



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2020 – 03:44 am BST

PDB ID : 3CJO
Title : Crystal structure of KSP in complex with inhibitor 30
Authors : Yan, Y.
Deposited on : 2008-03-13
Resolution : 2.28 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

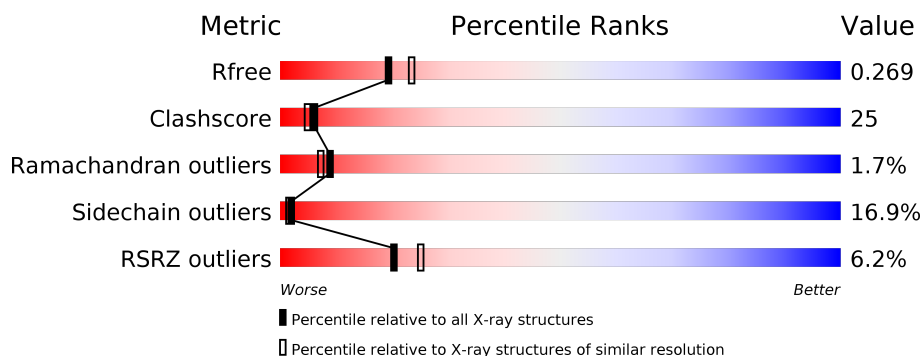
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 on 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	367	
1	B	367	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5633 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	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			
1	B	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

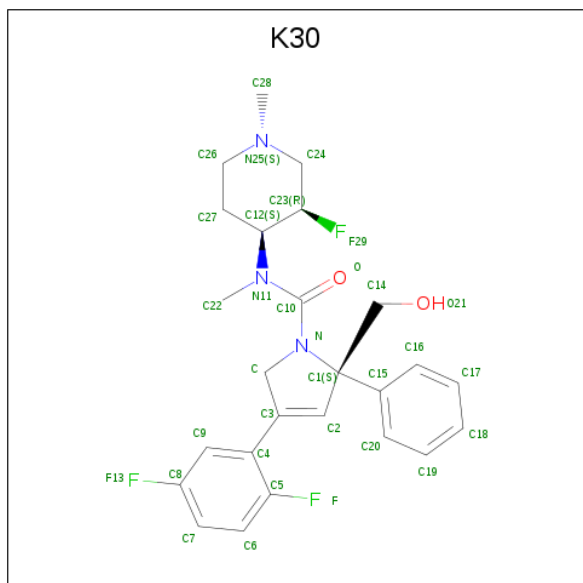
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is (2S)-4-(2,5-difluorophenyl)-N-[(3R,4S)-3-fluoro-1-methylpiperidin-4-yl]-2-(hydroxymethyl)-N-methyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (three-letter code: K30) (formula: C₂₅H₂₈F₃N₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			33	25	3	3	2		
4	B	1	Total	C	F	N	O	0	0
			33	25	3	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	178	Total	O	0	0
			178	178		
5	B	145	Total	O	0	0
			145	145		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

[illegible]

Chain B:

47% 34% 9% 10%

ALA SER GLN PRO ASN SER SER ALA LYS LYS GLU LYS LYS M18 R24 C25 R26 P27 F28 N29 L30 A31 R32 R33 K34 A35 S36 G117 A37 L40 V41 E42 C43 D44 V46 R47 K48 E49 V50 S51 V52 G55 G56 L57 K60 S61 S62 R63 R64 T65 V66 T67



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.76 Å 79.37 Å 158.85 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.28 29.32 – 2.28	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.28) 75.9 (29.32-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29 Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.181 , 0.261 0.186 , 0.269	Depositor DCC
R_{free} test set	1527 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5633	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0182e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K30, 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	0.66	0/2632	0.83	1/3559 (0.0%)
1	B	0.64	0/2632	0.84	1/3559 (0.0%)
All	All	0.65	0/5264	0.84	2/7118 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	LEU	CA-CB-CG	-5.58	102.46	115.30
1	A	293	LEU	CB-CG-CD1	5.07	119.62	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2594	0	2617	103	0
1	B	2594	0	2617	157	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	33	0	28	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	33	0	28	5	0
5	A	178	0	0	5	0
5	B	145	0	0	16	0
All	All	5633	0	5314	261	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 25.

All (261) 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:49:GLU:HG3	1:B:67:THR:HG22	1.20	1.08
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.33	1.06
1:B:40:ILE:HD13	1:B:340:SER:HA	1.40	1.00
1:A:318:ARG:HH11	1:A:318:ARG:HG2	1.23	1.00
1:B:190:ASN:HB2	1:B:192:ARG:HH12	1.34	0.90
1:B:173:ASN:O	1:B:220:LYS:HE2	1.71	0.90
1:B:312:ARG:HA	1:B:318:ARG:HD2	1.52	0.89
1:B:26:ARG:HH11	1:B:26:ARG:HG3	1.37	0.89
1:B:327:ARG:HH11	1:B:327:ARG:HB3	1.37	0.89
1:B:57:LEU:H	1:B:57:LEU:HD23	1.36	0.88
1:A:312:ARG:HA	1:A:318:ARG:HD2	1.56	0.86
1:A:327:ARG:HG3	1:A:327:ARG:HH11	1.40	0.86
1:B:49:GLU:CG	1:B:67:THR:HG22	2.04	0.85
1:B:318:ARG:HH11	1:B:318:ARG:HG2	1.37	0.85
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.60	0.84
1:B:72:PHE:HD1	1:B:76:THR:HG21	1.44	0.82
1:A:318:ARG:NH1	1:A:318:ARG:HG2	1.93	0.82
1:A:177:ASP:O	1:A:180:GLU:HG3	1.81	0.81
1:A:174:PRO:HG3	1:A:216:LYS:HD2	1.62	0.81
1:B:178:VAL:HG12	1:B:220:LYS:HG3	1.64	0.80
1:B:29:ASN:H	1:B:32:GLU:HG3	1.47	0.79
1:B:178:VAL:CG1	1:B:220:LYS:HG3	2.14	0.79
1:A:54:THR:CG2	1:A:64:LYS:HG3	2.13	0.77
1:B:52:VAL:HG21	1:B:347:LEU:CD2	2.14	0.77
1:A:247:GLU:OE1	1:A:255:LEU:HD23	1.86	0.76
1:B:287:ASN:HB3	5:B:706:HOH:O	1.84	0.76
1:B:327:ARG:NH1	1:B:327:ARG:HB3	2.02	0.74
1:B:187:ASP:OD2	1:B:189:ARG:HD2	1.87	0.74
1:B:271:ASN:HB3	5:B:617:HOH:O	1.89	0.73
1:B:57:LEU:CD2	1:B:57:LEU:H	2.01	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:HD2	1:B:175:SER:H	1.53	0.73
1:B:173:ASN:HD22	1:B:174:PRO:HD2	1.55	0.72
1:A:303:VAL:CG1	1:A:359:ILE:HG13	2.22	0.70
1:B:312:ARG:HA	1:B:318:ARG:CD	2.22	0.70
1:A:346:THR:HG21	5:A:620:HOH:O	1.92	0.69
1:B:173:ASN:HD21	1:B:175:SER:HB2	1.57	0.69
1:A:72:PHE:CD1	1:A:76:THR:HG21	2.28	0.69
1:A:92:GLU:O	1:A:97:TYR:HB2	1.92	0.69
1:B:162:GLU:OE2	1:B:221:ARG:NH1	2.25	0.69
1:A:248:THR:HA	1:A:253:GLU:O	1.92	0.69
1:B:40:ILE:CD1	1:B:340:SER:HA	2.20	0.68
1:B:354:HIS:O	1:B:357:LYS:HG3	1.94	0.68
1:A:57:LEU:O	1:A:61:SER:HB3	1.94	0.68
1:A:172:LEU:O	1:A:174:PRO:HD3	1.94	0.68
1:B:189:ARG:HG2	1:B:189:ARG:HH11	1.59	0.68
1:B:325:GLY:H	1:B:361:ASN:HD21	1.42	0.68
1:A:85:VAL:O	1:A:89:ILE:HG13	1.93	0.67
1:B:25:CYS:SG	1:B:41:VAL:HG21	2.34	0.67
1:B:305:ARG:HG3	1:B:305:ARG:HH11	1.59	0.67
1:B:57:LEU:O	1:B:61:SER:HB3	1.95	0.67
1:B:49:GLU:HG3	1:B:67:THR:CG2	2.12	0.67
1:B:318:ARG:HG2	1:B:318:ARG:NH1	2.03	0.67
1:A:327:ARG:HG3	1:A:327:ARG:NH1	2.09	0.66
1:B:190:ASN:HB2	1:B:192:ARG:NH1	2.09	0.66
1:B:44:ASP:O	1:B:48:LYS:N	2.28	0.65
1:B:317:THR:O	1:B:321:GLN:HB3	1.95	0.65
1:B:288:ILE:O	1:B:288:ILE:HG13	1.95	0.65
1:A:288:ILE:HG13	1:A:288:ILE:O	1.97	0.65
1:A:315:LYS:O	1:A:319:ILE:HG13	1.96	0.65
1:B:116:GLU:OE2	1:B:221:ARG:NH2	2.30	0.65
1:A:341:LEU:H	1:A:341:LEU:HD23	1.63	0.63
1:B:173:ASN:HD22	1:B:174:PRO:CD	2.10	0.63
1:A:106:GLN:HG2	1:A:109:THR:HG23	1.81	0.62
1:B:178:VAL:HG21	1:B:224:ALA:HA	1.81	0.62
1:B:174:PRO:CD	1:B:175:SER:H	2.12	0.61
1:B:245:MET:HB2	1:B:257:LYS:HB2	1.82	0.61
1:B:72:PHE:HB3	1:B:76:THR:OG1	2.00	0.61
1:B:51:SER:HB3	1:B:65:THR:OG1	2.00	0.60
1:A:171:LEU:O	1:A:220:LYS:HD3	2.01	0.60
1:A:38:HIS:NE2	5:A:662:HOH:O	2.32	0.60
1:B:86:VAL:HG21	1:B:135:ILE:HG12	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.67	0.60
1:B:312:ARG:HB3	1:B:312:ARG:NH1	2.17	0.59
1:A:44:ASP:OD2	1:A:47:ARG:HG3	2.02	0.59
1:B:189:ARG:NH1	1:B:189:ARG:HG2	2.17	0.59
1:B:184:MET:HE3	1:B:318:ARG:CZ	2.33	0.58
1:B:52:VAL:HG21	1:B:347:LEU:HD21	1.84	0.58
1:A:323:SER:O	1:A:330:THR:HG21	2.02	0.58
1:B:51:SER:HB2	1:B:63:ARG:HE	1.69	0.58
1:A:354:HIS:O	1:A:357:LYS:HG3	2.03	0.58
1:B:310:PRO:HA	5:B:674:HOH:O	2.02	0.57
1:A:192:ARG:HG3	1:A:192:ARG:O	2.04	0.57
1:B:178:VAL:HG12	1:B:220:LYS:CG	2.34	0.57
1:B:29:ASN:H	1:B:32:GLU:CG	2.17	0.57
1:A:158:VAL:HA	1:A:240:SER:O	2.04	0.57
1:A:29:ASN:O	1:A:33:ARG:HG2	2.04	0.57
1:B:78:GLN:HE21	1:B:78:GLN:HA	1.68	0.57
1:A:354:HIS:HD2	5:A:696:HOH:O	1.87	0.57
1:A:295:LEU:O	1:A:299:ILE:HG13	2.05	0.57
1:A:337:SER:OG	1:A:342:ASN:ND2	2.38	0.56
1:A:126:THR:OG1	1:A:129:GLU:HG3	2.06	0.56
1:A:44:ASP:CG	1:A:47:ARG:HG3	2.26	0.56
1:B:215:GLU:HA	4:B:603:K30:H22B	1.86	0.56
1:B:215:GLU:HG2	4:B:603:K30:H27A	1.85	0.56
1:A:45:PRO:HA	1:A:71:VAL:HG23	1.88	0.56
1:B:325:GLY:H	1:B:361:ASN:ND2	2.03	0.56
1:B:242:THR:OG1	1:B:260:LYS:HG3	2.06	0.56
1:B:339:ALA:HB3	1:B:342:ASN:HD22	1.71	0.56
1:B:312:ARG:HB3	1:B:312:ARG:HH11	1.70	0.56
1:A:209:GLU:HA	1:A:212:GLN:HE21	1.71	0.56
1:B:232:SER:O	5:B:733:HOH:O	2.17	0.55
1:A:129:GLU:O	1:A:131:PRO:HD3	2.06	0.55
1:A:172:LEU:HB3	1:A:202:ILE:HD11	1.88	0.55
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.88	0.55
1:A:40:ILE:HD13	1:A:343:LEU:HB2	1.89	0.55
1:B:57:LEU:HD11	5:B:649:HOH:O	2.07	0.54
1:A:136:ILE:N	1:A:137:PRO:HD2	2.22	0.54
1:B:24:ARG:HH12	1:B:78:GLN:HE22	1.55	0.54
1:B:246:LYS:HD3	1:B:254:GLU:OE1	2.07	0.54
1:B:62:SER:O	1:B:63:ARG:HB3	2.07	0.54
1:B:230:ALA:HB3	1:B:234:ARG:HD3	1.89	0.54
1:B:26:ARG:HG3	1:B:26:ARG:NH1	2.13	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LYS:HE2	1:B:262:ASN:HD21	1.73	0.54
1:B:209:GLU:O	1:B:213:ILE:HG13	2.07	0.54
1:A:211:TYR:OH	4:A:1:K30:H27	2.08	0.54
1:B:205:HIS:HD2	1:B:209:GLU:OE1	1.91	0.54
1:A:289:ASN:ND2	1:A:292:LEU:H	2.06	0.53
1:A:40:ILE:CD1	1:A:343:LEU:HB2	2.38	0.53
1:B:72:PHE:CD1	1:B:76:THR:HG21	2.35	0.53
1:A:287:ASN:N	5:A:647:HOH:O	2.42	0.53
1:B:30:LEU:HG	1:B:30:LEU:O	2.09	0.53
1:A:185:PHE:HE1	1:A:197:LYS:HB2	1.74	0.52
1:A:211:TYR:O	1:A:215:GLU:HG3	2.09	0.52
1:B:248:THR:HA	1:B:253:GLU:O	2.09	0.52
1:B:49:GLU:HG2	1:B:65:THR:HG22	1.91	0.52
1:B:117:GLY:O	4:B:603:K30:O21	2.27	0.52
1:A:160:LEU:HD22	1:A:239:PHE:HD2	1.75	0.52
1:A:322:ASP:O	1:A:326:GLY:HA3	2.08	0.52
1:A:326:GLY:O	1:A:361:ASN:HB2	2.08	0.52
1:B:27:PRO:HB3	1:B:74:ALA:HB1	1.90	0.52
1:A:128:GLU:OE1	1:A:207:LYS:HD3	2.09	0.52
1:B:173:ASN:ND2	1:B:174:PRO:HD2	2.23	0.52
1:B:328:THR:O	1:B:361:ASN:OD1	2.27	0.52
1:A:106:GLN:HG2	1:A:109:THR:CG2	2.39	0.52
1:B:269:SER:HA	1:B:292:LEU:HD21	1.91	0.52
1:B:121:PRO:HG3	5:B:739:HOH:O	2.10	0.51
1:A:28:PHE:HA	1:A:32:GLU:OE2	2.10	0.51
1:B:26:ARG:HH11	1:B:26:ARG:CG	2.17	0.51
1:B:117:GLY:C	1:B:118:GLU:HG3	2.30	0.51
1:B:305:ARG:HG3	1:B:305:ARG:NH1	2.23	0.51
1:B:257:LYS:HE3	5:B:664:HOH:O	2.09	0.51
4:A:1:K30:O	4:A:1:K30:H14A	2.10	0.51
1:B:28:PHE:HA	1:B:32:GLU:OE2	2.11	0.51
1:A:48:LYS:HA	1:A:71:VAL:HG22	1.92	0.51
1:A:161:LEU:CD1	1:A:319:ILE:HD13	2.41	0.50
1:A:271:ASN:C	1:A:271:ASN:HD22	2.14	0.50
1:B:93:VAL:HA	1:B:97:TYR:O	2.11	0.50
1:A:172:LEU:HB3	1:A:202:ILE:CD1	2.41	0.50
1:B:116:GLU:HB3	4:B:603:K30:F	2.02	0.50
1:B:146:LYS:HE3	5:B:672:HOH:O	2.12	0.50
1:B:147:LEU:HB3	1:B:154:PHE:CD2	2.47	0.50
1:B:173:ASN:HD22	1:B:173:ASN:C	2.14	0.50
1:A:289:ASN:HD22	1:A:292:LEU:H	1.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASN:HB2	5:B:691:HOH:O	2.12	0.50
1:A:341:LEU:HD23	1:A:341:LEU:N	2.26	0.49
1:B:186:ASP:O	1:B:188:PRO:HD3	2.12	0.49
1:A:38:HIS:ND1	1:A:38:HIS:O	2.46	0.49
1:B:230:ALA:O	1:B:234:ARG:HB2	2.13	0.49
1:B:29:ASN:N	1:B:32:GLU:HG3	2.21	0.49
1:A:134:GLY:O	1:A:137:PRO:HG2	2.13	0.48
1:B:312:ARG:CA	1:B:318:ARG:HD2	2.35	0.48
1:A:327:ARG:CG	1:A:327:ARG:NH1	2.77	0.48
1:B:111:LYS:HE3	1:B:266:LEU:O	2.13	0.48
1:A:139:THR:O	1:A:143:ILE:HG13	2.12	0.48
1:B:127:TRP:HB2	4:B:603:K30:H17	1.96	0.48
1:B:329:ARG:HB2	5:B:637:HOH:O	2.14	0.48
1:A:154:PHE:HA	1:A:244:HIS:O	2.14	0.47
1:B:29:ASN:O	1:B:31:ALA:N	2.47	0.47
1:B:147:LEU:CB	1:B:154:PHE:CE2	2.97	0.47
1:B:87:CYS:HB3	1:B:88:PRO:CD	2.44	0.47
1:A:342:ASN:O	1:A:346:THR:HG23	2.15	0.47
1:A:45:PRO:HA	1:A:71:VAL:CG2	2.45	0.47
1:B:339:ALA:HB3	1:B:342:ASN:ND2	2.30	0.47
1:B:49:GLU:HG2	1:B:65:THR:CG2	2.44	0.47
1:A:303:VAL:HG12	1:A:359:ILE:HG13	1.94	0.47
1:B:327:ARG:HA	1:B:362:LYS:HA	1.96	0.47
1:A:184:MET:HG3	1:A:196:ILE:HG13	1.97	0.46
1:A:192:ARG:HA	1:A:321:GLN:NE2	2.31	0.46
1:A:312:ARG:HA	1:A:318:ARG:CD	2.36	0.46
1:A:161:LEU:HD11	1:A:319:ILE:HD13	1.95	0.46
1:B:205:HIS:CD2	1:B:209:GLU:OE1	2.68	0.46
1:A:136:ILE:HG12	1:A:263:LEU:HD12	1.96	0.46
1:B:160:LEU:HB3	1:B:172:LEU:HG	1.98	0.46
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.97	0.46
1:A:130:ASP:HA	1:A:131:PRO:HD2	1.88	0.45
1:B:129:GLU:O	1:B:131:PRO:HD3	2.17	0.45
1:B:322:ASP:O	1:B:326:GLY:HA3	2.16	0.45
1:B:174:PRO:CD	1:B:175:SER:N	2.79	0.45
1:A:184:MET:HG3	1:A:196:ILE:CG1	2.47	0.45
1:A:241:VAL:O	1:A:241:VAL:HG13	2.16	0.45
1:B:147:LEU:HB3	1:B:154:PHE:CE2	2.51	0.45
1:B:28:PHE:CE2	1:B:37:ALA:HB1	2.52	0.45
1:B:293:LEU:HA	1:B:293:LEU:HD12	1.78	0.45
1:A:177:ASP:OD1	1:A:179:SER:OG	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:O	1:A:148:THR:HB	2.17	0.45
1:B:104:TYR:O	1:B:334:ALA:HA	2.16	0.45
1:B:207:LYS:C	1:B:209:GLU:H	2.20	0.45
1:B:18:ASN:HB2	1:B:360:LEU:HA	1.99	0.45
1:B:43:CYS:HB3	1:B:71:VAL:HG12	1.98	0.44
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.83	0.44
1:A:142:GLN:O	1:A:146:LYS:HG3	2.16	0.44
1:A:178:VAL:O	1:A:180:GLU:N	2.51	0.44
1:A:44:ASP:HB3	1:A:47:ARG:HB2	1.99	0.44
1:A:145:GLU:O	1:A:147:LEU:N	2.51	0.44
1:A:204:VAL:HG22	1:A:213:ILE:HD13	1.99	0.44
1:A:204:VAL:HG22	1:A:213:ILE:CD1	2.48	0.44
1:B:162:GLU:HA	1:B:236:HIS:O	2.18	0.44
1:B:33:ARG:HB2	1:B:33:ARG:HE	1.31	0.44
1:A:242:THR:OG1	1:A:260:LYS:HG3	2.18	0.44
1:B:257:LYS:HG3	5:B:664:HOH:O	2.17	0.44
1:B:161:LEU:HD22	1:B:196:ILE:HD13	2.00	0.43
1:B:323:SER:C	1:B:324:LEU:HG	2.37	0.43
1:A:160:LEU:HB3	1:A:172:LEU:HG	2.00	0.43
1:B:184:MET:HE3	1:B:318:ARG:NH2	2.33	0.43
1:B:362:LYS:HE3	1:B:362:LYS:HB3	1.55	0.43
1:B:40:ILE:HD12	1:B:343:LEU:HD23	2.00	0.43
1:A:257:LYS:HG3	1:A:257:LYS:HZ2	1.57	0.43
1:A:173:ASN:O	1:A:220:LYS:HE2	2.18	0.43
1:A:99:CYS:O	1:A:261:LEU:HA	2.18	0.43
1:B:52:VAL:O	1:B:63:ARG:HA	2.18	0.43
1:B:147:LEU:HB2	1:B:154:PHE:CE2	2.54	0.43
1:B:111:LYS:HB2	1:B:111:LYS:HE2	1.61	0.43
1:B:124:GLU:H	1:B:124:GLU:HG3	1.63	0.43
1:B:64:LYS:HD2	5:B:685:HOH:O	2.18	0.43
1:B:25:CYS:SG	1:B:41:VAL:CG2	3.07	0.42
1:B:297:ARG:HD3	5:B:607:HOH:O	2.19	0.42
1:B:308:HIS:CE1	5:B:660:HOH:O	2.73	0.42
1:B:57:LEU:N	1:B:57:LEU:CD2	2.74	0.42
1:A:22:VAL:HG22	1:A:333:ILE:HG12	2.01	0.42
1:A:87:CYS:N	1:A:88:PRO:HD2	2.34	0.42
1:B:165:ASN:O	1:B:165:ASN:ND2	2.53	0.42
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.49	0.42
1:B:184:MET:CE	1:B:318:ARG:CZ	2.97	0.42
1:B:325:GLY:HA2	1:B:360:LEU:O	2.19	0.42
1:B:292:LEU:HD12	1:B:292:LEU:HA	1.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG21	1:B:224:ALA:CA	2.48	0.42
1:B:79:ILE:O	1:B:79:ILE:HD12	2.20	0.42
1:A:184:MET:HB3	1:A:184:MET:HE2	1.83	0.42
1:A:53:ARG:HB2	1:A:63:ARG:NH2	2.34	0.42
1:B:308:HIS:HE1	5:B:660:HOH:O	2.03	0.42
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.96	0.41
1:B:246:LYS:HA	1:B:255:LEU:O	2.20	0.41
1:B:128:GLU:OE1	1:B:207:LYS:HE2	2.19	0.41
1:A:247:GLU:O	1:A:254:GLU:HA	2.21	0.41
1:B:169:PHE:CD2	1:B:178:VAL:O	2.74	0.41
1:B:308:HIS:HD2	5:B:737:HOH:O	2.02	0.41
1:A:305:ARG:NH2	5:A:675:HOH:O	2.36	0.41
1:B:309:VAL:HA	1:B:310:PRO:HD3	1.94	0.41
1:A:69:ASP:O	1:A:70:MET:HG3	2.21	0.41
1:B:117:GLY:O	1:B:118:GLU:HG3	2.20	0.41
1:B:70:MET:C	1:B:71:VAL:HG23	2.41	0.41
1:B:77:LYS:N	1:B:77:LYS:HD3	2.36	0.41
1:A:171:LEU:C	1:A:220:LYS:HD3	2.40	0.41
1:A:77:LYS:HD3	1:A:77:LYS:HA	1.92	0.41
1:A:87:CYS:HB3	1:A:88:PRO:CD	2.51	0.41
1:B:34:LYS:HB3	1:B:34:LYS:HE2	1.87	0.41
1:B:223:THR:O	1:B:227:LEU:HD13	2.22	0.40
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.36	0.40
1:A:357:LYS:HB3	1:A:357:LYS:HE2	1.50	0.40
1:B:130:ASP:HA	1:B:131:PRO:HD2	1.82	0.40
1:B:44:ASP:OD2	1:B:47:ARG:HB3	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	326/367 (89%)	302 (93%)	17 (5%)	7 (2%)	7	5
1	B	326/367 (89%)	310 (95%)	12 (4%)	4 (1%)	13	12
All	All	652/734 (89%)	612 (94%)	29 (4%)	11 (2%)	9	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	LYS
1	A	179	SER
1	B	30	LEU
1	B	189	ARG
1	A	145	GLU
1	A	150	ASN
1	A	189	ARG
1	A	312	ARG
1	B	149	ASP
1	B	36	SER
1	A	252	GLY

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	293/321 (91%)	246 (84%)	47 (16%)	2	2
1	B	293/321 (91%)	241 (82%)	52 (18%)	2	1
All	All	586/642 (91%)	487 (83%)	99 (17%)	2	1

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	19	ILE
1	A	22	VAL
1	A	34	LYS
1	A	36	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	49	GLU
1	A	57	LEU
1	A	62	SER
1	A	84	SER
1	A	89	ILE
1	A	122	ASN
1	A	126	THR
1	A	128	GLU
1	A	145	GLU
1	A	146	LYS
1	A	152	THR
1	A	160	LEU
1	A	161	LEU
1	A	175	SER
1	A	177	ASP
1	A	181	ARG
1	A	190	ASN
1	A	192	ARG
1	A	197	LYS
1	A	199	LEU
1	A	212	GLN
1	A	216	LYS
1	A	226	THR
1	A	249	THR
1	A	254	GLU
1	A	255	LEU
1	A	257	LYS
1	A	271	ASN
1	A	287	ASN
1	A	288	ILE
1	A	289	ASN
1	A	293	LEU
1	A	318	ARG
1	A	327	ARG
1	A	330	THR
1	A	341	LEU
1	A	343	LEU
1	A	346	THR
1	A	357	LYS
1	A	360	LEU
1	A	361	ASN
1	A	362	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	18	ASN
1	B	32	GLU
1	B	33	ARG
1	B	34	LYS
1	B	41	VAL
1	B	46	VAL
1	B	48	LYS
1	B	50	VAL
1	B	51	SER
1	B	52	VAL
1	B	57	LEU
1	B	60	LYS
1	B	62	SER
1	B	75	SER
1	B	76	THR
1	B	78	GLN
1	B	79	ILE
1	B	84	SER
1	B	89	ILE
1	B	115	MET
1	B	124	GLU
1	B	148	THR
1	B	171	LEU
1	B	173	ASN
1	B	176	SER
1	B	178	VAL
1	B	189	ARG
1	B	192	ARG
1	B	207	LYS
1	B	213	ILE
1	B	220	LYS
1	B	221	ARG
1	B	227	LEU
1	B	233	SER
1	B	246	LYS
1	B	247	GLU
1	B	289	ASN
1	B	293	LEU
1	B	302	LEU
1	B	312	ARG
1	B	318	ARG
1	B	327	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	329	ARG
1	B	337	SER
1	B	341	LEU
1	B	343	LEU
1	B	348	SER
1	B	350	LEU
1	B	357	LYS
1	B	360	LEU
1	B	361	ASN
1	B	362	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	150	ASN
1	A	173	ASN
1	A	212	GLN
1	A	229	ASN
1	A	262	ASN
1	A	271	ASN
1	A	289	ASN
1	A	308	HIS
1	A	321	GLN
1	A	342	ASN
1	A	354	HIS
1	A	361	ASN
1	B	78	GLN
1	B	141	HIS
1	B	142	GLN
1	B	165	ASN
1	B	173	ASN
1	B	205	HIS
1	B	212	GLN
1	B	244	HIS
1	B	262	ASN
1	B	287	ASN
1	B	289	ASN
1	B	308	HIS
1	B	342	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
3	ADP	B	600	2	24,29,29	2.26	8 (33%)	29,45,45	1.76	7 (24%)
4	K30	B	603	-	31,36,36	2.80	12 (38%)	35,53,53	2.67	17 (48%)
4	K30	A	1	-	31,36,36	2.86	13 (41%)	35,53,53	2.08	11 (31%)
3	ADP	A	601	2	24,29,29	2.29	6 (25%)	29,45,45	2.02	10 (34%)

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
3	ADP	B	600	2	-	2/12/32/32	0/3/3/3
4	K30	B	603	-	-	6/24/53/53	0/4/4/4
4	K30	A	1	-	-	3/24/53/53	0/4/4/4
3	ADP	A	601	2	-	0/12/32/32	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	K30	C1-C15	8.34	1.62	1.53
4	A	1	K30	C1-C15	8.29	1.62	1.53
3	A	601	ADP	O4'-C1'	8.13	1.52	1.41
3	B	600	ADP	O4'-C1'	6.50	1.50	1.41
4	A	1	K30	C4-C3	-5.77	1.43	1.49
4	A	1	K30	C1-C2	5.64	1.55	1.51
4	B	603	K30	C1-C2	5.40	1.55	1.51
4	B	603	K30	C6-C7	5.30	1.48	1.38
4	B	603	K30	C-C3	-4.94	1.43	1.50
4	B	603	K30	C2-C3	4.04	1.37	1.33
3	B	600	ADP	C2-N1	3.80	1.41	1.33
4	A	1	K30	C9-C4	3.77	1.45	1.39
3	B	600	ADP	C4-N3	3.54	1.40	1.35
4	A	1	K30	C26-N25	3.49	1.53	1.46
4	A	1	K30	C19-C20	3.49	1.46	1.38
3	A	601	ADP	C4-N3	3.47	1.40	1.35
4	B	603	K30	C26-N25	3.46	1.53	1.46
3	B	600	ADP	C8-N7	-3.41	1.28	1.34
4	A	1	K30	C24-N25	3.29	1.51	1.46
3	A	601	ADP	C2-N1	3.25	1.40	1.33
4	A	1	K30	O-C10	3.18	1.28	1.22
4	B	603	K30	C10-N11	2.94	1.42	1.35
3	A	601	ADP	PA-O1A	2.93	1.61	1.50
4	A	1	K30	C28-N25	2.92	1.53	1.46
3	A	601	ADP	C8-N7	-2.83	1.29	1.34
3	B	600	ADP	C2'-C1'	-2.71	1.49	1.53
4	A	1	K30	C17-C16	2.62	1.44	1.38
3	B	600	ADP	C2-N3	2.61	1.36	1.32
3	B	600	ADP	PB-O3B	-2.55	1.45	1.54
4	B	603	K30	C24-N25	2.48	1.50	1.46
4	A	1	K30	C-C3	-2.41	1.47	1.50
4	B	603	K30	C4-C5	2.32	1.42	1.38
4	B	603	K30	C28-N25	2.26	1.52	1.46
4	A	1	K30	C7-C8	2.25	1.41	1.37
3	B	600	ADP	O3'-C3'	-2.16	1.37	1.43
4	B	603	K30	C27-C26	2.16	1.58	1.52
4	A	1	K30	C12-N11	-2.15	1.43	1.47
3	A	601	ADP	C2'-C1'	2.09	1.56	1.53
4	B	603	K30	C-N	2.04	1.49	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	K30	N11-C10-N	8.92	127.52	114.78
3	A	601	ADP	C4-C5-N7	5.81	115.45	109.40
4	A	1	K30	C17-C16-C15	5.40	126.43	120.76
3	B	600	ADP	C5-C6-N6	4.62	127.38	120.35
4	A	1	K30	N11-C10-N	4.49	121.18	114.78
4	B	603	K30	C28-N25-C26	4.04	116.70	110.66
4	B	603	K30	O-C10-N	-3.97	115.06	123.75
4	A	1	K30	C4-C3-C2	3.60	133.57	126.90
3	A	601	ADP	O5'-C5'-C4'	-3.58	96.68	108.99
4	B	603	K30	C6-C7-C8	-3.54	114.70	118.36
4	B	603	K30	C28-N25-C24	-3.43	106.66	110.57
4	B	603	K30	C4-C3-C2	3.43	133.25	126.90
4	A	1	K30	C5-C4-C3	3.36	126.15	122.84
4	B	603	K30	C26-N25-C24	-3.26	107.17	110.16
4	B	603	K30	O-C10-N11	-3.15	116.91	124.17
3	A	601	ADP	N3-C2-N1	-3.12	123.80	128.68
4	B	603	K30	C26-C27-C12	2.97	114.57	109.91
3	A	601	ADP	O2'-C2'-C3'	-2.92	102.39	111.82
3	B	600	ADP	O3B-PB-O2B	2.92	118.78	107.64
3	B	600	ADP	C2'-C3'-C4'	2.84	108.16	102.64
4	B	603	K30	C6-C5-C4	-2.76	120.10	123.11
4	A	1	K30	F-C5-C4	2.75	124.33	119.67
4	B	603	K30	F29-C23-C12	-2.72	100.23	108.06
4	A	1	K30	C20-C15-C16	-2.62	114.08	117.97
4	A	1	K30	C18-C19-C20	2.59	124.13	120.19
3	B	600	ADP	O4'-C4'-C5'	2.58	117.87	109.37
4	A	1	K30	O-C10-N11	-2.58	118.23	124.17
4	B	603	K30	C20-C15-C16	-2.56	114.16	117.97
3	A	601	ADP	N6-C6-N1	2.54	123.84	118.57
3	B	600	ADP	O3'-C3'-C4'	-2.54	103.72	111.05
4	B	603	K30	F13-C8-C9	-2.49	114.70	118.25
3	A	601	ADP	C2-N1-C6	2.45	122.94	118.75
3	A	601	ADP	O3B-PB-O2B	2.44	116.95	107.64
4	B	603	K30	C19-C20-C15	2.38	123.26	120.76
3	A	601	ADP	O2B-PB-O1B	-2.31	101.62	110.68
3	B	600	ADP	C1'-N9-C4	-2.28	122.64	126.64
3	A	601	ADP	O4'-C4'-C3'	2.26	109.59	105.11
4	A	1	K30	C12-N11-C10	2.24	122.05	118.32
4	B	603	K30	C20-C15-C1	2.23	125.71	120.83
4	A	1	K30	C-C3-C4	-2.20	115.98	119.77
4	A	1	K30	C6-C5-C4	-2.16	120.75	123.11
4	B	603	K30	C4-C9-C8	2.14	121.54	117.98
3	A	601	ADP	O3'-C3'-C4'	-2.08	105.04	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	ADP	O5'-C5'-C4'	-2.06	101.90	108.99
4	B	603	K30	F-C5-C6	2.00	123.05	118.59

There are no chirality outliers.

All (11) torsion outliers are listed below:

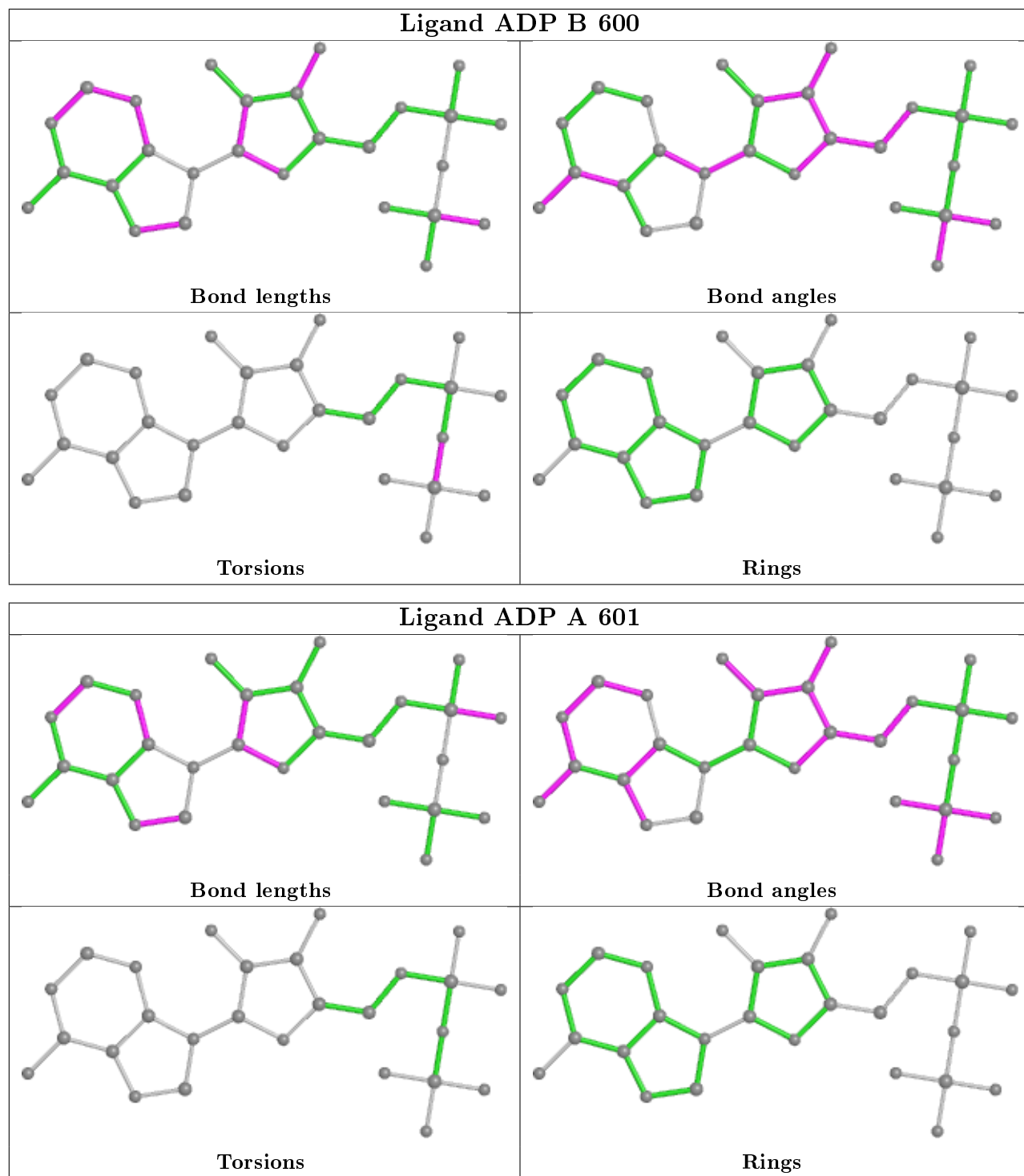
Mol	Chain	Res	Type	Atoms
3	B	600	ADP	PA-O3A-PB-O2B
3	B	600	ADP	PA-O3A-PB-O3B
4	A	1	K30	N-C10-N11-C12
4	B	603	K30	C15-C1-C14-O21
4	B	603	K30	N-C1-C14-O21
4	B	603	K30	N-C10-N11-C12
4	B	603	K30	O-C10-N11-C12
4	B	603	K30	N-C10-N11-C22
4	A	1	K30	C2-C3-C4-C5
4	B	603	K30	C2-C3-C4-C5
4	A	1	K30	N-C10-N11-C22

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	K30	5	0
4	A	1	K30	2	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	330/367 (89%)	0.12	25 (7%) 13 17	19, 36, 82, 98	0
1	B	330/367 (89%)	-0.06	16 (4%) 30 36	21, 39, 76, 109	0
All	All	660/734 (89%)	0.03	41 (6%) 20 25	19, 37, 80, 109	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	LYS	7.2
1	A	250	ILE	7.2
1	A	249	THR	6.0
1	A	57	LEU	5.8
1	A	251	ASP	5.5
1	A	35	ALA	4.3
1	B	34	LYS	3.9
1	A	255	LEU	3.9
1	B	35	ALA	3.8
1	A	248	THR	3.8
1	A	56	GLY	3.7
1	A	58	ALA	3.7
1	B	192	ARG	3.7
1	B	56	GLY	3.7
1	B	57	LEU	3.5
1	A	30	LEU	3.4
1	A	149	ASP	3.3
1	A	33	ARG	3.2
1	B	287	ASN	3.0
1	A	191	LYS	2.9
1	A	263	LEU	2.9
1	A	37	ALA	2.9
1	B	33	ARG	2.8
1	B	174	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	253	GLU	2.5
1	B	55	GLY	2.5
1	B	264	VAL	2.4
1	B	305	ARG	2.4
1	B	175	SER	2.4
1	A	178	VAL	2.4
1	A	135	ILE	2.4
1	A	101	ILE	2.3
1	A	305	ARG	2.3
1	B	31	ALA	2.3
1	B	288	ILE	2.3
1	A	190	ASN	2.2
1	A	264	VAL	2.2
1	B	104	TYR	2.1
1	A	192	ARG	2.0
1	B	103	ALA	2.0
1	A	136	ILE	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 carbohydrates in this entry.

6.4 Ligands ⓘ

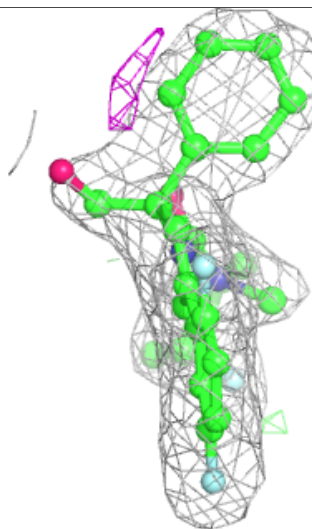
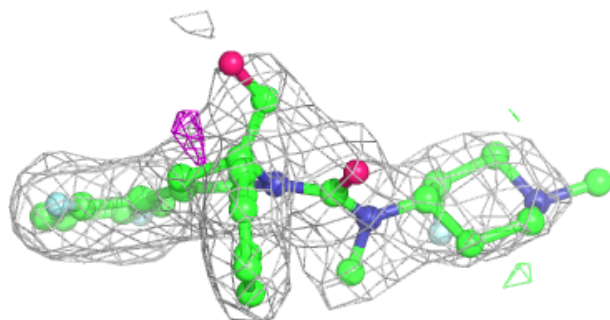
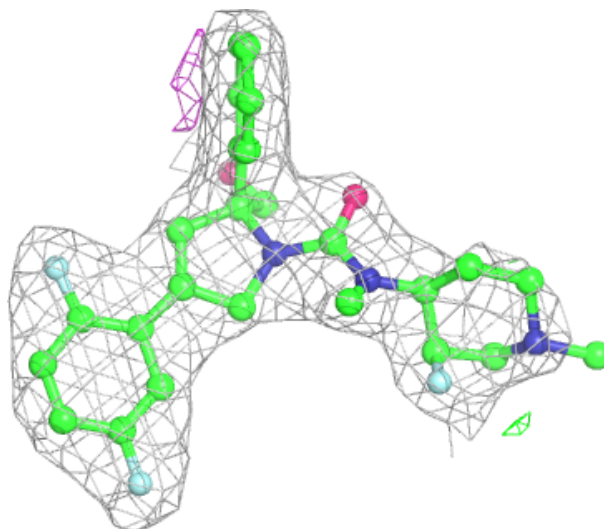
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	K30	A	1	33/33	0.95	0.15	27,35,61,66	0
4	K30	B	603	33/33	0.97	0.12	26,45,64,64	0
3	ADP	A	601	27/27	0.98	0.08	27,34,35,36	0
3	ADP	B	600	27/27	0.98	0.10	25,44,46,47	0
2	MG	B	602	1/1	0.98	0.33	30,30,30,30	0
2	MG	A	603	1/1	0.98	0.32	23,23,23,23	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.

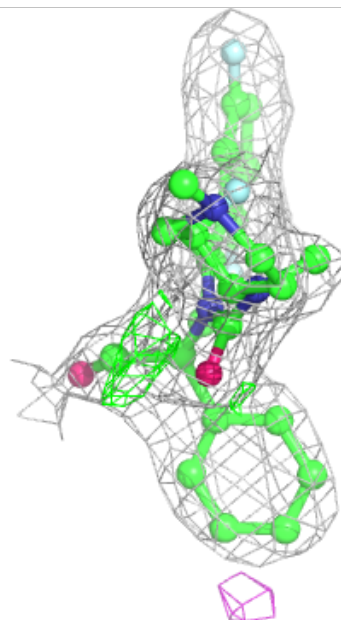
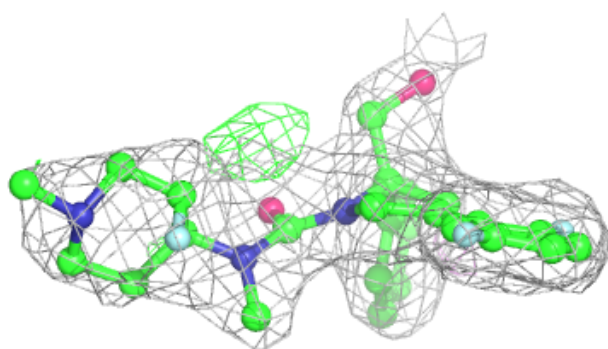
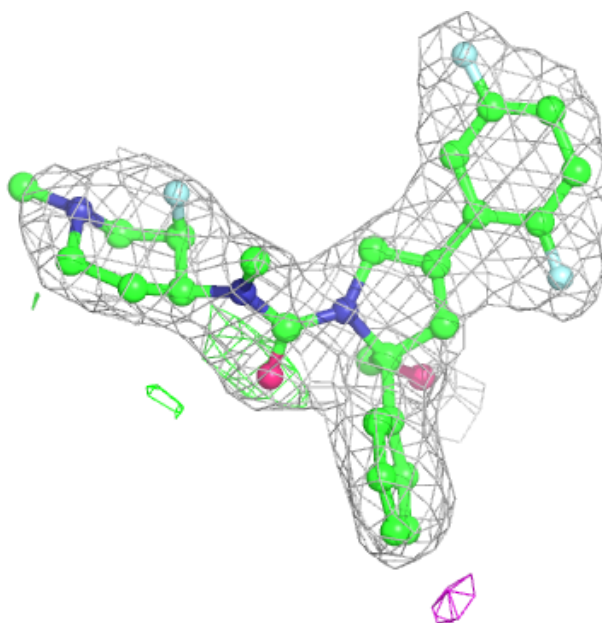
Electron density around K30 A 1:

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



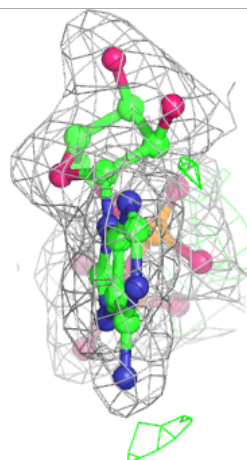
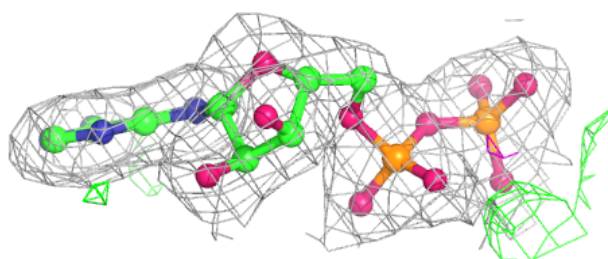
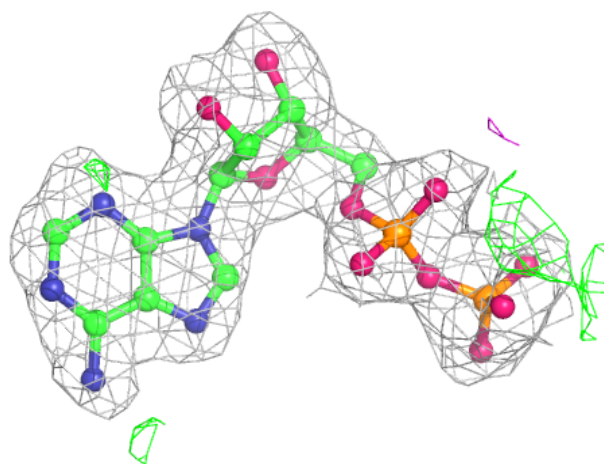
Electron density around K30 B 603:

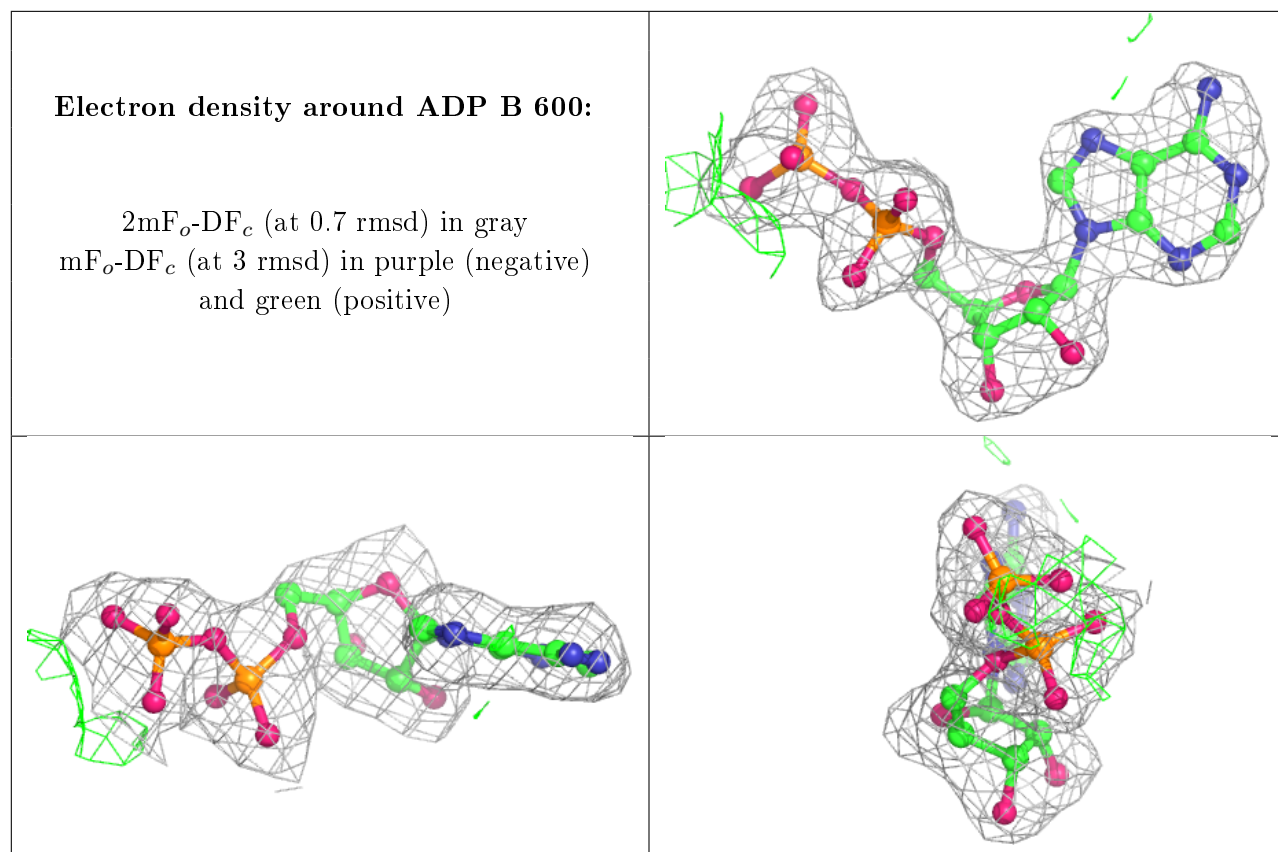
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 601:

$2mF_o-DF_c$ (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.