



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:16 AM UTC

PDB ID : 3L9H / pdb_00003l9h
Title : X-ray structure of mitotic kinesin-5 (KSP, KIF11, Eg5)in complex with the h
exahydro-2H-pyrano[3,2-c]quinoline EMD 534085
Authors : Knoechel, T.
Deposited on : 2010-01-05
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

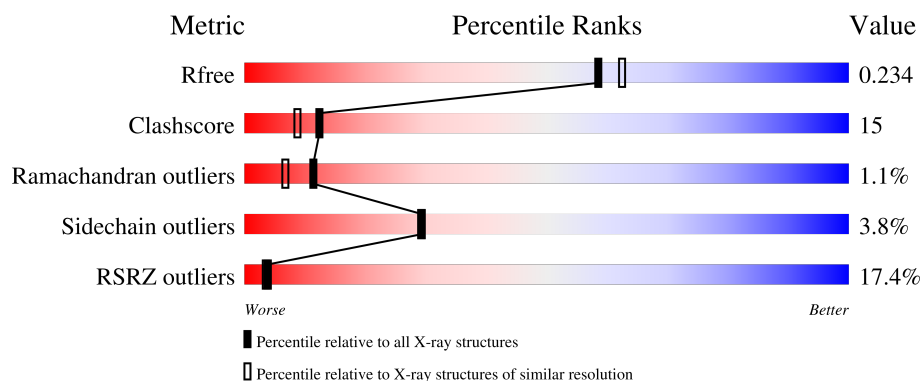
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	15% 65% 23% • 10%
1	B	368	17% 64% 23% • 10%

2 Entry composition [i](#)

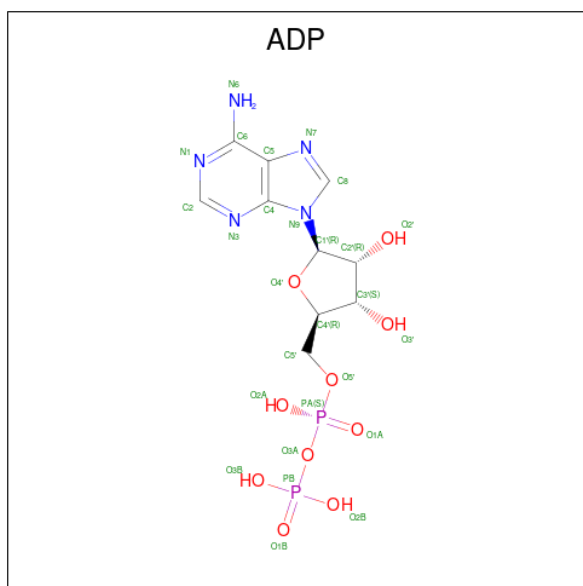
There are 4 unique types of molecules in this entry. The entry contains 5603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kinesin-like protein KIF11.

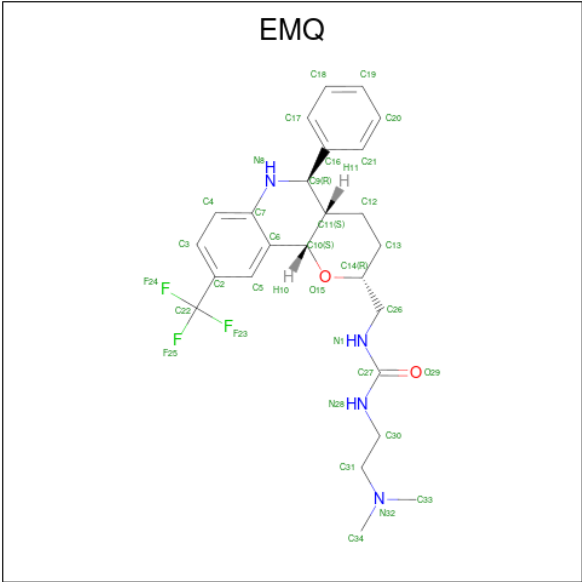
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2599	1628	453	508	10			
1	B	331	Total	C	N	O	S	0	0	0
			2599	1628	453	508	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is 1-[2-(dimethylamino)ethyl]-3-{[(2R,4aS,5R,10bS)-5-phenyl-9-(trifluoromethyl)-3,4,4a,5,6,10b-hexahydro-2H-pyrano[3,2-c]quinolin-2-yl]methyl}urea (CCD ID: EMQ) (formula: $C_{25}H_{31}F_3N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			34	25	3	4	2		
3	B	1	Total	C	F	N	O	0	0
			34	25	3	4	2		

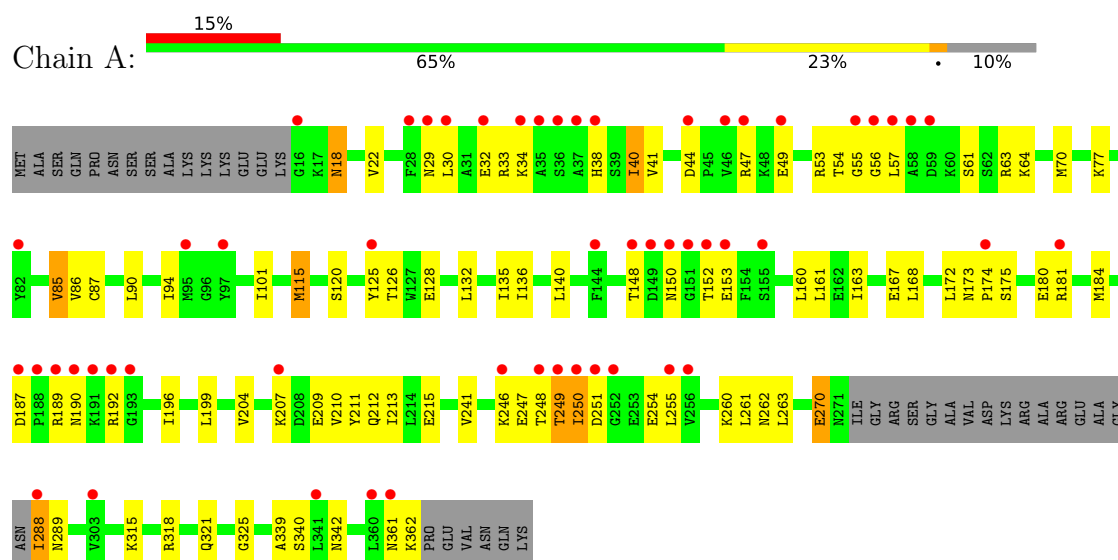
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total	O	0	0
			144	144		
4	B	139	Total	O	0	0
			139	139		

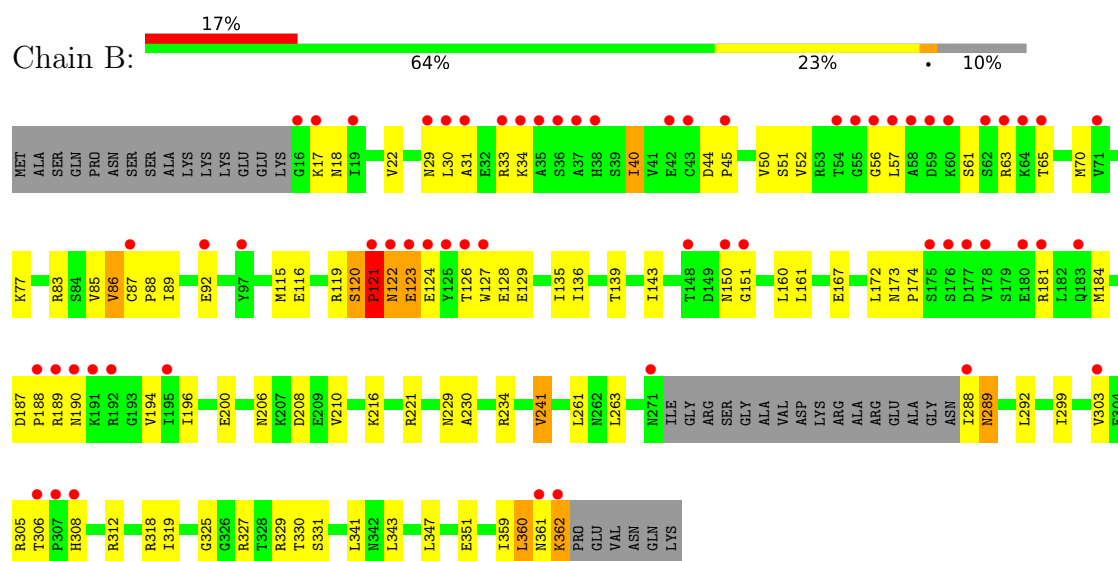
3 Residue-property plots [i](#)

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: Kinesin-like protein KIF11



• Molecule 1: Kinesin-like protein KIF11



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.95Å 79.72Å 69.51Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.0 (30.00-2.00) 87.9 (30.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.258 0.227 , 0.234	Depositor DCC
R_{free} test set	2638 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5603	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, EMQ

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	0.39	0/2637	0.94	8/3564 (0.2%)
1	B	0.38	0/2637	0.95	11/3564 (0.3%)
All	All	0.38	0/5274	0.94	19/7128 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	SER	CA-C-N	8.23	130.13	119.84
1	B	120	SER	C-N-CA	8.23	130.13	119.84
1	A	126	THR	N-CA-C	-7.97	100.24	110.53
1	B	86	VAL	N-CA-C	7.82	118.40	110.82
1	B	210	VAL	N-CA-C	7.35	117.87	110.23
1	B	135	ILE	N-CA-C	6.84	116.98	110.42
1	A	86	VAL	N-CA-C	6.28	116.91	110.82
1	B	85	VAL	N-CA-C	5.92	117.29	111.67
1	B	40	ILE	N-CA-C	-5.91	106.56	112.17
1	A	44	ASP	CA-C-N	5.65	125.76	119.32
1	A	44	ASP	C-N-CA	5.65	125.76	119.32
1	A	135	ILE	N-CA-C	5.62	115.81	110.42
1	B	150	ASN	N-CA-C	-5.60	102.23	110.52
1	B	44	ASP	CA-C-N	5.50	126.72	119.84
1	B	44	ASP	C-N-CA	5.50	126.72	119.84
1	A	40	ILE	N-CA-C	-5.48	107.64	112.90
1	B	126	THR	N-CA-C	-5.45	102.46	110.52
1	A	148	THR	N-CA-C	-5.36	106.00	112.54
1	A	41	VAL	N-CA-C	5.24	115.50	108.17

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	2599	0	2628	85	0
1	B	2599	0	2628	86	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	34	0	31	0	0
3	B	34	0	31	1	0
4	A	144	0	0	13	0
4	B	139	0	0	2	0
All	All	5603	0	5342	164	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 15.

All (164) 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:167:GLU:HG2	1:A:181:ARG:HH21	1.05	1.09
1:B:167:GLU:HG2	1:B:181:ARG:HH21	1.18	1.04
1:A:153:GLU:HB3	1:A:246:LYS:HB3	1.55	0.89
1:A:248:THR:HG22	1:A:254:GLU:HG2	1.57	0.84
1:A:249:THR:HG22	1:A:250:ILE:HD13	1.62	0.82
1:A:167:GLU:HG2	1:A:181:ARG:NH2	1.91	0.79
1:A:270:GLU:OE1	4:A:369:HOH:O	2.04	0.76
1:B:56:GLY:HA3	1:B:61:SER:HA	1.68	0.74
1:B:51:SER:HB3	1:B:63:ARG:HE	1.53	0.74
1:B:17:LYS:HG2	1:B:18:ASN:N	2.04	0.73
1:A:128:GLU:HG2	1:A:207:LYS:NZ	2.04	0.72
1:A:260:LYS:NZ	1:A:262:ASN:HD21	1.88	0.71
1:A:128:GLU:HG2	1:A:207:LYS:HZ2	1.55	0.71
1:B:167:GLU:CG	1:B:181:ARG:HH21	1.99	0.71
1:A:184:MET:HE2	1:A:318:ARG:CZ	2.21	0.71
1:B:18:ASN:ND2	1:B:360:LEU:HD22	2.06	0.70
1:A:173:ASN:ND2	1:A:175:SER:H	1.90	0.69
1:B:173:ASN:CG	1:B:200:GLU:HG3	2.17	0.69
1:B:87:CYS:HB2	1:B:88:PRO:HD3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.74	0.69
1:A:18:ASN:N	1:A:18:ASN:HD22	1.89	0.68
1:A:187:ASP:HB3	4:A:454:HOH:O	1.94	0.67
1:B:184:MET:HE2	1:B:318:ARG:CZ	2.25	0.67
1:B:83:ARG:HA	1:B:87:CYS:SG	2.35	0.66
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.78	0.65
1:A:56:GLY:C	1:A:57:LEU:HD22	2.22	0.65
1:B:30:LEU:HD22	1:B:33:ARG:HD2	1.79	0.65
1:A:29:ASN:OD1	1:A:32:GLU:HG3	1.97	0.65
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.27	0.64
1:B:167:GLU:HG2	1:B:181:ARG:NH2	2.03	0.62
1:A:339:ALA:HB3	1:A:342:ASN:ND2	2.14	0.62
1:B:57:LEU:O	1:B:61:SER:HB3	1.99	0.62
1:B:92:GLU:HG3	1:B:329:ARG:NH1	2.15	0.62
1:A:247:GLU:O	1:A:254:GLU:HA	1.99	0.61
1:A:189:ARG:C	4:A:454:HOH:O	2.42	0.61
1:A:161:LEU:HD22	1:A:196:ILE:HD13	1.82	0.61
1:B:327:ARG:HH12	1:B:362:LYS:HE2	1.66	0.60
1:B:241:VAL:HG13	1:B:261:LEU:HB3	1.84	0.60
1:A:77:LYS:HE3	4:A:394:HOH:O	2.01	0.59
1:B:115:MET:HE3	1:B:263:LEU:HB3	1.82	0.59
1:B:362:LYS:HB3	1:B:362:LYS:HZ3	1.68	0.59
1:A:249:THR:HG22	1:A:250:ILE:CD1	2.32	0.58
1:B:122:ASN:C	1:B:124:GLU:H	2.11	0.58
1:B:230:ALA:HB3	1:B:234:ARG:HD3	1.84	0.58
1:A:175:SER:HB3	1:B:34:LYS:NZ	2.19	0.58
1:B:306:THR:HG22	1:B:308:HIS:H	1.69	0.58
1:B:29:ASN:HD21	1:B:31:ALA:HB3	1.68	0.57
1:A:260:LYS:HZ1	1:A:262:ASN:HD21	1.50	0.57
1:A:270:GLU:HB3	4:A:369:HOH:O	2.05	0.57
1:A:190:ASN:N	4:A:454:HOH:O	2.37	0.56
1:B:30:LEU:C	1:B:30:LEU:HD13	2.31	0.56
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.87	0.56
1:B:17:LYS:HG2	1:B:18:ASN:H	1.70	0.56
1:A:40:ILE:HD13	1:A:340:SER:HA	1.87	0.56
1:A:288:ILE:HD12	1:A:288:ILE:N	2.21	0.55
1:B:206:ASN:OD1	1:B:208:ASP:HB2	2.06	0.55
1:A:187:ASP:CB	4:A:454:HOH:O	2.53	0.55
1:B:305:ARG:HH11	1:B:305:ARG:HG3	1.71	0.55
1:B:122:ASN:O	1:B:124:GLU:N	2.39	0.55
1:B:128:GLU:HB2	1:B:129:GLU:OE2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASN:O	1:B:33:ARG:HG2	2.08	0.54
1:A:18:ASN:N	1:A:18:ASN:ND2	2.55	0.53
1:A:251:ASP:HA	4:A:449:HOH:O	2.08	0.53
1:A:136:ILE:HG12	1:A:263:LEU:HD13	1.91	0.53
1:A:38:HIS:CD2	1:A:53:ARG:HH21	2.26	0.53
1:A:70:MET:HE1	1:A:85:VAL:HG12	1.90	0.53
1:B:50:VAL:O	1:B:65:THR:HA	2.09	0.53
1:A:54:THR:HG21	1:A:64:LYS:NZ	2.24	0.52
1:B:299:ILE:O	1:B:303:VAL:HG13	2.09	0.52
1:A:90:LEU:O	1:A:94:ILE:HG12	2.09	0.52
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.38	0.52
1:A:339:ALA:HB3	1:A:342:ASN:HD22	1.74	0.52
1:B:161:LEU:HD22	1:B:196:ILE:HD13	1.92	0.52
1:B:18:ASN:N	1:B:18:ASN:HD22	2.08	0.52
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.75	0.52
1:B:139:THR:O	1:B:143:ILE:HG13	2.09	0.51
1:B:30:LEU:HD13	1:B:30:LEU:O	2.10	0.51
1:A:207:LYS:C	1:A:209:GLU:H	2.19	0.51
1:B:241:VAL:CG1	1:B:261:LEU:HB3	2.40	0.51
1:A:362:LYS:HG3	4:A:460:HOH:O	2.10	0.51
1:A:53:ARG:HB2	1:A:63:ARG:HH22	1.75	0.50
1:A:172:LEU:O	1:A:174:PRO:HD3	2.12	0.50
1:B:161:LEU:HD21	1:B:319:ILE:HD13	1.94	0.50
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.77	0.50
1:A:53:ARG:HB2	1:A:63:ARG:NH2	2.27	0.49
1:B:120:SER:O	1:B:122:ASN:N	2.45	0.49
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.95	0.49
1:B:362:LYS:CB	1:B:362:LYS:NZ	2.75	0.49
1:A:57:LEU:O	1:A:61:SER:HB3	2.13	0.49
1:A:212:GLN:HG2	1:B:121:PRO:O	2.12	0.49
1:B:51:SER:OG	1:B:65:THR:HG22	2.12	0.49
1:B:305:ARG:HG3	1:B:305:ARG:NH1	2.27	0.49
1:A:175:SER:HB3	1:B:34:LYS:HZ3	1.77	0.49
1:B:33:ARG:HH11	1:B:33:ARG:HB2	1.77	0.48
1:A:184:MET:SD	1:A:315:LYS:HD2	2.53	0.48
1:B:115:MET:CE	1:B:263:LEU:HB3	2.43	0.48
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.44	0.47
1:A:204:VAL:HG22	1:A:213:ILE:CD1	2.45	0.47
1:B:119:ARG:HB2	3:B:602:EMQ:H30	1.96	0.47
1:B:327:ARG:HG2	1:B:327:ARG:NH1	2.29	0.47
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.45	0.46
1:B:52:VAL:O	1:B:63:ARG:HA	2.16	0.46
1:B:160:LEU:HB3	1:B:172:LEU:HG	1.97	0.46
1:B:89:ILE:O	1:B:92:GLU:HB2	2.16	0.46
1:B:173:ASN:OD1	1:B:200:GLU:HG3	2.16	0.46
1:A:175:SER:O	1:B:31:ALA:HB2	2.16	0.45
1:B:116:GLU:CD	1:B:221:ARG:HH12	2.24	0.45
1:A:325:GLY:H	1:A:361:ASN:HD21	1.63	0.45
1:A:160:LEU:HB3	1:A:172:LEU:HG	1.98	0.45
1:B:187:ASP:HA	1:B:188:PRO:HD3	1.86	0.45
1:B:92:GLU:HG3	1:B:329:ARG:HH11	1.80	0.45
1:A:215:GLU:OE1	1:B:121:PRO:O	2.35	0.44
1:A:63:ARG:HD2	4:A:401:HOH:O	2.17	0.44
1:B:86:VAL:O	1:B:87:CYS:C	2.58	0.44
1:B:122:ASN:C	1:B:124:GLU:N	2.76	0.44
1:A:184:MET:HE2	1:A:318:ARG:NH2	2.31	0.44
1:A:101:ILE:CG2	1:A:115:MET:HE1	2.48	0.44
1:A:150:ASN:C	1:A:152:THR:H	2.26	0.44
1:A:192:ARG:HG2	1:A:192:ARG:NH1	2.33	0.44
1:B:127:TRP:CZ2	1:B:128:GLU:HG2	2.53	0.44
1:A:174:PRO:O	1:B:30:LEU:HD12	2.18	0.43
1:B:77:LYS:HE2	4:B:430:HOH:O	2.18	0.43
1:B:289:ASN:HD22	1:B:292:LEU:H	1.64	0.43
1:A:260:LYS:HZ2	1:A:262:ASN:HD21	1.64	0.43
1:A:325:GLY:H	1:A:361:ASN:ND2	2.16	0.43
1:B:181:ARG:HH11	1:B:181:ARG:HG3	1.82	0.43
1:B:184:MET:HE3	1:B:194:VAL:HG11	2.00	0.43
1:B:128:GLU:HG3	4:B:448:HOH:O	2.17	0.43
1:A:270:GLU:CD	4:A:369:HOH:O	2.58	0.43
1:A:249:THR:HG22	1:A:250:ILE:N	2.34	0.43
1:A:163:ILE:HG12	1:A:168:LEU:HD23	2.01	0.43
1:A:22:VAL:HG11	1:A:70:MET:HE3	2.01	0.43
1:A:54:THR:HG21	1:A:64:LYS:HZ3	1.84	0.42
1:A:120:SER:HA	1:A:132:LEU:HD12	2.00	0.42
1:B:362:LYS:HB3	1:B:362:LYS:NZ	2.31	0.42
1:A:30:LEU:HG	1:A:33:ARG:HH22	1.82	0.42
1:A:136:ILE:O	1:A:140:LEU:HD23	2.19	0.42
1:B:229:ASN:HD22	1:B:229:ASN:N	2.17	0.42
1:A:173:ASN:HD21	1:A:175:SER:HB2	1.83	0.42
1:A:196:ILE:HG22	1:A:199:LEU:HB2	2.02	0.42
1:B:325:GLY:H	1:B:361:ASN:HD21	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD12	1:B:343:LEU:HD13	2.00	0.42
1:A:33:ARG:HB2	1:A:33:ARG:NH1	2.34	0.42
1:A:321:GLN:NE2	4:A:405:HOH:O	2.51	0.42
1:A:173:ASN:C	1:A:173:ASN:HD22	2.28	0.42
1:A:211:TYR:HD2	1:B:122:ASN:ND2	2.18	0.41
1:B:77:LYS:HE2	1:B:77:LYS:HB3	1.75	0.41
1:B:120:SER:HA	1:B:121:PRO:HD3	1.90	0.41
1:B:92:GLU:CG	1:B:329:ARG:NH1	2.82	0.41
1:A:136:ILE:O	1:A:140:LEU:CD2	2.69	0.41
1:B:18:ASN:HD21	1:B:360:LEU:HD22	1.83	0.41
1:A:47:ARG:HG2	1:A:49:GLU:CD	2.45	0.41
1:B:229:ASN:N	1:B:229:ASN:ND2	2.67	0.41
1:B:347:LEU:O	1:B:351:GLU:HG2	2.21	0.41
1:A:30:LEU:HG	1:A:33:ARG:NH2	2.36	0.41
1:A:207:LYS:HA	1:A:210:VAL:HG23	2.03	0.41
1:B:330:THR:CG2	1:B:331:SER:N	2.84	0.41
1:A:241:VAL:CG1	1:A:261:LEU:HB3	2.51	0.40
1:B:172:LEU:O	1:B:174:PRO:HD3	2.22	0.40
1:A:187:ASP:C	4:A:454:HOH:O	2.64	0.40
1:A:288:ILE:N	1:A:288:ILE:CD1	2.81	0.40
1:B:312:ARG:HA	1:B:318:ARG:CG	2.52	0.40
1:A:55:GLY:O	1:A:61:SER:HB2	2.21	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	327/368 (89%)	320 (98%)	6 (2%)	1 (0%)	36	35
1	B	327/368 (89%)	313 (96%)	8 (2%)	6 (2%)	6	3
All	All	654/736 (89%)	633 (97%)	14 (2%)	7 (1%)	11	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	PRO
1	A	249	THR
1	B	123	GLU
1	B	189	ARG
1	B	190	ASN
1	B	45	PRO
1	B	151	GLY

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	293/322 (91%)	281 (96%)	12 (4%)	27	26
1	B	293/322 (91%)	283 (97%)	10 (3%)	32	33
All	All	586/644 (91%)	564 (96%)	22 (4%)	29	29

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	34	LYS
1	A	85	VAL
1	A	87	CYS
1	A	115	MET
1	A	125	TYR
1	A	180	GLU
1	A	250	ILE
1	A	255	LEU
1	A	270	GLU
1	A	288	ILE
1	A	289	ASN
1	B	121	PRO
1	B	122	ASN
1	B	123	GLU
1	B	216	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	241	VAL
1	B	288	ILE
1	B	289	ASN
1	B	341	LEU
1	B	360	LEU
1	B	362	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	122	ASN
1	A	173	ASN
1	A	183	GLN
1	A	190	ASN
1	A	229	ASN
1	A	262	ASN
1	A	289	ASN
1	A	321	GLN
1	A	342	ASN
1	A	358	ASN
1	A	361	ASN
1	B	18	ASN
1	B	122	ASN
1	B	142	GLN
1	B	173	ASN
1	B	183	GLN
1	B	212	GLN
1	B	229	ASN
1	B	262	ASN
1	B	289	ASN
1	B	321	GLN
1	B	358	ASN
1	B	361	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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$
2	ADP	A	501	-	28,29,29	1.28	6 (21%)	43,45,45	1.14	2 (4%)
2	ADP	B	502	-	28,29,29	1.28	3 (10%)	43,45,45	1.13	2 (4%)
3	EMQ	B	602	-	37,37,37	1.41	5 (13%)	51,53,53	1.40	9 (17%)
3	EMQ	A	601	-	37,37,37	1.46	7 (18%)	51,53,53	1.08	2 (3%)

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	ADP	A	501	-	-	3/16/32/32	0/3/3/3
2	ADP	B	502	-	-	2/16/32/32	0/3/3/3
3	EMQ	B	602	-	-	4/21/46/46	0/4/4/4
3	EMQ	A	601	-	-	3/21/46/46	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	EMQ	C26-C14	3.63	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	EMQ	C9-N8	3.46	1.49	1.46
2	B	502	ADP	C2-N1	3.39	1.40	1.33
2	A	501	ADP	C2-N1	3.15	1.39	1.33
2	B	502	ADP	PA-O3A	-2.85	1.56	1.59
2	A	501	ADP	PA-O3A	-2.64	1.56	1.59
3	B	602	EMQ	C21-C16	2.56	1.43	1.39
3	B	602	EMQ	C13-C14	2.40	1.57	1.51
3	B	602	EMQ	C3-C2	2.28	1.43	1.39
3	A	601	EMQ	C21-C16	2.18	1.42	1.39
2	A	501	ADP	C8-N7	2.17	1.35	1.31
3	B	602	EMQ	C27-N1	2.15	1.39	1.35
3	A	601	EMQ	F23-C22	2.15	1.40	1.33
2	B	502	ADP	C6-N6	-2.14	1.28	1.34
2	A	501	ADP	C6-N6	-2.12	1.28	1.34
3	A	601	EMQ	F25-C22	2.07	1.40	1.33
2	A	501	ADP	C5-C6	2.06	1.46	1.41
3	B	602	EMQ	F24-C22	2.03	1.40	1.33
3	A	601	EMQ	C13-C14	2.03	1.56	1.51
3	A	601	EMQ	F24-C22	2.01	1.40	1.33
2	A	501	ADP	C1'-N9	2.01	1.51	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	EMQ	C14-O15-C10	-3.74	108.84	113.86
3	B	602	EMQ	N28-C27-N1	3.67	120.91	115.58
2	B	502	ADP	N3-C2-N1	-3.64	123.07	128.58
2	A	501	ADP	N3-C2-N1	-3.57	123.18	128.58
3	B	602	EMQ	C2-C5-C6	-3.38	118.92	122.53
2	A	501	ADP	C2-N1-C6	2.95	123.57	118.73
2	B	502	ADP	C2-N1-C6	2.88	123.46	118.73
3	B	602	EMQ	O29-C27-N28	-2.86	117.56	122.47
3	B	602	EMQ	C5-C6-C7	2.59	121.41	118.56
3	B	602	EMQ	C14-O15-C10	-2.52	110.48	113.86
3	B	602	EMQ	C34-N32-C33	-2.42	103.51	109.72
3	B	602	EMQ	C17-C16-C9	-2.39	116.99	120.78
3	A	601	EMQ	C2-C5-C6	-2.36	120.01	122.53
3	B	602	EMQ	C12-C11-C10	-2.23	107.67	110.43
3	B	602	EMQ	F23-C22-C2	-2.06	108.49	112.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

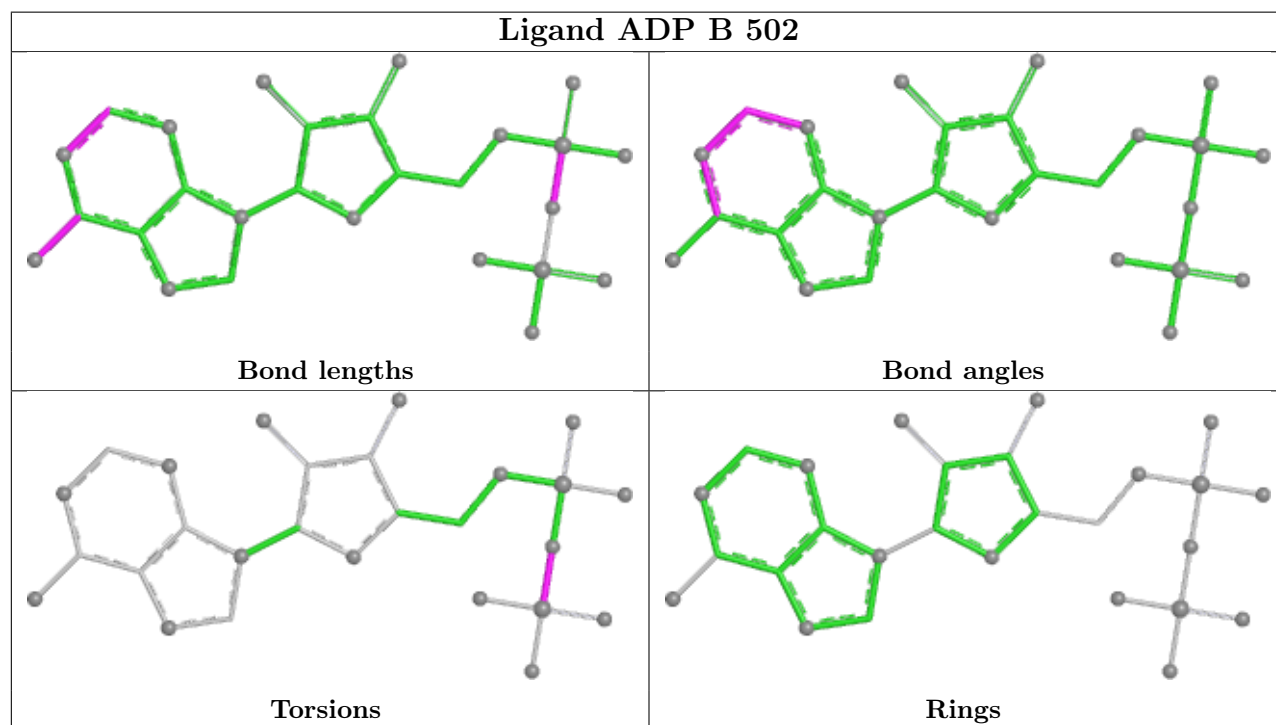
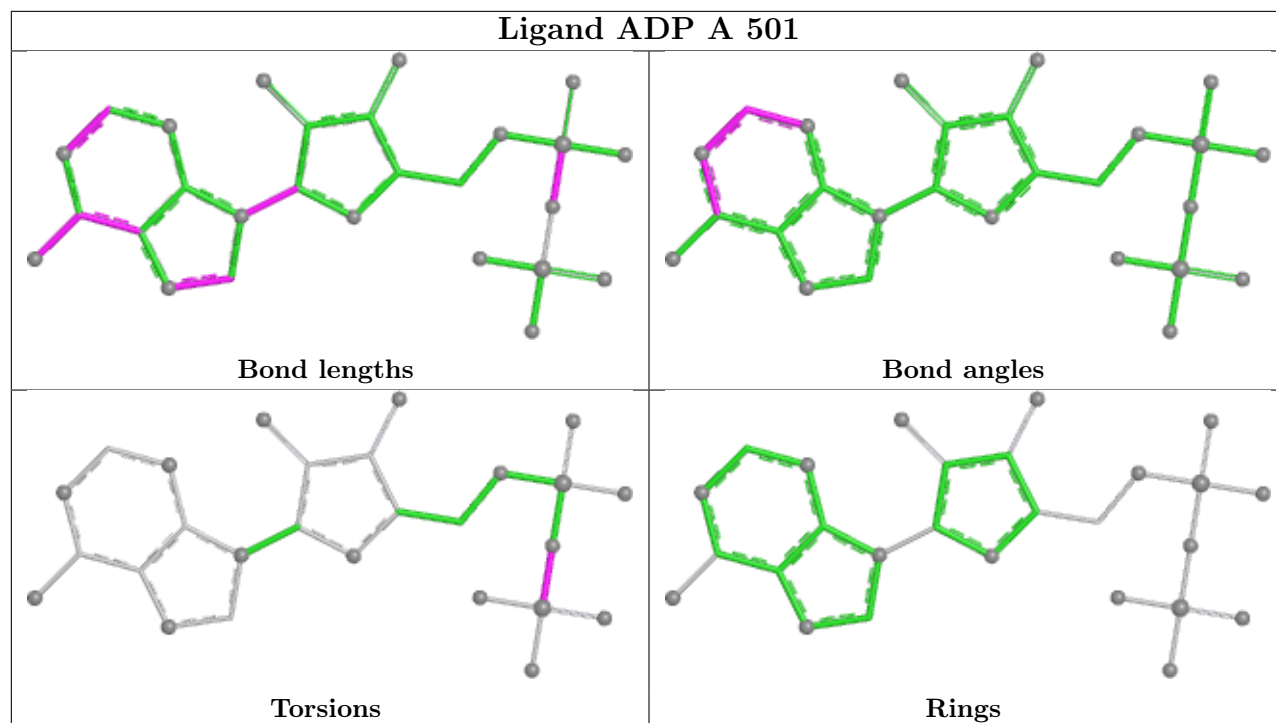
Mol	Chain	Res	Type	Atoms
2	A	501	ADP	PA-O3A-PB-O3B
2	B	502	ADP	PA-O3A-PB-O3B
3	A	601	EMQ	C13-C14-C26-N1
3	B	602	EMQ	N28-C30-C31-N32
3	A	601	EMQ	N28-C30-C31-N32
3	A	601	EMQ	O15-C14-C26-N1
3	B	602	EMQ	C30-C31-N32-C34
3	B	602	EMQ	C30-C31-N32-C33
2	A	501	ADP	PA-O3A-PB-O1B
2	A	501	ADP	PA-O3A-PB-O2B
2	B	502	ADP	PA-O3A-PB-O2B
3	B	602	EMQ	O15-C14-C26-N1

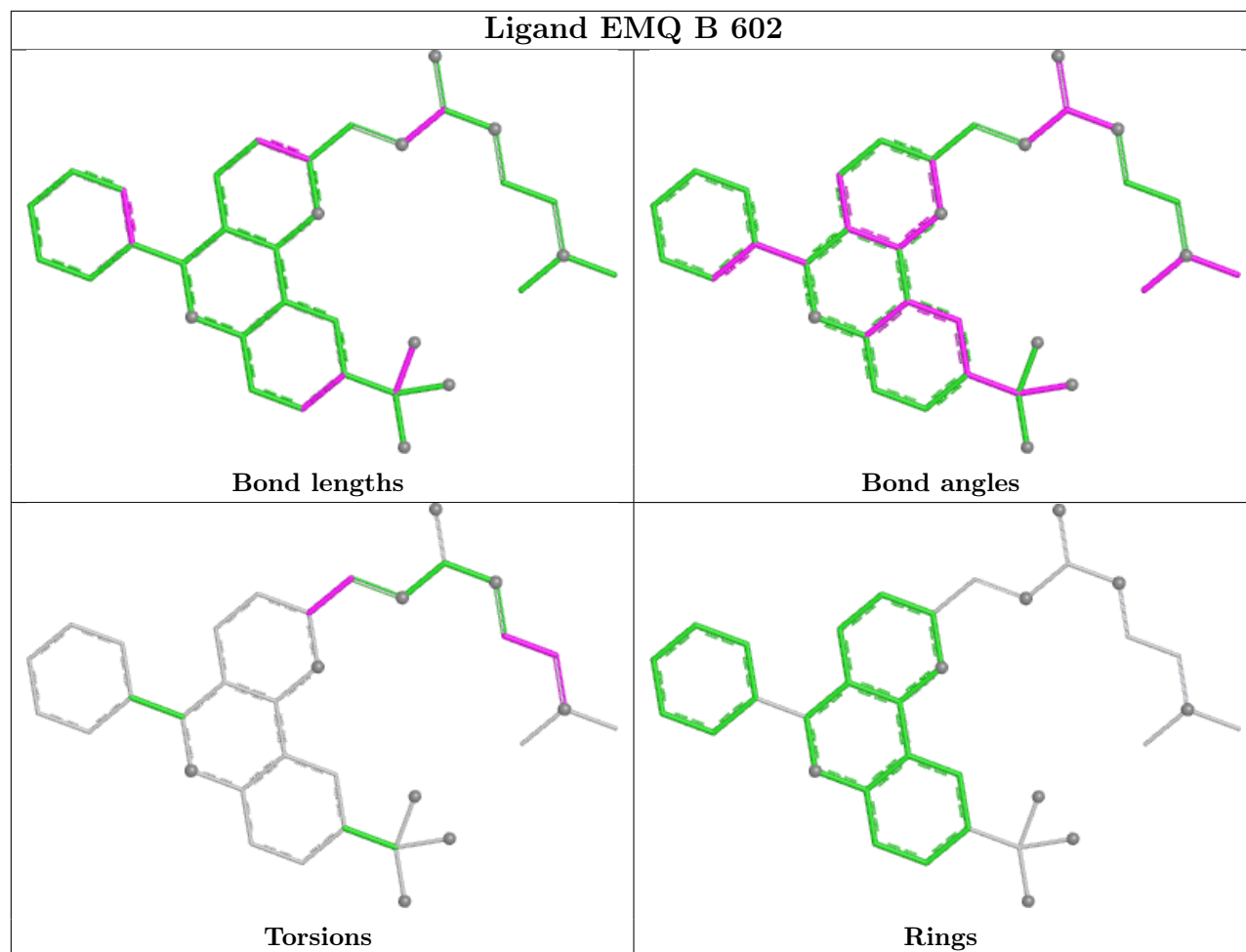
There are no ring outliers.

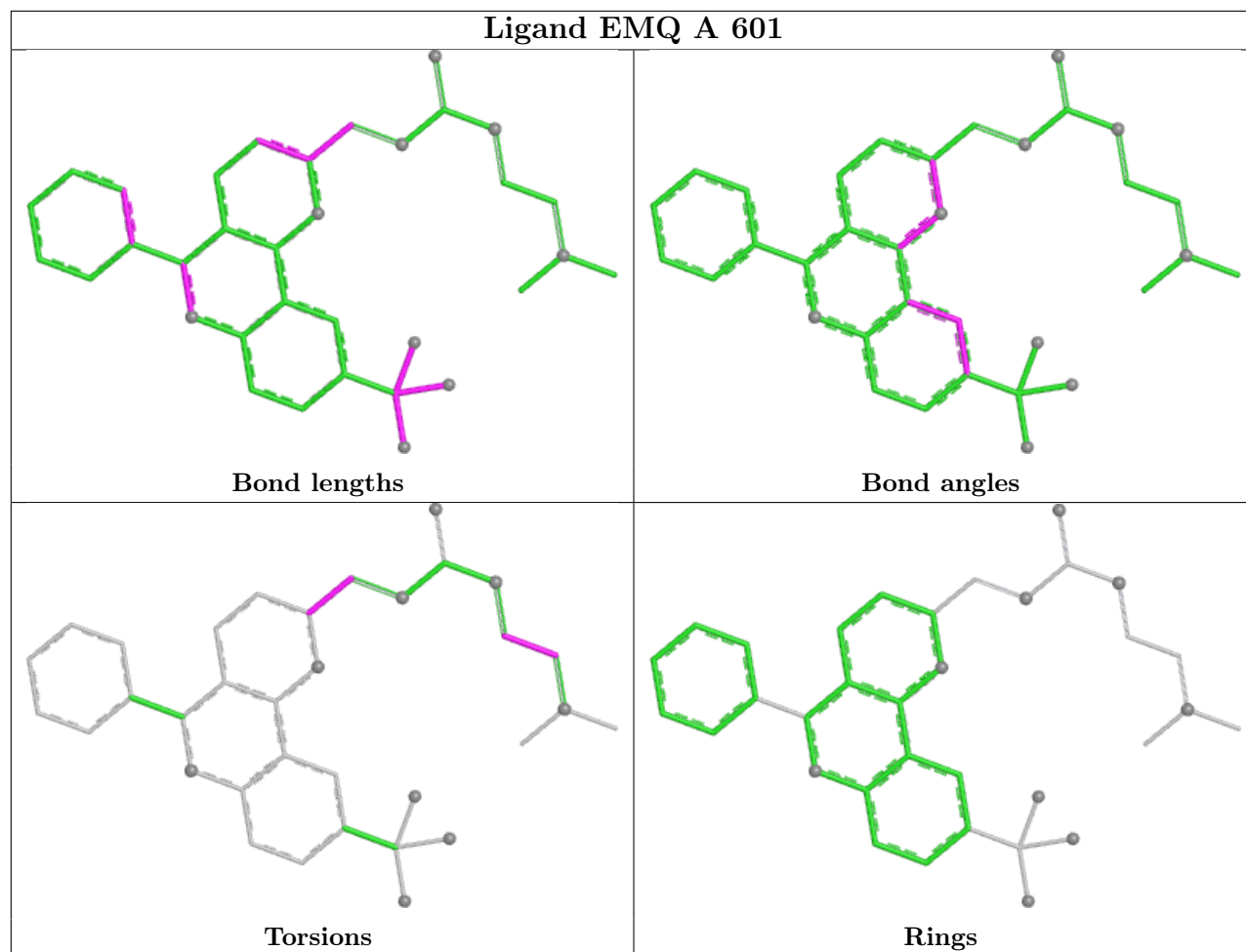
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	EMQ	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/368 (89%)	0.91	54 (16%)  	19, 36, 62, 68	0
1	B	331/368 (89%)	0.88	61 (18%)  	20, 38, 60, 66	0
All	All	662/736 (89%)	0.89	115 (17%)  	19, 37, 61, 68	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	SER	7.0
1	B	57	LEU	6.6
1	A	37	ALA	6.6
1	A	56	GLY	5.5
1	B	58	ALA	5.4
1	A	248	THR	5.2
1	A	250	ILE	5.1
1	B	31	ALA	5.1
1	A	192	ARG	4.9
1	A	249	THR	4.7
1	A	251	ASP	4.2
1	B	121	PRO	4.2
1	B	150	ASN	4.1
1	A	38	HIS	4.0
1	B	35	ALA	4.0
1	B	303	VAL	3.9
1	A	150	ASN	3.9
1	A	151	GLY	3.8
1	A	59	ASP	3.8
1	B	181	ARG	3.8
1	A	16	GLY	3.8
1	A	30	LEU	3.7
1	A	252	GLY	3.7
1	A	28	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	174	PRO	3.7
1	B	55	GLY	3.6
1	A	34	LYS	3.6
1	A	153	GLU	3.5
1	B	34	LYS	3.5
1	A	57	LEU	3.5
1	A	190	ASN	3.5
1	B	175	SER	3.5
1	B	16	GLY	3.4
1	B	178	VAL	3.4
1	B	307	PRO	3.4
1	A	58	ALA	3.4
1	A	255	LEU	3.4
1	A	188	PRO	3.3
1	A	35	ALA	3.3
1	B	54	THR	3.3
1	B	65	THR	3.2
1	A	191	LYS	3.2
1	B	37	ALA	3.1
1	A	360	LEU	3.1
1	B	56	GLY	3.1
1	B	361	ASN	3.1
1	A	256	VAL	3.1
1	B	97	TYR	3.1
1	B	288	ILE	3.1
1	A	189	ARG	3.0
1	B	362	LYS	3.0
1	B	192	ARG	3.0
1	A	303	VAL	3.0
1	B	92	GLU	2.9
1	A	97	TYR	2.9
1	A	193	GLY	2.9
1	B	308	HIS	2.9
1	A	55	GLY	2.9
1	B	59	ASP	2.9
1	A	288	ILE	2.9
1	B	189	ARG	2.8
1	B	17	LYS	2.8
1	A	144	PHE	2.8
1	B	148	THR	2.8
1	B	271	ASN	2.8
1	B	188	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	19	ILE	2.8
1	B	126	THR	2.7
1	A	152	THR	2.7
1	A	246	LYS	2.7
1	B	123	GLU	2.6
1	B	38	HIS	2.6
1	B	190	ASN	2.6
1	B	62	SER	2.6
1	B	71	VAL	2.5
1	B	125	TYR	2.5
1	A	181	ARG	2.5
1	B	63	ARG	2.5
1	B	30	LEU	2.5
1	B	122	ASN	2.5
1	A	207	LYS	2.5
1	A	47	ARG	2.5
1	A	44	ASP	2.4
1	B	191	LYS	2.4
1	B	124	GLU	2.4
1	B	60	LYS	2.4
1	B	306	THR	2.4
1	A	32	GLU	2.3
1	B	42	GLU	2.3
1	A	341	LEU	2.3
1	A	148	THR	2.3
1	B	180	GLU	2.3
1	B	43	CYS	2.3
1	B	176	SER	2.2
1	A	361	ASN	2.2
1	B	29	ASN	2.2
1	B	87	CYS	2.2
1	B	33	ARG	2.2
1	B	64	LYS	2.2
1	A	29	ASN	2.2
1	B	177	ASP	2.2
1	A	125	TYR	2.2
1	B	195	ILE	2.1
1	B	36	SER	2.1
1	A	82	TYR	2.1
1	B	183	GLN	2.1
1	A	187	ASP	2.1
1	B	127	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	49	GLU	2.1
1	A	95	MET	2.1
1	A	149	ASP	2.1
1	B	45	PRO	2.1
1	A	155	SER	2.1
1	A	46	VAL	2.0
1	B	151	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

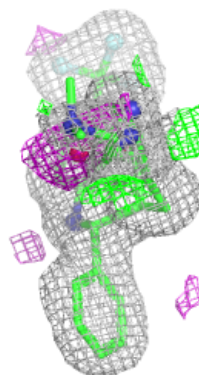
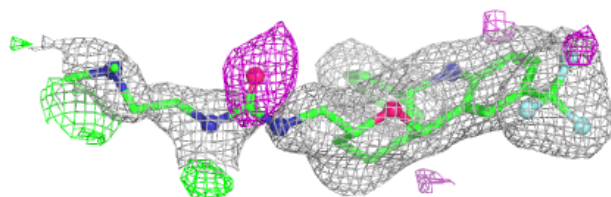
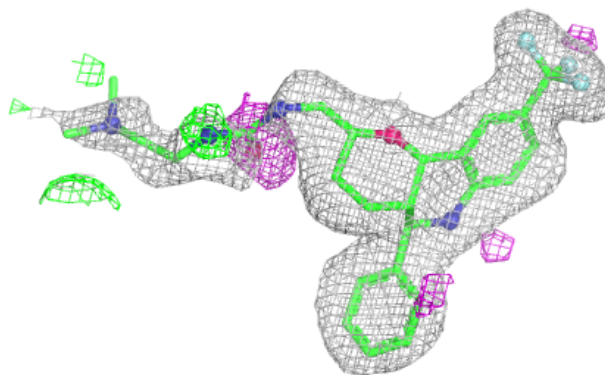
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EMQ	B	602	34/34	0.89	0.13	28,35,65,67	0
3	EMQ	A	601	34/34	0.93	0.11	25,32,58,59	0
2	ADP	A	501	27/27	0.97	0.07	21,27,30,32	0
2	ADP	B	502	27/27	0.97	0.08	25,37,47,48	0

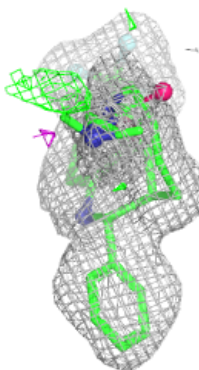
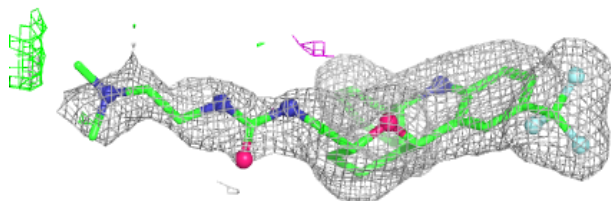
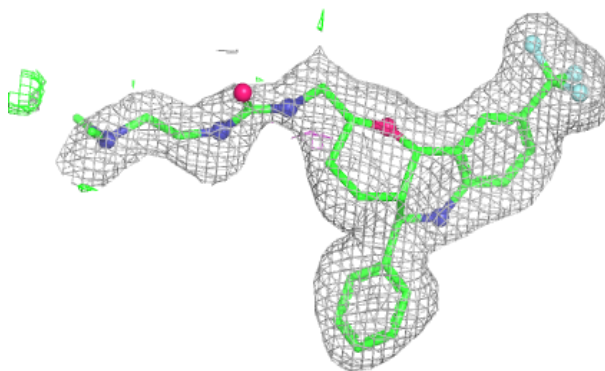
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EMQ B 602:

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

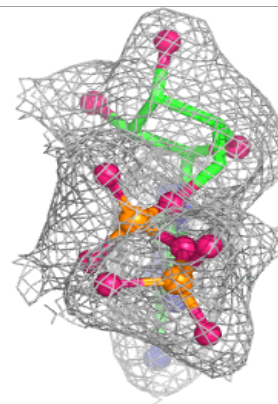
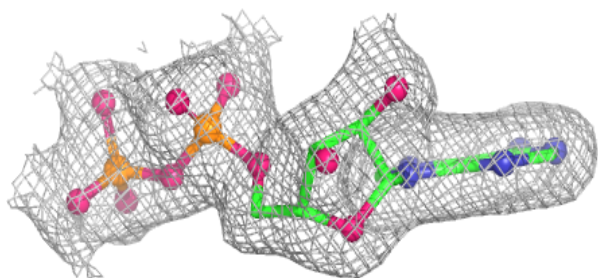
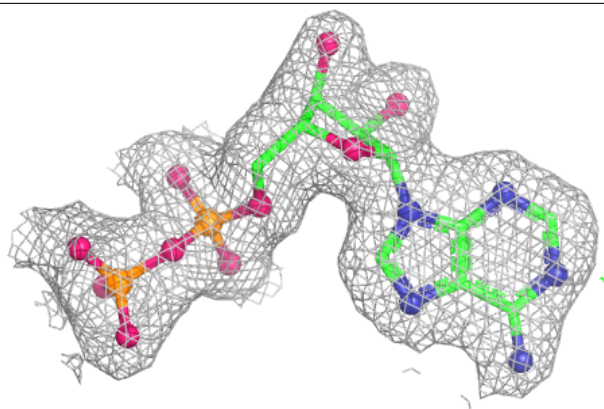
**Electron density around EMQ A 601:**

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

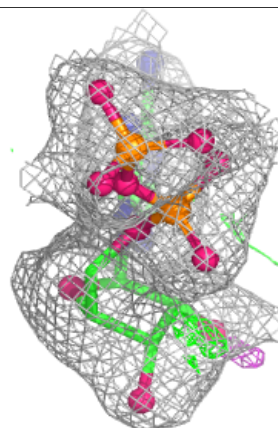
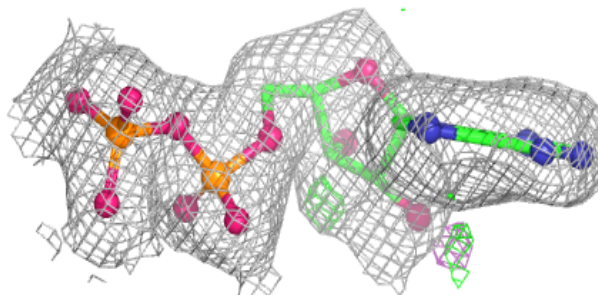
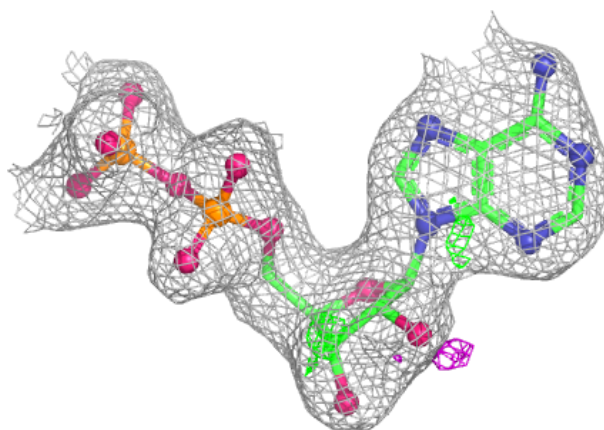


Electron density around ADP A 501:

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

**Electron density around ADP B 502:**

$2mF_o-DF_c$ (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.