Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 09:17 AM EST

PDB ID	:	1KI6
Title	:	CRYSTAL STRUCTURE OF THYMIDINE KINASE FROM HERPES SIMPLEX VIRUS TYPE I COMPLEXED WITH A 5-IODOURACIL ANHYDROHEXITOL NUCLEOSIDE
Authors	:	Champness, J.N.; Bennett, M.S.; Wien, F.; Herdewijn, P.; Ostrowski, T.; Summers, W.C.; Sanderson, M.R.
Deposited on	:	1998-05-18
Resolution	:	2.37 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:

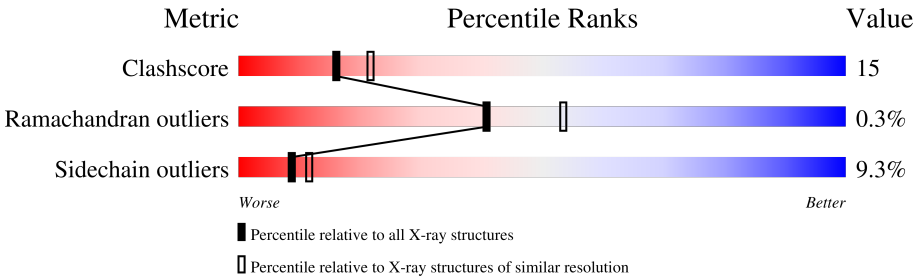
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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))
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	331	63% 24% • 9%
2	B	331	60% 27% 5% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4946 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 THYMIDINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2300	1467	402	416	15	0	0	0

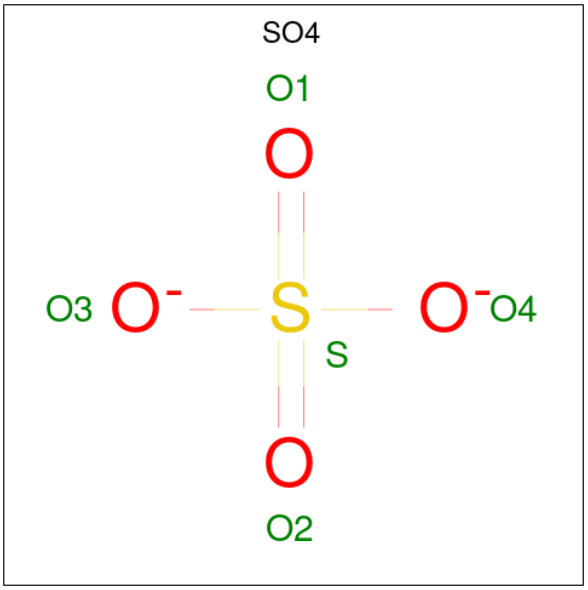
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ALA	PRO	conflict	UNP P03176

- Molecule 2 is a protein called THYMIDINE KINASE.

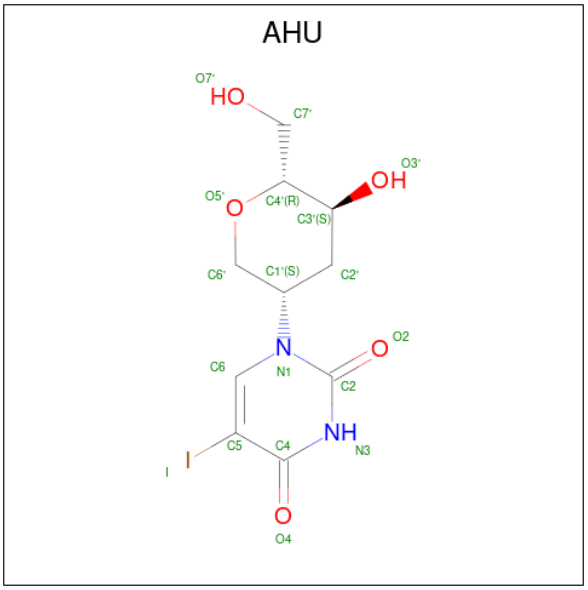
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	304	2325	1485	406	419	15	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is 1',5'-ANHYDRO-2',3'-DIDEOXY-2'-(5-IODOURACIL-1-YL)-D-ABABINO-HEXITOL (three-letter code: AHU) (formula: $C_{10}H_{13}IN_2O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C I N O 18 10 1 2 5	0	0
4	B	1	Total C I N O 18 10 1 2 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	135	Total O 135 135	0	0
5	B	140	Total O 140 140	0	0

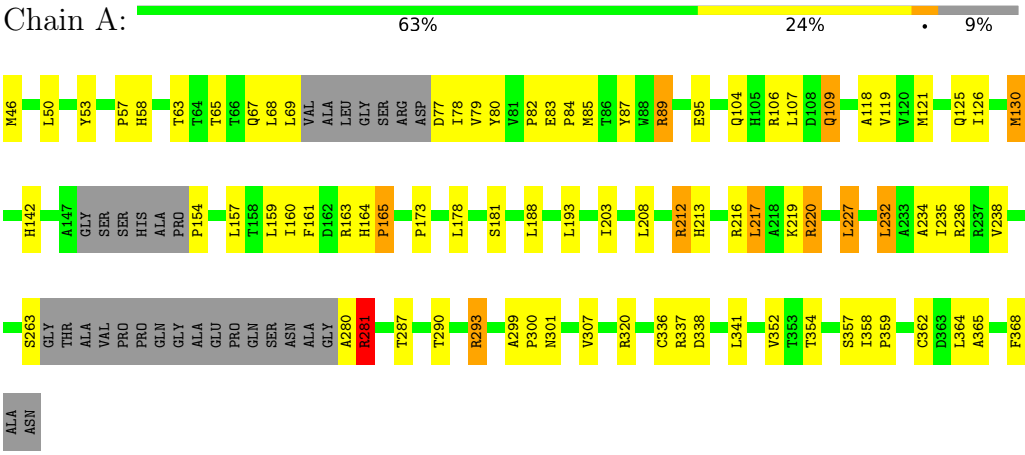
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

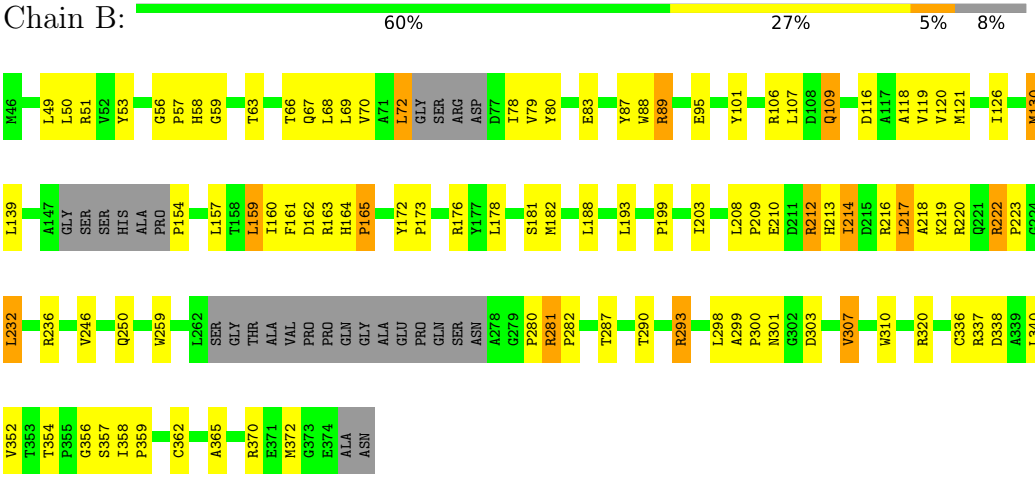
- Molecule 1: THYMIDINE KINASE

Chain A:



- Molecule 2: THYMIDINE KINASE

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	113.60Å 116.40Å 108.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.37	Depositor
% Data completeness (in resolution range)	88.0 (12.00-2.37)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.38Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.223 , 0.317	Depositor
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.009	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
Total number of atoms	4946	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, AHU

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	0.71	1/2351 (0.0%)	0.78	1/3207 (0.0%)
2	B	0.72	1/2377 (0.0%)	0.78	1/3244 (0.0%)
All	All	0.72	2/4728 (0.0%)	0.78	2/6451 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	MET	C-N	8.48	1.50	1.34
2	B	336	CYS	CB-SG	-5.26	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	154	PRO	N-CA-CB	6.18	110.72	103.30
1	A	154	PRO	N-CA-CB	5.47	109.86	103.30

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	2300	0	2313	65	0
2	B	2325	0	2343	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	18	0	12	3	0
4	B	18	0	12	1	0
5	A	135	0	0	5	0
5	B	140	0	0	6	0
All	All	4946	0	4680	136	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 (136) 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:126:ILE:HD11	2:B:126:ILE:HD11	1.56	0.88
2:B:232:LEU:HD13	2:B:236:ARG:HD2	1.66	0.77
2:B:59:GLY:HA3	2:B:217:LEU:HD22	1.67	0.76
1:A:69:LEU:HD23	1:A:337:ARG:HG2	1.68	0.75
4:B:2:AHU:O7'	4:B:2:AHU:H6'1	1.86	0.75
1:A:232:LEU:HD13	1:A:236:ARG:HD2	1.68	0.74
2:B:70:VAL:HG21	2:B:80:TYR:HB2	1.69	0.74
1:A:219:LYS:O	1:A:220:ARG:HD2	1.90	0.71
2:B:72:LEU:HD22	2:B:337:ARG:HD3	1.72	0.71
2:B:106:ARG:HG3	2:B:106:ARG:HH11	1.57	0.68
1:A:106:ARG:HH11	1:A:106:ARG:HG3	1.59	0.67
1:A:119:VAL:HG12	2:B:119:VAL:HG12	1.76	0.66
1:A:68:LEU:HB3	1:A:337:ARG:HG3	1.77	0.66
2:B:51:ARG:NH2	2:B:199:PRO:O	2.29	0.65
2:B:159:LEU:HD13	2:B:161:PHE:CZ	2.32	0.65
2:B:358:ILE:HB	2:B:359:PRO:HD3	1.78	0.64
1:A:193:LEU:HD13	2:B:193:LEU:HD13	1.80	0.64
1:A:164:HIS:CD2	1:A:165:PRO:HD2	2.33	0.64
2:B:121:MET:HG3	2:B:181:SER:HB2	1.81	0.62
1:A:163:ARG:HD2	5:A:562:HOH:O	2.00	0.62
2:B:210:GLU:O	2:B:214:ILE:HD13	2.00	0.62
1:A:142:HIS:HE1	5:A:615:HOH:O	1.84	0.61
1:A:217:LEU:HD13	1:A:227:LEU:HD23	1.82	0.60
2:B:83:GLU:HG2	2:B:88:TRP:CH2	2.36	0.60
1:A:159:LEU:HD13	1:A:161:PHE:CZ	2.36	0.59
1:A:217:LEU:HD12	1:A:232:LEU:HG	1.84	0.59
2:B:370:ARG:NH1	5:B:643:HOH:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ILE:HD11	2:B:160:ILE:HG13	1.85	0.59
2:B:79:VAL:HG23	2:B:157:LEU:HD11	1.84	0.58
1:A:263:SER:OG	1:A:293:ARG:NH1	2.36	0.58
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.85	0.57
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.40	0.57
1:A:163:ARG:NH1	5:A:775:HOH:O	2.38	0.56
1:A:87:TYR:HB2	1:A:372:MET:HG2	1.88	0.55
2:B:119:VAL:HG23	5:B:684:HOH:O	2.06	0.55
2:B:320:ARG:O	2:B:320:ARG:HG2	2.07	0.55
2:B:69:LEU:HD11	2:B:341:LEU:HG	1.89	0.55
1:A:118:ALA:HA	1:A:181:SER:O	2.06	0.55
2:B:121:MET:HE2	2:B:176:ARG:HG3	1.87	0.54
1:A:63:THR:O	1:A:67:GLN:HG2	2.07	0.54
2:B:63:THR:O	2:B:67:GLN:HG2	2.07	0.54
2:B:69:LEU:HD22	2:B:340:LEU:CD2	2.38	0.54
1:A:78:ILE:HD11	1:A:160:ILE:HG13	1.90	0.54
2:B:69:LEU:HD22	2:B:340:LEU:HD23	1.89	0.53
2:B:118:ALA:HB1	5:B:559:HOH:O	2.07	0.53
2:B:58:HIS:HD1	2:B:172:TYR:HH	1.57	0.53
1:A:337:ARG:NH1	1:A:338:ASP:OD1	2.42	0.53
1:A:135:THR:O	1:A:139:LEU:HB2	2.09	0.53
1:A:352:VAL:HB	1:A:357:SER:HB2	1.91	0.52
2:B:246:VAL:O	2:B:250:GLN:HG3	2.07	0.52
1:A:58:HIS:HB3	4:A:1:AHU:H3'	1.91	0.52
2:B:222:ARG:HG3	2:B:223:PRO:HD2	1.91	0.52
2:B:56:GLY:O	2:B:163:ARG:NH2	2.42	0.52
2:B:135:THR:O	2:B:139:LEU:HB2	2.10	0.51
1:A:104:GLN:HB3	5:A:528:HOH:O	2.10	0.51
1:A:57:PRO:HB3	1:A:235:ILE:HG23	1.93	0.51
2:B:214:ILE:CD1	2:B:232:LEU:HD12	2.41	0.51
1:A:85:MET:HE2	1:A:89:ARG:CG	2.40	0.51
1:A:212:ARG:HH12	1:A:216:ARG:CZ	2.24	0.51
2:B:208:LEU:O	2:B:236:ARG:NH2	2.43	0.51
2:B:298:LEU:HB2	5:B:687:HOH:O	2.11	0.51
1:A:208:LEU:O	1:A:236:ARG:NH2	2.42	0.50
1:A:212:ARG:HH22	1:A:216:ARG:NH2	2.10	0.50
1:A:213:HIS:CE1	1:A:232:LEU:HD21	2.46	0.50
1:A:246:VAL:O	1:A:250:GLN:HG3	2.12	0.50
2:B:72:LEU:CD2	2:B:337:ARG:HD3	2.42	0.50
1:A:65:THR:HG21	1:A:336:CYS:HB3	1.95	0.49
2:B:121:MET:CE	2:B:176:ARG:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:HIS:O	1:A:217:LEU:HB2	2.12	0.49
2:B:49:LEU:N	2:B:350:THR:O	2.42	0.48
2:B:301:ASN:OD1	2:B:303:ASP:HB2	2.13	0.48
2:B:109:GLN:HE21	2:B:109:GLN:N	2.11	0.48
1:A:320:ARG:O	1:A:320:ARG:HG2	2.13	0.48
2:B:287:THR:O	2:B:290:THR:HG22	2.14	0.48
1:A:109:GLN:HE21	1:A:109:GLN:N	2.12	0.48
2:B:66:THR:OG1	2:B:80:TYR:CE1	2.62	0.48
1:A:125:GLN:NE2	4:A:1:AHU:O4	2.27	0.48
1:A:280:ALA:O	1:A:281:ARG:HB3	2.14	0.47
1:A:58:HIS:H	1:A:58:HIS:HD1	1.61	0.47
2:B:78:ILE:HD11	2:B:160:ILE:CG1	2.44	0.47
2:B:352:VAL:HB	2:B:357:SER:HB2	1.96	0.47
2:B:106:ARG:HG3	2:B:106:ARG:NH1	2.26	0.47
1:A:287:THR:O	1:A:290:THR:HG22	2.15	0.47
2:B:53:TYR:HB2	2:B:203:ILE:HD13	1.96	0.47
2:B:116:ASP:O	2:B:120:VAL:HG23	2.15	0.47
2:B:218:ALA:HA	2:B:227:LEU:HD13	1.95	0.47
1:A:364:LEU:HD12	2:B:310:TRP:CZ2	2.50	0.47
1:A:84:PRO:HG3	1:A:368:PHE:HZ	1.81	0.46
1:A:89:ARG:HD2	1:A:95:GLU:OE1	2.16	0.46
2:B:70:VAL:HG22	2:B:78:ILE:HG12	1.97	0.46
2:B:337:ARG:NH1	2:B:338:ASP:OD1	2.48	0.46
1:A:65:THR:HG21	1:A:336:CYS:CB	2.46	0.46
1:A:106:ARG:HG3	1:A:106:ARG:NH1	2.26	0.46
2:B:87:TYR:HB2	2:B:372:MET:HG2	1.99	0.45
1:A:83:GLU:HA	1:A:84:PRO:HD3	1.70	0.45
1:A:79:VAL:HG23	1:A:157:LEU:HD11	1.97	0.45
2:B:188:LEU:HD23	2:B:188:LEU:HA	1.73	0.45
1:A:299:ALA:O	1:A:301:ASN:N	2.49	0.45
2:B:57:PRO:HB2	2:B:213:HIS:HE1	1.82	0.45
2:B:214:ILE:HD12	2:B:232:LEU:HD12	1.98	0.45
1:A:371:GLU:OE2	2:B:307:VAL:HG22	2.17	0.44
2:B:164:HIS:CG	2:B:165:PRO:HD2	2.52	0.44
2:B:162:ASP:O	2:B:163:ARG:HB2	2.16	0.44
2:B:222:ARG:NH1	5:B:675:HOH:O	2.41	0.44
2:B:68:LEU:HB3	2:B:337:ARG:HG3	2.00	0.44
2:B:101:TYR:CZ	2:B:225:GLU:HG3	2.54	0.43
2:B:209:PRO:HD3	5:B:606:HOH:O	2.17	0.43
2:B:66:THR:HG1	2:B:80:TYR:HE1	1.57	0.43
1:A:53:TYR:HB2	1:A:203:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD21	1:A:161:PHE:HZ	1.84	0.43
1:A:164:HIS:CG	1:A:165:PRO:CD	3.02	0.43
2:B:208:LEU:HD11	2:B:212:ARG:NH1	2.34	0.43
2:B:281:ARG:HA	2:B:282:PRO:HD3	1.89	0.43
1:A:234:ALA:O	1:A:238:VAL:HG23	2.19	0.43
1:A:130:MET:HB3	1:A:131:PRO:HD3	2.00	0.42
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.77	0.42
1:A:259:TRP:CH2	1:A:293:ARG:HG2	2.54	0.42
1:A:80:TYR:CE2	1:A:82:PRO:HB3	2.54	0.42
1:A:220:ARG:HA	5:A:698:HOH:O	2.18	0.42
1:A:85:MET:HE2	1:A:89:ARG:HG2	2.01	0.42
2:B:232:LEU:O	2:B:236:ARG:HG3	2.19	0.42
1:A:79:VAL:HG11	1:A:365:ALA:HB3	2.02	0.42
1:A:58:HIS:CB	4:A:1:AHU:H3'	2.49	0.42
2:B:79:VAL:HG11	2:B:365:ALA:HB3	2.02	0.42
2:B:83:GLU:HG2	2:B:88:TRP:CZ3	2.55	0.42
2:B:130:MET:HB3	2:B:131:PRO:HD3	2.03	0.41
2:B:259:TRP:CH2	2:B:293:ARG:HG2	2.55	0.41
2:B:109:GLN:CA	2:B:109:GLN:NE2	2.83	0.41
2:B:216:ARG:HH21	2:B:220:ARG:HD2	1.84	0.41
1:A:119:VAL:HG12	2:B:119:VAL:CG1	2.47	0.41
2:B:299:ALA:HB1	2:B:300:PRO:CD	2.51	0.41
1:A:109:GLN:NE2	1:A:109:GLN:CA	2.84	0.41
2:B:356:GLY:C	2:B:359:PRO:HD2	2.41	0.41
2:B:89:ARG:HD2	2:B:95:GLU:OE1	2.21	0.40
2:B:232:LEU:CD1	2:B:236:ARG:HD2	2.45	0.40
2:B:299:ALA:HB1	2:B:300:PRO:HD2	2.03	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	292/331 (88%)	277 (95%)	13 (4%)	2 (1%)	22 30
2	B	296/331 (89%)	284 (96%)	12 (4%)	0	100 100
All	All	588/662 (89%)	561 (95%)	25 (4%)	2 (0%)	41 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ARG
1	A	300	PRO

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	241/263 (92%)	220 (91%)	21 (9%)	10 14
2	B	243/264 (92%)	219 (90%)	24 (10%)	8 10
All	All	484/527 (92%)	439 (91%)	45 (9%)	9 11

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

Mol	Chain	Res	Type
1	A	50	LEU
1	A	77	ASP
1	A	89	ARG
1	A	107	LEU
1	A	109	GLN
1	A	121	MET
1	A	130	MET
1	A	165	PRO
1	A	173	PRO
1	A	178	LEU
1	A	212	ARG
1	A	217	LEU
1	A	220	ARG
1	A	227	LEU

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Mol	Chain	Res	Type
1	A	232	LEU
1	A	281	ARG
1	A	293	ARG
1	A	307	VAL
1	A	341	LEU
1	A	354	THR
1	A	362	CYS
2	B	50	LEU
2	B	72	LEU
2	B	89	ARG
2	B	107	LEU
2	B	109	GLN
2	B	130	MET
2	B	159	LEU
2	B	165	PRO
2	B	173	PRO
2	B	178	LEU
2	B	182	MET
2	B	212	ARG
2	B	214	ILE
2	B	217	LEU
2	B	219	LYS
2	B	222	ARG
2	B	232	LEU
2	B	280	PRO
2	B	281	ARG
2	B	293	ARG
2	B	307	VAL
2	B	341	LEU
2	B	354	THR
2	B	362	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	142	HIS
1	A	342	GLN
2	B	109	GLN
2	B	142	HIS
2	B	221	GLN
2	B	323	HIS

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Mol	Chain	Res	Type
2	B	342	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	AHU	A	1	-	19,19,19	1.25	2 (10%)	24,27,27	2.43	14 (58%)
3	SO4	B	4	-	4,4,4	1.29	0	6,6,6	0.95	0
3	SO4	A	3	-	4,4,4	0.93	0	6,6,6	0.81	0
4	AHU	B	2	-	19,19,19	2.74	7 (36%)	24,27,27	2.85	14 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHU	A	1	-	-	1/6/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AHU	B	2	-	-	0/6/19/19	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	AHU	C2-N3	-7.16	1.25	1.38
4	B	2	AHU	C3'-C4'	-4.51	1.44	1.52
4	B	2	AHU	C2'-C1'	-4.33	1.44	1.53
4	A	1	AHU	O3'-C3'	-3.50	1.35	1.43
4	B	2	AHU	C7'-C4'	3.37	1.63	1.51
4	B	2	AHU	C6'-C1'	-3.37	1.46	1.51
4	B	2	AHU	C2-N1	-3.07	1.33	1.38
4	B	2	AHU	O7'-C7'	2.25	1.51	1.42
4	A	1	AHU	C6-C5	-2.08	1.29	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	AHU	O5'-C4'-C3'	-7.84	96.49	109.64
4	A	1	AHU	C4-C5-I	4.39	125.80	118.54
4	B	2	AHU	O5'-C4'-C7'	4.16	113.73	107.20
4	A	1	AHU	C7'-C4'-C3'	-3.98	107.98	113.54
4	B	2	AHU	O4-C4-N3	-3.92	112.60	120.12
4	B	2	AHU	C4-C5-I	3.52	124.36	118.54
4	A	1	AHU	O3'-C3'-C4'	-3.49	102.62	110.01
4	B	2	AHU	C1'-N1-C6	3.41	125.16	119.77
4	B	2	AHU	C7'-C4'-C3'	3.32	118.17	113.54
4	B	2	AHU	O3'-C3'-C4'	-3.16	103.32	110.01
4	A	1	AHU	N3-C2-N1	-3.12	110.74	114.89
4	B	2	AHU	C1'-N1-C2	-3.01	113.41	117.13
4	A	1	AHU	O5'-C4'-C7'	2.94	111.82	107.20
4	A	1	AHU	O4-C4-N3	-2.91	114.55	120.12
4	A	1	AHU	O3'-C3'-C2'	2.83	116.97	109.94
4	A	1	AHU	C2'-C3'-C4'	2.83	114.44	110.77
4	A	1	AHU	O7'-C7'-C4'	-2.79	101.72	111.29
4	B	2	AHU	O5'-C6'-C1'	-2.69	107.37	111.47
4	B	2	AHU	C5-C4-N3	2.64	118.26	113.86
4	A	1	AHU	O5'-C4'-C3'	-2.52	105.42	109.64
4	B	2	AHU	C3'-C2'-C1'	2.51	115.34	112.39
4	B	2	AHU	N3-C2-N1	2.43	118.12	114.89
4	A	1	AHU	C1'-N1-C2	-2.39	114.18	117.13
4	A	1	AHU	C6-N1-C2	2.21	123.53	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	AHU	O2-C2-N1	2.20	125.71	122.79
4	A	1	AHU	C5-C6-N1	2.18	125.03	121.85
4	B	2	AHU	C2'-C3'-C4'	2.05	113.42	110.77
4	B	2	AHU	C6-C5-C4	-2.01	115.11	119.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	AHU	O5'-C4'-C7'-O7'

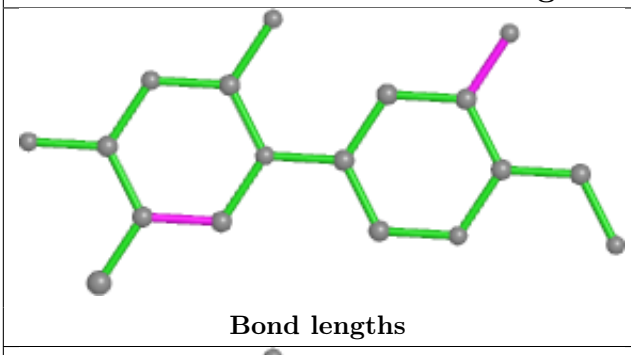
There are no ring outliers.

2 monomers are involved in 4 short contacts:

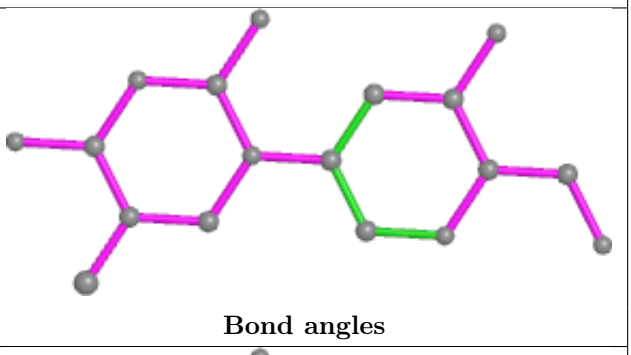
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	AHU	3	0
4	B	2	AHU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

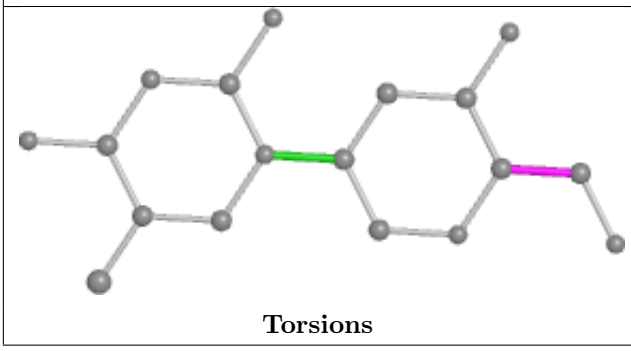
Ligand AHU A 1



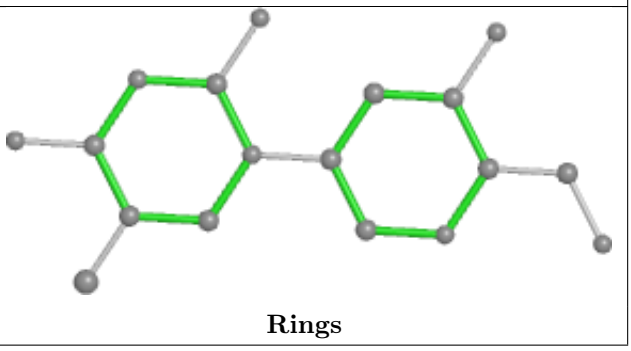
Bond lengths



Bond angles

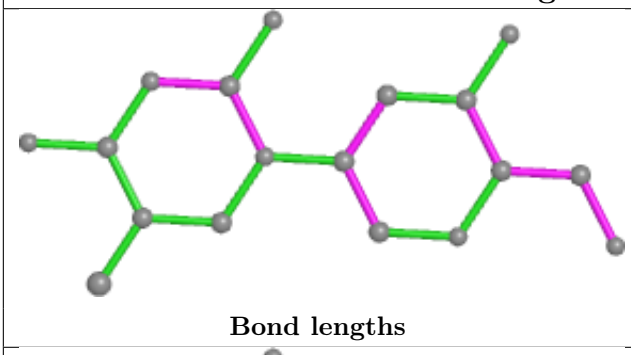


Torsions

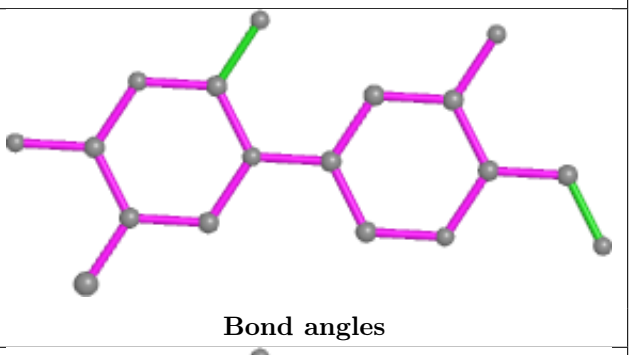


Rings

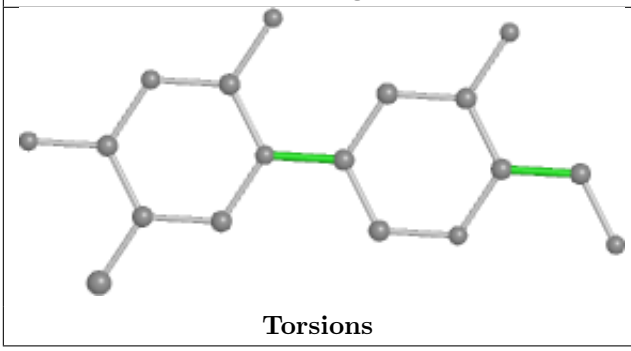
Ligand AHU B 2



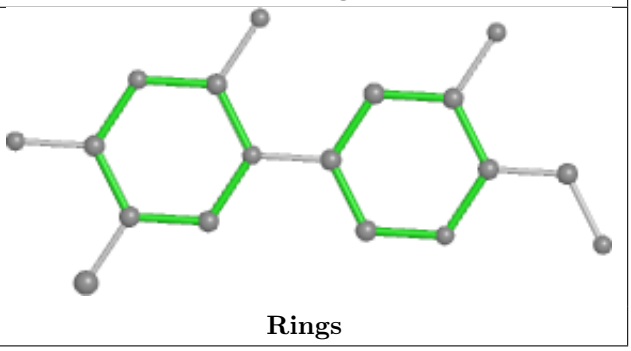
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.