



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:06 PM UTC

PDB ID : 6RGY / pdb_00006rgy
Title : Revisiting pH-gated conformational switch. Complex HK853-RR468 pH 7.5
Authors : Mideros-Mora, C.; Casino, P.; Marina, A.
Deposited on : 2019-04-18
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

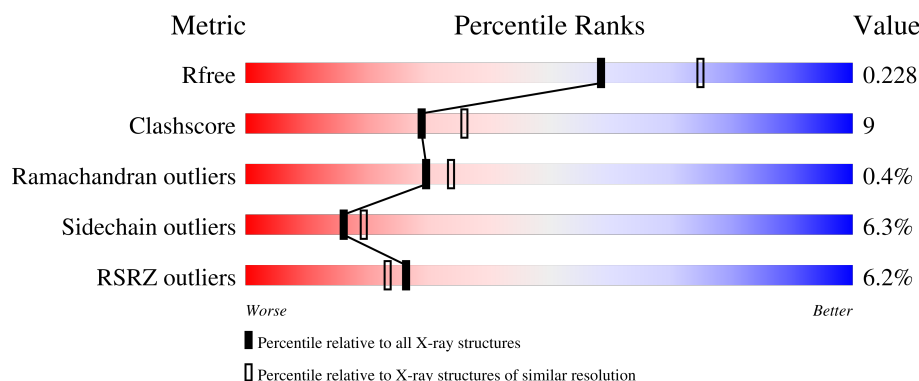
1 Overall quality at a glance

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	258	10% 76% 13% • 9%
1	B	258	4% 75% 13% • 9%
2	C	122	3% 80% 14% • •
2	D	122	3% 80% 18% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	204	-	-	X	-
4	SO4	D	203	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5990 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.

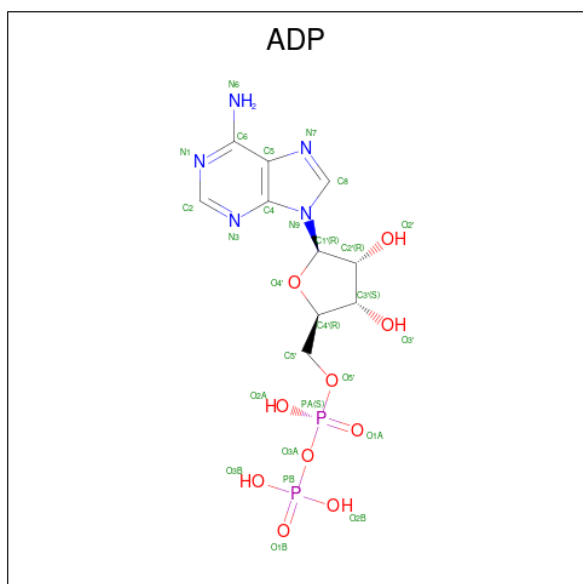
- Molecule 1 is a protein called Osmosensitive K⁺ channel histidine kinase KdpD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	1	0
			1822	1167	309	343	3			
1	B	236	Total	C	N	O	S	0	2	0
			1844	1178	311	352	3			

- Molecule 2 is a protein called Response regulator.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	C	120	Total	Be	C	F	N	O	S	0	0	0
			940	1	605	3	153	174	4			
2	D	121	Total	Be	C	F	N	O	S	0	0	0
			948	1	609	3	151	180	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

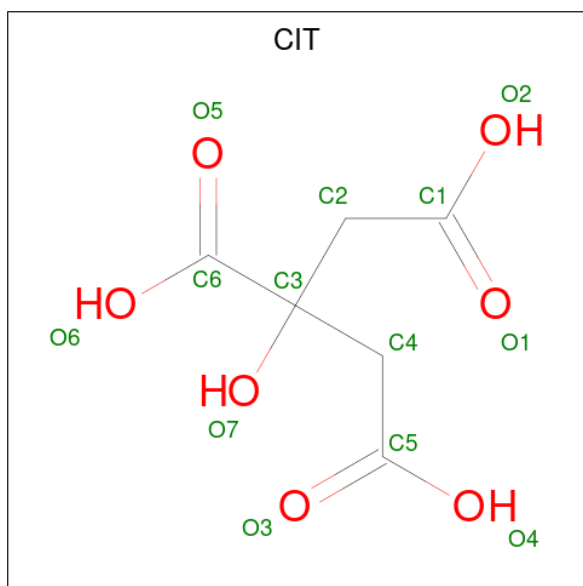
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	93	Total	O	0	0
			93	93		

Continued on next page...

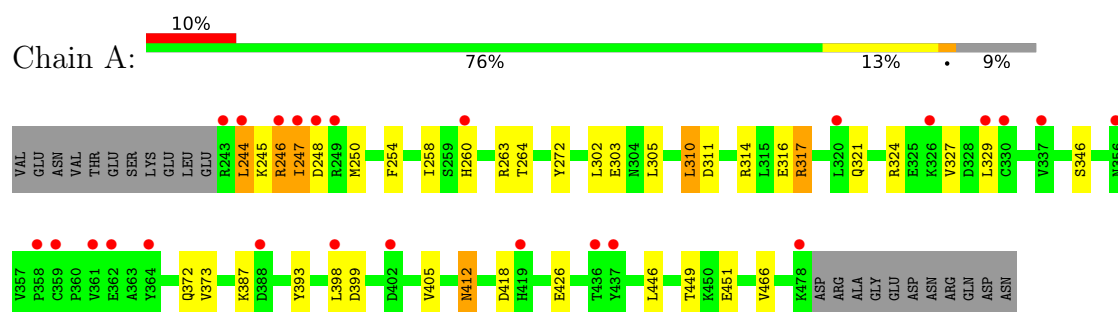
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	86	Total 86	O 86	0	0
7	C	57	Total 57	O 57	0	0
7	D	66	Total 66	O 66	0	0

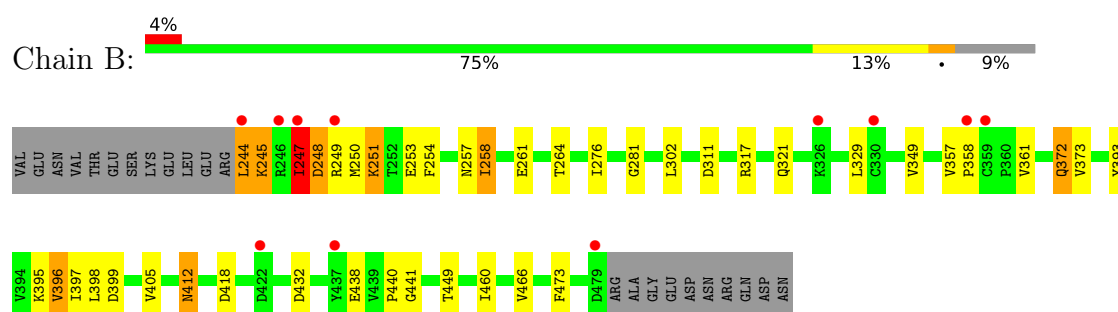
3 Residue-property plots [i](#)

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.

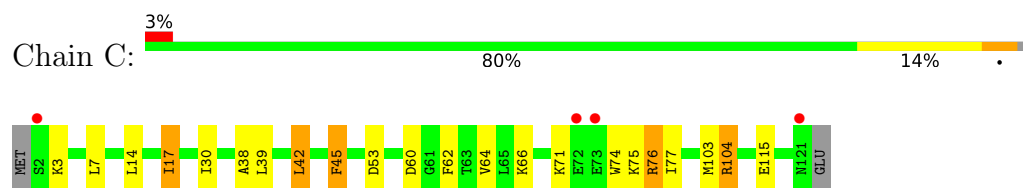
- Molecule 1: Osmosensitive K⁺ channel histidine kinase KdpD



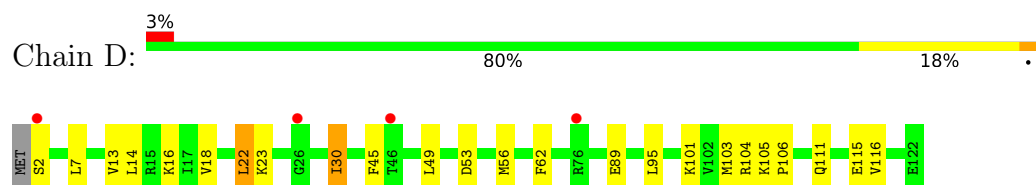
- Molecule 1: Osmosensitive K⁺ channel histidine kinase KdpD



- Molecule 2: Response regulator



- Molecule 2: Response regulator



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.47Å 92.71Å 174.52Å 90.00° 93.39° 90.00°	Depositor
Resolution (Å)	87.11 – 2.20 87.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (87.11-2.20) 99.7 (87.11-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.186 , 0.227 (Not available) , 0.228	Depositor DCC
R_{free} test set	2793 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, SO4, CIT, BFD

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	1.31	4/1857 (0.2%)	1.14	2/2526 (0.1%)
1	B	1.30	6/1881 (0.3%)	1.14	5/2555 (0.2%)
2	C	1.35	1/940 (0.1%)	1.16	5/1264 (0.4%)
2	D	1.35	4/948 (0.4%)	1.19	3/1274 (0.2%)
All	All	1.32	15/5626 (0.3%)	1.15	15/7619 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	THR	N-CA	-7.67	1.40	1.46
2	D	23	LYS	C-O	-6.05	1.16	1.24
2	D	30	ILE	C-O	-6.00	1.17	1.24
2	D	95	LEU	CA-C	5.58	1.60	1.52
1	A	264	THR	C-O	-5.53	1.19	1.24
1	B	281	GLY	C-O	-5.46	1.18	1.24
2	D	111	GLN	C-O	-5.39	1.17	1.24
1	B	258	ILE	C-O	-5.36	1.18	1.24
1	B	372	GLN	CA-C	5.34	1.59	1.52
1	A	303	GLU	C-O	-5.27	1.18	1.24
1	A	263	ARG	C-O	-5.18	1.18	1.24
1	A	446	LEU	C-O	-5.12	1.17	1.24
1	B	276	ILE	C-O	-5.12	1.18	1.24
1	B	264	THR	CA-C	5.10	1.58	1.52
2	C	17	ILE	C-O	-5.10	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	71	LYS	N-CA-C	-7.24	98.41	109.85
2	D	62	PHE	N-CA-C	-6.21	104.59	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	LYS	N-CA-C	-6.15	99.63	109.96
2	D	56	MET	CA-C-N	-6.07	114.51	120.52
2	D	56	MET	C-N-CA	-6.07	114.51	120.52
1	B	438	GLU	CA-C-N	-5.82	118.40	122.59
1	B	438	GLU	C-N-CA	-5.82	118.40	122.59
1	B	248	ASP	N-CA-C	-5.62	105.54	112.90
2	C	77	ILE	CA-C-N	-5.49	114.30	119.85
2	C	77	ILE	C-N-CA	-5.49	114.30	119.85
1	A	248	ASP	N-CA-C	-5.33	105.63	111.82
2	C	62	PHE	N-CA-C	-5.15	105.74	111.36
1	B	253	GLU	N-CA-C	-5.08	105.83	111.36
1	B	396	VAL	N-CA-CB	5.06	117.06	110.99
2	C	45	PHE	N-CA-C	5.03	116.46	108.96

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	1822	0	1790	39	0
1	B	1844	0	1828	29	0
2	C	940	0	975	18	0
2	D	948	0	974	13	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
4	C	15	0	0	2	0
4	D	20	0	0	3	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	D	13	0	5	0	0
7	A	93	0	0	1	0
7	B	86	0	0	1	0
7	C	57	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	66	0	0	1	0
All	All	5990	0	5596	98	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 9.

All (98) 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)
2:C:76:ARG:HH11	2:C:76:ARG:HG2	1.25	0.97
1:A:247:ILE:HG23	1:A:250:MET:H	1.27	0.96
1:A:310:LEU:HD13	1:A:314:ARG:NH2	1.82	0.94
1:A:246:ARG:NH2	1:A:246:ARG:HB2	1.81	0.94
1:A:246:ARG:HB2	1:A:246:ARG:CZ	2.00	0.90
2:C:74:TRP:O	2:C:76:ARG:N	2.10	0.83
1:A:247:ILE:HG23	1:A:250:MET:N	1.95	0.82
2:C:76:ARG:HG2	2:C:76:ARG:NH1	1.94	0.81
1:A:254:PHE:CZ	1:A:258:ILE:HD11	2.19	0.76
1:A:246:ARG:HG3	1:A:247:ILE:H	1.52	0.74
1:B:248:ASP:OD1	1:B:251:LYS:NZ	2.21	0.71
1:A:310:LEU:HD13	1:A:314:ARG:HH22	1.53	0.71
2:D:104:ARG:CZ	4:D:203:SO4:O2	2.39	0.70
1:A:247:ILE:HG22	1:A:250:MET:CG	2.20	0.70
1:B:261[A]:GLU:HG2	1:B:440:PRO:HB2	1.73	0.70
1:B:329:LEU:CD2	1:B:405:VAL:HG11	2.22	0.70
1:B:261[A]:GLU:CG	1:B:440:PRO:HB2	2.22	0.69
1:A:247:ILE:CG2	1:A:250:MET:HG3	2.23	0.68
1:B:247:ILE:CG2	1:B:250:MET:H	2.08	0.67
1:A:246:ARG:HG3	1:A:247:ILE:N	2.09	0.67
1:B:244:LEU:O	1:B:245:LYS:HB2	1.94	0.67
1:A:310:LEU:HD13	1:A:314:ARG:CZ	2.25	0.66
1:B:247:ILE:HG23	1:B:250:MET:H	1.62	0.65
1:B:247:ILE:HG23	1:B:249:ARG:N	2.12	0.65
1:B:254:PHE:CZ	1:B:258:ILE:HD11	2.32	0.64
1:B:373:VAL:HG13	1:B:449:THR:HG23	1.79	0.64
1:A:412:ASN:H	1:A:412:ASN:HD22	1.47	0.62
2:C:76:ARG:HH11	2:C:76:ARG:CG	2.07	0.62
1:A:310:LEU:HD11	1:A:314:ARG:NH1	2.17	0.60
1:A:329:LEU:CD2	1:A:405:VAL:HG11	2.33	0.58
2:C:103:MET:HE3	2:C:115:GLU:HG3	1.86	0.58
2:D:18:VAL:HG12	2:D:22:LEU:HD22	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:HA	1:A:316:GLU:OE2	2.03	0.58
1:A:247:ILE:HG22	1:A:250:MET:HB2	1.86	0.57
1:B:395:LYS:HE3	1:B:397:ILE:HD11	1.86	0.57
2:D:103:MET:HE1	2:D:115:GLU:HG3	1.87	0.57
2:C:74:TRP:C	2:C:76:ARG:H	2.13	0.56
1:B:412:ASN:HD22	1:B:412:ASN:H	1.55	0.55
1:A:247:ILE:HG22	1:A:250:MET:CB	2.36	0.55
1:A:393:TYR:H	1:A:412:ASN:HD21	1.54	0.54
1:A:311:ASP:OD2	1:A:372:GLN:NE2	2.40	0.54
1:A:244:LEU:N	1:A:244:LEU:HD12	2.22	0.54
1:A:317:ARG:HD3	7:A:645:HOH:O	2.06	0.54
2:D:13:VAL:HG23	4:D:204:SO4:O3	2.08	0.53
1:B:361:VAL:HG11	1:B:398:LEU:HD21	1.91	0.53
1:A:310:LEU:HD11	1:A:314:ARG:HH12	1.74	0.53
1:B:247:ILE:HG23	1:B:249:ARG:H	1.72	0.53
1:A:329:LEU:HD23	1:A:405:VAL:HG11	1.91	0.53
1:A:247:ILE:HG22	1:A:250:MET:HG3	1.85	0.53
1:A:246:ARG:CG	1:A:247:ILE:N	2.71	0.52
1:A:310:LEU:CD1	1:A:314:ARG:NH1	2.73	0.52
1:A:244:LEU:N	1:A:244:LEU:CD1	2.73	0.52
2:C:38:ALA:O	2:C:42:LEU:HD22	2.10	0.52
1:B:247:ILE:HG22	1:B:250:MET:HB2	1.91	0.51
2:C:30:ILE:HD12	2:C:30:ILE:N	2.26	0.51
1:B:393:TYR:H	1:B:412:ASN:HD21	1.59	0.51
1:A:398:LEU:HD23	1:A:399:ASP:N	2.26	0.50
2:C:76:ARG:CD	7:C:331:HOH:O	2.60	0.50
2:C:30:ILE:HD13	2:C:45:PHE:CE2	2.47	0.50
1:B:247:ILE:HG22	1:B:250:MET:CB	2.43	0.49
1:A:247:ILE:CG2	1:A:250:MET:CG	2.85	0.49
2:C:14:LEU:C	2:C:14:LEU:HD13	2.38	0.49
1:B:398:LEU:HD23	1:B:399:ASP:N	2.27	0.49
1:B:329:LEU:HD22	1:B:405:VAL:HG11	1.94	0.48
1:B:244:LEU:HD13	1:B:244:LEU:HA	1.77	0.47
1:B:257:ASN:HB3	1:B:441:GLY:O	2.14	0.47
1:B:311:ASP:OD2	1:B:372:GLN:NE2	2.48	0.47
2:C:104:ARG:HG3	4:C:204:SO4:O2	2.16	0.46
1:A:310:LEU:CD1	1:A:314:ARG:CZ	2.93	0.46
2:C:104:ARG:HD3	7:C:345:HOH:O	2.16	0.46
1:B:247:ILE:CG2	1:B:250:MET:N	2.78	0.45
2:D:14:LEU:C	2:D:14:LEU:HD13	2.41	0.45
2:D:104:ARG:NH2	4:D:203:SO4:O2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:LYS:NZ	7:D:304:HOH:O	2.50	0.45
1:A:373:VAL:HG13	1:A:449:THR:HG23	1.99	0.44
1:A:260:HIS:NE2	4:A:502:SO4:O2	2.50	0.44
2:D:103:MET:CE	2:D:115:GLU:HG3	2.46	0.44
2:D:103:MET:HE1	2:D:115:GLU:CG	2.47	0.44
1:B:398:LEU:HD23	1:B:398:LEU:C	2.43	0.44
1:B:357:VAL:HG22	1:B:358:PRO:HD2	1.98	0.44
1:B:460:ILE:HA	1:B:473:PHE:O	2.18	0.43
2:C:39:LEU:HA	2:C:42:LEU:HD23	2.00	0.43
1:A:451:GLU:HA	1:A:451:GLU:OE1	2.18	0.43
2:C:76:ARG:HD3	7:C:331:HOH:O	2.19	0.43
1:B:317:ARG:NH2	7:B:605:HOH:O	2.51	0.43
2:C:60:ASP:O	2:C:64:VAL:HG23	2.18	0.43
1:B:247:ILE:HG22	1:B:250:MET:H	1.83	0.43
2:C:104:ARG:NH2	4:C:204:SO4:O1	2.52	0.43
1:A:272:TYR:CE1	2:C:17:ILE:HB	2.54	0.42
2:D:30:ILE:HD13	2:D:45:PHE:CE2	2.54	0.42
2:D:49:LEU:CD2	2:D:116:VAL:HG13	2.50	0.42
1:A:247:ILE:CG2	1:A:250:MET:HB2	2.50	0.42
2:D:105:LYS:HA	2:D:106:PRO:C	2.45	0.42
1:A:247:ILE:CG2	1:A:250:MET:CB	2.97	0.41
2:D:30:ILE:N	2:D:30:ILE:HD12	2.36	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.94	0.40
1:A:412:ASN:HD22	1:A:412:ASN:N	2.11	0.40
1:B:247:ILE:HG22	1:B:250:MET:CG	2.51	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	235/258 (91%)	229 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	236/258 (92%)	227 (96%)	7 (3%)	2 (1%)	16	16
2	C	117/122 (96%)	112 (96%)	4 (3%)	1 (1%)	14	14
2	D	118/122 (97%)	114 (97%)	4 (3%)	0	100	100
All	All	706/760 (93%)	682 (97%)	21 (3%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	75	LYS
1	B	245	LYS
1	B	247	ILE

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	194/232 (84%)	178 (92%)	16 (8%)	10	12
1	B	201/232 (87%)	190 (94%)	11 (6%)	19	24
2	C	103/109 (94%)	97 (94%)	6 (6%)	18	22
2	D	104/109 (95%)	99 (95%)	5 (5%)	23	30
All	All	602/682 (88%)	564 (94%)	38 (6%)	16	19

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	LEU
1	A	245	LYS
1	A	246	ARG
1	A	247	ILE
1	A	302	LEU
1	A	305	LEU
1	A	310	LEU
1	A	317	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	321	GLN
1	A	324	ARG
1	A	327	VAL
1	A	346	SER
1	A	412	ASN
1	A	418	ASP
1	A	426	GLU
1	A	466	VAL
1	B	244	LEU
1	B	247	ILE
1	B	251	LYS
1	B	302	LEU
1	B	321	GLN
1	B	349	VAL
1	B	396	VAL
1	B	412	ASN
1	B	418	ASP
1	B	432	ASP
1	B	466	VAL
2	C	3	LYS
2	C	7	LEU
2	C	42	LEU
2	C	66	LYS
2	C	76	ARG
2	C	104	ARG
2	D	2	SER
2	D	7	LEU
2	D	22	LEU
2	D	89	GLU
2	D	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	HIS
1	A	412	ASN
1	B	260	HIS
1	B	347	HIS
1	B	412	ASN
2	C	69	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	BFD	C	53	2,5	8,11,12	5.03	3 (37%)	2,15,17	2.57	1 (50%)
2	BFD	D	53	2,5	8,11,12	4.70	3 (37%)	2,15,17	2.33	1 (50%)

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	BFD	C	53	2,5	-	1/5/11/13	-
2	BFD	D	53	2,5	-	1/5/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	53	BFD	F3-BE	8.55	1.73	1.54
2	D	53	BFD	F3-BE	8.13	1.72	1.54
2	C	53	BFD	F2-BE	7.92	1.71	1.54
2	C	53	BFD	F1-BE	7.91	1.71	1.54
2	D	53	BFD	F2-BE	7.53	1.71	1.54
2	D	53	BFD	F1-BE	6.97	1.69	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	53	BFD	OD2-CG-CB	-3.58	116.33	124.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	53	BFD	OD2-CG-CB	-3.12	117.39	124.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	53	BFD	CA-CB-CG-OD1
2	D	53	BFD	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
4	SO4	B	504	-	4,4,4	0.52	0	6,6,6	0.36	0
3	ADP	B	501	-	28,29,29	1.80	7 (25%)	43,45,45	1.91	17 (39%)
4	SO4	C	202	-	4,4,4	0.53	0	6,6,6	0.40	0
4	SO4	B	502	-	4,4,4	0.40	0	6,6,6	0.53	0
4	SO4	D	204	-	4,4,4	0.57	0	6,6,6	0.71	0
4	SO4	D	202	-	4,4,4	0.54	0	6,6,6	0.33	0
4	SO4	A	503	-	4,4,4	0.46	0	6,6,6	0.62	0
4	SO4	B	503	-	4,4,4	0.58	0	6,6,6	0.16	0
4	SO4	C	204	-	4,4,4	0.42	0	6,6,6	0.60	0
4	SO4	D	205	-	4,4,4	0.63	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	203	-	4,4,4	0.43	0	6,6,6	0.49	0
6	CIT	D	206	-	12,12,12	1.07	0	17,17,17	1.97	3 (17%)
4	SO4	C	203	-	4,4,4	0.51	0	6,6,6	0.22	0
4	SO4	A	502	-	4,4,4	0.58	0	6,6,6	0.25	0
3	ADP	A	501	-	28,29,29	2.08	8 (28%)	43,45,45	1.86	14 (32%)
4	SO4	A	504	-	4,4,4	0.54	0	6,6,6	0.36	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	ADP	B	501	-	-	3/16/32/32	0/3/3/3
6	CIT	D	206	-	-	10/16/16/16	-
3	ADP	A	501	-	-	2/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ADP	PA-O3A	7.21	1.67	1.59
3	B	501	ADP	C5-C4	4.21	1.46	1.39
3	A	501	ADP	C5-C4	4.09	1.46	1.39
3	A	501	ADP	C5-N7	-3.97	1.31	1.39
3	B	501	ADP	C5-N7	-3.93	1.31	1.39
3	B	501	ADP	C8-N7	3.42	1.38	1.31
3	B	501	ADP	PA-O3A	3.39	1.63	1.59
3	B	501	ADP	C2'-C1'	-2.69	1.45	1.53
3	A	501	ADP	C8-N9	-2.44	1.33	1.37
3	A	501	ADP	C2-N1	2.36	1.38	1.33
3	A	501	ADP	C2'-C1'	-2.36	1.46	1.53
3	A	501	ADP	C8-N7	2.23	1.36	1.31
3	A	501	ADP	C4-N9	-2.13	1.33	1.37
3	B	501	ADP	PB-O1B	-2.11	1.43	1.50
3	B	501	ADP	C2-N1	2.02	1.37	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	206	CIT	O7-C3-C6	-5.39	101.31	108.96
3	A	501	ADP	C4-N9-C8	4.18	110.13	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	ADP	O3A-PB-O1B	-3.83	90.91	111.04
3	A	501	ADP	N3-C4-N9	3.68	133.43	127.17
3	B	501	ADP	C4-N9-C1'	-3.61	118.19	126.63
6	D	206	CIT	O6-C6-C3	3.55	119.94	113.14
3	A	501	ADP	N6-C6-N1	3.37	125.88	118.38
3	B	501	ADP	N3-C2-N1	-3.36	123.49	128.58
3	B	501	ADP	O2B-PB-O1B	3.36	123.93	110.83
3	B	501	ADP	C5-C4-N3	-3.26	122.22	126.72
3	B	501	ADP	O2A-PA-O1A	2.91	126.00	112.44
3	A	501	ADP	O3B-PB-O1B	2.88	122.06	110.83
3	B	501	ADP	O3A-PB-O1B	-2.88	95.90	111.04
3	A	501	ADP	C2-N1-C6	2.78	123.30	118.73
3	A	501	ADP	O2A-PA-O1A	2.77	125.33	112.44
3	A	501	ADP	C5-C4-N3	-2.76	122.91	126.72
3	B	501	ADP	C2-N1-C6	2.75	123.25	118.73
3	A	501	ADP	C4-N9-C1'	-2.73	120.25	126.63
3	B	501	ADP	C1'-N9-C8	2.73	133.15	127.09
3	B	501	ADP	N3-C4-N9	2.46	131.35	127.17
3	B	501	ADP	O2A-PA-O3A	2.45	113.89	107.27
3	A	501	ADP	N9-C8-N7	-2.41	110.52	113.94
3	A	501	ADP	O3A-PA-O1A	-2.40	103.49	110.70
3	A	501	ADP	O3B-PB-O2B	2.37	116.70	107.80
3	B	501	ADP	O3A-PA-O1A	-2.30	103.78	110.70
3	B	501	ADP	N6-C6-N1	2.26	123.41	118.38
3	B	501	ADP	C2-N3-C4	2.25	117.34	111.83
3	A	501	ADP	N3-C2-N1	-2.21	125.24	128.58
6	D	206	CIT	C4-C3-C2	2.19	114.94	109.31
3	B	501	ADP	N9-C8-N7	-2.16	110.87	113.94
3	B	501	ADP	O3B-PB-O2B	2.16	115.89	107.80
3	B	501	ADP	C3'-C2'-C1'	2.05	105.35	101.46
3	A	501	ADP	C5-C4-N9	-2.03	103.60	105.81
3	B	501	ADP	C4-C5-N7	-2.02	108.28	110.58

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	PA-O3A-PB-O3B
3	B	501	ADP	PA-O3A-PB-O2B
6	D	206	CIT	O7-C3-C4-C5
6	D	206	CIT	O7-C3-C6-O5
6	D	206	CIT	O7-C3-C6-O6

Continued on next page...

Continued from previous page...

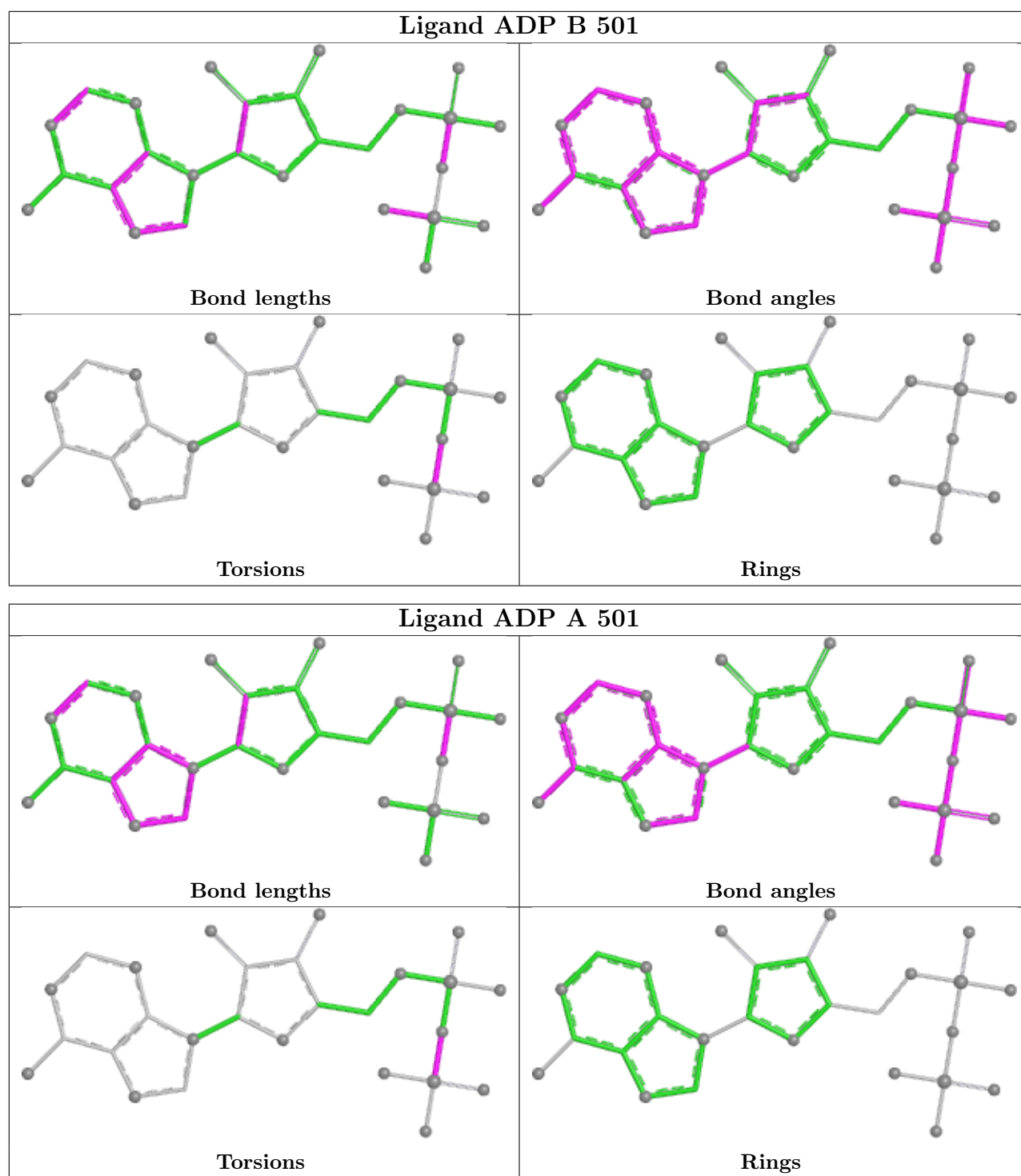
Mol	Chain	Res	Type	Atoms
6	D	206	CIT	C4-C3-C6-O5
6	D	206	CIT	C4-C3-C6-O6
6	D	206	CIT	C2-C3-C4-C5
6	D	206	CIT	C6-C3-C4-C5
6	D	206	CIT	C1-C2-C3-C6
6	D	206	CIT	C2-C3-C6-O6
3	B	501	ADP	PA-O3A-PB-O3B
6	D	206	CIT	C2-C3-C6-O5
3	A	501	ADP	PA-O3A-PB-O2B
3	B	501	ADP	PA-O3A-PB-O1B

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	204	SO4	1	0
4	C	204	SO4	2	0
4	D	203	SO4	2	0
4	A	502	SO4	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	236/258 (91%)	0.52	25 (10%) 11 8	20, 56, 99, 130	6 (2%)
1	B	236/258 (91%)	0.45	11 (4%) 36 33	20, 55, 94, 120	9 (3%)
2	C	119/122 (97%)	0.13	4 (3%) 48 45	32, 52, 91, 104	0
2	D	120/122 (98%)	0.24	4 (3%) 49 46	35, 53, 96, 110	0
All	All	711/760 (93%)	0.39	44 (6%) 26 23	20, 55, 96, 130	15 (2%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	5.9
1	B	247	ILE	5.8
1	A	247	ILE	5.3
1	B	244	LEU	5.3
1	B	246	ARG	4.6
1	A	243	ARG	4.3
1	A	330	CYS	3.7
1	A	402	ASP	3.6
1	A	337	VAL	3.6
1	A	326	LYS	3.5
1	A	437	TYR	3.4
1	A	356	ASN	3.3
1	B	479	ASP	3.0
1	A	359	CYS	2.9
1	A	246	ARG	2.9
2	D	2	SER	2.9
1	B	359	CYS	2.9
2	C	2	SER	2.8
2	C	73	GLU	2.8
1	B	249	ARG	2.7
1	B	422	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	46	THR	2.6
2	D	26	GLY	2.6
1	A	358	PRO	2.6
1	A	361	VAL	2.6
2	C	72	GLU	2.6
1	A	478	LYS	2.6
1	B	326	LYS	2.6
1	A	249	ARG	2.5
1	A	398	LEU	2.4
1	B	437	TYR	2.3
1	A	260	HIS	2.3
1	A	364	TYR	2.3
1	B	330	CYS	2.2
2	D	76	ARG	2.2
1	B	358	PRO	2.2
1	A	320	LEU	2.1
1	A	419	HIS	2.1
2	C	121	ASN	2.1
1	A	362	GLU	2.1
1	A	329	LEU	2.1
1	A	248	ASP	2.1
1	A	436	THR	2.0
1	A	388	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BFD	C	53	12/13	0.93	0.08	33,39,43,46	0
2	BFD	D	53	12/13	0.94	0.08	35,39,41,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

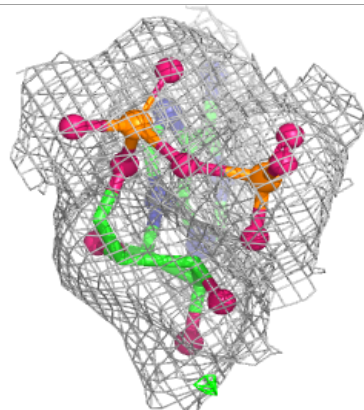
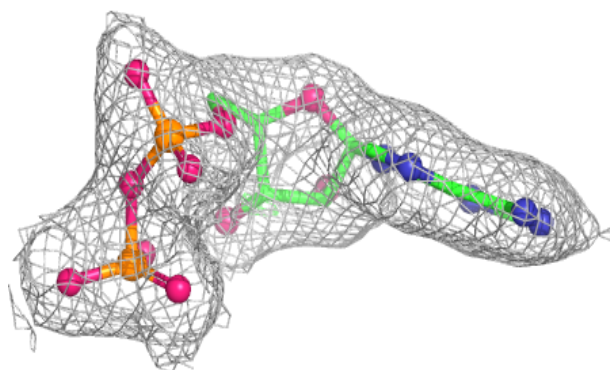
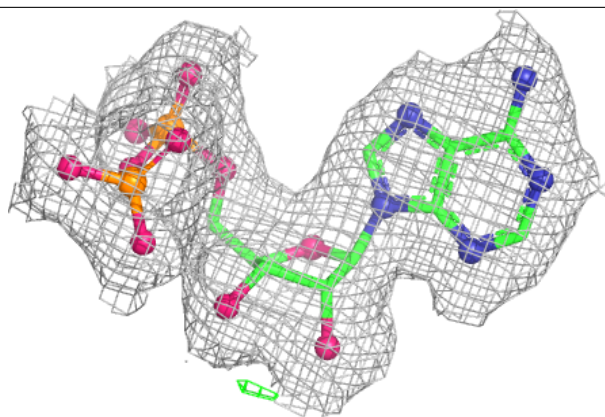
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CIT	D	206	13/13	0.67	0.14	83,100,108,108	0
4	SO4	C	203	5/5	0.76	0.08	103,109,110,122	0
4	SO4	A	502	5/5	0.80	0.13	85,100,101,105	0
4	SO4	D	205	5/5	0.82	0.14	81,83,96,100	0
4	SO4	A	503	5/5	0.84	0.10	73,75,84,88	0
4	SO4	B	504	5/5	0.86	0.10	82,93,98,99	0
4	SO4	D	202	5/5	0.86	0.12	80,91,97,102	0
4	SO4	A	504	5/5	0.88	0.10	77,83,95,100	0
4	SO4	B	502	5/5	0.89	0.09	75,76,82,84	0
4	SO4	C	204	5/5	0.91	0.09	73,74,78,79	0
4	SO4	D	203	5/5	0.91	0.09	61,74,76,81	0
4	SO4	B	503	5/5	0.92	0.09	78,80,92,94	0
4	SO4	D	204	5/5	0.94	0.08	67,69,75,81	0
4	SO4	C	202	5/5	0.96	0.08	66,67,72,74	0
3	ADP	A	501	27/27	0.98	0.05	35,39,45,45	0
3	ADP	B	501	27/27	0.98	0.05	35,39,45,46	0
5	MG	D	201	1/1	0.99	0.03	41,41,41,41	0
5	MG	C	201	1/1	0.99	0.04	42,42,42,42	0

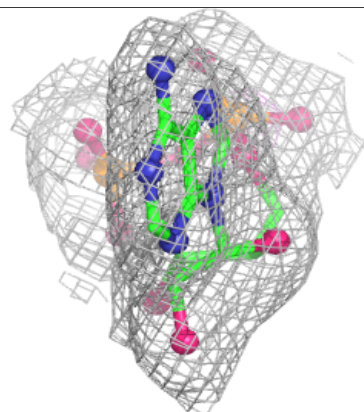
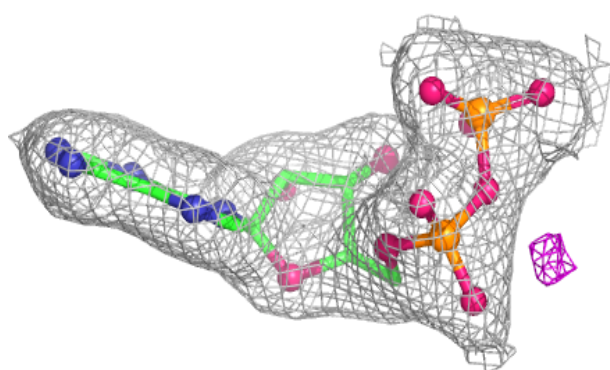
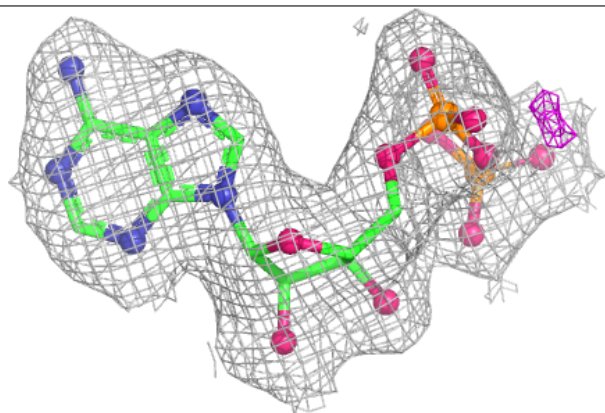
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 501:

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

**Electron density around ADP B 501:**

$2mF_o-DF_c$ (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.