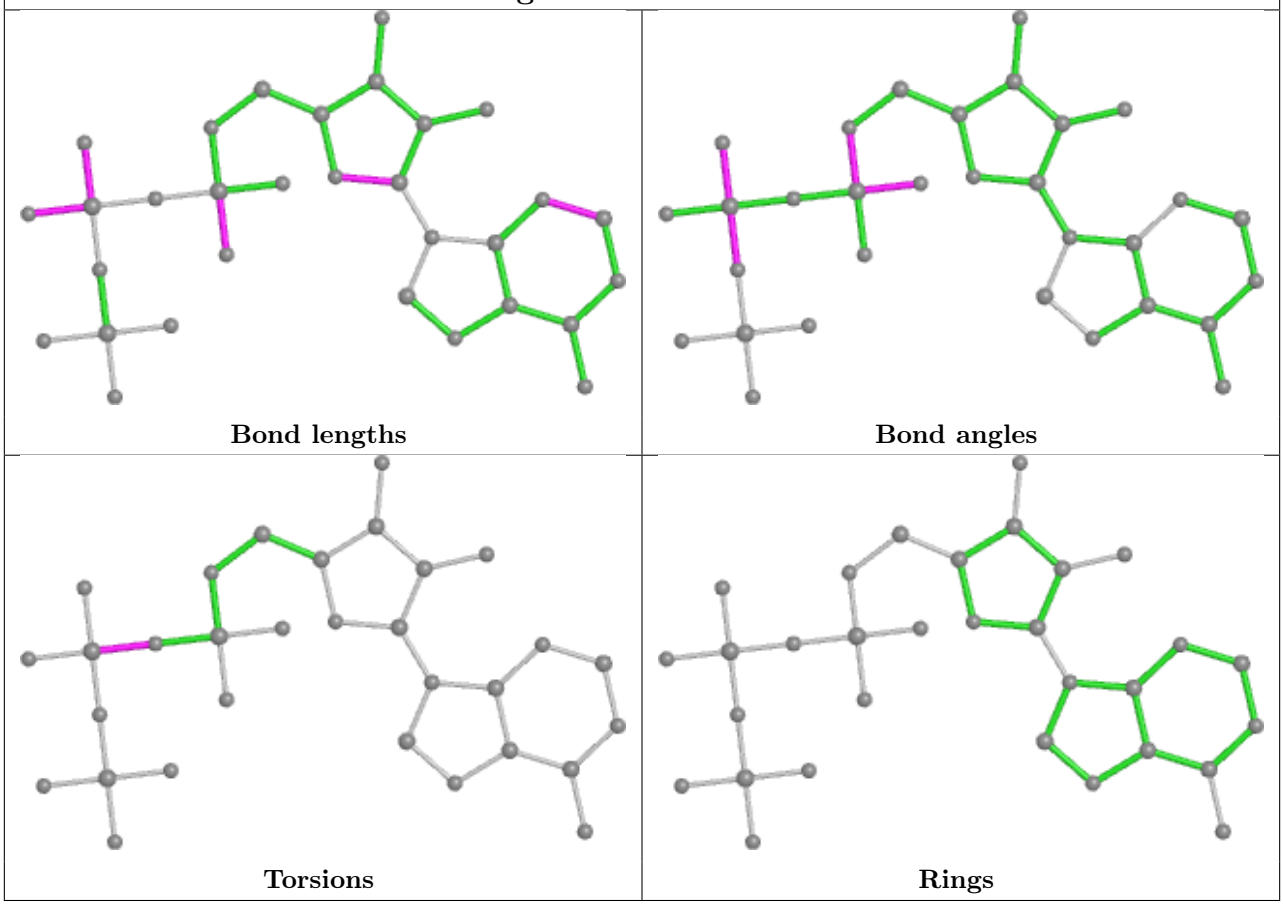
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1694	AD9	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 AD9 A 1694



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	203:ASN	C	204:GLN	N	1.09
1	A	204:GLN	C	205:ALA	N	1.05

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	692/788 (87%)	-0.14	25 (3%) 42 49	20, 41, 70, 125	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	GLN	10.2
1	A	205	ALA	9.1
1	A	206	ASN	8.7
1	A	203	ASN	7.1
1	A	500	ASN	5.2
1	A	207	GLY	5.2
1	A	208	SER	5.0
1	A	209	GLY	4.5
1	A	623	LYS	3.8
1	A	525	ILE	3.6
1	A	299	ALA	3.5
1	A	44	ARG	2.8
1	A	66	ASP	2.6
1	A	496	LYS	2.6
1	A	290	ALA	2.6
1	A	249	SER	2.4
1	A	442	CYS	2.4
1	A	495	LEU	2.3
1	A	692	PHE	2.2
1	A	469	LEU	2.2
1	A	622	LYS	2.1
1	A	131	ARG	2.1
1	A	334	VAL	2.1
1	A	67	GLY	2.0
1	A	42	LYS	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)

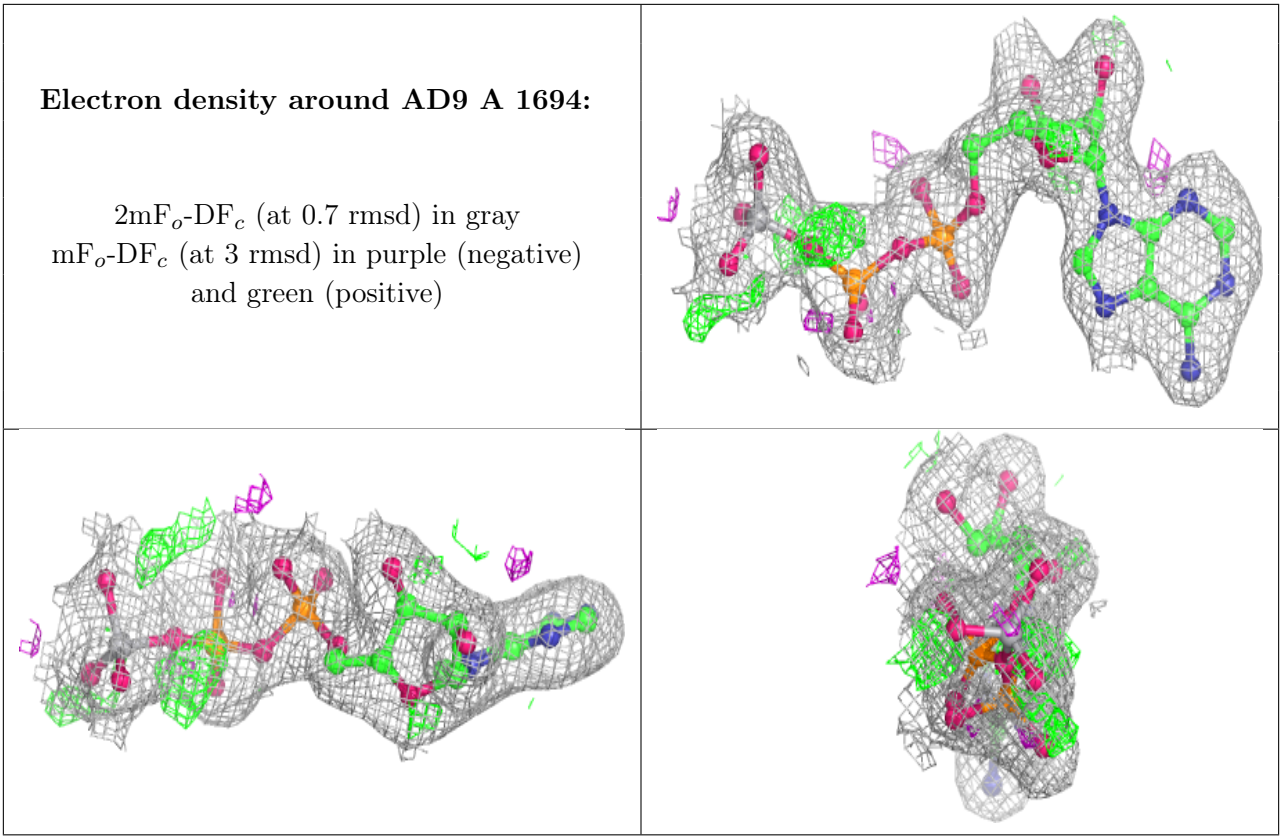
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AD9	A	1694	31/31	0.98	0.11	21,29,38,49	0
3	MG	A	1695	1/1	0.98	0.20	28,28,28,28	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 AD9 A 1694:

$2mF_o$-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.