



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:52 AM UTC

PDB ID : 1KI7 / pdb_00001ki7
Title : CRYSTAL STRUCTURE OF THYMIDINE KINASE FROM HERPES SIMPLEX VIRUS TYPE I COMPLEXED WITH 5-IODODEOXYURIDINE
Authors : Champness, J.N.; Bennett, M.S.; Wien, F.; Visse, R.; Summers, W.C.; Sander-son, M.R.
Deposited on : 1998-05-15
Resolution : 2.20 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

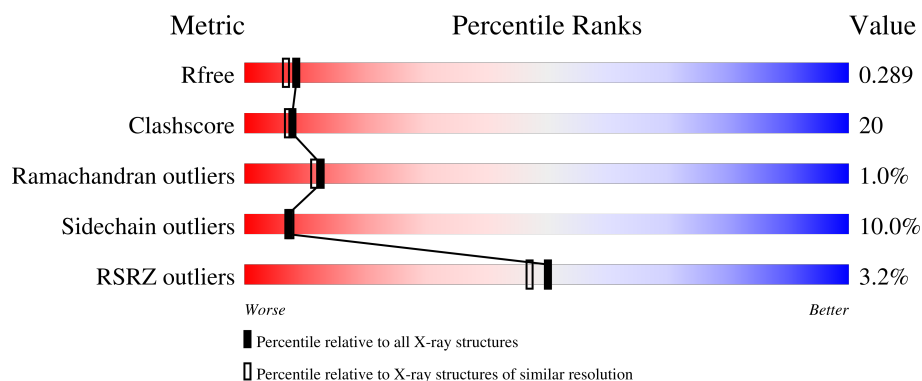
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	331	
1	B	331	

2 Entry composition [i](#)

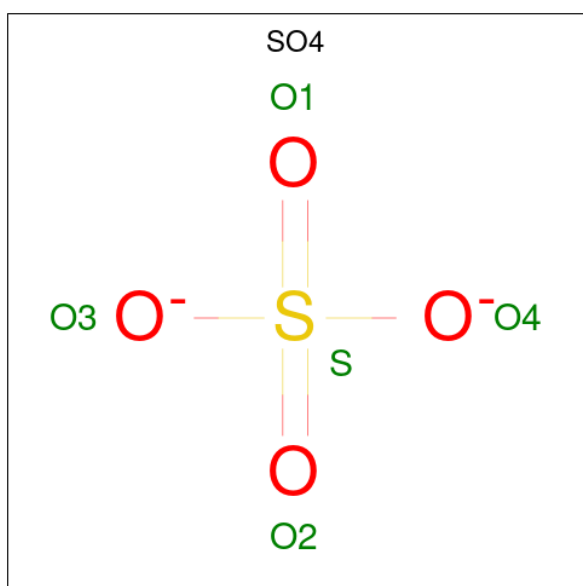
There are 4 unique types of molecules in this entry. The entry contains 4878 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

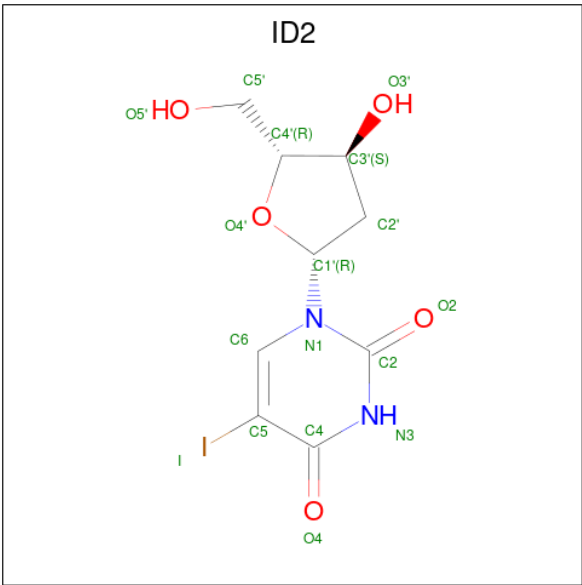
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	3
			2313	1473	407	418	15			
1	B	312	Total	C	N	O	S	0	0	3
			2360	1504	415	426	15			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 5-IODODEOXYURIDINE (CCD ID: ID2) (formula: C₉H₁₁IN₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	0	0
			17	9	1	2	5		
3	B	1	Total	C	I	N	O	0	0
			17	9	1	2	5		

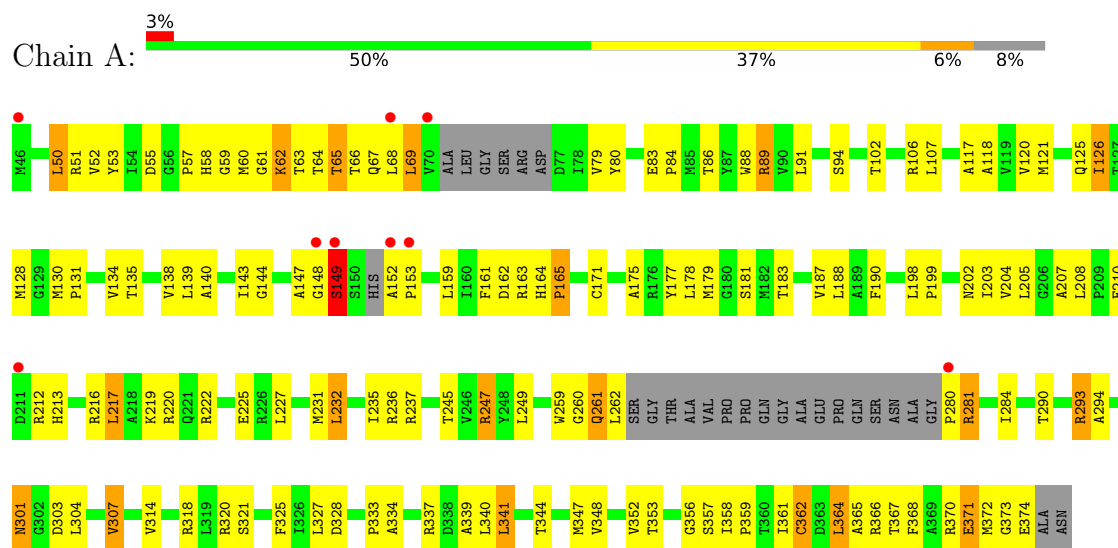
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	70	Total	O	0	0
			70	70		

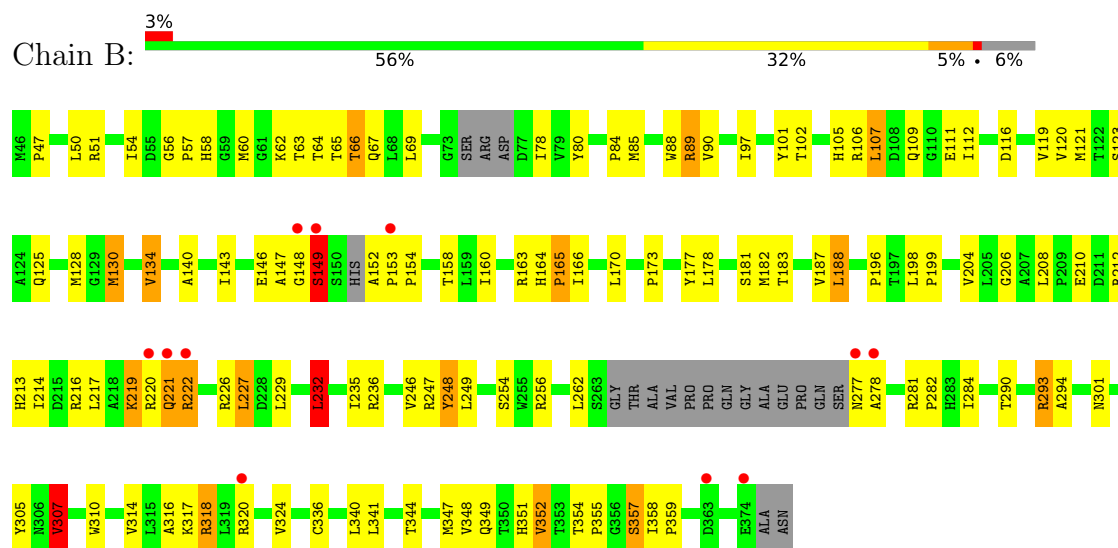
3 Residue-property plots [i](#)

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: THYMIDINE KINASE



• Molecule 1: THYMIDINE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.60Å 116.60Å 108.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.20 12.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.0 (12.00-2.20) 96.8 (12.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.21Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.206 , 0.286 0.226 , 0.289	Depositor DCC
R_{free} test set	3588 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4878	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 5.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ID2

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	0.91	2/2366 (0.1%)	1.15	18/3231 (0.6%)
1	B	0.95	3/2414 (0.1%)	1.16	20/3298 (0.6%)
All	All	0.93	5/4780 (0.1%)	1.16	38/6529 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	SER	C-N	-5.57	1.25	1.33
1	A	261	GLN	C-N	-5.54	1.25	1.33
1	B	177	TYR	C-O	-5.28	1.18	1.24
1	A	284	ILE	C-O	-5.26	1.17	1.24
1	B	232	LEU	C-O	-5.12	1.18	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ARG	N-CA-C	-8.43	100.79	112.25
1	B	152	ALA	CA-C-N	7.83	128.45	120.38
1	B	152	ALA	C-N-CA	7.83	128.45	120.38
1	A	307	VAL	CB-CA-C	-7.60	102.08	112.04
1	A	91	LEU	N-CA-C	7.50	120.11	111.11
1	A	280	PRO	N-CA-CB	7.03	110.73	103.00
1	B	177	TYR	N-CA-C	-6.82	103.78	111.14
1	A	373	GLY	N-CA-C	-6.74	103.44	112.14
1	A	294	ALA	CA-C-N	6.64	126.34	119.56
1	A	294	ALA	C-N-CA	6.64	126.34	119.56
1	B	307	VAL	CB-CA-C	-6.62	103.49	111.97
1	A	177	TYR	N-CA-C	-6.25	104.54	111.36
1	A	231	MET	N-CA-C	-6.19	104.61	111.36
1	B	222	ARG	N-CA-C	-6.09	101.12	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	TYR	N-CA-C	-6.03	101.99	110.50
1	B	210	GLU	N-CA-C	6.01	117.50	111.07
1	B	294	ALA	CA-C-N	5.99	125.67	119.56
1	B	294	ALA	C-N-CA	5.99	125.67	119.56
1	B	89	ARG	N-CA-C	5.82	121.09	113.30
1	A	128	MET	N-CA-C	5.77	117.57	111.28
1	B	221	GLN	N-CA-C	5.67	117.92	109.59
1	A	171	CYS	N-CA-C	5.60	117.08	110.97
1	A	371	GLU	N-CA-C	5.59	117.18	111.14
1	B	147	ALA	N-CA-C	-5.55	98.98	110.80
1	B	281	ARG	CA-C-N	-5.51	115.06	120.52
1	B	281	ARG	C-N-CA	-5.51	115.06	120.52
1	A	67	GLN	N-CA-C	-5.45	105.34	111.28
1	B	352	VAL	N-CA-C	-5.43	100.78	109.20
1	B	140	ALA	N-CA-C	5.38	121.71	109.81
1	B	293	ARG	N-CA-C	-5.35	107.30	112.97
1	B	357	SER	N-CA-C	-5.29	105.69	111.82
1	A	210	GLU	N-CA-C	5.27	116.72	110.97
1	A	334	ALA	N-CA-C	-5.25	105.20	111.03
1	B	351	HIS	N-CA-C	-5.21	103.80	110.53
1	A	65	THR	N-CA-C	-5.20	108.20	114.75
1	B	248	TYR	N-CA-C	-5.18	104.89	111.11
1	A	120	VAL	N-CA-C	-5.01	105.82	110.53
1	A	126	ILE	N-CA-C	-5.00	105.67	110.72

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	2313	0	2319	95	0
1	B	2360	0	2374	94	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	17	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	10	4	0
4	A	91	0	0	6	0
4	B	70	0	0	1	0
All	All	4878	0	4714	186	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 20.

All (186) 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:65:THR:HG21	1:B:336:CYS:HB2	1.57	0.84
1:B:121:MET:HB3	1:B:182:MET:HE2	1.59	0.83
1:A:68:LEU:HB3	1:A:337:ARG:HD3	1.64	0.80
1:B:246:VAL:HG21	1:B:324:VAL:HG21	1.65	0.79
1:A:69:LEU:HG	1:A:340:LEU:HD23	1.67	0.76
1:A:217:LEU:HD12	1:A:232:LEU:HG	1.67	0.76
1:A:293:ARG:HH11	1:A:293:ARG:HG3	1.53	0.73
1:A:130:MET:HB3	1:A:131:PRO:HD3	1.71	0.73
1:B:66:THR:HG23	1:B:160:ILE:HG21	1.69	0.72
1:B:66:THR:HG23	1:B:160:ILE:CG2	2.19	0.71
1:A:232:LEU:O	1:A:236:ARG:HG3	1.89	0.71
1:B:222:ARG:NH1	3:B:2:ID2:H5'2	2.05	0.71
1:B:247:ARG:HD2	1:B:282:PRO:HD3	1.73	0.70
1:B:232:LEU:O	1:B:236:ARG:HG3	1.92	0.70
1:B:63:THR:O	1:B:67:GLN:HG2	1.92	0.70
1:B:341:LEU:O	1:B:341:LEU:HD13	1.94	0.69
1:B:358:ILE:HB	1:B:359:PRO:HD3	1.75	0.68
1:B:69:LEU:HD11	1:B:341:LEU:HD23	1.76	0.67
1:B:217:LEU:HD13	1:B:227:LEU:CD1	2.25	0.67
1:B:109:GLN:HB3	1:B:111:GLU:HG3	1.78	0.66
1:A:83:GLU:HG2	1:A:88:TRP:CH2	2.32	0.65
1:B:69:LEU:HD22	1:B:340:LEU:CD2	2.28	0.64
1:A:213:HIS:CE1	1:A:232:LEU:HD21	2.33	0.63
1:A:301:ASN:HD21	1:A:303:ASP:HB2	1.62	0.63
1:B:78:ILE:HG12	1:B:158:THR:HB	1.79	0.63
1:A:356:GLY:O	1:A:359:PRO:HD2	1.98	0.62
1:B:262:LEU:HD11	1:B:284:ILE:HG12	1.82	0.62
1:A:51:ARG:NH2	1:A:199:PRO:O	2.32	0.61
1:A:118:ALA:HA	1:A:181:SER:O	1.99	0.61
1:B:107:LEU:HA	1:B:112:ILE:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:O	1:A:344:THR:HB	2.01	0.60
1:A:149:SER:OG	1:A:348:VAL:HG13	2.01	0.60
1:A:117:ALA:O	1:A:121:MET:HB2	2.02	0.60
1:B:65:THR:HG21	1:B:336:CYS:CB	2.29	0.59
1:B:217:LEU:HD13	1:B:227:LEU:HD11	1.85	0.59
1:B:248:TYR:HB2	1:B:282:PRO:HG2	1.84	0.59
1:B:314:VAL:O	1:B:318:ARG:HG2	2.04	0.58
1:A:62:LYS:NZ	1:A:62:LYS:HB2	2.19	0.57
1:B:125:GLN:HE22	3:B:2:ID2:HN3	1.51	0.57
1:B:116:ASP:O	1:B:120:VAL:HG23	2.05	0.57
1:B:277:ASN:CG	1:B:278:ALA:H	2.13	0.57
1:A:63:THR:HA	1:A:66:THR:HG22	1.86	0.57
1:A:207:ALA:HB3	1:A:328:ASP:HA	1.87	0.57
1:B:97:ILE:HD11	1:B:128:MET:HE1	1.87	0.57
1:A:55:ASP:O	1:A:205:LEU:HA	2.05	0.56
1:B:262:LEU:HD23	1:B:293:ARG:HG2	1.87	0.56
1:B:50:LEU:HD12	1:B:158:THR:HG23	1.88	0.56
1:B:56:GLY:O	1:B:163:ARG:NH2	2.39	0.56
1:B:101:TYR:HB3	1:B:226:ARG:HG2	1.87	0.56
1:B:97:ILE:HD12	3:B:2:ID2:O4'	2.06	0.55
1:B:85:MET:HE1	1:B:222:ARG:HD2	1.88	0.55
1:B:51:ARG:NH2	1:B:199:PRO:O	2.39	0.55
1:A:69:LEU:HD22	1:A:337:ARG:HG3	1.89	0.55
1:A:301:ASN:HD21	1:A:303:ASP:CB	2.18	0.55
1:B:66:THR:HG21	1:B:80:TYR:CE1	2.42	0.55
1:A:125:GLN:HE22	3:A:1:ID2:HN3	1.55	0.55
1:A:61:GLY:O	1:A:65:THR:HG23	2.06	0.54
1:A:352:VAL:HB	1:A:357:SER:HB2	1.89	0.54
1:A:356:GLY:C	1:A:359:PRO:HD2	2.33	0.53
1:B:85:MET:O	1:B:89:ARG:HG2	2.09	0.53
1:A:53:TYR:HB2	1:A:203:ILE:HD13	1.90	0.53
1:A:301:ASN:HD21	1:A:303:ASP:CG	2.17	0.53
1:A:352:VAL:HB	1:A:357:SER:CB	2.39	0.53
1:A:63:THR:HG23	2:A:3:SO4:O1	2.08	0.52
4:A:525:HOH:O	1:B:317:LYS:HD2	2.09	0.52
1:B:64:THR:O	1:B:67:GLN:HB2	2.10	0.52
1:A:222:ARG:HG3	3:A:1:ID2:H4'	1.91	0.52
1:B:219:LYS:HB2	1:B:219:LYS:NZ	2.24	0.52
1:B:84:PRO:HG2	1:B:88:TRP:CE2	2.45	0.52
1:B:247:ARG:HG3	1:B:277:ASN:HD21	1.75	0.52
1:B:262:LEU:HD23	1:B:293:ARG:CG	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASN:HD22	1:A:301:ASN:C	2.17	0.51
1:A:222:ARG:HG2	1:A:225:GLU:OE1	2.10	0.51
1:A:219:LYS:HB2	1:A:220:ARG:HH11	1.76	0.51
1:B:164:HIS:CD2	1:B:165:PRO:HD2	2.45	0.51
1:B:58:HIS:H	1:B:58:HIS:CD2	2.29	0.51
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.94	0.50
1:A:314:VAL:O	1:A:318:ARG:HG2	2.12	0.50
1:A:372:MET:CE	1:B:307:VAL:HG13	2.42	0.50
1:A:152:ALA:HB1	1:A:153:PRO:HD2	1.92	0.50
1:B:47:PRO:HG2	1:B:352:VAL:CG2	2.42	0.49
1:B:310:TRP:O	1:B:314:VAL:HG23	2.12	0.49
1:B:213:HIS:CE1	1:B:232:LEU:HD21	2.47	0.49
1:A:69:LEU:HD11	1:A:341:LEU:HD22	1.94	0.49
1:B:69:LEU:HD23	1:B:160:ILE:HD13	1.93	0.49
1:A:368:PHE:C	1:A:368:PHE:CD1	2.91	0.48
1:B:149:SER:HB3	1:B:349:GLN:HE21	1.78	0.48
1:A:62:LYS:HB2	1:A:62:LYS:HZ2	1.77	0.48
1:B:121:MET:HG3	1:B:181:SER:HB2	1.94	0.48
1:B:214:ILE:HG12	1:B:229:LEU:HD22	1.95	0.48
1:B:149:SER:HB3	1:B:349:GLN:NE2	2.28	0.48
1:B:217:LEU:CD1	1:B:232:LEU:HG	2.44	0.48
1:B:143:ILE:HG13	1:B:198:LEU:HD13	1.96	0.48
1:B:66:THR:CG2	1:B:80:TYR:CE1	2.96	0.48
1:B:69:LEU:HD23	1:B:160:ILE:CD1	2.44	0.48
1:B:232:LEU:O	1:B:235:ILE:HG22	2.13	0.48
1:A:63:THR:HG22	1:A:162:ASP:OD2	2.14	0.47
1:B:148:GLY:H	1:B:349:GLN:HB2	1.79	0.47
1:B:208:LEU:O	1:B:236:ARG:NH2	2.44	0.47
1:A:293:ARG:O	1:A:293:ARG:HG2	2.15	0.47
1:A:262:LEU:N	4:A:598:HOH:O	2.47	0.47
1:A:83:GLU:HG2	1:A:88:TRP:CZ3	2.49	0.47
1:A:293:ARG:HG3	1:A:293:ARG:NH1	2.26	0.47
1:B:102:THR:OG1	1:B:226:ARG:NH2	2.47	0.47
1:B:153:PRO:CB	1:B:154:PRO:HD2	2.44	0.47
1:A:144:GLY:O	1:A:199:PRO:HG3	2.14	0.46
1:A:281:ARG:N	1:A:281:ARG:HD2	2.31	0.46
1:A:162:ASP:O	1:A:163:ARG:HB2	2.15	0.46
1:A:175:ALA:O	1:A:179:MET:HG2	2.15	0.46
1:B:69:LEU:HD22	1:B:340:LEU:HD23	1.96	0.46
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.50	0.46
1:A:57:PRO:HB3	1:A:235:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ILE:HG13	1:B:116:ASP:CB	2.45	0.46
1:B:344:THR:O	1:B:347:MET:HB2	2.15	0.46
1:A:58:HIS:H	1:A:58:HIS:CD2	2.33	0.46
1:A:83:GLU:OE1	1:A:222:ARG:NH1	2.49	0.45
1:A:301:ASN:ND2	1:A:303:ASP:HB2	2.31	0.45
1:A:86:THR:HB	1:A:372:MET:HA	1.98	0.45
1:A:102:THR:O	1:A:106:ARG:HG3	2.16	0.45
1:A:138:VAL:HG21	1:B:310:TRP:HB3	1.99	0.45
1:A:147:ALA:O	1:A:148:GLY:C	2.60	0.45
1:A:62:LYS:NZ	1:A:62:LYS:CB	2.80	0.45
1:A:327:LEU:HD11	1:A:339:ALA:HB3	1.99	0.45
1:A:66:THR:HG23	1:A:80:TYR:CE1	2.52	0.45
1:A:79:VAL:HG11	1:A:365:ALA:CB	2.47	0.45
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.52	0.45
1:B:249:LEU:HD11	1:B:316:ALA:HA	1.99	0.45
1:A:86:THR:OG1	1:A:374:GLU:HG3	2.17	0.44
1:A:143:ILE:HD12	4:A:536:HOH:O	2.17	0.44
1:A:320:ARG:HG3	1:A:321:SER:N	2.31	0.44
4:A:567:HOH:O	1:B:130:MET:HA	2.16	0.44
1:A:216:ARG:O	1:A:217:LEU:C	2.61	0.44
1:B:57:PRO:HB2	1:B:213:HIS:HE1	1.82	0.44
1:B:149:SER:OG	1:B:347:MET:O	2.34	0.44
1:A:245:THR:O	1:A:249:LEU:HG	2.17	0.44
1:B:66:THR:HG23	1:B:160:ILE:HG22	1.95	0.44
1:A:213:HIS:O	1:A:217:LEU:HB2	2.17	0.44
1:A:140:ALA:HA	1:A:198:LEU:HD21	2.00	0.43
1:A:204:VAL:HA	1:A:325:PHE:O	2.18	0.43
1:B:153:PRO:HB3	1:B:154:PRO:HD2	2.00	0.43
1:A:62:LYS:HG2	4:A:613:HOH:O	2.18	0.43
1:A:135:THR:O	1:A:139:LEU:HB2	2.17	0.43
1:A:213:HIS:NE2	1:A:232:LEU:HD21	2.33	0.43
1:B:54:ILE:HD13	1:B:204:VAL:HB	2.01	0.43
1:B:112:ILE:HG13	1:B:116:ASP:HB3	1.99	0.43
1:B:352:VAL:HB	1:B:357:SER:HB2	2.00	0.43
1:B:102:THR:O	1:B:105:HIS:HB3	2.19	0.43
1:A:259:TRP:C	1:A:261:GLN:H	2.26	0.43
1:A:367:THR:O	1:A:370:ARG:HG2	2.19	0.43
1:B:354:THR:HG22	1:B:355:PRO:HD2	2.01	0.43
1:A:204:VAL:HG22	1:A:325:PHE:HB2	1.99	0.43
1:A:327:LEU:CD1	1:A:339:ALA:HB3	2.48	0.43
1:B:316:ALA:O	1:B:320:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HD13	1:A:52:VAL:CG2	2.49	0.42
1:A:362:CYS:O	1:A:366:ARG:HG3	2.18	0.42
1:B:284:ILE:HG22	4:B:533:HOH:O	2.19	0.42
1:B:60:MET:HE1	1:B:206:GLY:HA3	2.00	0.42
1:B:217:LEU:HD11	1:B:232:LEU:HG	2.01	0.42
1:A:159:LEU:HD13	1:A:161:PHE:CZ	2.54	0.42
1:A:57:PRO:O	1:A:60:MET:HE2	2.20	0.42
1:B:102:THR:O	1:B:106:ARG:HG3	2.19	0.42
1:A:89:ARG:O	1:A:94:SER:HA	2.18	0.42
1:A:202:ASN:CG	1:A:347:MET:HB3	2.45	0.42
3:B:2:ID2:O5'	3:B:2:ID2:H6	2.19	0.42
1:A:84:PRO:HG2	1:A:88:TRP:CE2	2.55	0.42
1:A:372:MET:HE1	1:B:307:VAL:HG13	2.02	0.41
1:A:371:GLU:OE2	1:B:307:VAL:HG22	2.20	0.41
1:B:58:HIS:O	1:B:213:HIS:NE2	2.42	0.41
1:B:146:GLU:OE2	1:B:348:VAL:HG11	2.20	0.41
1:B:183:THR:O	1:B:187:VAL:HG23	2.19	0.41
1:B:188:LEU:HD12	1:B:188:LEU:HA	1.94	0.41
1:A:208:LEU:O	1:A:236:ARG:NH2	2.53	0.41
1:A:183:THR:O	1:A:187:VAL:HG23	2.21	0.41
1:B:248:TYR:HA	1:B:282:PRO:HD2	2.02	0.41
1:A:126:ILE:CD1	1:A:190:PHE:HE1	2.34	0.41
1:A:361:ILE:O	1:A:364:LEU:HB3	2.21	0.41
1:B:166:ILE:O	1:B:170:LEU:HB3	2.20	0.41
1:B:217:LEU:C	1:B:219:LYS:H	2.28	0.41
1:B:246:VAL:HG11	1:B:324:VAL:HG23	2.02	0.41
1:A:69:LEU:CG	1:A:340:LEU:HD23	2.45	0.41
1:A:165:PRO:HA	4:A:628:HOH:O	2.20	0.41
1:A:281:ARG:HD2	1:A:281:ARG:H	1.85	0.41
1:A:59:GLY:O	1:A:216:ARG:HB2	2.21	0.40
1:A:247:ARG:HH11	1:A:247:ARG:HG2	1.87	0.40
1:B:219:LYS:O	1:B:221:GLN:N	2.54	0.40
1:B:130:MET:O	1:B:134:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	297/331 (90%)	278 (94%)	17 (6%)	2 (1%)	18	19
1	B	304/331 (92%)	284 (93%)	16 (5%)	4 (1%)	9	8
All	All	601/662 (91%)	562 (94%)	33 (6%)	6 (1%)	12	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	B	220	ARG
1	B	149	SER
1	B	227	LEU
1	A	260	GLY
1	B	90	VAL

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	242/264 (92%)	215 (89%)	27 (11%)	6	5
1	B	247/264 (94%)	225 (91%)	22 (9%)	9	10
All	All	489/528 (93%)	440 (90%)	49 (10%)	7	7

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	62	LYS
1	A	64	THR
1	A	69	LEU
1	A	89	ARG
1	A	107	LEU
1	A	134	VAL
1	A	149	SER
1	A	165	PRO
1	A	178	LEU
1	A	188	LEU
1	A	212	ARG
1	A	217	LEU
1	A	227	LEU
1	A	232	LEU
1	A	237	ARG
1	A	247	ARG
1	A	281	ARG
1	A	290	THR
1	A	301	ASN
1	A	304	LEU
1	A	307	VAL
1	A	333	PRO
1	A	341	LEU
1	A	353	THR
1	A	362	CYS
1	A	364	LEU
1	B	62	LYS
1	B	66	THR
1	B	107	LEU
1	B	119	VAL
1	B	123	SER
1	B	130	MET
1	B	134	VAL
1	B	165	PRO
1	B	173	PRO
1	B	178	LEU
1	B	188	LEU
1	B	196	PRO
1	B	212	ARG
1	B	216	ARG
1	B	219	LYS
1	B	232	LEU

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Mol	Chain	Res	Type
1	B	254	SER
1	B	256	ARG
1	B	290	THR
1	B	301	ASN
1	B	307	VAL
1	B	318	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	105	HIS
1	A	125	GLN
1	A	142	HIS
1	A	301	ASN
1	A	323	HIS
1	A	331	GLN
1	A	351	HIS
1	B	58	HIS
1	B	105	HIS
1	B	125	GLN
1	B	142	HIS
1	B	202	ASN
1	B	277	ASN
1	B	306	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SO4	A	3	-	4,4,4	0.84	0	6,6,6	0.62	0
3	ID2	A	1	-	18,18,18	1.26	2 (11%)	26,26,26	1.69	5 (19%)
3	ID2	B	2	-	18,18,18	1.64	3 (16%)	26,26,26	1.44	4 (15%)
2	SO4	B	4	-	4,4,4	0.78	0	6,6,6	0.76	0

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	ID2	A	1	-	-	0/6/18/18	0/2/2/2
3	ID2	B	2	-	-	0/6/18/18	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	ID2	C3'-C4'	-3.73	1.43	1.53
3	B	2	ID2	O3'-C3'	-3.51	1.36	1.43
3	A	1	ID2	O3'-C3'	-2.91	1.37	1.43
3	A	1	ID2	C4-C5	-2.82	1.39	1.45
3	B	2	ID2	C6-C5	2.21	1.41	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	ID2	O4'-C1'-C2'	-3.95	98.87	106.25
3	A	1	ID2	O2-C2-N1	3.74	127.67	122.80
3	B	2	ID2	N3-C2-N1	3.53	119.48	114.89
3	B	2	ID2	O4'-C1'-C2'	-3.42	99.86	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	ID2	O4'-C1'-N1	-2.61	103.24	107.86
3	A	1	ID2	O4'-C1'-N1	-2.49	103.45	107.86
3	A	1	ID2	C4'-O4'-C1'	2.48	115.41	109.51
3	A	1	ID2	C4-N3-C2	2.32	130.38	127.34
3	B	2	ID2	C6-N1-C2	-2.05	119.26	121.30

There are no chirality outliers.

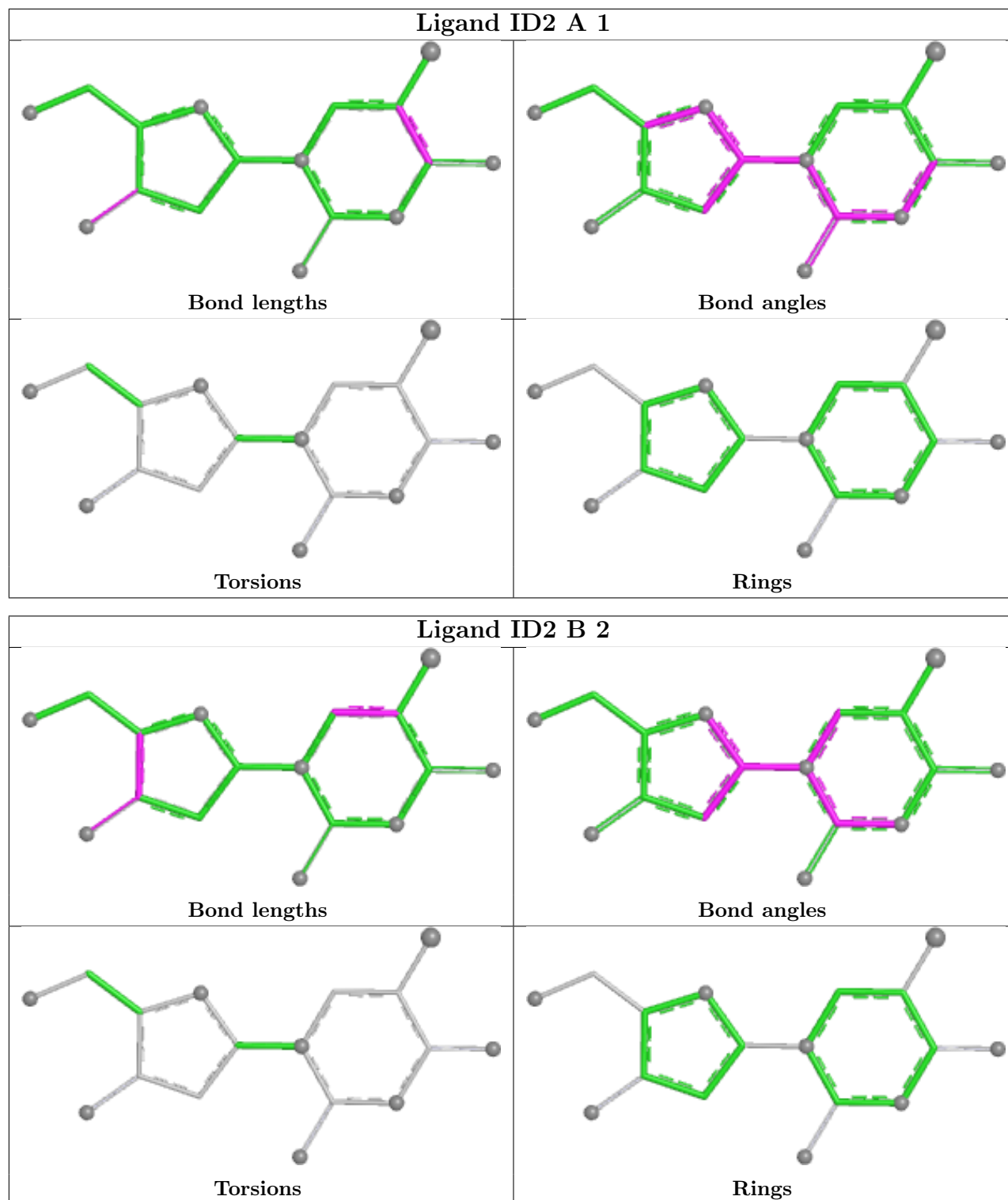
There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	SO4	1	0
3	A	1	ID2	2	0
3	B	2	ID2	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	305/331 (92%)	0.05	9 (2%) 52 49	4, 16, 31, 45	0
1	B	312/331 (94%)	0.07	11 (3%) 47 44	5, 15, 31, 43	0
All	All	617/662 (93%)	0.06	20 (3%) 50 47	4, 15, 31, 45	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	GLN	4.8
1	B	148	GLY	4.3
1	B	153	PRO	3.8
1	A	148	GLY	3.6
1	B	278	ALA	3.6
1	B	149	SER	3.3
1	B	222	ARG	3.3
1	A	152	ALA	3.3
1	A	68	LEU	3.1
1	A	280	PRO	3.1
1	B	220	ARG	3.1
1	A	149	SER	3.0
1	B	277	ASN	3.0
1	B	374	GLU	2.8
1	A	70	VAL	2.6
1	A	153	PRO	2.5
1	A	211	ASP	2.5
1	A	46	MET	2.5
1	B	320	ARG	2.0
1	B	363	ASP	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](#)

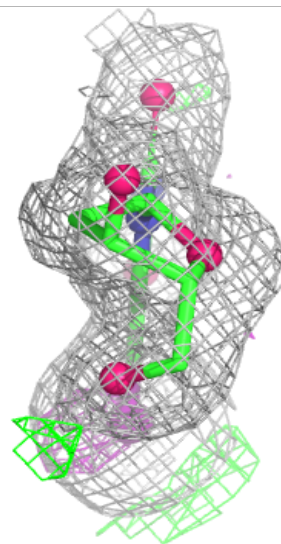
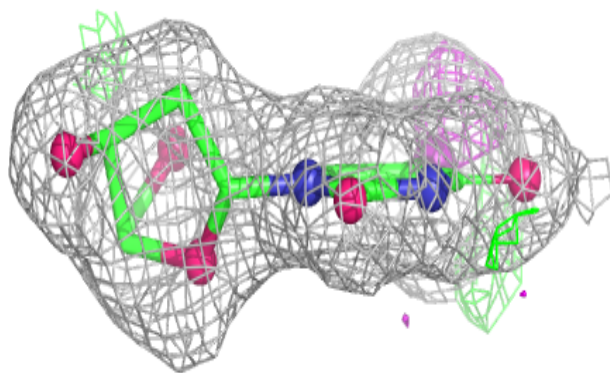
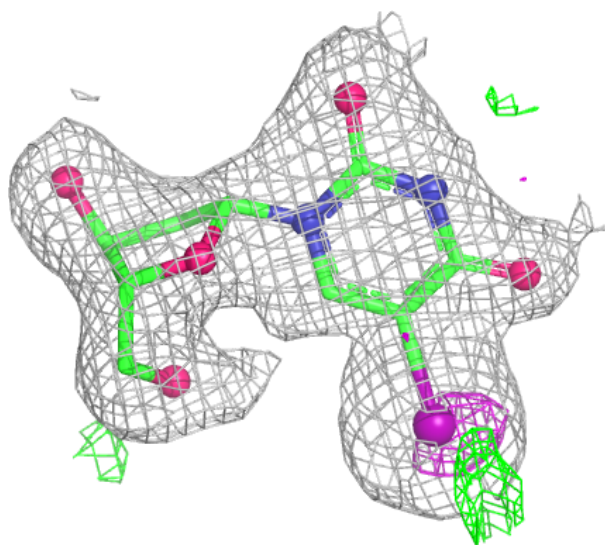
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	SO4	A	3	5/5	0.96	0.07	21,22,24,26	0
2	SO4	B	4	5/5	0.97	0.06	12,13,15,17	0
3	ID2	A	1	17/17	0.99	0.05	5,11,13,15	0
3	ID2	B	2	17/17	0.99	0.06	2,5,15,21	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.

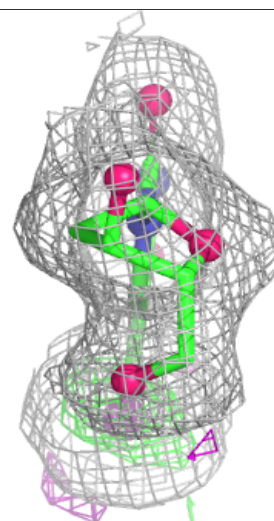
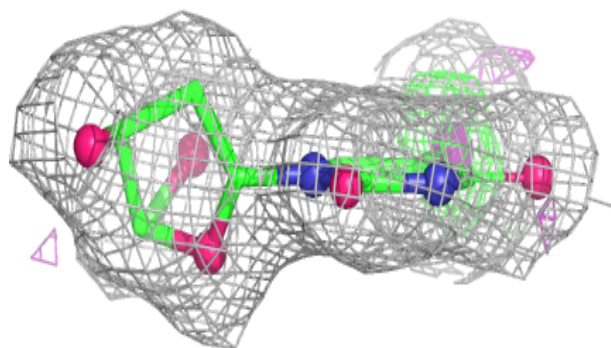
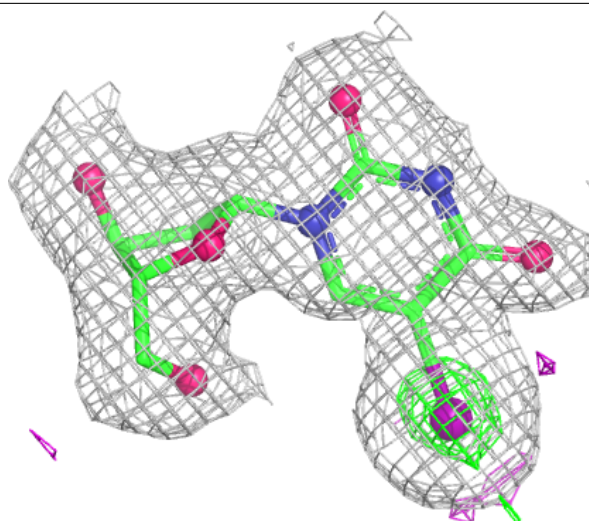
Electron density around ID2 A 1:

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



Electron density around ID2 B 2:

$2mF_o-DF_c$ (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.