WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2025 – 09:05 AM EST

PDB ID	:	2VYP
Title	:	Rabbit-muscle G-actin in complex with myxobacterial rhizopodin
Authors	:	Hagelueken, G.; Albrecht, S.C.; Steinmetz, H.; Jansen, R.; Heinz, D.W.; Kalesse, M.; Schubert, W.-D.
Deposited on	:	2008-07-25
Resolution	:	2.35 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.35 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	Percentile Ranks	Value
Rfree		0.306
Clashscore		9
Ramachandran outliers		0.4%
Sidechain outliers		1.2%
RSRZ outliers		20.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
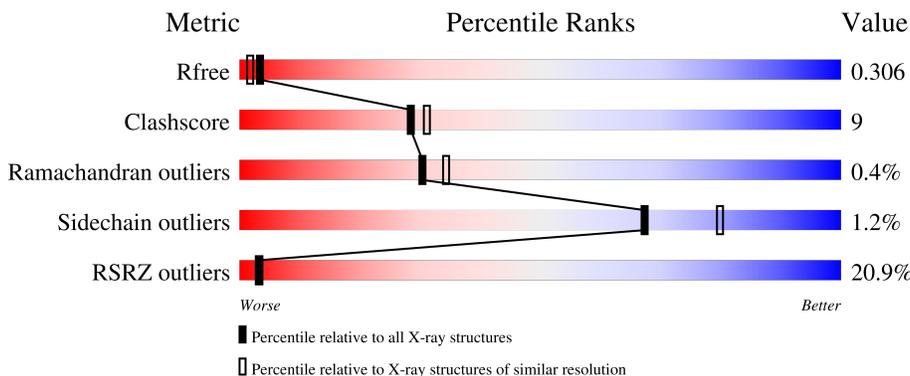
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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%

| Mol	Chain	Length	Quality of chain
1	A	377	17% ... 82% ... 11% · 5%
1	B	377	21% ... 71% ... 16% · 12%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5844 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 ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	4	0
			2823	1790	472	541	20			
1	B	330	Total	C	N	O	S	0	5	1
			2613	1664	432	496	21			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is RHIZOPODIN (three-letter code: RH9) (formula: $C_{78}H_{124}N_4O_{22}$).

RH9
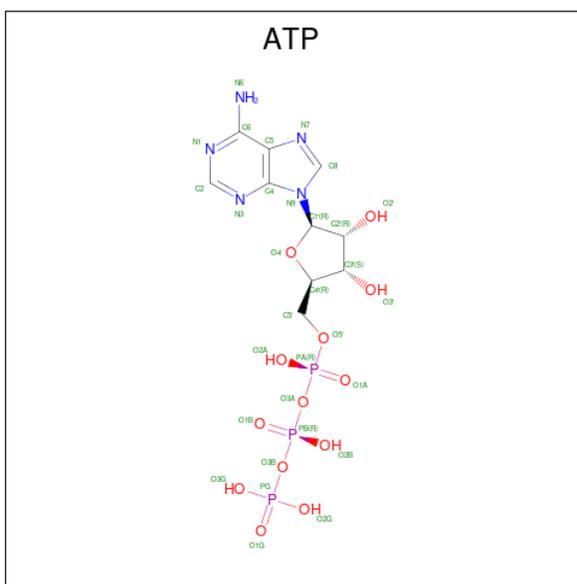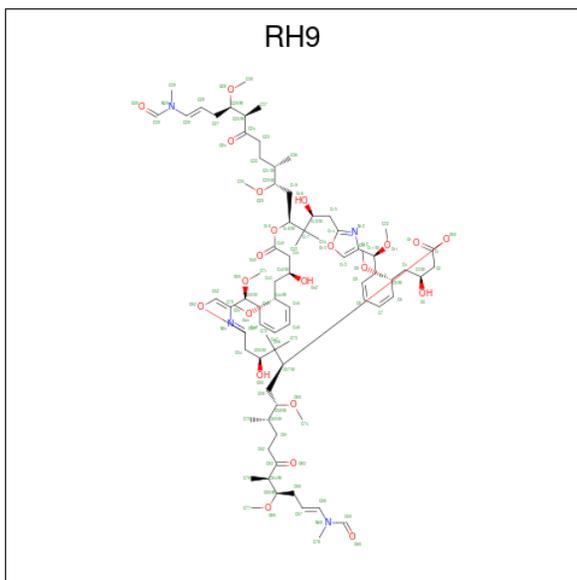
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	104	78	4	22	0	0

- Molecule 5 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).

HEZ
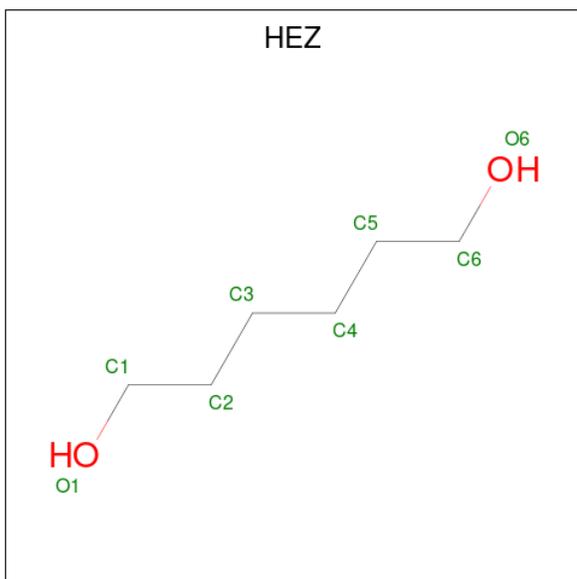
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	C 6	O 2	0	0
5	A	1	Total 8	C 6	O 2	0	0
5	A	1	Total 8	C 6	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	152	Total 152	O 152	0	0
6	B	62	Total 62	O 62	0	0

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. 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. 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: ACTIN, ALPHA SKELETAL MUSCLE

Chain A:

• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain B:
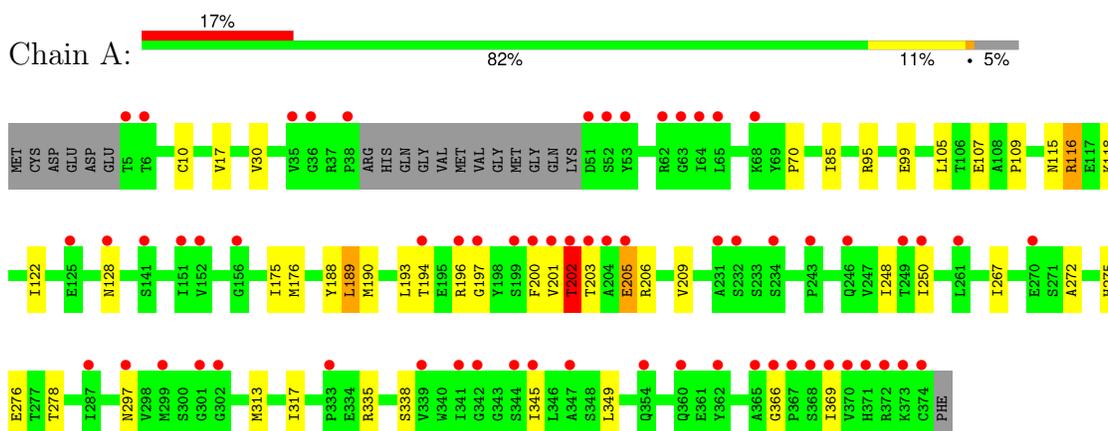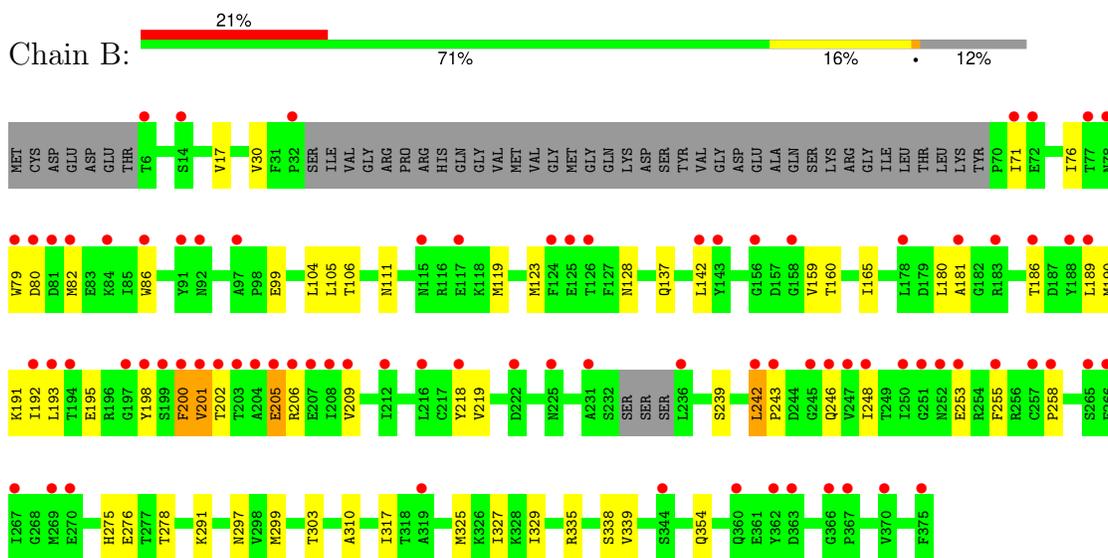
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.65Å 194.86Å 53.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.41 – 2.35 19.41 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.41-2.35) 99.7 (19.41-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.12 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.241 0.273 , 0.306	Depositor DCC
R_{free} test set	1759 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5844	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ATP, HEZ, RH9

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	0.86	0/2892	0.83	1/3920 (0.0%)
1	B	0.76	1/2685 (0.0%)	0.75	1/3637 (0.0%)
All	All	0.81	1/5577 (0.0%)	0.79	2/7557 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	ASP	C-O	13.96	1.49	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ARG	CG-CD-NE	-5.62	100.00	111.80
1	B	242	LEU	N-CA-C	5.48	125.80	111.00

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	2823	0	2801	34	0
1	B	2613	0	2588	63	0
2	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	12	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	104	0	124	2	0
5	A	24	0	42	1	0
6	A	152	0	0	1	0
6	B	62	0	0	1	0
All	All	5844	0	5579	98	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 9.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:O	1:B:209:VAL:HG22	1.69	0.93
1:B:190:MET:HE2	1:B:209:VAL:HG21	1.48	0.92
1:B:242:LEU:HD21	1:B:248:ILE:CD1	2.02	0.89
1:A:107:GLU:OE1	1:A:116:ARG:HD2	1.86	0.76
1:B:200:PHE:O	1:B:202:THR:HG22	1.85	0.75
1:A:193:LEU:HD21	1:A:250:ILE:HG21	1.69	0.73
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.69	0.73
1:B:190:MET:HE2	1:B:209:VAL:CG2	2.20	0.71
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.71	0.70
1:A:95[B]:ARG:NH1	6:A:2025:HOH:O	2.25	0.69
1:A:278:THR:HG21	1:A:297:ASN:HD21	1.58	0.68
1:A:201:VAL:N	1:A:205:GLU:HG3	2.12	0.65
1:B:104:LEU:C	1:B:104:LEU:HD23	2.17	0.64
1:A:193:LEU:HD21	1:A:250:ILE:CG2	2.27	0.64
1:B:278:THR:HG21	1:B:297:ASN:HD21	1.63	0.63
1:B:291:LYS:HG2	1:B:325:MET:SD	2.39	0.63
1:B:111:ASN:HD21	1:B:119[B]:MET:HE1	1.63	0.63
1:B:190:MET:CE	1:B:206:ARG:HB2	2.29	0.62
1:B:242:LEU:HD21	1:B:248:ILE:HD12	1.81	0.62
1:A:202:THR:HG22	1:A:203:THR:H	1.65	0.61
1:B:99[B]:GLU:HG3	1:B:128:ASN:HB3	1.83	0.61
1:B:198:TYR:CZ	1:B:248:ILE:HG23	2.36	0.61
1:B:206:ARG:O	1:B:209:VAL:CG2	2.47	0.60
1:B:202:THR:HG23	1:B:205:GLU:HB2	1.81	0.60
1:B:299[A]:MET:HE1	1:B:310:ALA:HA	1.84	0.60
1:B:105:LEU:HD13	1:B:119[A]:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MET:HE1	1:B:206:ARG:HB2	1.84	0.59
1:B:105:LEU:HD13	1:B:119[A]:MET:CE	2.33	0.58
1:B:278:THR:CG2	1:B:297:ASN:HD21	2.15	0.58
1:A:313:MET:HE3	1:A:317:ILE:HG12	1.85	0.58
1:A:272:ALA:HB1	1:A:276:GLU:HB2	1.87	0.57
1:A:196:ARG:N	1:A:197:GLY:HA2	2.21	0.56
1:A:202:THR:HG22	1:A:203:THR:N	2.21	0.56
1:B:242:LEU:HD21	1:B:248:ILE:HD11	1.86	0.55
1:B:202:THR:HG23	1:B:205:GLU:CB	2.36	0.55
1:B:105:LEU:HD11	1:B:123:MET:HG3	1.88	0.54
1:A:349:LEU:HD22	5:A:1378:HEZ:H22	1.90	0.54
1:A:366:GLY:O	1:A:369:ILE:HG22	2.09	0.52
1:B:242:LEU:HD23	1:B:246:GLN:O	2.09	0.52
1:A:313:MET:HE3	1:A:317:ILE:CG1	2.40	0.52
1:B:190:MET:CE	1:B:209:VAL:HG21	2.32	0.52
1:B:142:LEU:HD22	1:B:165:ILE:HB	1.92	0.51
1:B:335:ARG:HA	1:B:338:SER:OG	2.10	0.51
1:B:219:VAL:HG22	1:B:258:PRO:HB2	1.92	0.51
1:B:71:ILE:HG13	1:B:82:MET:HE1	1.92	0.50
1:B:186:THR:HG23	1:B:209:VAL:HG23	1.93	0.50
1:A:190:MET:O	1:A:194:THR:HG23	2.12	0.49
1:B:303:THR:O	1:B:303:THR:HG22	2.12	0.49
1:B:106:THR:HB	1:B:137:GLN:HG3	1.94	0.48
1:B:86:TRP:CD2	1:B:123:MET:HE1	2.49	0.48
1:B:191:LYS:O	1:B:195:GLU:N	2.40	0.48
1:A:118:LYS:HE3	1:A:122:ILE:HD11	1.96	0.48
1:B:189:LEU:HD12	1:B:193:LEU:HD13	1.96	0.48
1:B:17:VAL:O	1:B:30:VAL:HA	2.14	0.47
1:A:201:VAL:HG13	1:A:202:THR:H	1.80	0.47
1:A:99[B]:GLU:HG3	1:A:128:ASN:HB3	1.97	0.47
1:A:107:GLU:CD	1:A:116:ARG:HD2	2.35	0.47
1:A:70:PRO:HG2	1:A:85:ILE:CD1	2.42	0.46
1:B:190:MET:HE2	1:B:206:ARG:HB2	1.96	0.46
1:A:109:PRO:HB3	1:A:175:ILE:HD13	1.97	0.46
1:B:190:MET:HE1	1:B:206:ARG:CB	2.45	0.46
1:B:299[A]:MET:CE	1:B:329:ILE:HG21	2.46	0.46
1:B:200:PHE:O	1:B:201:VAL:C	2.53	0.46
1:B:189:LEU:CD1	1:B:192:ILE:HD11	2.43	0.46
1:B:76:ILE:HD12	1:B:119[B]:MET:HE3	1.97	0.46
1:A:188:TYR:CD1	1:A:267:ILE:HG22	2.52	0.45
1:A:275:HIS:CD2	1:A:275:HIS:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:HD23	1:B:181:ALA:N	2.32	0.44
1:A:189:LEU:HD22	1:A:193:LEU:CD1	2.46	0.44
1:A:345:ILE:HD13	4:A:1377:RH9:H2C2	2.00	0.44
1:A:10:CYS:HB3	1:A:105:LEU:HD23	2.00	0.44
1:B:137:GLN:HG2	1:B:339:VAL:HG11	1.99	0.44
1:B:317:ILE:HG22	1:B:327:ILE:HD12	2.00	0.44
1:A:205:GLU:O	1:A:209:VAL:HG23	2.18	0.43
1:B:198:TYR:OH	1:B:248:ILE:HG23	2.17	0.43
1:B:239:SER:HA	1:B:248:ILE:O	2.18	0.43
1:A:190:MET:HG2	1:A:209:VAL:HG21	2.01	0.43
1:B:189:LEU:O	1:B:193:LEU:HD13	2.19	0.43
1:B:192:ILE:HD13	1:B:253:GLU:HB3	2.01	0.43
1:B:299[A]:MET:HE1	1:B:329:ILE:HG21	2.01	0.43
1:A:335:ARG:HA	1:A:338:SER:OG	2.19	0.43
1:B:189:LEU:HD12	1:B:192:ILE:CD1	2.44	0.43
1:A:200:PHE:HZ	1:A:248:ILE:HD13	1.84	0.42
1:B:186:THR:HG22	1:B:190:MET:HE3	2.01	0.42
1:B:275:HIS:CE1	1:B:276:GLU:HG3	2.53	0.42
1:B:186:THR:CG2	1:B:209:VAL:HG23	2.49	0.42
1:B:201:VAL:HG12	1:B:201:VAL:O	2.19	0.42
1:B:104:LEU:HD23	1:B:105:LEU:N	2.35	0.42
1:B:354[B]:GLN:NE2	6:B:2058:HOH:O	2.52	0.42
1:A:99[B]:GLU:CG	1:A:128:ASN:HB3	2.49	0.42
1:B:218:TYR:O	1:B:255:PHE:HA	2.19	0.42
1:A:17:VAL:O	1:A:30:VAL:HA	2.20	0.42
1:B:76:ILE:HG21	1:B:79:TRP:CZ3	2.55	0.41
1:B:159:VAL:HG22	1:B:160:THR:N	2.35	0.41
1:A:175:ILE:O	1:A:176[A]:MET:CE	2.68	0.41
1:B:105:LEU:HD11	1:B:123:MET:CG	2.50	0.41
4:A:1377:RH9:H67	4:A:1377:RH9:H781	1.69	0.40
1:B:76:ILE:HD12	1:B:119[B]:MET:CE	2.51	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	358/377 (95%)	348 (97%)	9 (2%)	1 (0%)	37	43
1	B	329/377 (87%)	316 (96%)	11 (3%)	2 (1%)	22	24
All	All	687/754 (91%)	664 (97%)	20 (3%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	THR
1	B	201	VAL
1	B	243	PRO

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/320 (96%)	303 (98%)	5 (2%)	58	71
1	B	284/320 (89%)	282 (99%)	2 (1%)	81	89
All	All	592/640 (92%)	585 (99%)	7 (1%)	67	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	116	ARG
1	A	189	LEU
1	A	202	THR
1	A	205	GLU
1	B	200	PHE
1	B	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	275	HIS
1	A	297	ASN
1	B	225	ASN
1	B	275	HIS
1	B	297	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 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	#$|Z| > 2$
4	RH9	A	1377	-	92,106,106	1.31	9 (9%)	98,142,142	1.68	12 (12%)
5	HEZ	A	1380	-	7,7,7	0.43	0	6,6,6	0.24	0
2	ATP	A	1375	3	28,33,33	1.26	2 (7%)	34,52,52	1.27	4 (11%)
5	HEZ	A	1379	-	7,7,7	0.44	0	6,6,6	0.48	0
5	HEZ	A	1378	-	7,7,7	0.23	0	6,6,6	0.40	0
2	ATP	B	1377	3	28,33,33	1.28	2 (7%)	34,52,52	1.38	4 (11%)

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	RH9	A	1377	-	-	4/142/154/154	0/2/3/3
5	HEZ	A	1380	-	-	3/5/5/5	-
2	ATP	A	1375	3	-	2/18/38/38	0/3/3/3
5	HEZ	A	1379	-	-	2/5/5/5	-
5	HEZ	A	1378	-	-	1/5/5/5	-
2	ATP	B	1377	3	-	1/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1377	RH9	C54-C53	5.52	1.53	1.49
4	A	1377	RH9	O18-C40	4.48	1.46	1.34
4	A	1377	RH9	O58-C1	4.10	1.45	1.34
2	B	1377	ATP	PB-O3B	3.87	1.63	1.59
2	A	1375	ATP	PB-O3B	3.81	1.63	1.59
4	A	1377	RH9	C69-N68	-3.74	1.28	1.36
2	B	1377	ATP	C2-N3	3.47	1.37	1.32
4	A	1377	RH9	C30-N29	-3.37	1.29	1.36
4	A	1377	RH9	C15-C16	-3.01	1.50	1.53
4	A	1377	RH9	C15-C14	2.61	1.51	1.49
2	A	1375	ATP	C2-N3	2.45	1.35	1.32
4	A	1377	RH9	O18-C18	-2.29	1.42	1.46
4	A	1377	RH9	O63-C63	2.13	1.25	1.21

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1377	RH9	C58-C57-C56	8.30	122.06	115.88
4	A	1377	RH9	O18-C40-C41	4.76	119.96	111.43
4	A	1377	RH9	C49-C48-C47	-4.56	119.64	125.44
4	A	1377	RH9	C10-C9-C8	-4.14	120.17	125.44
4	A	1377	RH9	C34-C17-C33	3.89	114.28	109.17
4	A	1377	RH9	O58-C57-C58	3.50	114.44	106.97
2	B	1377	ATP	O3G-PG-O2G	3.39	120.50	107.80
4	A	1377	RH9	C49-C50-C51	-3.10	109.40	113.08
2	A	1375	ATP	C4'-O4'-C1'	-2.95	107.22	109.92
2	B	1377	ATP	N3-C2-N1	-2.95	124.67	128.67
2	B	1377	ATP	O4'-C1'-N9	2.89	112.58	108.75
2	B	1377	ATP	O2B-PB-O3A	2.76	114.73	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1377	RH9	O58-C1-C2	2.66	116.21	111.43
2	A	1375	ATP	O2A-PA-O3A	2.35	113.63	107.27
2	A	1375	ATP	O2A-PA-O1A	2.23	122.80	112.44
2	A	1375	ATP	N3-C2-N1	-2.19	125.69	128.67
4	A	1377	RH9	O20-C20-C21	2.16	113.47	108.27
4	A	1377	RH9	C73-C56-C55	2.10	112.86	108.94
4	A	1377	RH9	C4-C3-C2	-2.09	108.69	112.96
4	A	1377	RH9	O40-C40-C41	-2.04	119.92	124.65

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1377	RH9	C45-C44-O44-C70
5	A	1379	HEZ	C2-C3-C4-C5
5	A	1380	HEZ	C2-C3-C4-C5
4	A	1377	RH9	C73-C56-C57-O58
4	A	1377	RH9	C33-C17-C18-O18
5	A	1378	HEZ	C2-C3-C4-C5
4	A	1377	RH9	C55-C56-C57-O58
2	A	1375	ATP	C5'-O5'-PA-O1A
2	B	1377	ATP	C5'-O5'-PA-O1A
5	A	1379	HEZ	C4-C5-C6-O6
5	A	1380	HEZ	O1-C1-C2-C3
5	A	1380	HEZ	C4-C5-C6-O6
2	A	1375	ATP	PG-O3B-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1377	RH9	2	0
5	A	1378	HEZ	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 RH9 A 1377	
Bond lengths	Bond angles
Torsions	Rings

Ligand ATP A 1375	
Bond lengths	Bond angles
Torsions	Rings

Ligand ATP B 1377

Bond lengths

Bond angles

Torsions

Rings
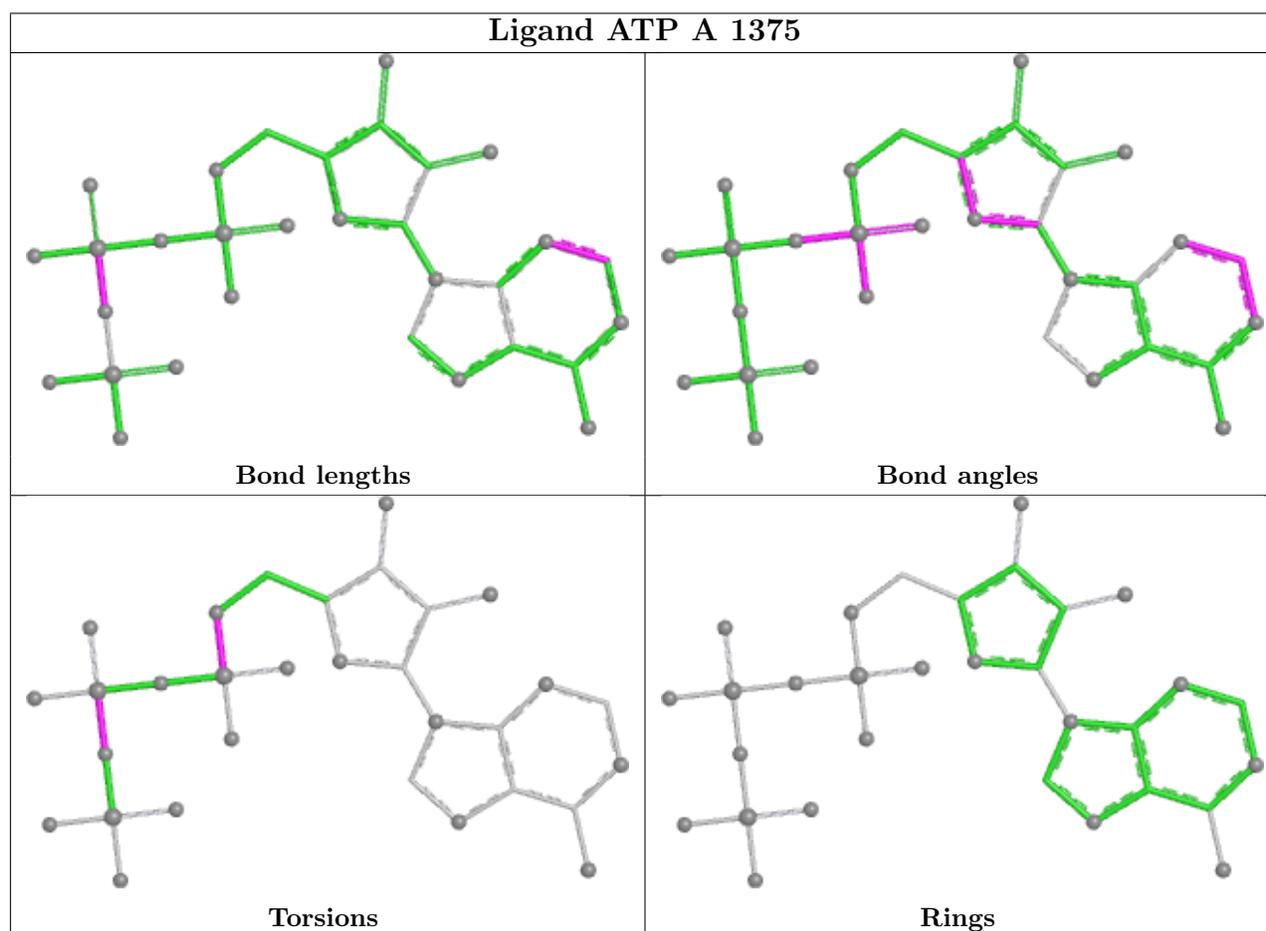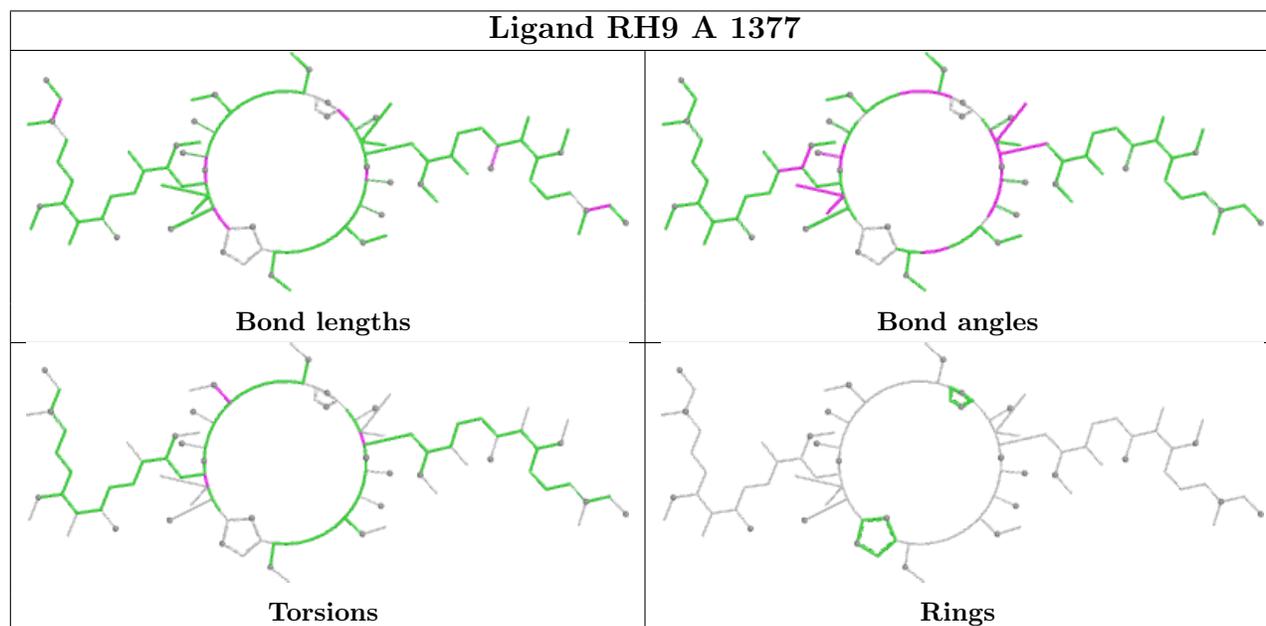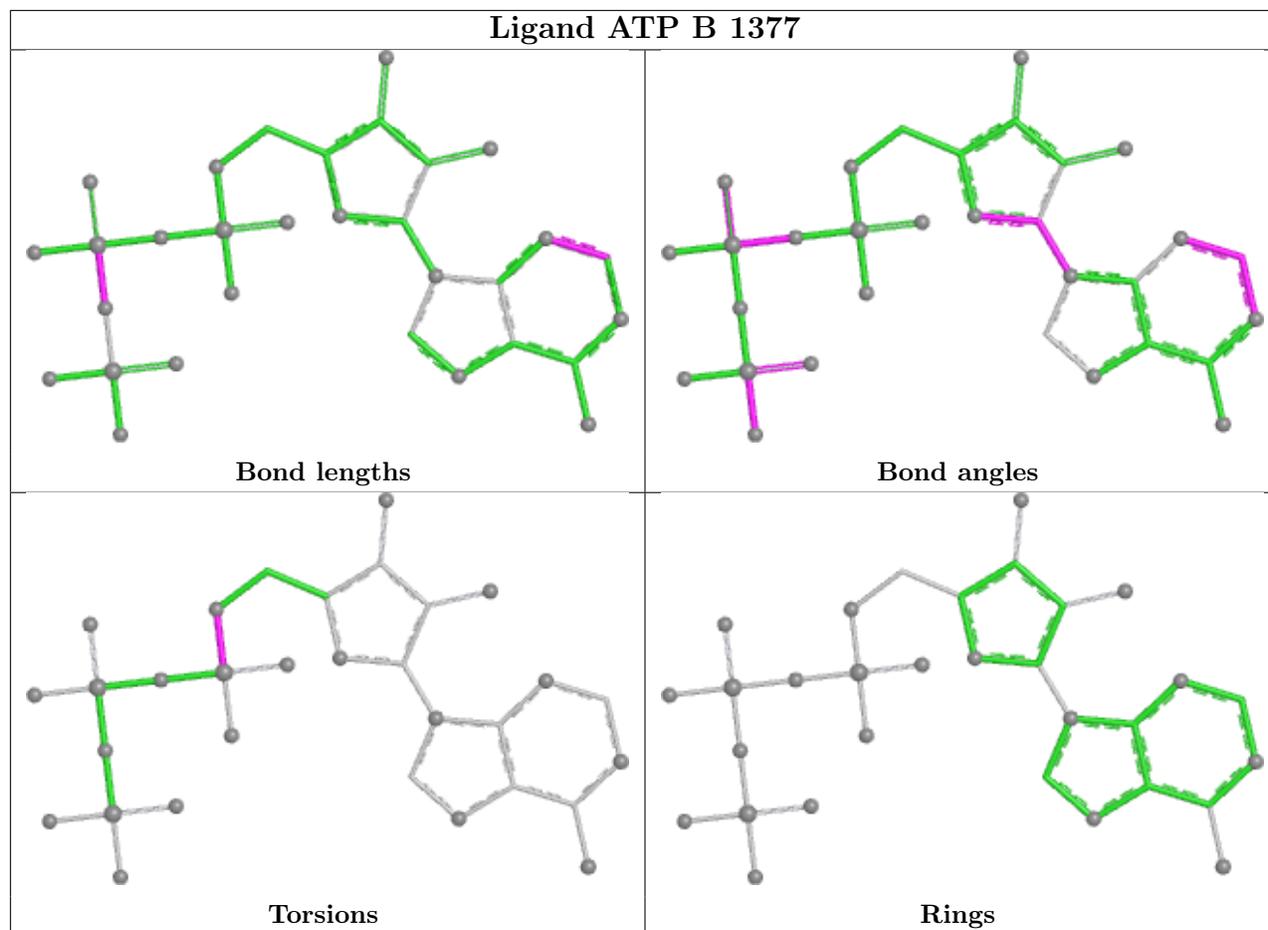
5.7 Other polymers ⓘ

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 ⓘ

Warning: The R factor obtained from EDS is 0.2756, which does not match the depositor's R factor of 0.186. Please interpret the results in this section carefully.

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(Å²)	Q<0.9
1	A	358/377 (94%)	1.33	63 (17%)	4	5	30, 54, 69, 89	5 (1%)
1	B	330/377 (87%)	1.45	81 (24%)	2	2	29, 55, 65, 75	5 (1%)
All	All	688/754 (91%)	1.39	144 (20%)	3	3	29, 55, 66, 89	10 (1%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	5.3
1	A	203	THR	5.3
1	A	366	GLY	5.1
1	B	193	LEU	4.6
1	B	363	ASP	4.2
1	A	65	LEU	4.2
1	B	204	ALA	4.0
1	A	53	TYR	3.9
1	A	365	ALA	3.9
1	B	200	PHE	3.9
1	A	371	HIS	3.9
1	B	79	TRP	3.8
1	A	370	VAL	3.8
1	B	91	TYR	3.8
1	B	80	ASP	3.8
1	A	369	ILE	3.7
1	A	199	SER	3.6
1	A	51	ASP	3.5
1	A	200	PHE	3.5
1	A	201	VAL	3.5
1	A	368	SER	3.4
1	B	247	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	6	THR	3.3
1	A	38	PRO	3.3
1	B	251	GLY	3.3
1	B	209	VAL	3.3
1	B	84	LYS	3.3
1	B	81	ASP	3.3
1	B	245	GLY	3.3
1	B	199	SER	3.3
1	A	250	ILE	3.2
1	A	367	PRO	3.2
1	B	236	LEU	3.2
1	A	204	ALA	3.2
1	A	372	ARG	3.2
1	B	186	THR	3.2
1	B	77	THR	3.2
1	B	216	LEU	3.1
1	A	374	CYS	3.0
1	B	252	ASN	3.0
1	A	287	ILE	3.0
1	B	203	THR	3.0
1	A	64	ILE	3.0
1	B	192	ILE	3.0
1	B	189	LEU	3.0
1	A	232	SER	2.9
1	A	234	SER	2.9
1	B	158	GLY	2.9
1	B	188	TYR	2.9
1	B	194	THR	2.9
1	B	78	ASN	2.9
1	B	201	VAL	2.8
1	B	125	GLU	2.8
1	B	86	TRP	2.8
1	A	205	GLU	2.8
1	B	178	LEU	2.8
1	B	212	ILE	2.8
1	A	333	PRO	2.8
1	A	5	THR	2.8
1	A	362	TYR	2.8
1	A	339	VAL	2.7
1	A	249	THR	2.7
1	A	243	PRO	2.7
1	A	52	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	205	GLU	2.6
1	A	62	ARG	2.6
1	A	202	THR	2.6
1	A	128	ASN	2.6
1	B	269	MET	2.6
1	B	225	ASN	2.6
1	A	261	LEU	2.5
1	B	198	TYR	2.5
1	A	345	ILE	2.5
1	B	246	GLN	2.5
1	B	197	GLY	2.5
1	B	202	THR	2.5
1	B	231	ALA	2.5
1	B	14	SER	2.5
1	B	344	SER	2.5
1	A	197	GLY	2.5
1	B	92	ASN	2.5
1	A	360	GLN	2.5
1	B	360	GLN	2.5
1	B	32	PRO	2.5
1	B	143	TYR	2.4
1	A	156	GLY	2.4
1	B	255	PHE	2.4
1	A	373	LYS	2.4
1	B	366	GLY	2.4
1	B	242	LEU	2.4
1	A	344	SER	2.4
1	A	347	ALA	2.4
1	B	97	ALA	2.4
1	A	270	GLU	2.4
1	B	183	ARG	2.4
1	B	248	ILE	2.3
1	B	206	ARG	2.3
1	A	302	GLY	2.3
1	B	71	ILE	2.3
1	A	297	ASN	2.3
1	B	117	GLU	2.3
1	B	253	GLU	2.3
1	A	6[A]	THR	2.3
1	B	257	CYS	2.3
1	A	63	GLY	2.3
1	B	72	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	2.2
1	B	319	ALA	2.2
1	B	208	ILE	2.2
1	B	375	PHE	2.2
1	B	265	SER	2.2
1	B	267	ILE	2.2
1	A	152	VAL	2.2
1	B	370	VAL	2.2
1	B	222	ASP	2.2
1	A	125	GLU	2.2
1	A	301	GLY	2.2
1	A	35	VAL	2.2
1	A	299	MET	2.2
1	A	342	GLY	2.1
1	B	207	GLU	2.1
1	B	142	LEU	2.1
1	B	367	PRO	2.1
1	A	194	THR	2.1
1	B	362	TYR	2.1
1	B	258	PRO	2.1
1	B	218	TYR	2.1
1	B	270	GLU	2.1
1	B	250	ILE	2.1
1	B	115	ASN	2.1
1	A	341	ILE	2.1
1	A	354	GLN	2.1
1	B	243	PRO	2.1
1	A	231	ALA	2.1
1	B	82	MET	2.1
1	B	126	THR	2.1
1	B	156	GLY	2.0
1	A	141	SER	2.0
1	A	151	ILE	2.0
1	A	196	ARG	2.0
1	B	124	PHE	2.0
1	B	266	PHE	2.0
1	A	68	LYS	2.0
1	A	246	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	CA	B	1379	1/1	0.72	0.16	96,96,96,96	0
5	HEZ	A	1380	8/8	0.72	0.17	76,77,82,84	0
5	HEZ	A	1379	8/8	0.80	0.15	70,71,73,74	0
2	ATP	B	1377	31/31	0.91	0.12	53,61,68,69	0
5	HEZ	A	1378	8/8	0.91	0.13	31,36,46,47	1
4	RH9	A	1377	104/104	0.93	0.09	33,42,48,50	0
3	CA	B	1376	1/1	0.94	0.10	61,61,61,61	0
2	ATP	A	1375	31/31	0.97	0.08	33,39,41,42	0
3	CA	B	1378	1/1	0.98	0.04	54,54,54,54	0
3	CA	A	1376	1/1	0.99	0.03	35,35,35,35	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 ATP B 1377:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
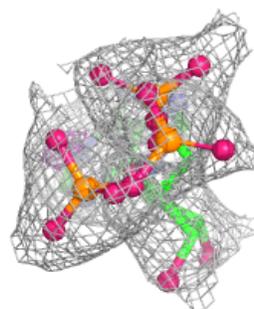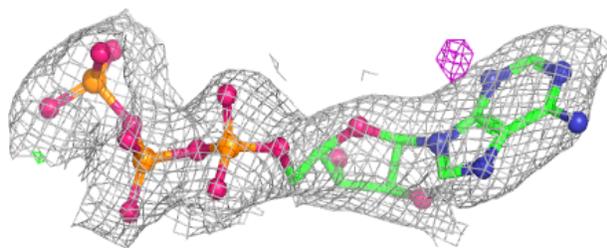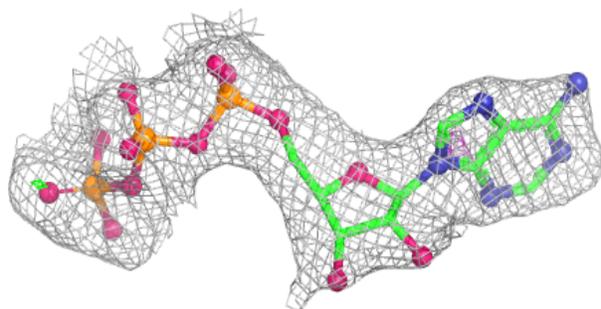
Electron density around RH9 A 1377:

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

Electron density around ATP A 1375:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
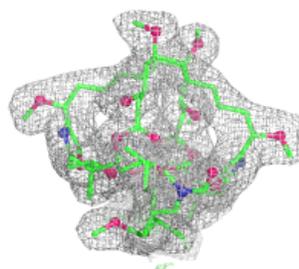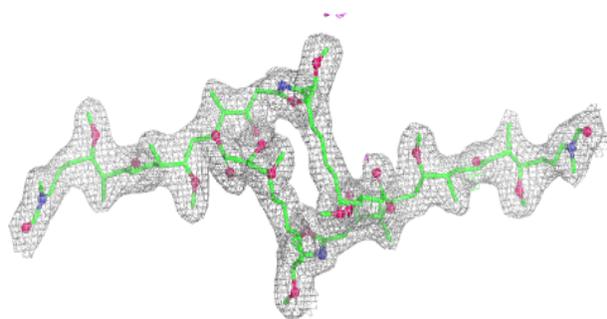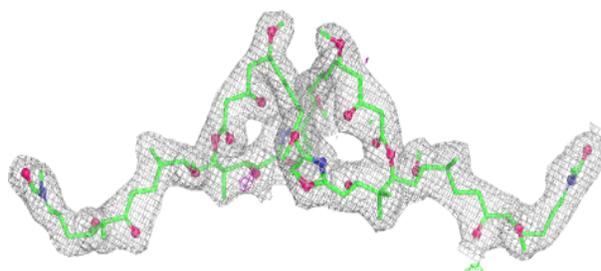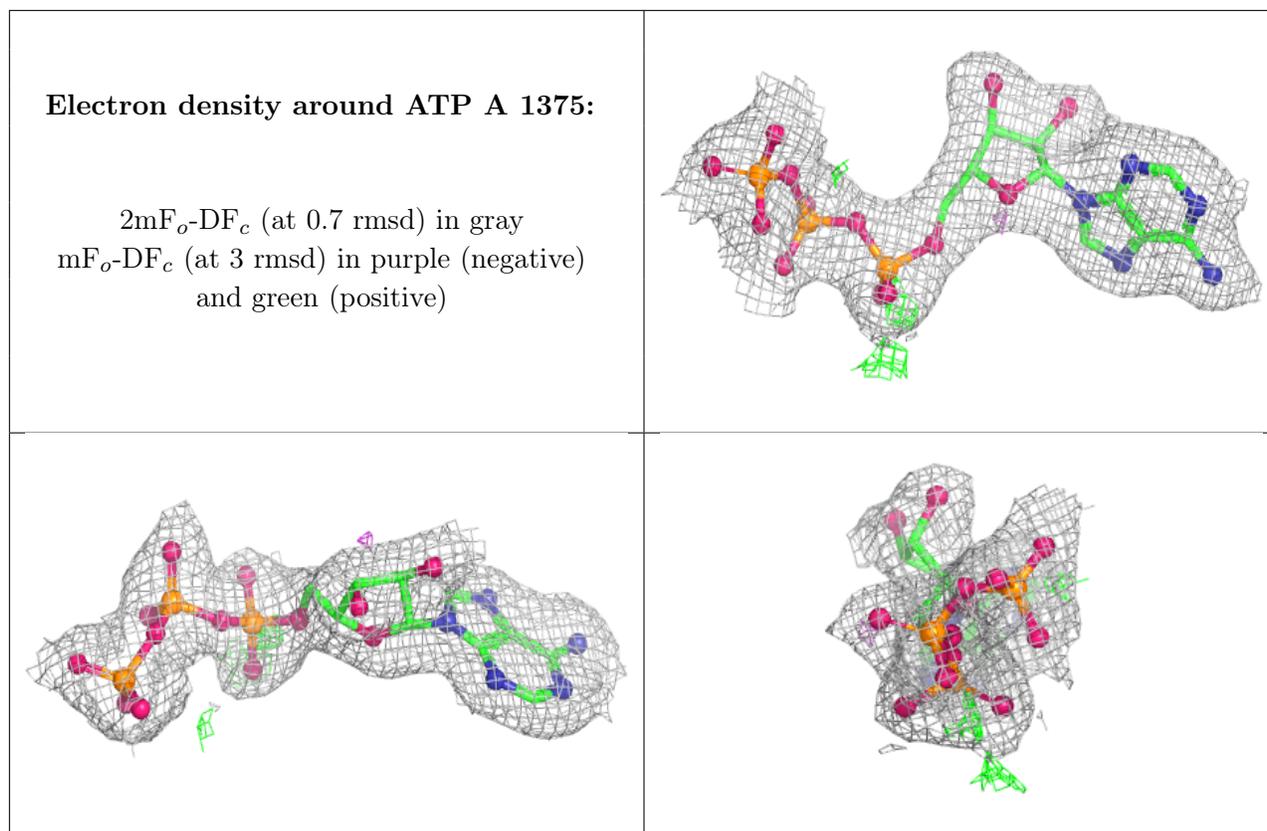
6.5 Other polymers (i)

There are no such residues in this entry.