Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 05:25 pm BST

PDB ID	:	6RH0 / pdb_00006rh0
Title	:	Revisiting pH-gated conformational switch. Complex HK853-RR468 pH 5.5
Authors	:	Mideros-Mora, C.; Casino, P.; Marina, A.
Deposited on	:	2019-04-18
Resolution	:	2.87 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 (i) 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 (i)) were used in the production of this report:

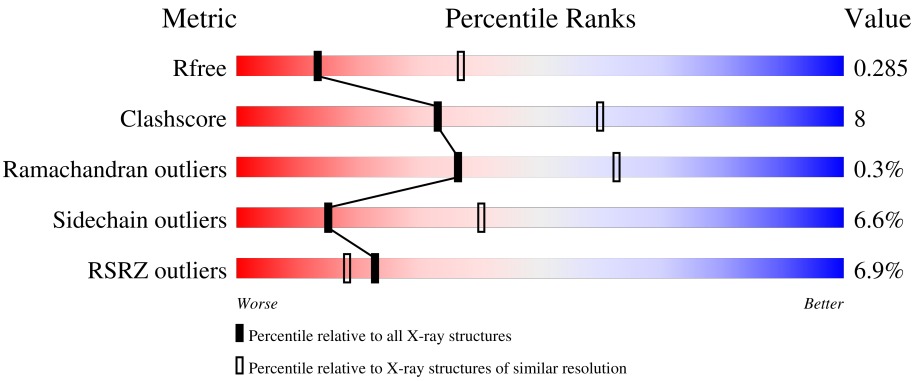
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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% 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	8% 67% 18% 9%
1	B	258	9% 83% 7% 9%
2	C	122	2% 94%
2	D	122	2% 93% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5805 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.

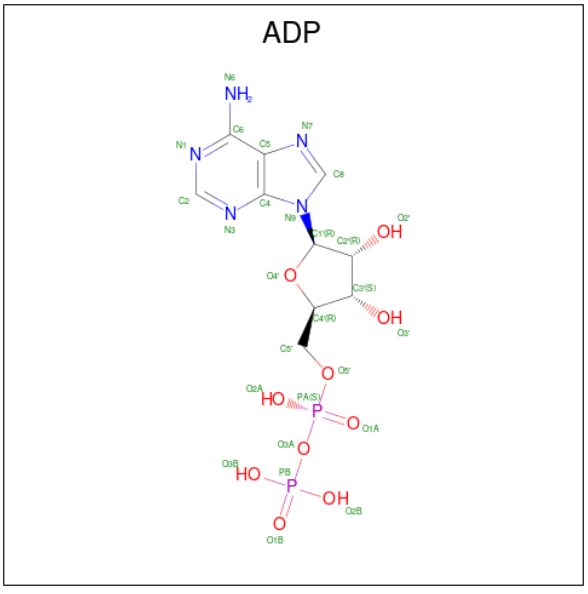
- Molecule 1 is a protein called Sensor histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1835	1172	309	351	3			
1	B	235	Total	C	N	O	S	0	0	0
			1811	1152	306	350	3			

- Molecule 2 is a protein called Response regulator.

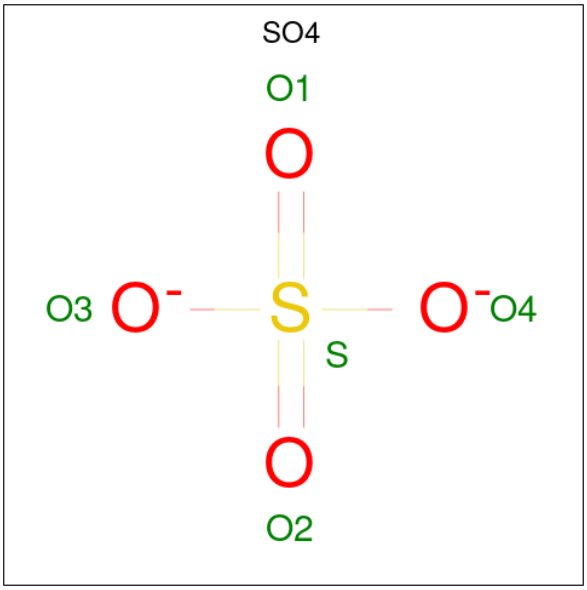
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	120	Total	C	N	O	S	0	0	0
			944	609	153	178	4			
2	D	121	Total	C	N	O	S	0	0	0
			945	610	154	177	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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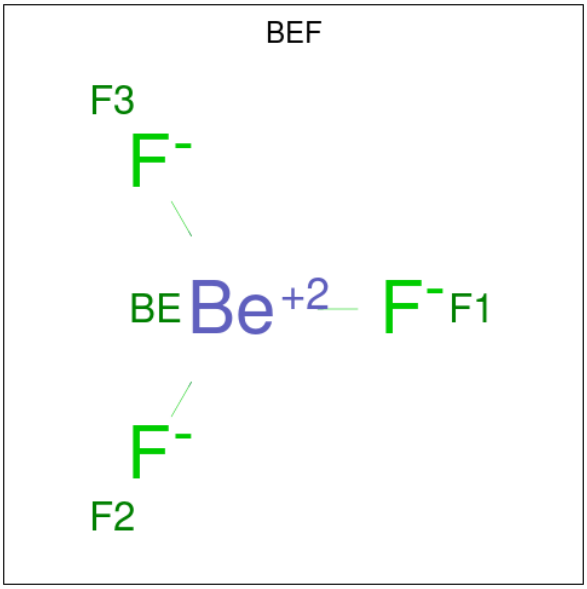
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

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

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

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Be F 4 1 3	0	0
6	D	1	Total Be F 4 1 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	44	Total O 44 44	0	0

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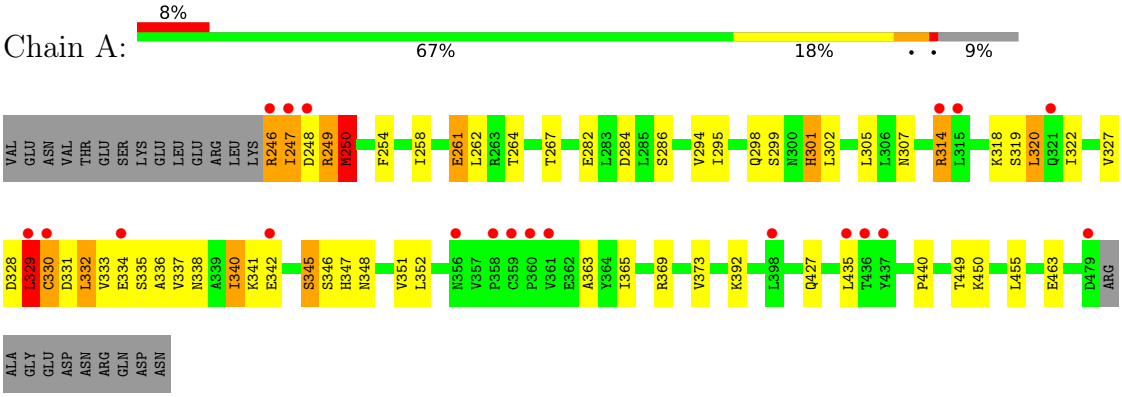
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	44	Total O 44 44	0	0
7	C	30	Total O 30 30	0	0
7	D	28	Total O 28 28	0	0

3 Residue-property plots

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.

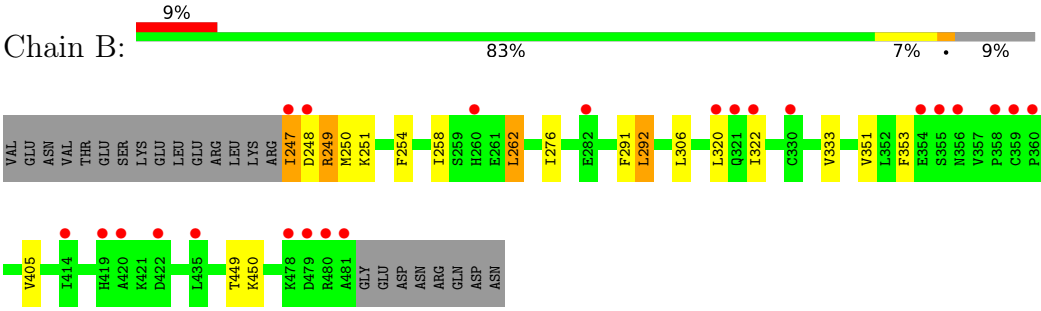
• Molecule 1: Sensor histidine kinase

Chain A:



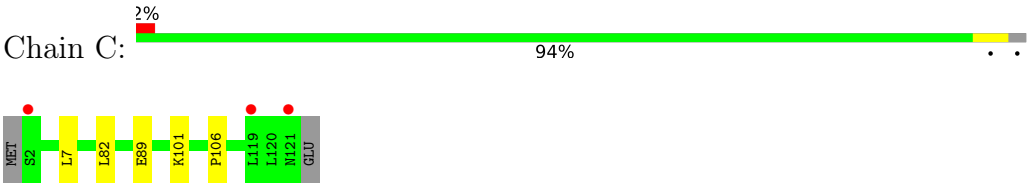
• Molecule 1: Sensor histidine kinase

Chain B:



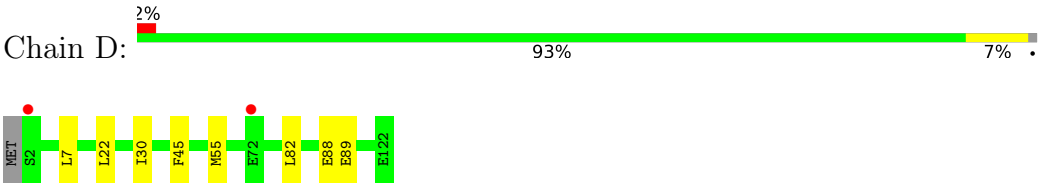
• Molecule 2: Response regulator

Chain C:



• Molecule 2: Response regulator

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	68.62Å 92.93Å 174.34Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	49.21 – 2.87 49.21 – 2.87	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.21-2.87) 97.2 (49.21-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.240 , 0.287 0.241 , 0.285	Depositor DCC
R_{free} test set	1279 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5805	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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, BEF, ADP, MG

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	1.01	0/1867	0.92	10/2535 (0.4%)
1	B	0.62	0/1842	0.79	0/2506
2	C	0.52	0/957	0.73	0/1288
2	D	0.54	0/958	0.76	1/1290 (0.1%)
All	All	0.75	0/5624	0.82	11/7619 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	ASP	N-CA-C	-7.57	104.94	112.97
1	A	301	HIS	N-CA-C	-7.15	103.42	111.14
1	A	250	MET	N-CA-C	-7.04	102.81	111.40
1	A	261	GLU	N-CA-C	6.51	118.46	111.36
1	A	249	ARG	N-CA-C	-6.25	106.20	113.88
1	A	307	ASN	N-CA-C	-5.46	105.34	112.23
1	A	264	THR	CA-C-N	-5.43	114.22	119.87
1	A	264	THR	C-N-CA	-5.43	114.22	119.87
1	A	284	ASP	N-CA-C	-5.31	103.61	110.19
1	A	334	GLU	N-CA-C	-5.29	105.60	111.36
2	D	55	MET	N-CA-C	5.09	116.56	108.67

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	1835	0	1820	64	0
1	B	1811	0	1761	23	0
2	C	944	0	984	2	0
2	D	945	0	982	3	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	25	0	0	0	0
4	D	15	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
7	A	44	0	0	1	0
7	B	44	0	0	0	0
7	C	30	0	0	0	0
7	D	28	0	0	0	0
All	All	5805	0	5571	87	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 8.

All (87) 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:329:LEU:HD11	1:A:365:ILE:CD1	1.60	1.31
1:A:329:LEU:CD1	1:A:365:ILE:HD11	1.67	1.24
1:A:246:ARG:CD	1:A:247:ILE:H	1.56	1.19
1:A:246:ARG:HG2	1:A:247:ILE:HG22	1.32	1.10
1:A:246:ARG:HD2	1:A:247:ILE:N	1.68	1.08
1:A:246:ARG:HD2	1:A:247:ILE:H	0.92	1.04
1:A:337:VAL:HG13	1:A:351:VAL:HG11	1.43	0.99
1:A:329:LEU:HD11	1:A:365:ILE:HD11	0.99	0.96
1:B:247:ILE:HG23	1:B:249:ARG:HD3	1.48	0.95
1:A:247:ILE:HG23	1:A:250:MET:HG3	1.49	0.91
1:A:246:ARG:HH21	1:A:246:ARG:HG3	1.38	0.88
1:A:247:ILE:CG2	1:A:250:MET:HG3	2.06	0.85
1:A:337:VAL:HG13	1:A:351:VAL:CG1	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:HIS:HB3	7:A:629:HOH:O	1.78	0.83
1:A:254:PHE:CZ	1:A:258:ILE:HD11	2.15	0.82
1:A:331:ASP:OD1	1:A:332:LEU:N	2.13	0.82
1:A:246:ARG:CD	1:A:247:ILE:N	2.36	0.80
1:A:329:LEU:HD11	1:A:365:ILE:HD13	1.63	0.79
1:B:247:ILE:HG21	1:B:249:ARG:NE	1.97	0.79
1:B:249:ARG:CD	1:B:249:ARG:H	1.97	0.78
1:A:329:LEU:O	1:A:333:VAL:HG23	1.88	0.74
1:A:314:ARG:HG3	1:A:319:SER:HB2	1.68	0.73
1:A:332:LEU:C	1:A:332:LEU:HD23	2.15	0.72
1:A:246:ARG:HG2	1:A:247:ILE:CG2	2.18	0.69
1:A:340:ILE:HG12	1:A:340:ILE:O	1.91	0.69
1:A:246:ARG:HG3	1:A:246:ARG:NH2	2.07	0.67
1:A:246:ARG:CG	1:A:247:ILE:N	2.58	0.67
1:B:247:ILE:CG2	1:B:249:ARG:HD3	2.21	0.67
1:B:247:ILE:HG23	1:B:248:ASP:H	1.60	0.66
1:B:254:PHE:CZ	1:B:258:ILE:HD11	2.31	0.66
1:B:249:ARG:HD3	1:B:249:ARG:H	1.59	0.65
1:A:328:ASP:OD1	1:A:330:CYS:HB2	1.96	0.65
1:A:314:ARG:CG	1:A:319:SER:HB2	2.26	0.64
1:A:246:ARG:HH12	1:A:427:GLN:NE2	2.02	0.57
1:A:320:LEU:HD21	1:A:369:ARG:NE	2.19	0.56
1:B:258:ILE:O	1:B:262:LEU:HB2	2.06	0.56
1:A:320:LEU:HD21	1:A:369:ARG:CZ	2.35	0.55
1:A:373:VAL:HG13	1:A:449:THR:HG23	1.88	0.54
1:A:247:ILE:CG1	1:A:249:ARG:CB	2.85	0.54
1:B:247:ILE:CG2	1:B:249:ARG:CD	2.86	0.54
1:B:373:VAL:HG13	1:B:449:THR:HG23	1.90	0.54
1:A:329:LEU:HD22	1:A:363:ALA:HB3	1.90	0.53
1:A:295:ILE:O	1:A:299:SER:OG	2.26	0.53
1:A:247:ILE:HG12	1:A:249:ARG:CB	2.38	0.52
1:A:262:LEU:HD12	1:B:306:LEU:HD21	1.92	0.51
1:A:314:ARG:NH2	2:D:88:GLU:HG3	2.26	0.50
1:B:258:ILE:HG23	1:B:262:LEU:HD22	1.95	0.48
1:A:337:VAL:CG1	1:A:351:VAL:CG1	2.88	0.48
1:A:335:SER:O	1:A:336:ALA:C	2.55	0.48
1:A:246:ARG:CG	1:A:247:ILE:H	2.13	0.48
1:A:247:ILE:HG13	1:A:249:ARG:H	1.78	0.48
1:B:247:ILE:CG2	1:B:249:ARG:NE	2.72	0.48
1:A:322:ILE:HD11	1:A:455:LEU:HB3	1.95	0.48
1:A:261:GLU:HG3	1:A:440:PRO:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ILE:CG1	1:A:249:ARG:H	2.28	0.47
1:A:246:ARG:HG2	1:A:247:ILE:N	2.30	0.47
1:A:345:SER:C	1:A:347:HIS:N	2.72	0.47
1:A:340:ILE:HD11	1:A:351:VAL:HG21	1.96	0.46
1:A:328:ASP:O	1:A:330:CYS:N	2.48	0.46
1:A:333:VAL:O	1:A:337:VAL:HG23	2.15	0.46
1:A:294:VAL:O	1:A:298:GLN:HG2	2.15	0.46
1:A:247:ILE:HG21	1:A:250:MET:HG3	1.95	0.46
1:B:247:ILE:HG23	1:B:248:ASP:N	2.29	0.46
2:D:30:ILE:HD13	2:D:45:PHE:CE2	2.49	0.46
1:A:328:ASP:C	1:A:330:CYS:N	2.72	0.46
1:A:332:LEU:HD23	1:A:332:LEU:O	2.16	0.45
1:B:276:ILE:HD11	1:B:291:PHE:HB3	1.98	0.45
2:D:30:ILE:HD13	2:D:45:PHE:CZ	2.52	0.45
1:A:246:ARG:NH2	1:A:246:ARG:CG	2.75	0.44
1:A:247:ILE:HG13	1:A:249:ARG:N	2.32	0.44
1:A:348:ASN:O	1:A:392:LYS:HD3	2.18	0.44
1:A:254:PHE:CE1	1:A:258:ILE:HD11	2.51	0.44
1:B:249:ARG:CD	1:B:249:ARG:N	2.72	0.43
1:A:327:VAL:HG22	1:A:328:ASP:N	2.33	0.43
1:A:328:ASP:C	1:A:330:CYS:H	2.25	0.43
1:A:331:ASP:C	1:A:333:VAL:N	2.73	0.43
1:B:247:ILE:HG23	1:B:249:ARG:CD	2.32	0.43
1:B:248:ASP:H	1:B:249:ARG:HD3	1.82	0.43
1:A:262:LEU:HD12	1:B:306:LEU:CD2	2.48	0.43
1:B:247:ILE:HG21	1:B:249:ARG:HE	1.81	0.42
1:B:333:VAL:HG21	1:B:353:PHE:CE1	2.55	0.42
1:A:329:LEU:CD2	1:A:363:ALA:HB3	2.49	0.42
1:A:342:GLU:O	1:A:345:SER:OG	2.38	0.42
1:B:276:ILE:HD13	1:B:292:LEU:CD1	2.50	0.41
1:A:267:THR:HG23	2:C:106:PRO:HA	2.02	0.41
1:A:267:THR:HA	2:C:106:PRO:HB3	2.03	0.40
1:B:258:ILE:CG2	1:B:262:LEU:HD22	2.51	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	232/258 (90%)	217 (94%)	14 (6%)	1 (0%)	30 56
1	B	233/258 (90%)	226 (97%)	6 (3%)	1 (0%)	30 56
2	C	118/122 (97%)	115 (98%)	3 (2%)	0	100 100
2	D	119/122 (98%)	117 (98%)	2 (2%)	0	100 100
All	All	702/760 (92%)	675 (96%)	25 (4%)	2 (0%)	36 62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	ILE
1	A	329	LEU

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	201/232 (87%)	179 (89%)	22 (11%)	6 18
1	B	194/232 (84%)	184 (95%)	10 (5%)	21 50
2	C	106/110 (96%)	102 (96%)	4 (4%)	29 61
2	D	105/110 (96%)	101 (96%)	4 (4%)	29 61
All	All	606/684 (89%)	566 (93%)	40 (7%)	15 40

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	247	ILE
1	A	250	MET
1	A	282	GLU
1	A	286	SER
1	A	302	LEU
1	A	305	LEU
1	A	314	ARG
1	A	318	LYS
1	A	320	LEU
1	A	329	LEU
1	A	330	CYS
1	A	332	LEU
1	A	338	ASN
1	A	340	ILE
1	A	341	LYS
1	A	345	SER
1	A	346	SER
1	A	352	LEU
1	A	435	LEU
1	A	450	LYS
1	A	463	GLU
1	B	247	ILE
1	B	249	ARG
1	B	250	MET
1	B	251	LYS
1	B	262	LEU
1	B	292	LEU
1	B	320	LEU
1	B	351	VAL
1	B	405	VAL
1	B	450	LYS
2	C	7	LEU
2	C	82	LEU
2	C	89	GLU
2	C	101	LYS
2	D	7	LEU
2	D	22	LEU
2	D	82	LEU
2	D	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	ASN
1	A	304	ASN
1	A	338	ASN
1	A	350	ASN
1	A	356	ASN
1	A	379	ASN
1	A	427	GLN
1	B	278	ASN
1	B	301	HIS
1	B	304	ASN
1	B	338	ASN
1	B	350	ASN
1	B	356	ASN
1	B	376	ASN
1	B	379	ASN
2	C	36	GLN
2	C	121	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

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	C	206	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	C	205	-	4,4,4	0.32	0	6,6,6	0.04	0
4	SO4	D	202	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	B	502	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	B	503	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	C	204	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	D	203	-	4,4,4	0.32	0	6,6,6	0.05	0
6	BEF	C	207	2	0,3,3	-	-	-		
4	SO4	A	503	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	D	204	-	4,4,4	0.32	0	6,6,6	0.04	0
6	BEF	D	205	2	0,3,3	-	-	-		
4	SO4	C	202	-	4,4,4	0.33	0	6,6,6	0.04	0
3	ADP	B	501	-	27,29,29	1.43	4 (14%)	42,45,45	1.98	11 (26%)
3	ADP	A	501	-	27,29,29	1.42	4 (14%)	42,45,45	1.99	11 (26%)
4	SO4	C	203	-	4,4,4	0.32	0	6,6,6	0.05	0
4	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.04	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	-	-	1/16/32/32	0/3/3/3
3	ADP	A	501	-	-	2/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ADP	C5-C4	4.72	1.47	1.39
3	A	501	ADP	C5-C4	4.65	1.47	1.39
3	B	501	ADP	C5-C6	2.84	1.49	1.41
3	A	501	ADP	C5-C6	2.80	1.48	1.41
3	A	501	ADP	C8-N7	2.40	1.36	1.31
3	B	501	ADP	C8-N7	2.39	1.36	1.31
3	B	501	ADP	C5-N7	-2.32	1.34	1.39
3	A	501	ADP	C5-N7	-2.31	1.34	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	ADP	C5-C4-N3	-6.22	118.64	126.75
3	B	501	ADP	C5-C4-N3	-6.15	118.72	126.75
3	A	501	ADP	N3-C4-N9	4.84	135.06	127.08
3	B	501	ADP	N3-C4-N9	4.83	135.05	127.08
3	A	501	ADP	C2-N3-C4	4.07	121.37	111.75
3	B	501	ADP	C2-N3-C4	4.04	121.30	111.75
3	A	501	ADP	N3-C2-N1	-3.70	122.81	128.60
3	B	501	ADP	N3-C2-N1	-3.69	122.83	128.60
3	A	501	ADP	C4-C5-N7	-3.43	106.44	110.62
3	B	501	ADP	C4-C5-N7	-3.42	106.45	110.62
3	A	501	ADP	C5-N7-C8	3.10	107.92	103.51
3	B	501	ADP	C5-N7-C8	3.09	107.89	103.51
3	B	501	ADP	C4-N9-C8	2.63	108.58	105.73
3	A	501	ADP	C4-N9-C8	2.56	108.51	105.73
3	B	501	ADP	C3'-C2'-C1'	2.41	106.00	101.43
3	A	501	ADP	C3'-C2'-C1'	2.32	105.84	101.43
3	B	501	ADP	C6-C5-N7	2.32	136.34	132.02
3	A	501	ADP	PA-O3A-PB	-2.31	124.92	132.83
3	A	501	ADP	C6-C5-N7	2.28	136.27	132.02
3	A	501	ADP	N9-C8-N7	-2.25	110.83	113.91
3	B	501	ADP	N9-C8-N7	-2.25	110.84	113.91
3	B	501	ADP	PA-O3A-PB	-2.12	125.56	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	ADP	PB-O3A-PA-O5'
3	A	501	ADP	PA-O3A-PB-O2B
3	A	501	ADP	PA-O3A-PB-O3B

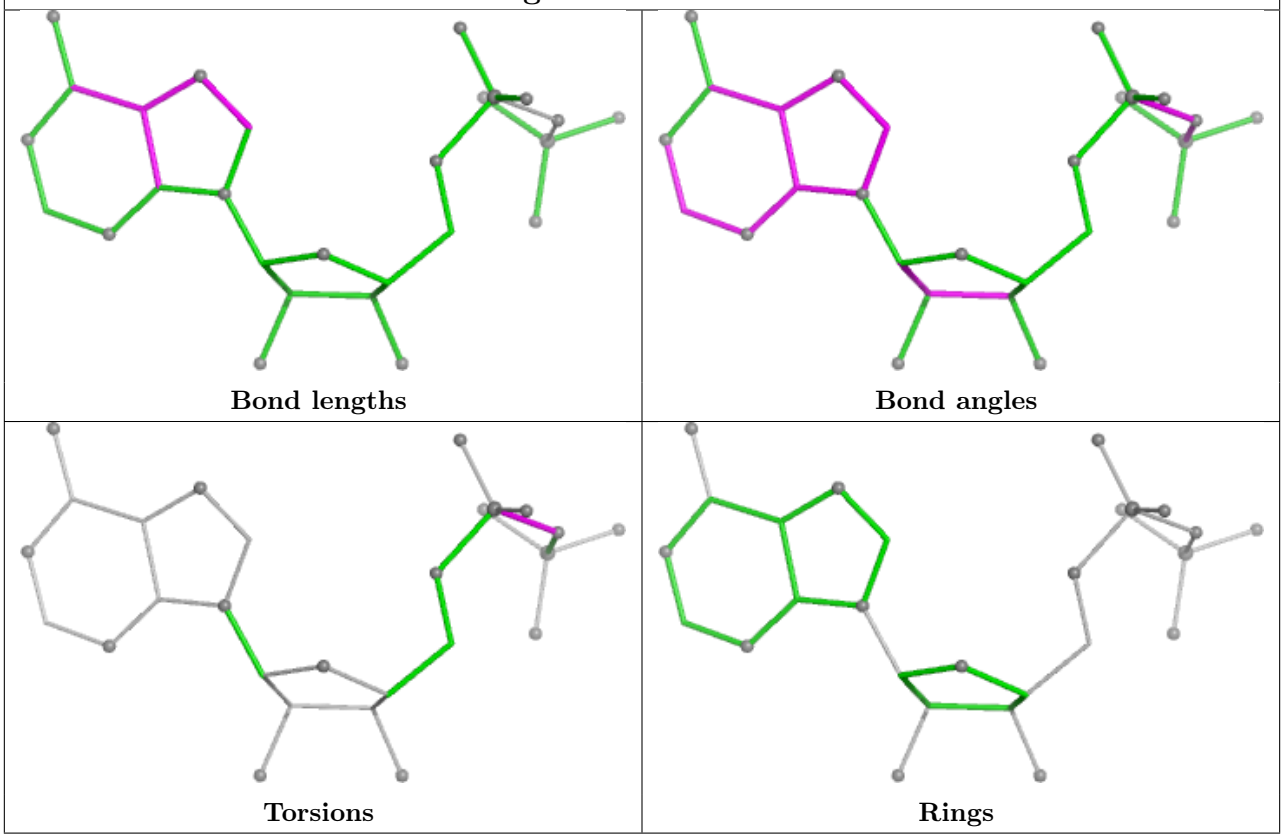
There are no ring outliers.

No monomer is involved in short contacts.

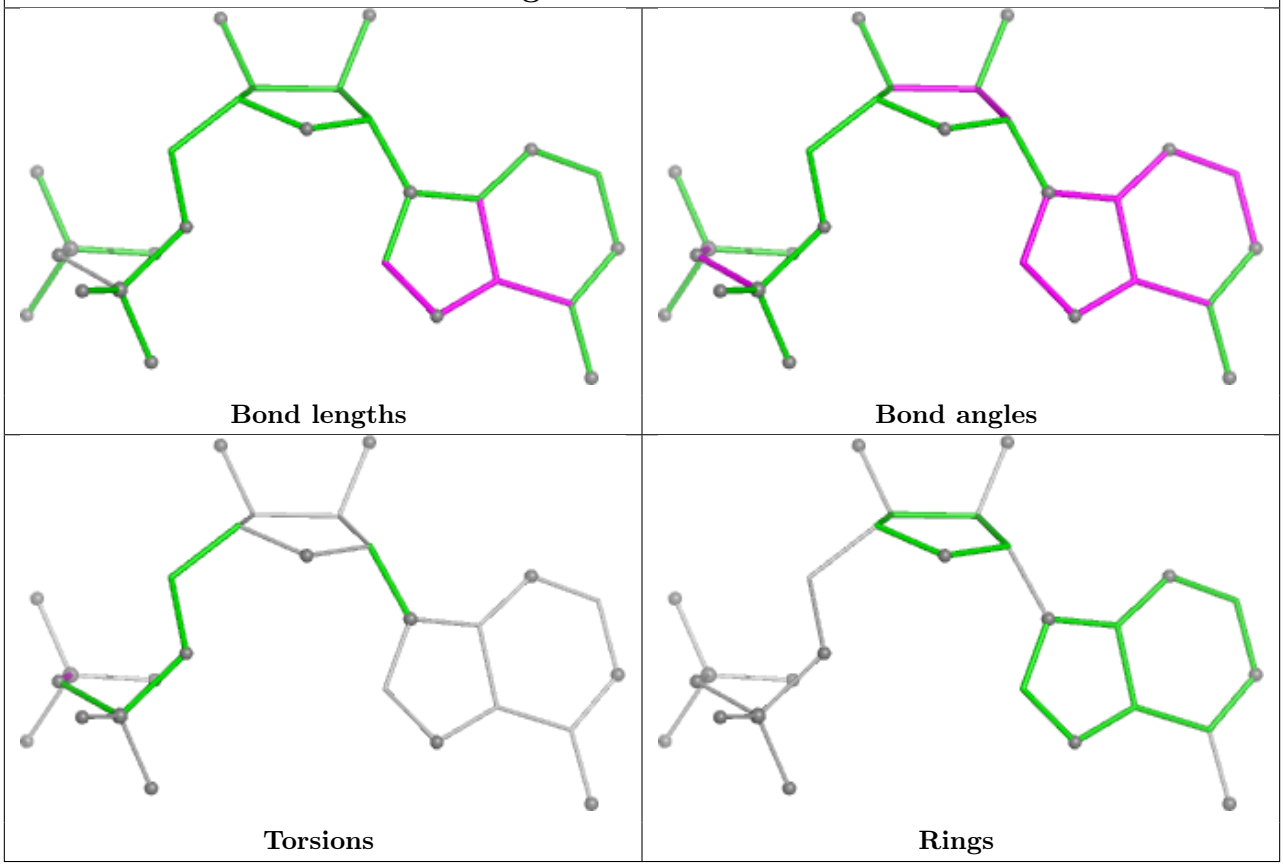
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADP B 501



Ligand ADP A 501



5.7 Other polymers (i)

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

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, 95^{th} 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	234/258 (90%)	0.87	20 (8%) 16 13	34, 68, 101, 125	0
1	B	235/258 (91%)	0.99	24 (10%) 12 10	36, 67, 102, 121	0
2	C	120/122 (98%)	0.62	3 (2%) 58 49	38, 59, 93, 113	0
2	D	121/122 (99%)	0.72	2 (1%) 69 61	41, 62, 96, 106	0
All	All	710/760 (93%)	0.84	49 (6%) 23 18	34, 64, 101, 125	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	ALA	5.7
1	B	479	ASP	4.7
1	B	247	ILE	4.7
1	B	330	CYS	4.0
1	A	247	ILE	3.9
1	B	322	ILE	3.8
2	C	2	SER	3.5
1	A	330	CYS	3.4
1	B	414	ILE	3.1
1	A	437	TYR	3.1
1	B	359	CYS	3.1
2	C	119	LEU	3.0
2	D	72	GLU	2.8
1	B	480	ARG	2.8
2	D	2	SER	2.8
1	B	321	GLN	2.8
1	A	334	GLU	2.7
1	B	356	ASN	2.7
1	A	359	CYS	2.7
1	A	356	ASN	2.7
1	A	436	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	358	PRO	2.7
1	A	361	VAL	2.6
1	B	364	TYR	2.6
1	A	435	LEU	2.5
1	A	321	GLN	2.5
1	B	354	GLU	2.5
1	A	358	PRO	2.4
1	B	435	LEU	2.4
1	A	248	ASP	2.4
1	B	320	LEU	2.3
1	A	246	ARG	2.3
1	A	398	LEU	2.3
1	B	422	ASP	2.2
1	A	315	LEU	2.2
2	C	121	ASN	2.2
1	A	360	PRO	2.2
1	B	355	SER	2.2
1	B	260	HIS	2.2
1	B	419	HIS	2.2
1	B	360	PRO	2.1
1	B	248	ASP	2.1
1	A	329	LEU	2.1
1	A	314	ARG	2.1
1	B	420	ALA	2.1
1	B	478	LYS	2.1
1	A	479	ASP	2.0
1	A	342	GLU	2.0
1	B	282	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

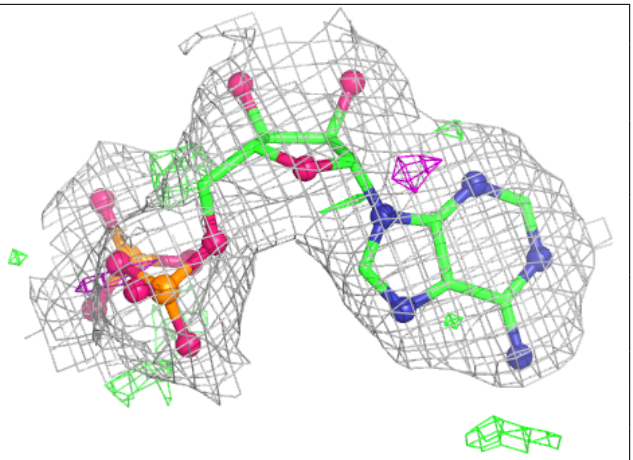
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

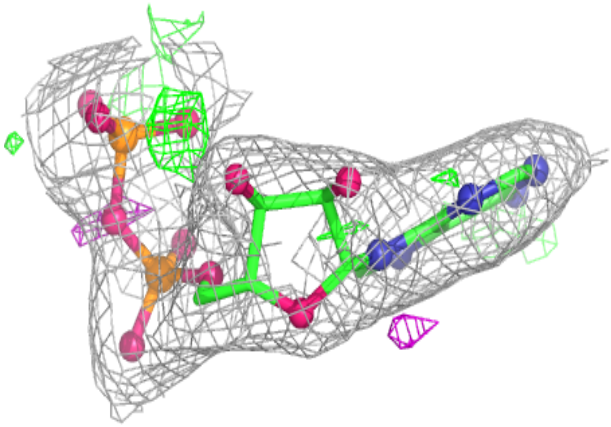
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BEF	D	205	4/4	0.72	0.25	44,45,46,46	4
4	SO4	C	205	5/5	0.74	0.13	100,100,101,101	0
4	SO4	D	204	5/5	0.79	0.12	108,108,109,109	0
4	SO4	B	503	5/5	0.81	0.15	90,90,91,91	0
4	SO4	A	503	5/5	0.82	0.17	80,80,81,81	0
4	SO4	B	502	5/5	0.82	0.21	86,86,86,86	0
4	SO4	C	206	5/5	0.84	0.14	94,95,95,95	0
4	SO4	C	203	5/5	0.85	0.16	77,77,78,78	0
4	SO4	A	502	5/5	0.87	0.16	91,91,92,92	0
4	SO4	C	204	5/5	0.87	0.14	96,97,97,97	0
4	SO4	C	202	5/5	0.88	0.13	68,68,69,69	0
4	SO4	D	203	5/5	0.89	0.15	72,73,73,73	0
6	BEF	C	207	4/4	0.90	0.16	51,53,54,54	4
4	SO4	D	202	5/5	0.91	0.14	69,69,69,70	0
5	MG	D	201	1/1	0.92	0.15	46,46,46,46	0
3	ADP	A	501	27/27	0.92	0.11	42,43,44,44	0
5	MG	C	201	1/1	0.92	0.12	37,37,37,37	0
3	ADP	B	501	27/27	0.93	0.10	43,44,44,45	0

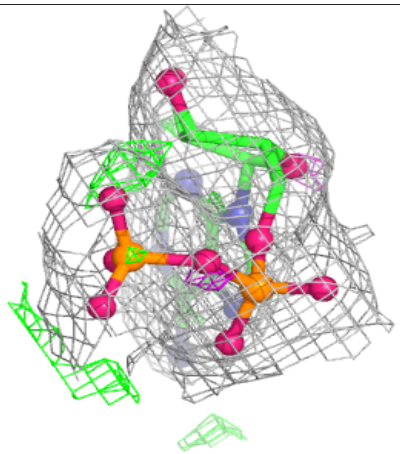
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

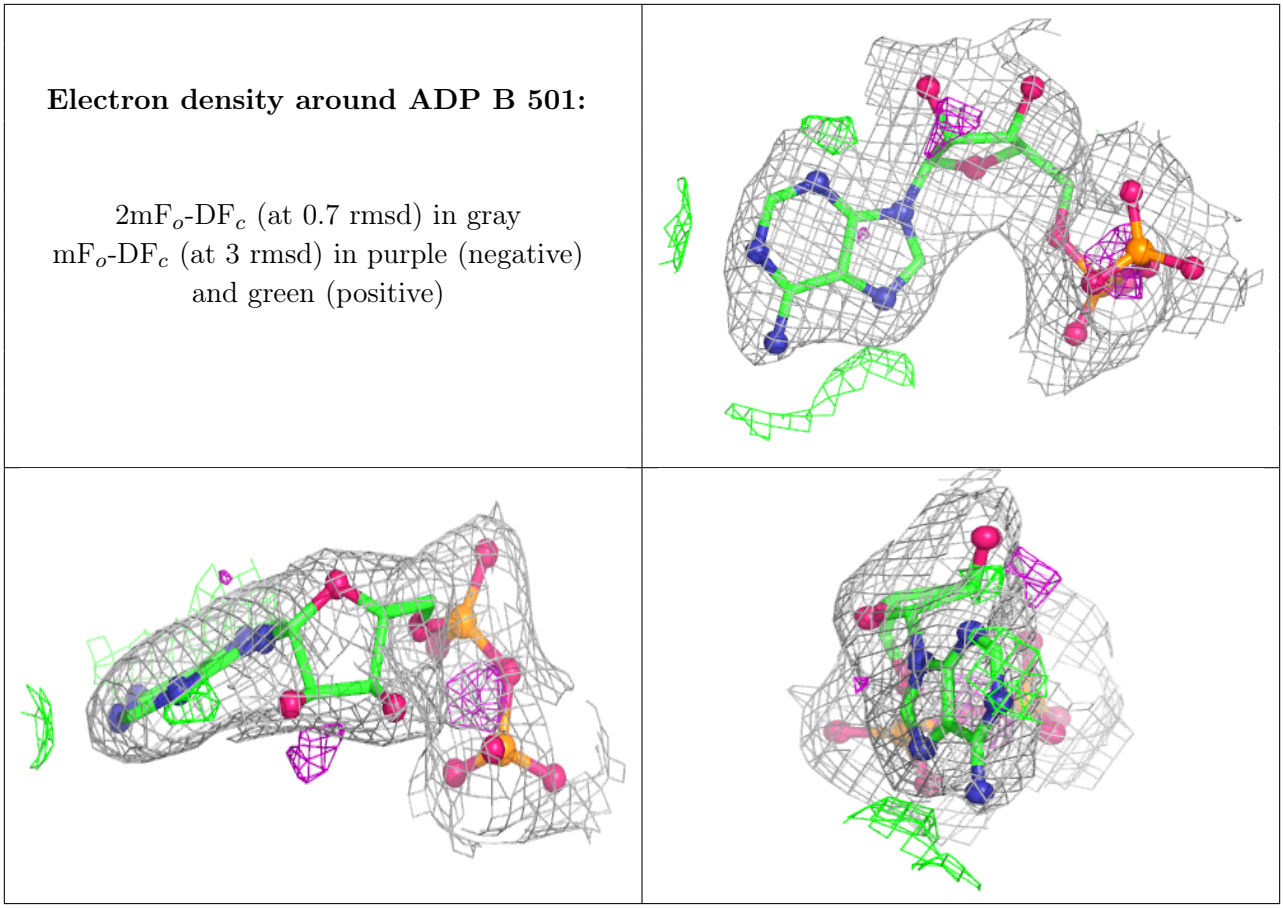






Electron density around ADP B 501:

$2mF_o$-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

There are no such residues in this entry.