



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 11:03 AM UTC

PDB ID : 2WOG / pdb_00002wog
Title : Intermediate and final states of human kinesin Eg5 in complex with S-trityl-L-cysteine
Authors : Kaan, H.Y.K.; Ulaganathan, V.; Hackney, D.D.; Kozielski, F.
Deposited on : 2009-07-23
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

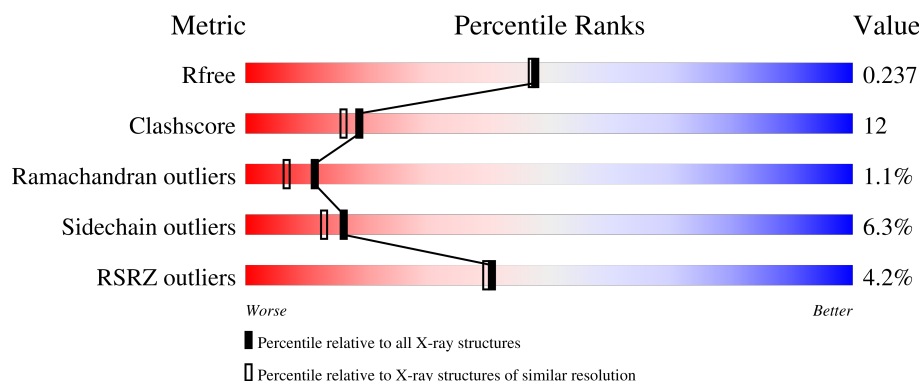
1 Overall quality at a glance

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	4% 76% 13% • 10%
1	B	368	4% 71% 14% • • 11%
1	C	368	4% 67% 19% • 10%

2 Entry composition [i](#)

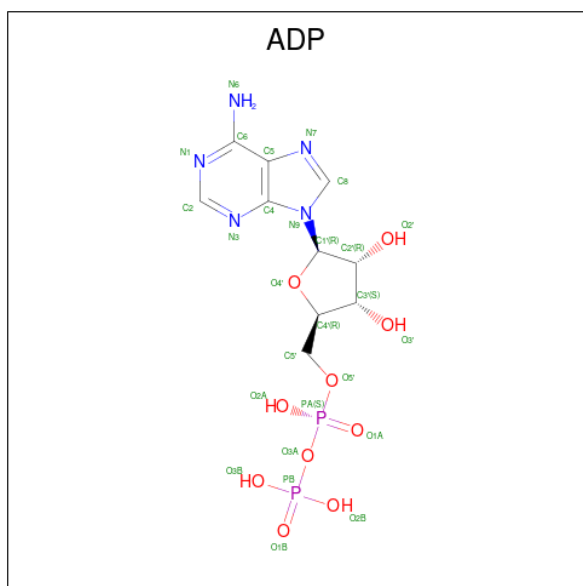
There are 5 unique types of molecules in this entry. The entry contains 9044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	333	Total	C	N	O	S	0	15	0
			2701	1697	468	524	12			
1	B	328	Total	C	N	O	S	0	23	0
			2706	1712	465	518	11			
1	C	330	Total	C	N	O	S	0	9	0
			2637	1656	457	514	10			

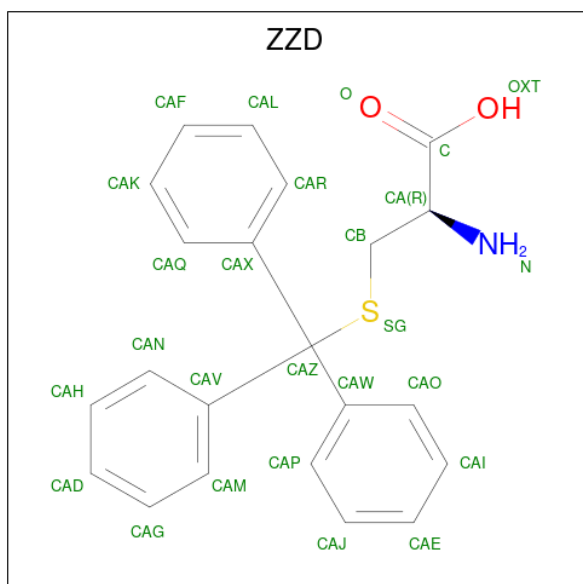
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is S-TRITYL-L-CYSTEINE (CCD ID: ZSD) (formula: C₂₂H₂₁NO₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 26 22 1 2 1	0	0
4	B	1	Total C N O S 26 22 1 2 1	0	0
4	C	1	Total C N O S 26 22 1 2 1	0	0

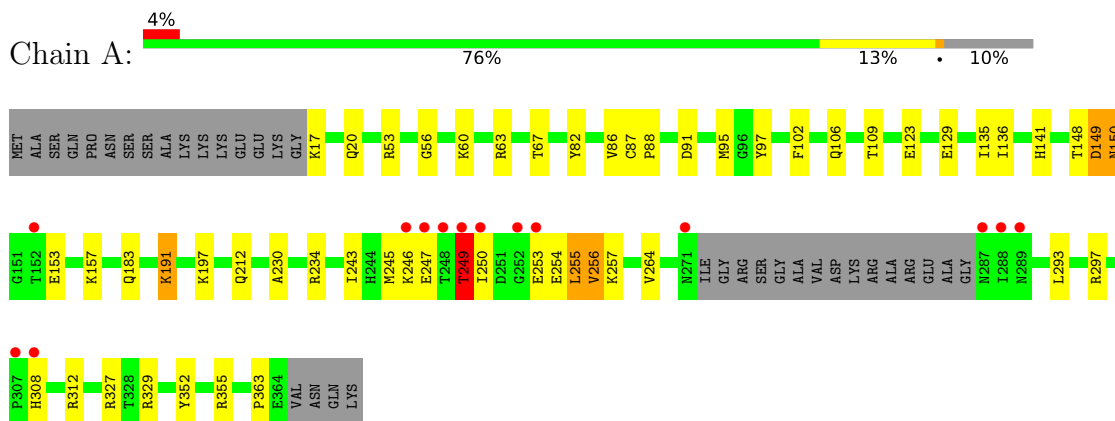
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	309	Total O 309 309	0	0
5	B	318	Total O 318 318	0	0
5	C	211	Total O 211 211	0	0

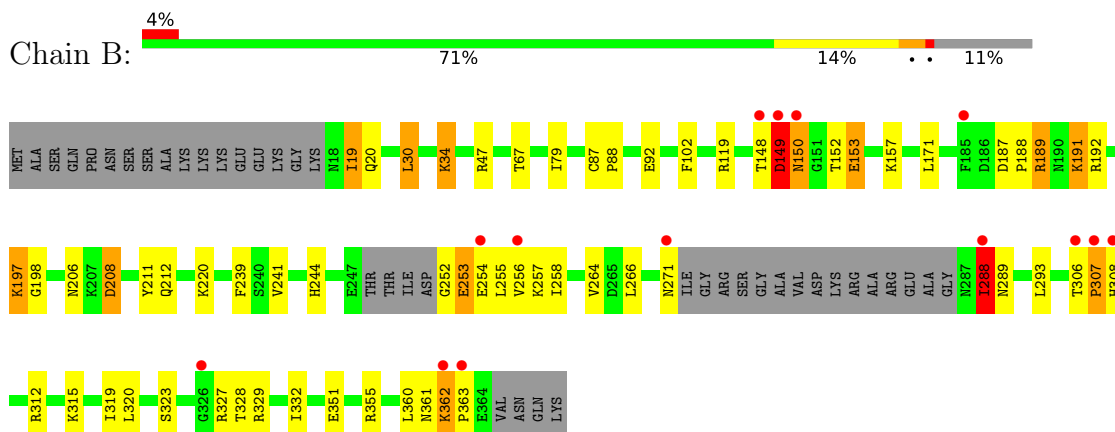
3 Residue-property plots [i](#)

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.

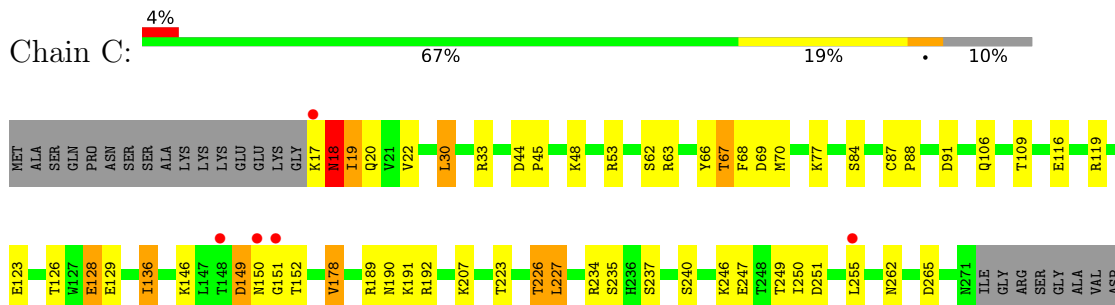
• Molecule 1: KINESIN-LIKE PROTEIN KIF11



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.50Å 96.50Å 124.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.16 – 2.00 29.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.16-2.00) 99.8 (29.16-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.155 , 0.218 (Not available) , 0.237	Depositor DCC
R_{free} test set	4351 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.029 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9044	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: ZZD, MG, ADP

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	0.72	0/2786	0.93	4/3763 (0.1%)
1	B	0.72	0/2815	0.99	7/3800 (0.2%)
1	C	0.71	0/2703	0.99	9/3652 (0.2%)
All	All	0.71	0/8304	0.97	20/11215 (0.2%)

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	B	1	0

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	VAL	N-CA-C	-10.54	93.31	108.48
1	B	257[A]	LYS	N-CA-C	-9.62	93.72	109.40
1	B	257[B]	LYS	N-CA-C	-9.62	93.72	109.40
1	B	257[A]	LYS	N-CA-CB	-7.62	97.56	110.83
1	B	257[B]	LYS	N-CA-CB	-7.62	97.56	110.83
1	C	178	VAL	CB-CA-C	-7.34	97.77	111.79
1	B	256	VAL	CB-CA-C	-7.18	99.92	110.62
1	A	136	ILE	CA-C-N	-6.94	111.84	119.19
1	A	136	ILE	C-N-CA	-6.94	111.84	119.19
1	C	62	SER	N-CA-C	6.66	120.15	110.42
1	C	337	SER	N-CA-C	-6.50	101.10	110.40
1	C	149	ASP	N-CA-C	6.30	124.21	110.80
1	C	306	THR	N-CA-C	6.29	116.84	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ILE	CA-C-N	-6.17	112.65	119.19
1	C	136	ILE	C-N-CA	-6.17	112.65	119.19
1	A	191	LYS	N-CA-C	5.53	122.57	110.80
1	C	44	ASP	CA-C-N	5.16	125.20	119.32
1	C	44	ASP	C-N-CA	5.16	125.20	119.32
1	A	123	GLU	N-CA-C	5.10	120.65	113.56
1	B	288	ILE	CB-CA-C	-5.01	103.07	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	150[B]	ASN	CA

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	2701	0	2765	53	0
1	B	2706	0	2796	78	0
1	C	2637	0	2688	68	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	26	0	20	1	0
4	B	26	0	20	0	0
4	C	26	0	20	0	0
5	A	309	0	0	18	0
5	B	318	0	0	17	0
5	C	211	0	0	10	0
All	All	9044	0	8345	197	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 12.

All (197) 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:220[A]:LYS:CE	5:B:2160:HOH:O	1.73	1.32
1:B:102[B]:PHE:CZ	1:B:320[B]:LEU:HD12	1.64	1.31
1:B:327:ARG:O	1:B:363:PRO:HA	1.50	1.12
1:C:30:LEU:HD23	1:C:33:ARG:HH21	1.06	1.12
1:B:208:ASP:HB3	5:B:2200:HOH:O	1.54	1.05
1:A:246:LYS:HA	5:A:2227:HOH:O	1.58	1.04
1:C:30:LEU:CD2	1:C:33:ARG:HH21	1.71	1.03
1:B:92:GLU:HG2	5:B:2095:HOH:O	1.60	1.02
1:B:102[B]:PHE:CZ	1:B:320[B]:LEU:CD1	2.45	1.00
1:B:197[A]:LYS:HD3	1:B:198:GLY:N	1.77	0.99
1:B:92:GLU:OE2	1:B:329:ARG:HD2	1.63	0.99
1:C:48[B]:LYS:HE2	1:C:68:PHE:O	1.62	0.99
1:C:17:LYS:O	1:C:19:ILE:HG22	1.64	0.98
1:B:102[B]:PHE:HZ	1:B:320[B]:LEU:HD12	1.21	0.98
1:B:312:ARG:HG2	5:B:2267:HOH:O	1.61	0.97
1:B:220[A]:LYS:HE2	5:B:2160:HOH:O	1.41	0.97
1:C:30:LEU:HD23	1:C:33:ARG:NH2	1.83	0.94
1:C:249[B]:THR:HG22	1:C:251[B]:ASP:H	1.33	0.93
1:B:254[B]:GLU:HA	1:B:254[B]:GLU:OE1	1.68	0.92
1:A:88:PRO:HG3	1:C:249[B]:THR:HG21	1.52	0.92
1:C:66:TYR:OH	1:C:351:GLU:OE1	1.89	0.90
1:A:88:PRO:HG3	1:C:249[B]:THR:CG2	2.01	0.89
1:C:289:ASN:O	1:C:293:LEU:HD13	1.69	0.89
1:B:220[A]:LYS:HE3	5:B:2160:HOH:O	1.48	0.89
1:B:206[B]:ASN:HD21	1:B:208:ASP:CG	1.79	0.89
1:C:17:LYS:HE2	5:C:2178:HOH:O	1.72	0.88
1:C:123[B]:GLU:HA	1:C:123[B]:GLU:OE2	1.73	0.87
1:B:191:LYS:HE3	1:B:191:LYS:H	1.40	0.86
1:B:319:ILE:HG22	1:B:320[B]:LEU:CD2	2.06	0.85
1:B:191:LYS:H	1:B:191:LYS:CE	1.93	0.82
1:C:123[B]:GLU:OE2	1:C:123[B]:GLU:CA	2.27	0.82
1:B:47[B]:ARG:NH1	5:B:2042:HOH:O	2.11	0.81
1:A:247:GLU:HG2	5:A:2226:HOH:O	1.81	0.80
1:B:361:ASN:CG	5:B:2271:HOH:O	2.24	0.80
1:B:319:ILE:HG22	1:B:320[B]:LEU:HD22	1.63	0.80
1:C:251[B]:ASP:OD1	5:C:2161:HOH:O	1.99	0.80
1:B:47[B]:ARG:NE	5:B:2041:HOH:O	2.14	0.80
1:B:92:GLU:OE2	1:B:329:ARG:CD	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:SER:O	1:C:328:THR:HG21	1.85	0.77
1:C:192[B]:ARG:NH2	1:C:324:LEU:O	2.17	0.76
1:C:362:LYS:HB2	1:C:363:PRO:HD2	1.66	0.76
1:C:226:THR:HG22	1:C:227:LEU:HD13	1.70	0.73
1:C:22:VAL:HG11	1:C:70:MET:HE3	1.70	0.73
1:B:361:ASN:HB3	5:B:2271:HOH:O	1.90	0.72
1:A:308:HIS:HB2	5:A:2253:HOH:O	1.90	0.72
1:A:247:GLU:CG	5:A:2226:HOH:O	2.39	0.70
1:B:206[B]:ASN:OD1	1:B:208:ASP:OD1	2.11	0.69
1:C:149:ASP:O	1:C:150:ASN:C	2.37	0.67
1:C:17:LYS:O	1:C:18:ASN:ND2	2.27	0.67
1:B:362:LYS:HD2	1:B:362:LYS:N	2.10	0.66
1:C:329:ARG:NH2	5:C:2181:HOH:O	2.28	0.65
1:B:244:HIS:CD2	1:B:258:ILE:HG12	2.32	0.65
1:B:220[B]:LYS:HE2	5:B:2160:HOH:O	1.96	0.65
1:A:355:ARG:NH2	5:A:2291:HOH:O	2.28	0.65
1:C:17:LYS:C	1:C:19:ILE:H	2.05	0.65
1:C:48[B]:LYS:CE	1:C:68:PHE:O	2.42	0.65
1:C:304:GLU:O	1:C:306:THR:N	2.30	0.64
1:B:197[A]:LYS:HD3	1:B:198:GLY:H	1.62	0.64
1:A:141:HIS:ND1	5:A:2129:HOH:O	2.30	0.64
1:A:256:VAL:HA	5:A:2227:HOH:O	1.98	0.64
1:B:67[A]:THR:HG22	5:B:2296:HOH:O	1.97	0.63
1:C:289:ASN:O	1:C:293:LEU:CD1	2.44	0.63
1:A:86:VAL:HG21	1:A:135:ILE:HG12	1.81	0.62
1:C:306:THR:HG23	1:C:307:PRO:HD2	1.82	0.61
1:B:254[B]:GLU:OE1	1:B:254[B]:GLU:CA	2.44	0.61
1:C:249[B]:THR:HG22	1:C:250:ILE:N	2.17	0.60
1:C:312:ARG:HH11	1:C:312:ARG:HB3	1.66	0.60
1:B:102[B]:PHE:CE1	1:B:320[B]:LEU:CD1	2.84	0.60
1:C:235:SER:O	5:C:2152:HOH:O	2.16	0.60
1:B:239:PHE:HE1	1:B:241[A]:VAL:CG2	2.15	0.59
1:A:88:PRO:HG3	1:C:249[B]:THR:HG23	1.82	0.59
1:A:352:TYR:O	1:A:355:ARG:HG2	2.02	0.59
1:B:327:ARG:HA	1:B:362:LYS:O	2.02	0.59
1:A:95[A]:MET:HA	1:A:95[A]:MET:HE2	1.84	0.59
1:B:206[B]:ASN:ND2	1:B:208:ASP:CG	2.59	0.59
1:B:252:GLY:O	1:B:253:GLU:HG3	2.04	0.58
1:C:249[B]:THR:CG2	1:C:250:ILE:N	2.66	0.58
1:B:323:SER:HA	1:B:328:THR:HB	1.86	0.58
1:B:361:ASN:CB	5:B:2271:HOH:O	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47[B]:ARG:NH1	5:B:2038:HOH:O	2.36	0.57
1:B:206[B]:ASN:ND2	1:B:208:ASP:OD2	2.36	0.57
1:B:288:ILE:O	1:B:289:ASN:ND2	2.35	0.57
1:B:149:ASP:N	1:B:149:ASP:OD1	2.34	0.56
1:A:183[A]:GLN:HG3	5:A:2159:HOH:O	2.05	0.56
1:A:293:LEU:HD21	1:A:297[A]:ARG:NH2	2.21	0.56
1:C:106:GLN:HG2	1:C:109:THR:HG23	1.87	0.55
1:A:87[B]:CYS:HB3	1:A:88:PRO:HD3	1.89	0.54
1:C:223:THR:O	1:C:226:THR:HB	2.07	0.54
1:A:148:THR:CG2	1:A:149:ASP:N	2.71	0.53
1:A:246:LYS:HZ2	1:A:254[B]:GLU:CD	2.16	0.53
1:B:361:ASN:HB2	5:B:2303:HOH:O	2.08	0.53
1:A:148:THR:O	1:A:150[B]:ASN:ND2	2.41	0.53
1:C:234:ARG:NH1	5:C:2150:HOH:O	2.34	0.53
1:C:240:SER:OG	1:C:262:ASN:ND2	2.41	0.53
1:A:312:ARG:HG3	5:A:2114:HOH:O	2.07	0.53
1:C:17:LYS:C	1:C:19:ILE:N	2.67	0.53
1:B:87[A]:CYS:HB2	1:B:88:PRO:HD3	1.90	0.53
1:A:148:THR:O	1:A:149:ASP:C	2.51	0.52
1:B:252:GLY:O	1:B:253:GLU:CB	2.57	0.52
1:B:239:PHE:HE1	1:B:241[A]:VAL:HG22	1.75	0.52
1:B:191:LYS:CD	1:B:191:LYS:N	2.72	0.52
1:C:67:THR:HG22	1:C:361:ASN:OD1	2.09	0.52
1:B:306:THR:HB	1:B:307:PRO:HD2	1.91	0.52
1:B:319:ILE:HG22	1:B:320[B]:LEU:HD23	1.89	0.52
1:C:67:THR:CG2	1:C:361:ASN:OD1	2.58	0.52
1:C:17:LYS:O	1:C:19:ILE:N	2.43	0.51
1:B:148:THR:O	1:B:149:ASP:O	2.26	0.51
1:B:351:GLU:O	1:B:355:ARG:HG3	2.10	0.51
1:B:87[B]:CYS:HB3	1:B:88:PRO:HD3	1.91	0.51
1:A:254[B]:GLU:OE2	1:A:256:VAL:HG23	2.09	0.51
1:A:257:LYS:NZ	5:A:2228:HOH:O	2.43	0.50
1:C:315:LYS:HE3	5:C:2096:HOH:O	2.10	0.50
1:A:246:LYS:NZ	1:A:254[B]:GLU:CD	2.69	0.50
1:B:197[A]:LYS:CD	1:B:198:GLY:N	2.64	0.50
1:C:67:THR:HG21	1:C:361:ASN:HA	1.92	0.50
1:A:67[B]:THR:HG23	5:A:2288:HOH:O	2.10	0.50
1:A:56:GLY:O	1:A:60:LYS:HE3	2.12	0.50
1:B:30:LEU:O	1:B:34:LYS:HE2	2.12	0.50
1:B:191:LYS:H	1:B:191:LYS:CD	2.25	0.50
1:C:48[A]:LYS:HD3	1:C:69:ASP:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:SER:HB3	1:C:265:ASP:HB3	1.94	0.49
1:C:45:PRO:HB3	5:C:2045:HOH:O	2.11	0.49
1:C:303:VAL:C	1:C:305:ARG:H	2.21	0.49
1:A:148:THR:HG22	1:A:149:ASP:N	2.28	0.48
1:A:106:GLN:HG2	1:A:109:THR:HG23	1.96	0.48
1:B:191:LYS:N	1:B:191:LYS:HD3	2.29	0.48
1:B:252:GLY:O	1:B:253:GLU:CG	2.62	0.48
1:C:128:GLU:OE2	1:C:207:LYS:HE2	2.13	0.48
1:A:20:GLN:HE22	1:A:329:ARG:HH21	1.60	0.47
1:A:293:LEU:HD21	1:A:297[A]:ARG:CZ	2.45	0.47
1:B:102[A]:PHE:HB3	1:B:264:VAL:HB	1.96	0.47
1:B:288:ILE:C	1:B:289:ASN:HD22	2.22	0.47
1:B:119:ARG:HD2	1:B:211:TYR:HE2	1.81	0.46
1:A:249:THR:OG1	1:A:255:LEU:HD21	2.16	0.46
1:A:327:ARG:O	1:A:363:PRO:HA	2.16	0.46
1:B:152:THR:HG22	1:B:153:GLU:O	2.15	0.46
1:C:91:ASP:OD1	1:C:146:LYS:NZ	2.47	0.46
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.96	0.46
1:A:91:ASP:O	1:A:95[B]:MET:HG3	2.16	0.46
1:A:230:ALA:HB3	1:A:234:ARG:HD2	1.98	0.45
1:A:255:LEU:C	5:A:2227:HOH:O	2.59	0.45
1:A:257:LYS:HE2	5:A:2229:HOH:O	2.16	0.45
1:B:212[B]:GLN:HG3	5:B:2205:HOH:O	2.16	0.45
1:C:67:THR:HG21	5:C:2028:HOH:O	2.16	0.45
1:A:87[B]:CYS:HB3	1:A:88:PRO:CD	2.47	0.45
1:B:187:ASP:OD1	1:B:188:PRO:HD2	2.16	0.45
1:C:116:GLU:HG2	1:C:136:ILE:HD12	1.99	0.45
1:C:126:THR:OG1	1:C:129:GLU:HG2	2.17	0.45
1:C:149:ASP:O	1:C:151:GLY:N	2.49	0.45
1:A:88:PRO:CG	1:C:249[B]:THR:HG23	2.47	0.44
1:A:106:GLN:HG2	1:A:109:THR:CG2	2.47	0.44
1:B:119:ARG:HD2	1:B:211:TYR:CE2	2.52	0.44
1:B:148:THR:O	1:B:149:ASP:C	2.55	0.44
1:C:20:GLN:OE1	1:C:70:MET:HE2	2.18	0.44
1:C:309:VAL:CG1	1:C:311:TYR:CE2	3.01	0.44
1:B:191:LYS:CE	1:B:191:LYS:N	2.73	0.44
1:C:106:GLN:HG2	1:C:109:THR:CG2	2.48	0.44
1:A:82:TYR:CE1	1:A:87[A]:CYS:SG	3.10	0.44
1:C:309:VAL:HG12	1:C:311:TYR:CE2	2.53	0.44
4:A:1365:ZZD:CAO	4:A:1365:ZZD:HB1C	2.47	0.44
1:B:102[A]:PHE:CD1	1:B:266:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:HA	1:C:63:ARG:HD3	2.01	0.43
1:A:88:PRO:CG	1:C:249[B]:THR:CG2	2.86	0.43
1:B:315:LYS:HE3	5:B:2154:HOH:O	2.18	0.43
1:B:19[A]:ILE:HD12	1:B:20:GLN:O	2.19	0.43
1:A:102:PHE:HB3	1:A:264:VAL:HB	2.00	0.43
1:B:19[A]:ILE:CD1	1:B:332:ILE:HG13	2.49	0.43
1:B:189[B]:ARG:CG	1:B:189[B]:ARG:HH11	2.32	0.42
1:A:243:ILE:HG22	1:A:245:MET:HG3	2.00	0.42
1:A:53:ARG:HA	1:A:63:ARG:HD3	2.01	0.42
1:A:293:LEU:HD11	5:A:2252:HOH:O	2.20	0.42
1:A:293:LEU:O	1:A:297[A]:ARG:HG3	2.19	0.42
1:A:97:TYR:CZ	5:A:2296:HOH:O	2.67	0.42
1:B:288:ILE:C	1:B:289:ASN:ND2	2.78	0.42
1:A:95[A]:MET:HE3	5:A:2092:HOH:O	2.20	0.42
1:A:56:GLY:O	1:A:60:LYS:CE	2.68	0.42
1:A:148:THR:CG2	1:A:149:ASP:H	2.32	0.41
1:C:18:ASN:OD1	1:C:326:GLY:O	2.38	0.41
1:C:291:SER:HA	1:C:314:SER:HB2	2.01	0.41
1:B:252:GLY:O	1:B:253:GLU:HB2	2.20	0.41
1:B:362:LYS:N	1:B:362:LYS:CD	2.82	0.41
1:C:309:VAL:HA	1:C:310:PRO:HD3	1.47	0.41
1:C:322:ASP:HB3	5:C:2115:HOH:O	2.21	0.41
1:A:355:ARG:NH1	5:A:2292:HOH:O	2.42	0.41
1:B:271:ASN:C	1:B:271:ASN:HD22	2.29	0.41
1:C:309:VAL:HG11	1:C:311:TYR:CZ	2.56	0.41
1:C:22:VAL:CG1	1:C:70:MET:HB2	2.51	0.40
1:B:119:ARG:HD3	1:B:211:TYR:OH	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	344/368 (94%)	337 (98%)	4 (1%)	3 (1%)	14	9
1	B	344/368 (94%)	336 (98%)	2 (1%)	6 (2%)	7	3
1	C	335/368 (91%)	320 (96%)	12 (4%)	3 (1%)	14	9
All	All	1023/1104 (93%)	993 (97%)	18 (2%)	12 (1%)	11	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	B	149	ASP
1	B	253	GLU
1	C	18	ASN
1	C	305	ARG
1	A	191	LYS
1	B	150[A]	ASN
1	B	150[B]	ASN
1	B	288	ILE
1	C	190	ASN
1	B	307	PRO
1	A	249	THR

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	311/322 (97%)	296 (95%)	15 (5%)	23	21
1	B	314/322 (98%)	290 (92%)	24 (8%)	12	9
1	C	301/322 (94%)	277 (92%)	24 (8%)	11	8
All	All	926/966 (96%)	863 (93%)	63 (7%)	16	11

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS

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Mol	Chain	Res	Type
1	A	129	GLU
1	A	150[A]	ASN
1	A	150[B]	ASN
1	A	153	GLU
1	A	157[A]	LYS
1	A	157[C]	LYS
1	A	197[A]	LYS
1	A	197[B]	LYS
1	A	212	GLN
1	A	249	THR
1	A	250	ILE
1	A	253	GLU
1	A	255	LEU
1	A	256	VAL
1	B	19[A]	ILE
1	B	19[B]	ILE
1	B	30	LEU
1	B	34	LYS
1	B	79	ILE
1	B	149	ASP
1	B	150[A]	ASN
1	B	150[B]	ASN
1	B	153	GLU
1	B	157	LYS
1	B	171	LEU
1	B	189[A]	ARG
1	B	189[B]	ARG
1	B	191	LYS
1	B	192	ARG
1	B	197[A]	LYS
1	B	197[B]	LYS
1	B	208	ASP
1	B	255	LEU
1	B	288	ILE
1	B	293	LEU
1	B	308	HIS
1	B	360	LEU
1	B	362	LYS
1	C	18	ASN
1	C	19	ILE
1	C	30	LEU
1	C	67	THR

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Mol	Chain	Res	Type
1	C	77[A]	LYS
1	C	77[B]	LYS
1	C	84	SER
1	C	119	ARG
1	C	128	GLU
1	C	152	THR
1	C	178	VAL
1	C	189	ARG
1	C	191	LYS
1	C	226	THR
1	C	227	LEU
1	C	246	LYS
1	C	247	GLU
1	C	255	LEU
1	C	289	ASN
1	C	312	ARG
1	C	322	ASP
1	C	337	SER
1	C	341	LEU
1	C	357	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	20	GLN
1	A	98	ASN
1	A	165	ASN
1	A	190	ASN
1	A	205	HIS
1	A	262	ASN
1	A	321	GLN
1	B	122	ASN
1	B	183	GLN
1	B	205	HIS
1	B	262	ASN
1	B	271	ASN
1	B	287	ASN
1	B	289	ASN
1	B	321	GLN
1	C	122	ASN
1	C	165	ASN
1	C	183	GLN

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Mol	Chain	Res	Type
1	C	244	HIS
1	C	262	ASN
1	C	271	ASN
1	C	289	ASN
1	C	321	GLN
1	C	354	HIS

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 9 ligands modelled in this entry, 3 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
2	ADP	C	600	3	28,29,29	1.36	4 (14%)	43,45,45	1.92	10 (23%)
4	ZZD	C	1364	-	27,28,28	0.79	0	33,38,38	0.88	1 (3%)
2	ADP	B	600	3	28,29,29	1.49	5 (17%)	43,45,45	1.87	9 (20%)
4	ZZD	B	1365	-	27,28,28	0.79	0	33,38,38	0.83	0
4	ZZD	A	1365	-	27,28,28	0.79	0	33,38,38	0.87	1 (3%)
2	ADP	A	600	3	28,29,29	1.33	3 (10%)	43,45,45	1.74	10 (23%)

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	C	600	3	-	0/16/32/32	0/3/3/3
4	ZZD	C	1364	-	-	1/28/28/28	0/3/3/3
2	ADP	B	600	3	-	0/16/32/32	0/3/3/3
4	ZZD	B	1365	-	-	1/28/28/28	0/3/3/3
4	ZZD	A	1365	-	-	1/28/28/28	0/3/3/3
2	ADP	A	600	3	-	1/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ADP	C5-C4	4.84	1.47	1.39
2	C	600	ADP	C5-C4	4.68	1.47	1.39
2	A	600	ADP	C5-C4	3.83	1.45	1.39
2	B	600	ADP	C5-N7	-2.77	1.34	1.39
2	C	600	ADP	C5-C6	2.71	1.48	1.41
2	A	600	ADP	PA-O3A	2.71	1.62	1.59
2	B	600	ADP	C5-C6	2.67	1.48	1.41
2	A	600	ADP	C5-C6	2.56	1.48	1.41
2	C	600	ADP	C8-N7	2.23	1.36	1.31
2	B	600	ADP	C4-N9	-2.18	1.33	1.37
2	C	600	ADP	C5-N7	-2.08	1.35	1.39
2	B	600	ADP	C8-N9	-2.04	1.34	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ADP	C5-C4-N3	-5.66	118.92	126.72
2	B	600	ADP	N3-C4-N9	5.18	135.98	127.17
2	A	600	ADP	C5-C4-N3	-4.88	120.00	126.72
2	C	600	ADP	C5-C4-N3	-4.70	120.25	126.72
2	A	600	ADP	N3-C4-N9	4.41	134.67	127.17
2	C	600	ADP	N3-C4-N9	4.37	134.60	127.17
2	C	600	ADP	C4-N9-C8	4.29	110.24	105.74
2	C	600	ADP	N3-C2-N1	-4.28	122.11	128.58
2	B	600	ADP	C4-N9-C8	3.66	109.58	105.74
2	A	600	ADP	C4-N9-C8	3.51	109.42	105.74
2	C	600	ADP	C2-N3-C4	3.48	120.33	111.83
2	C	600	ADP	C4-C5-N7	-3.38	106.72	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ADP	N3-C2-N1	-3.35	123.51	128.58
2	A	600	ADP	C2-N3-C4	3.30	119.89	111.83
2	C	600	ADP	C2-N1-C6	3.25	124.08	118.73
2	B	600	ADP	C4-C5-N7	-3.20	106.92	110.58
2	B	600	ADP	C2-N3-C4	3.18	119.59	111.83
2	C	600	ADP	N9-C8-N7	-2.99	109.70	113.94
2	C	600	ADP	C5-N7-C8	2.98	108.14	103.45
2	A	600	ADP	C4-C5-N7	-2.64	107.56	110.58
2	B	600	ADP	C5-N7-C8	2.64	107.60	103.45
2	B	600	ADP	N3-C2-N1	-2.63	124.60	128.58
2	C	600	ADP	C6-C5-N7	2.58	137.07	132.09
2	B	600	ADP	N9-C8-N7	-2.37	110.58	113.94
4	C	1364	ZZD	CAW-CAZ-CAV	-2.28	104.72	111.04
4	A	1365	ZZD	CAW-CAZ-CAV	-2.24	104.84	111.04
2	A	600	ADP	N9-C8-N7	-2.20	110.81	113.94
2	A	600	ADP	C6-C5-N7	2.19	136.31	132.09
2	A	600	ADP	C5-N7-C8	2.18	106.88	103.45
2	B	600	ADP	N6-C6-N1	2.09	123.02	118.38
2	A	600	ADP	O3B-PB-O2B	2.04	115.47	107.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1365	ZZD	CAR-CAX-CAZ-SG
2	A	600	ADP	PA-O3A-PB-O2B
4	A	1365	ZZD	CAR-CAX-CAZ-SG
4	C	1364	ZZD	CAR-CAX-CAZ-SG

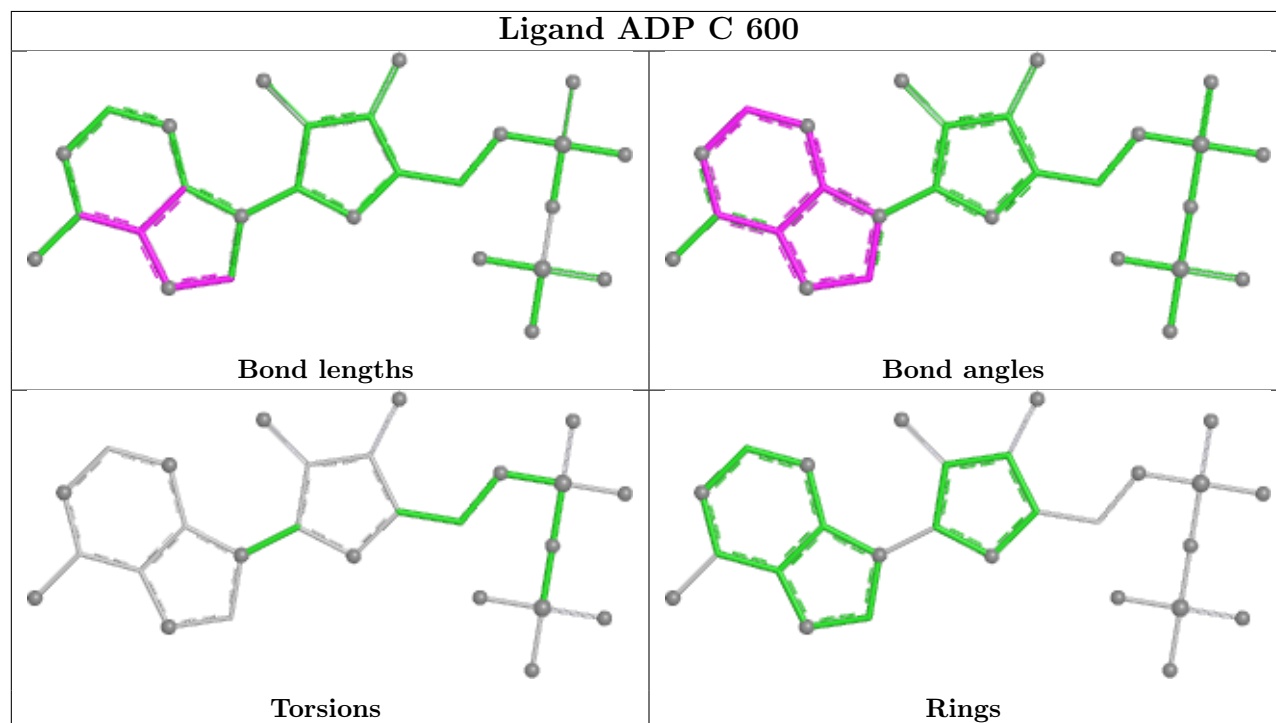
There are no ring outliers.

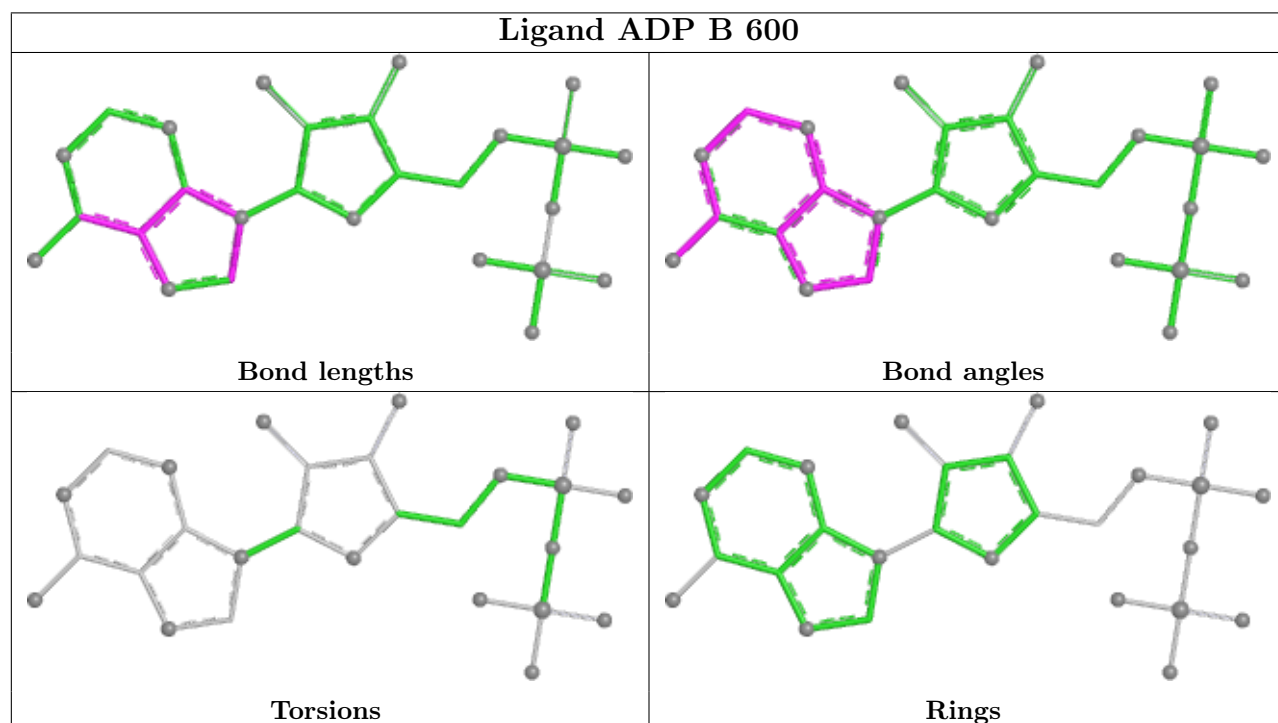
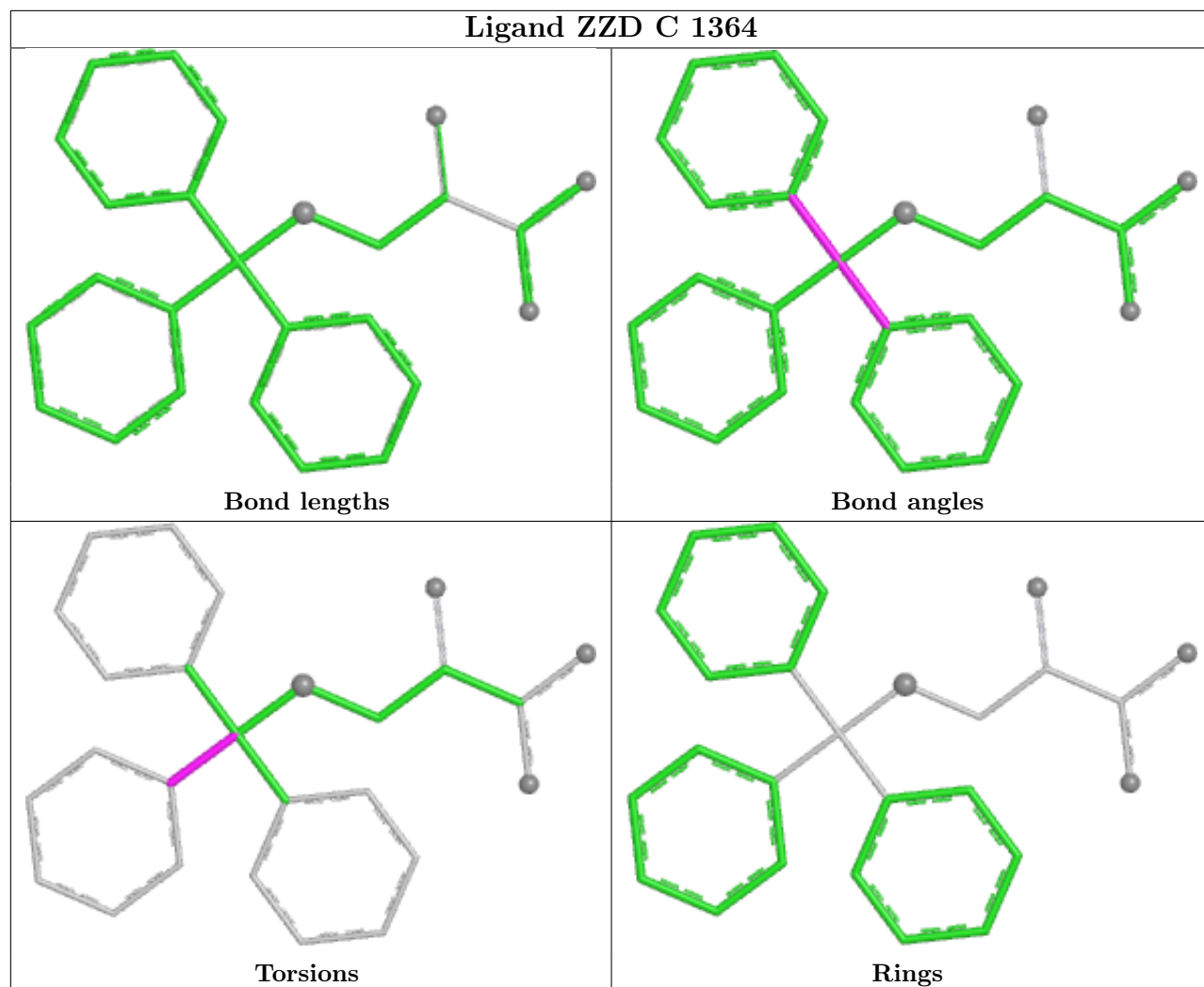
1 monomer is involved in 1 short contact:

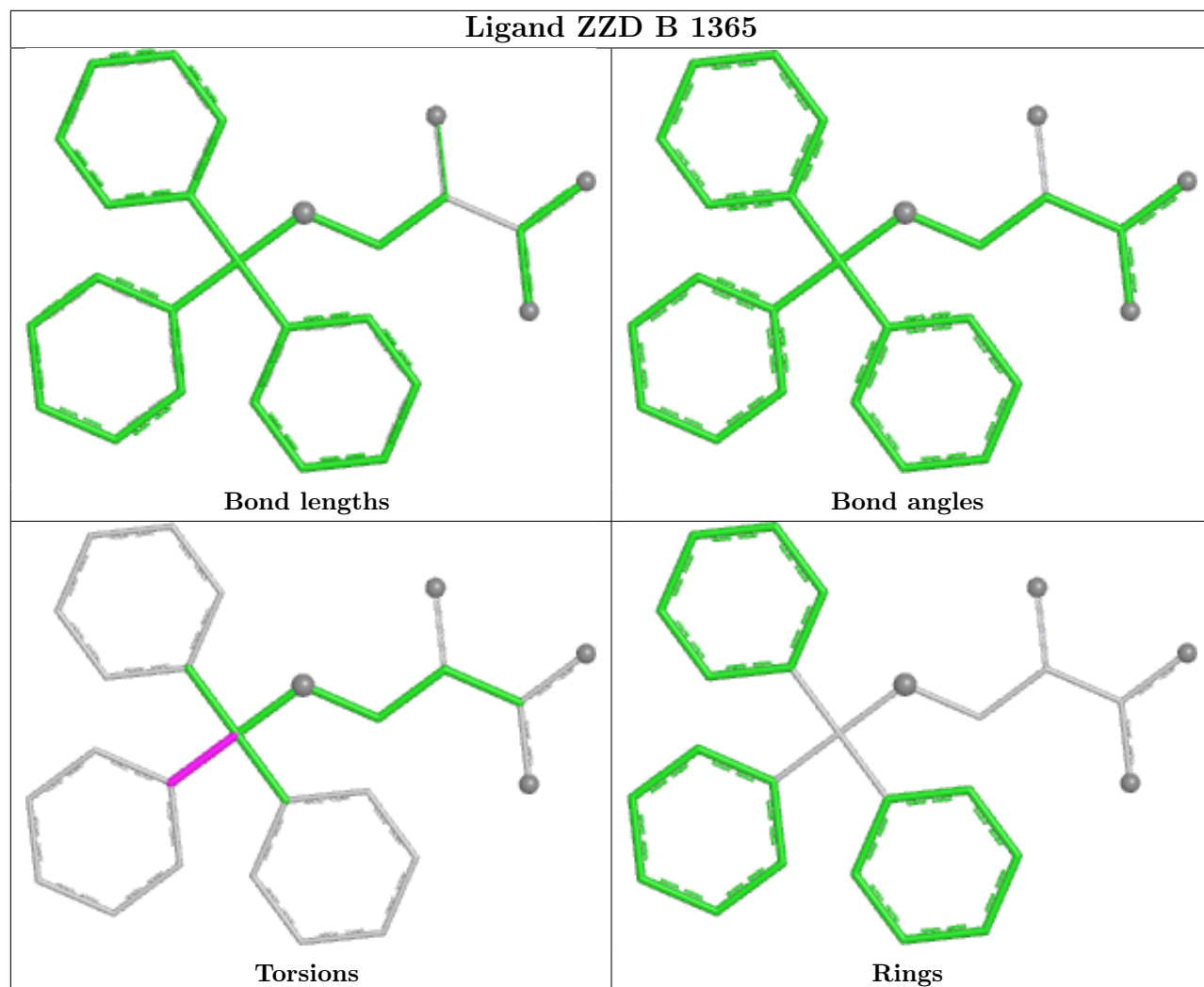
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1365	ZZD	1	0

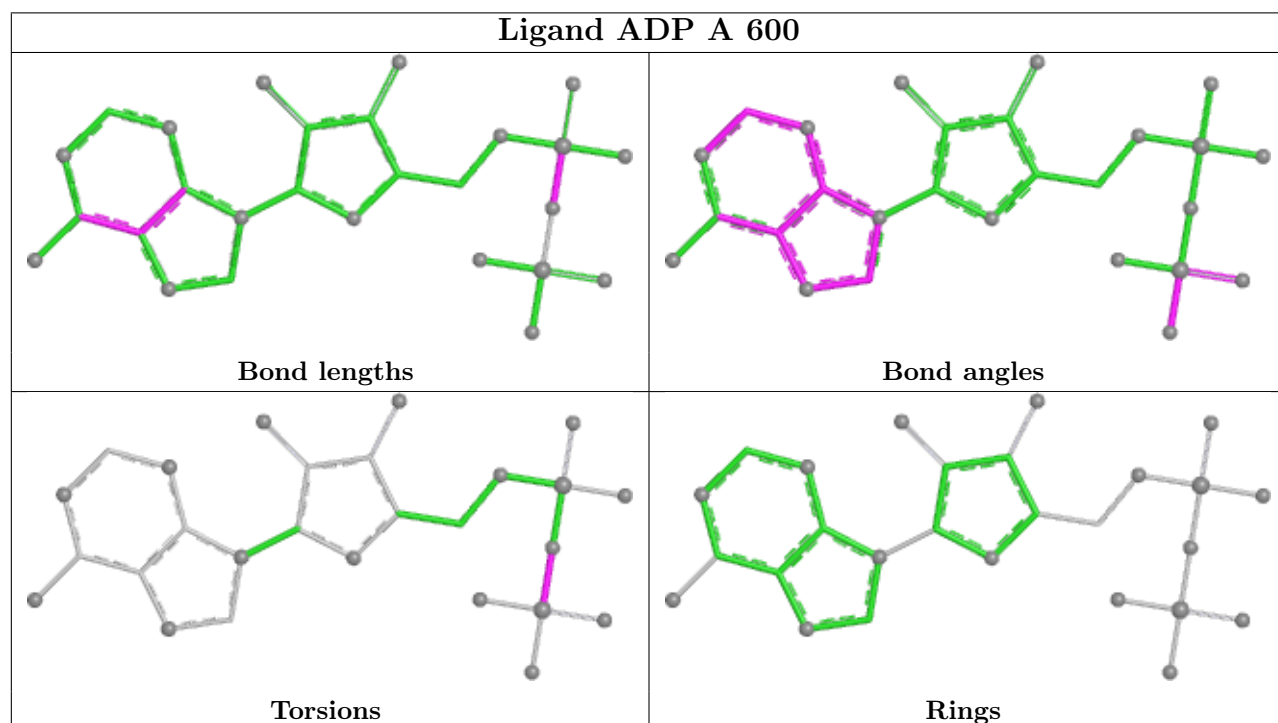
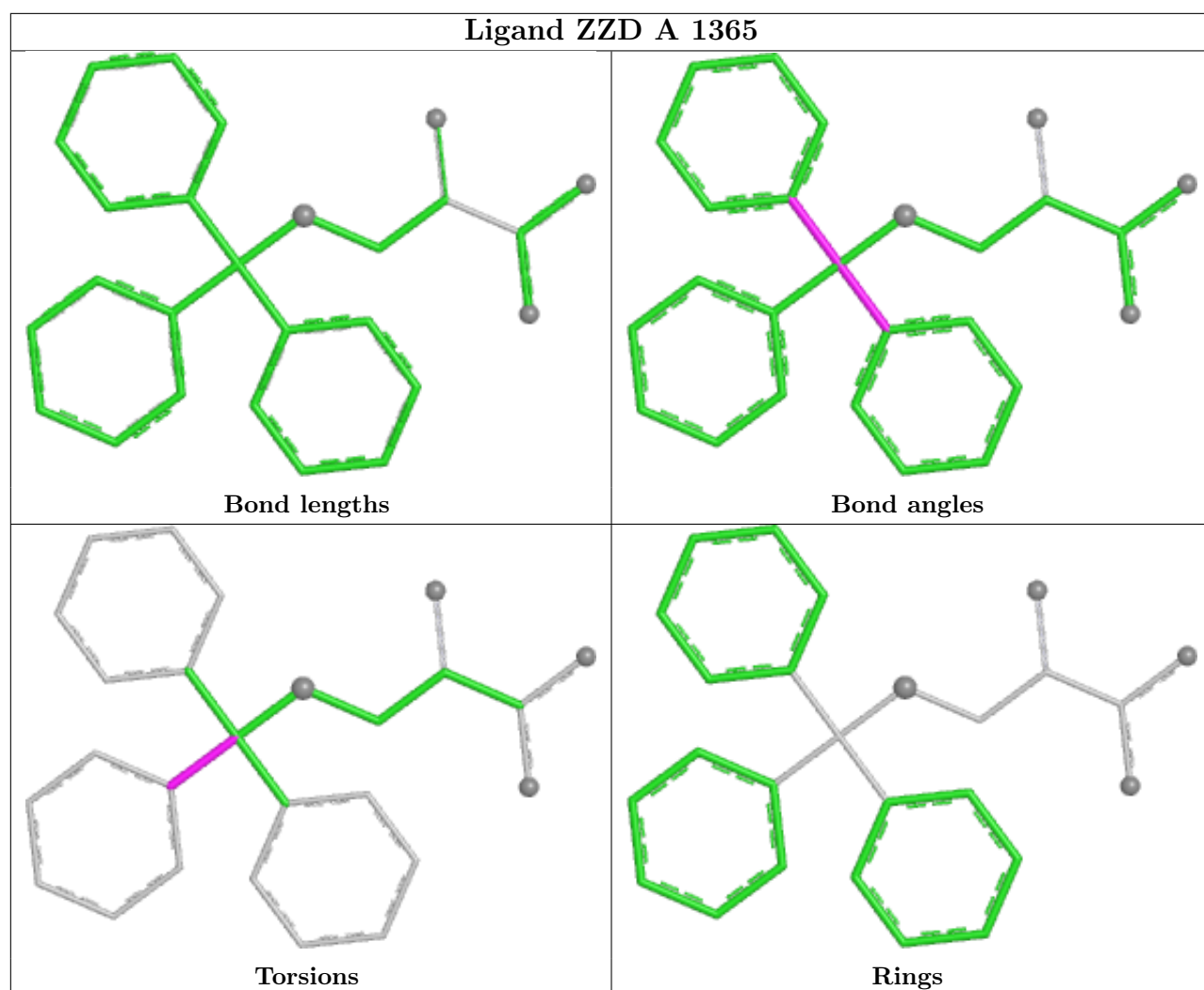
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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 ⓘ

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	333/368 (90%)	-0.31	14 (4%)	40	39	11, 27, 61, 91	15 (4%)
1	B	328/368 (89%)	-0.29	14 (4%)	40	39	13, 27, 61, 82	23 (7%)
1	C	330/368 (89%)	0.09	14 (4%)	40	39	19, 37, 65, 79	9 (2%)
All	All	991/1104 (89%)	-0.17	42 (4%)	40	39	11, 31, 63, 91	47 (4%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	ASP	9.4
1	B	363	PRO	6.4
1	A	250	ILE	5.9
1	C	255	LEU	4.4
1	C	305	ARG	4.2
1	A	288	ILE	4.1
1	A	289	ASN	3.9
1	B	288	ILE	3.9
1	B	362	LYS	3.5
1	C	17	LYS	3.5
1	A	252	GLY	3.4
1	A	248	THR	3.4
1	A	287	ASN	3.3
1	A	249	THR	3.3
1	C	293	LEU	3.2
1	B	148	THR	3.1
1	C	363	PRO	3.1
1	B	254[A]	GLU	3.0
1	C	303	VAL	2.9
1	A	247	GLU	2.8
1	B	307	PRO	2.8
1	B	150[A]	ASN	2.8
1	C	307	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	327	ARG	2.6
1	B	308	HIS	2.6
1	B	271	ASN	2.6
1	C	148	THR	2.5
1	B	326	GLY	2.5
1	A	308	HIS	2.5
1	C	304	GLU	2.4
1	C	308	HIS	2.4
1	A	271	ASN	2.3
1	A	307	PRO	2.2
1	A	246	LYS	2.2
1	C	306	THR	2.2
1	B	185[A]	PHE	2.1
1	C	150	ASN	2.1
1	B	306	THR	2.1
1	C	151	GLY	2.1
1	B	256	VAL	2.1
1	A	152	THR	2.0
1	A	253	GLU	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($\text{\AA}^2$)	Q<0.9
4	ZZD	C	1364	26/26	0.88	0.10	29,43,53,57	0
4	ZZD	B	1365	26/26	0.92	0.07	20,31,44,48	0
4	ZZD	A	1365	26/26	0.92	0.07	27,35,46,48	0
3	MG	A	601	1/1	0.93	0.04	21,21,21,21	0

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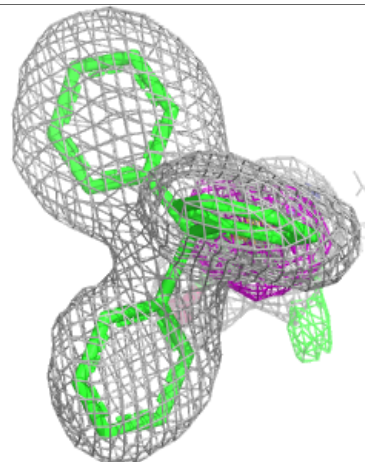
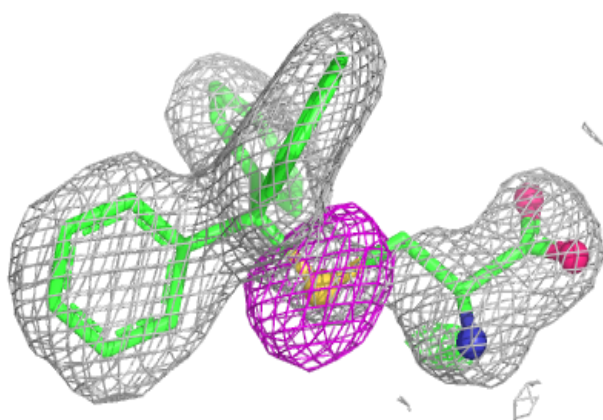
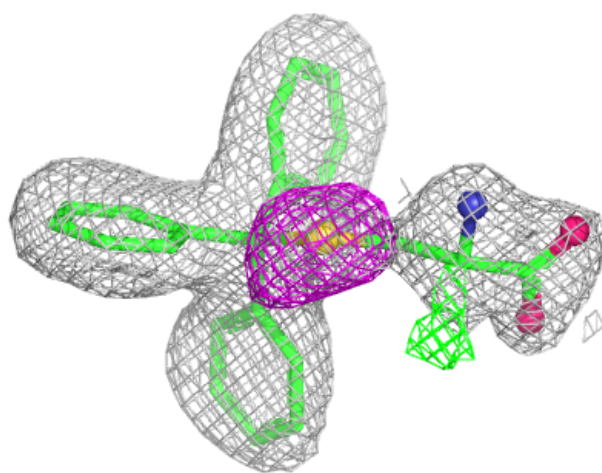
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	B	600	27/27	0.99	0.03	16,23,27,31	0
2	ADP	C	600	27/27	0.99	0.04	24,32,36,37	0
2	ADP	A	600	27/27	0.99	0.04	15,24,28,34	0
3	MG	C	601	1/1	1.00	0.02	31,31,31,31	0
3	MG	B	601	1/1	1.00	0.01	20,20,20,20	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.

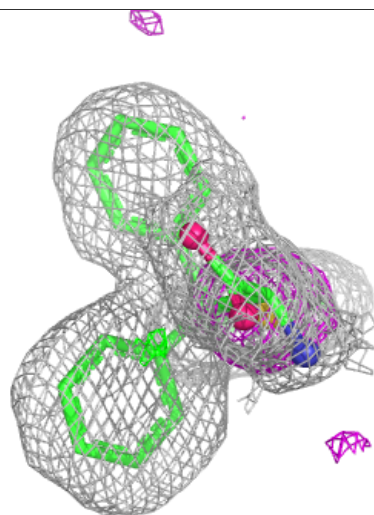
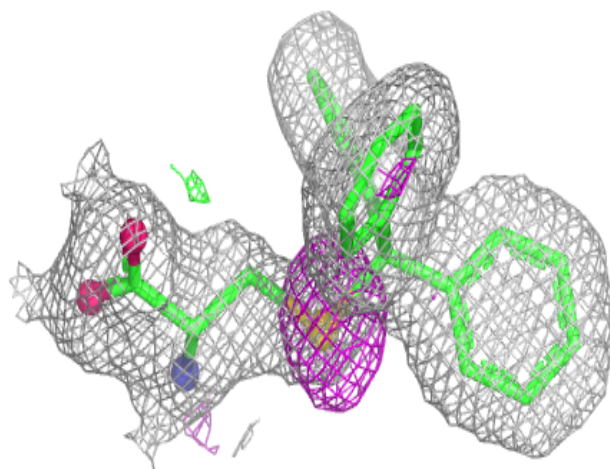
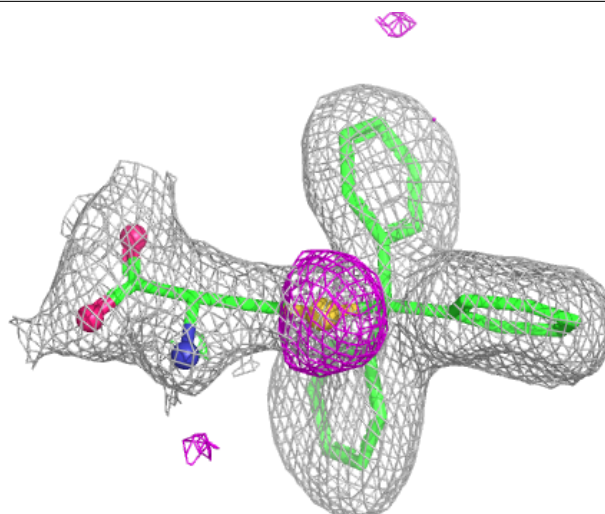
Electron density around ZSD C 1364:

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



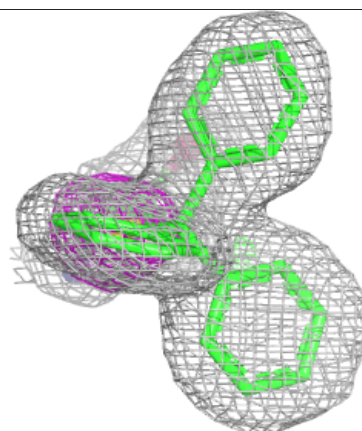
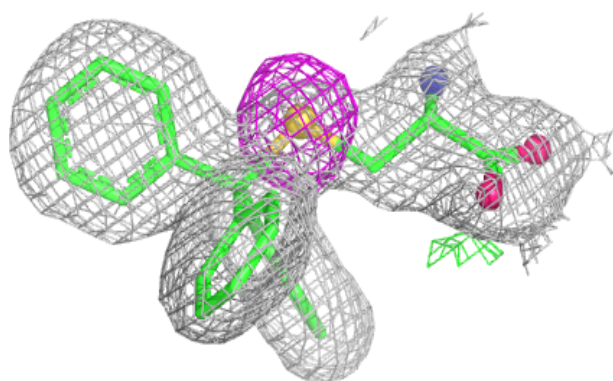
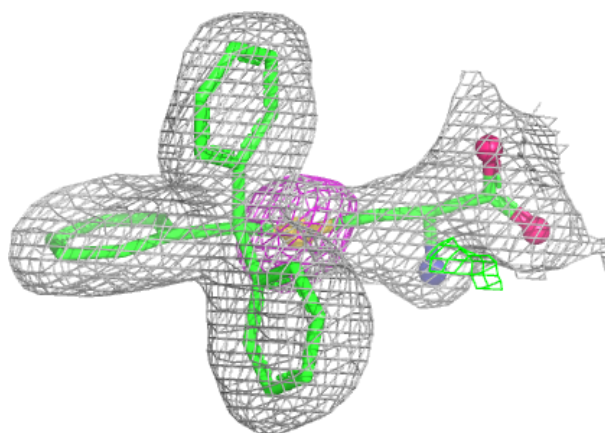
Electron density around ZSD B 1365:

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



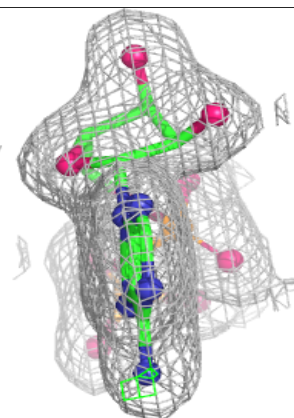
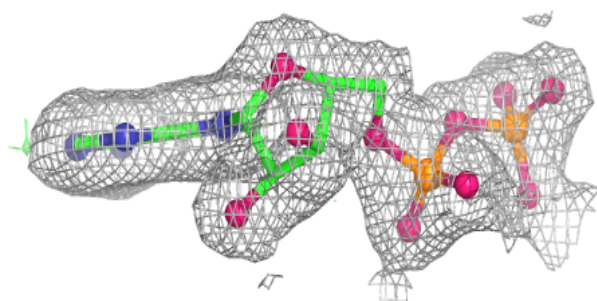
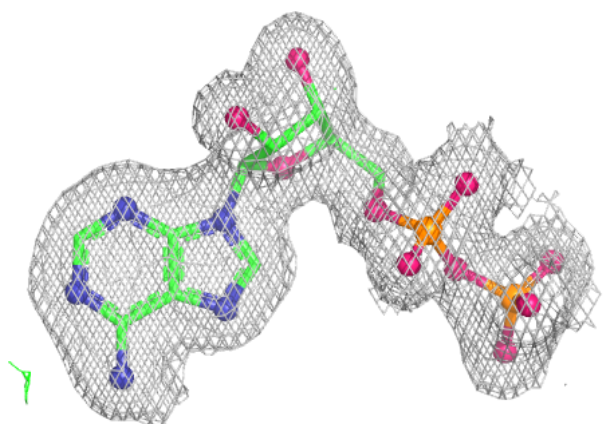
Electron density around ZZZ A 1365:

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



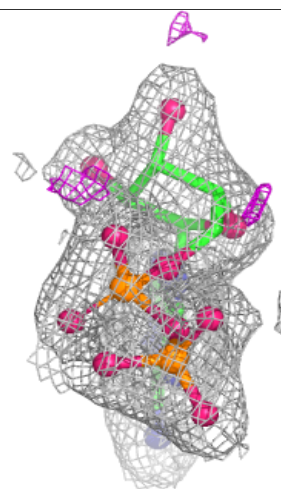
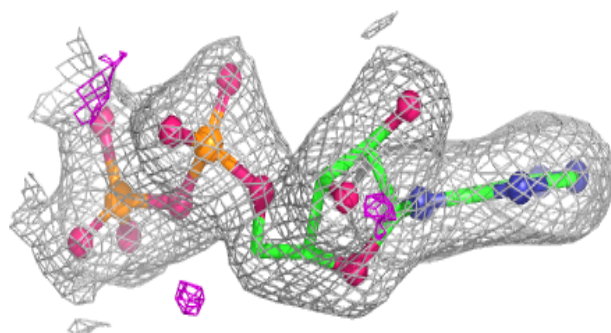
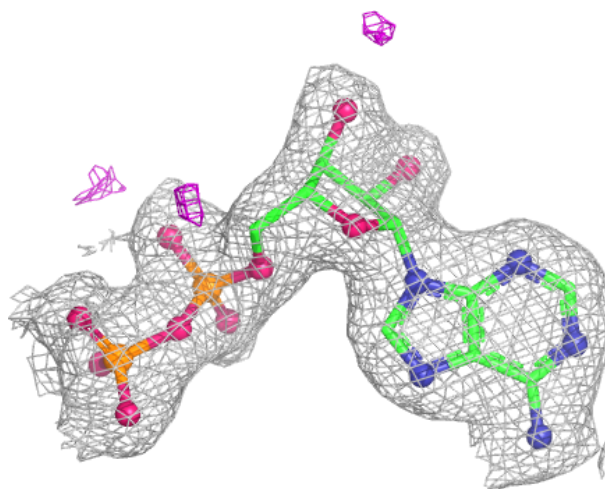
Electron density around ADP B 600:

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



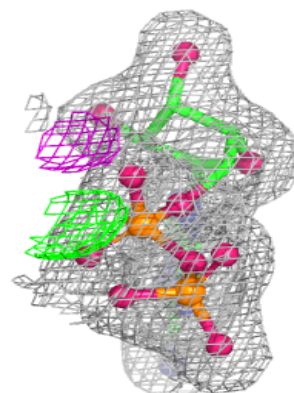
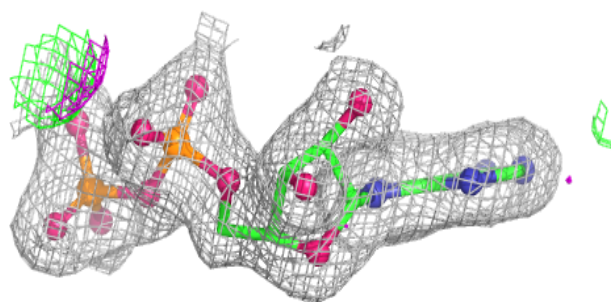
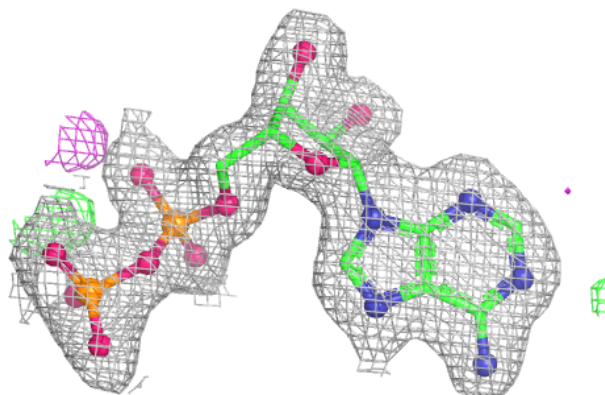
Electron density around ADP C 600:

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



Electron density around ADP A 600:

$2mF_o-DF_c$ (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.