wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 05:53 AM EDT

PDB ID	:	4JAV / pdb_00004jav
Title	:	Structural basis of a rationally rewired protein-protein interface (HK853wt and RR468mutant V13P, L14I, I17M and N21V)
Authors	:	Podgornaia, A.I.; Casino, P.; Marina, A.; Laub, M.T.
Deposited on	:	2013-02-19
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

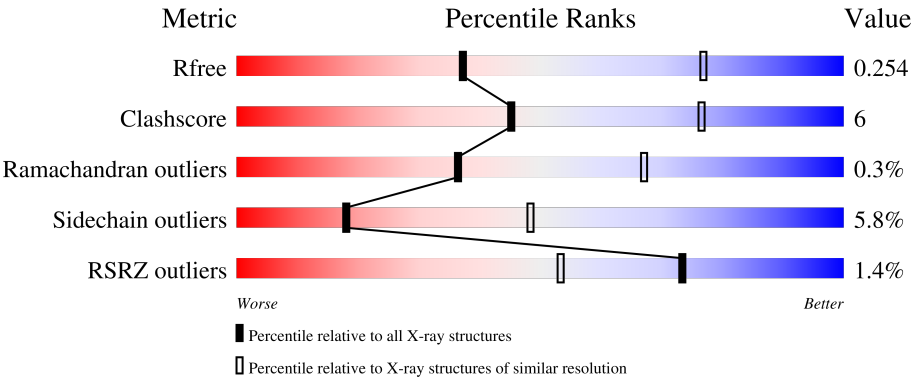
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	78% 16% • 5%
1	B	258	3% 79% 13% • 5%
2	C	122	87% 11% ••
2	D	122	2% 87% 11% ••

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
3	SO4	B	503	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5944 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 Histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1968	1253	333	379	3			
1	B	244	Total	C	N	O	S	0	1	0
			1953	1243	333	374	3			

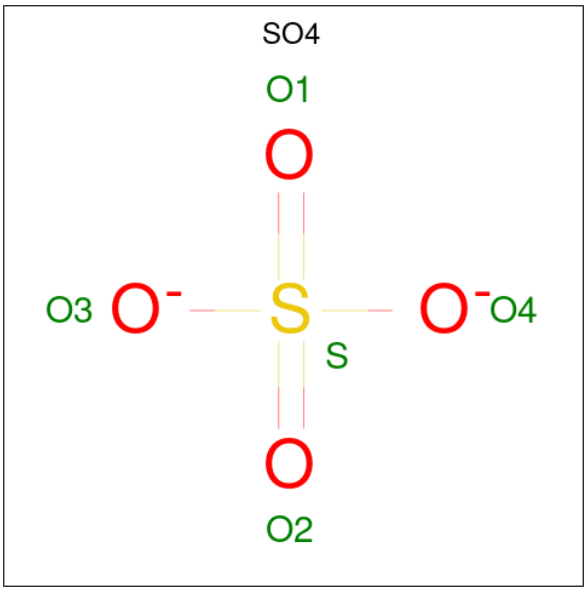
- Molecule 2 is a protein called Response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	121	Total	C	N	O	S	0	0	0
			961	620	155	181	5			
2	D	120	Total	C	N	O	S	0	2	0
			957	619	154	179	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	13	PRO	VAL	engineered mutation	UNP Q9WYT9
C	14	ILE	LEU	engineered mutation	UNP Q9WYT9
C	17	MET	ILE	engineered mutation	UNP Q9WYT9
C	21	VAL	ASN	engineered mutation	UNP Q9WYT9
D	13	PRO	VAL	engineered mutation	UNP Q9WYT9
D	14	ILE	LEU	engineered mutation	UNP Q9WYT9
D	17	MET	ILE	engineered mutation	UNP Q9WYT9
D	21	VAL	ASN	engineered mutation	UNP Q9WYT9

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

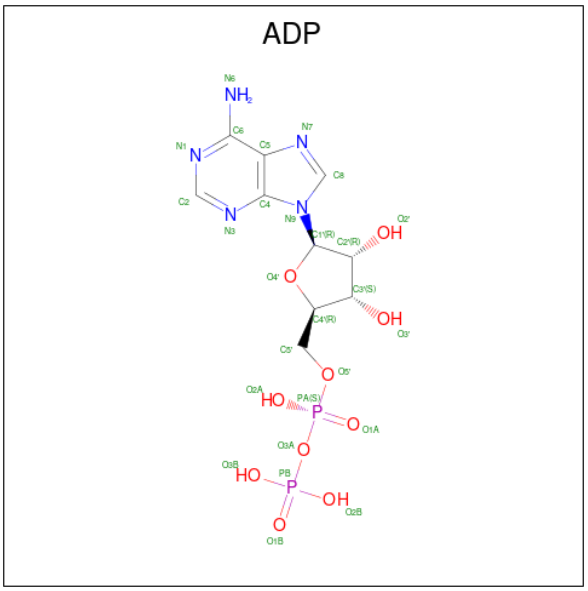


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

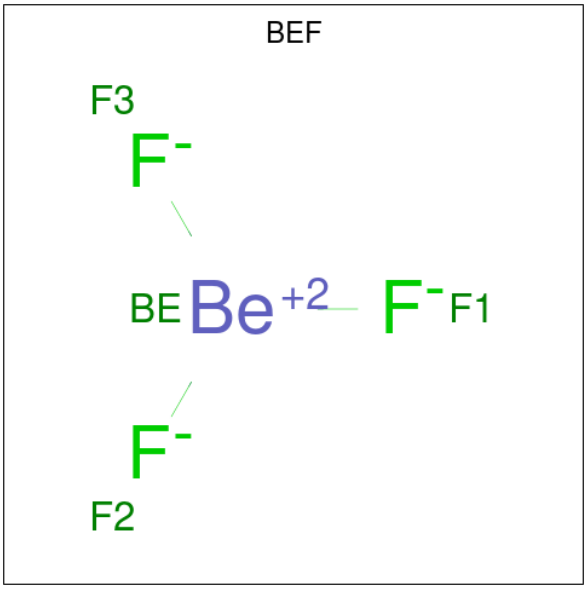


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 8 is water.

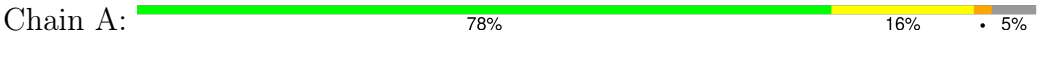
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	8	Total O 8 8	0	0
8	B	1	Total O 1 1	0	0
8	C	4	Total O 4 4	0	0

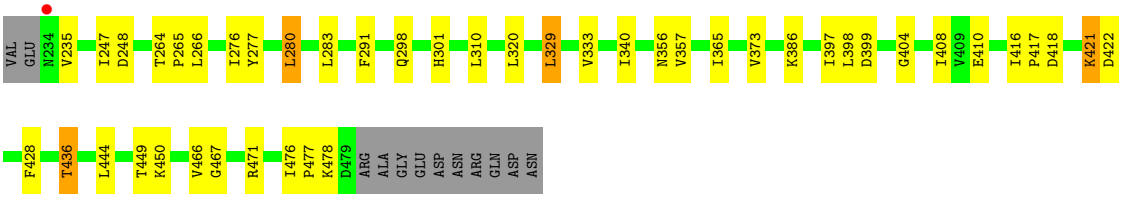
3 Residue-property plots (i)

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: Histidine kinase

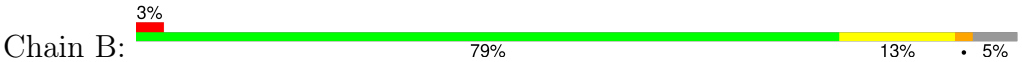
Chain A:

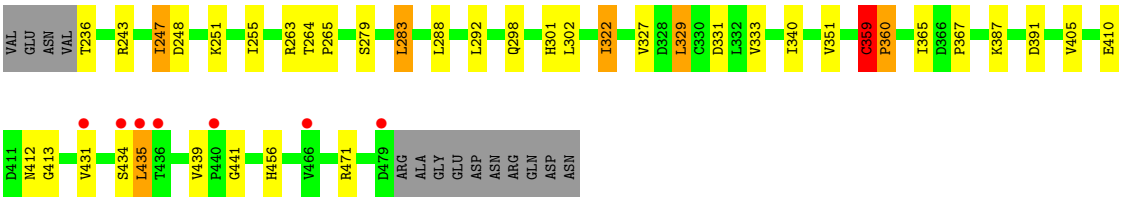




• Molecule 1: Histidine kinase

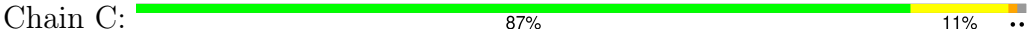
Chain B:

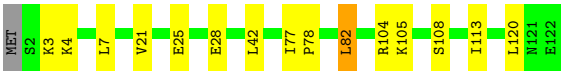




• Molecule 2: Response regulator

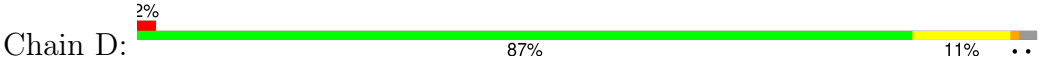
Chain C:

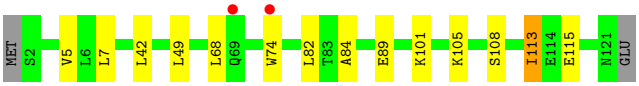




• Molecule 2: Response regulator

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.32Å 143.93Å 138.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.55 – 3.10 44.55 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.55-3.10) 99.8 (44.55-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.253 0.202 , 0.254	Depositor DCC
R_{free} test set	1129 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5944	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, ADP, MG, CL, BEF

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	0.35	0/2000	0.80	0/2705
1	B	0.38	0/1988	0.93	5/2688 (0.2%)
2	C	0.34	0/975	0.81	2/1308 (0.2%)
2	D	0.37	0/977	0.83	0/1312
All	All	0.36	0/5940	0.85	7/8013 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	412	ASN	N-CA-C	-16.07	83.04	109.24
1	B	412	ASN	CB-CA-C	10.04	126.32	109.75
1	B	413	GLY	N-CA-C	-8.05	99.51	111.19
2	C	108	SER	CA-C-N	6.18	126.36	119.32
2	C	108	SER	C-N-CA	6.18	126.36	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	359	CYS	Peptide

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	1968	0	1989	22	0
1	B	1953	0	1976	37	0
2	C	961	0	1011	7	0
2	D	957	0	1015	6	0
3	A	10	0	0	0	0
3	B	15	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	B	1	0	0	0	0
7	C	4	0	0	0	0
7	D	4	0	0	0	0
8	A	8	0	0	0	0
8	B	1	0	0	0	0
8	C	4	0	0	0	0
All	All	5944	0	6015	70	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 6.

The worst 5 of 70 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:387:LYS:CE	1:B:435:LEU:HD11	1.69	1.21
1:B:387:LYS:HZ3	1:B:435:LEU:HD21	1.14	1.07
1:B:387:LYS:HE3	1:B:435:LEU:HD11	1.43	0.99
1:B:387:LYS:NZ	1:B:435:LEU:HD21	1.81	0.94
1:B:387:LYS:HE2	1:B:435:LEU:HD11	1.47	0.94

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	244/258 (95%)	237 (97%)	7 (3%)	0	100 100
1	B	243/258 (94%)	233 (96%)	8 (3%)	2 (1%)	16 47
2	C	119/122 (98%)	118 (99%)	1 (1%)	0	100 100
2	D	120/122 (98%)	117 (98%)	3 (2%)	0	100 100
All	All	726/760 (96%)	705 (97%)	19 (3%)	2 (0%)	36 67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	360	PRO
1	B	359	CYS

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	221/232 (95%)	206 (93%)	15 (7%)	14 42
1	B	219/232 (94%)	205 (94%)	14 (6%)	16 44
2	C	109/110 (99%)	105 (96%)	4 (4%)	30 61
2	D	110/110 (100%)	105 (96%)	5 (4%)	24 56
All	All	659/684 (96%)	621 (94%)	38 (6%)	18 48

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	435	LEU
2	D	82	LEU
2	C	7	LEU
2	C	104	ARG
2	D	113	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	300	ASN
1	B	301	HIS
2	D	36	GLN
1	B	350	ASN
1	A	301	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\#\|Z\|>2$
5	ADP	A	504	4	28,29,29	1.47	5 (17%)	43,45,45	1.80	9 (20%)
3	SO4	A	502	4	4,4,4	0.44	0	6,6,6	0.12	0
3	SO4	A	501	-	4,4,4	0.42	0	6,6,6	0.11	0
3	SO4	B	503	-	4,4,4	0.42	0	6,6,6	0.07	0
3	SO4	B	501	-	4,4,4	0.42	0	6,6,6	0.08	0
5	ADP	B	505	4	28,29,29	1.45	4 (14%)	43,45,45	1.84	11 (25%)
3	SO4	B	502	-	4,4,4	0.41	0	6,6,6	0.11	0
7	BEF	C	202	2	0,3,3	-	-	-		
7	BEF	D	202	2	0,3,3	-	-	-		

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
5	ADP	B	505	4	-	1/16/32/32	0/3/3/3
5	ADP	A	504	4	-	1/16/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	ADP	C5-C4	4.87	1.47	1.39
5	A	504	ADP	C5-C4	4.86	1.47	1.39
5	B	505	ADP	C5-C6	2.84	1.48	1.41
5	A	504	ADP	C5-C6	2.72	1.48	1.41
5	A	504	ADP	C5-N7	-2.53	1.34	1.39

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	505	ADP	C5-C4-N3	-5.93	118.55	126.72
5	A	504	ADP	C5-C4-N3	-5.80	118.74	126.72
5	B	505	ADP	N3-C4-N9	4.66	135.10	127.17
5	A	504	ADP	N3-C4-N9	4.59	134.97	127.17
5	B	505	ADP	C2-N3-C4	3.79	121.08	111.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	ADP	PA-O3A-PB-O3B
5	B	505	ADP	PB-O3A-PA-O2A

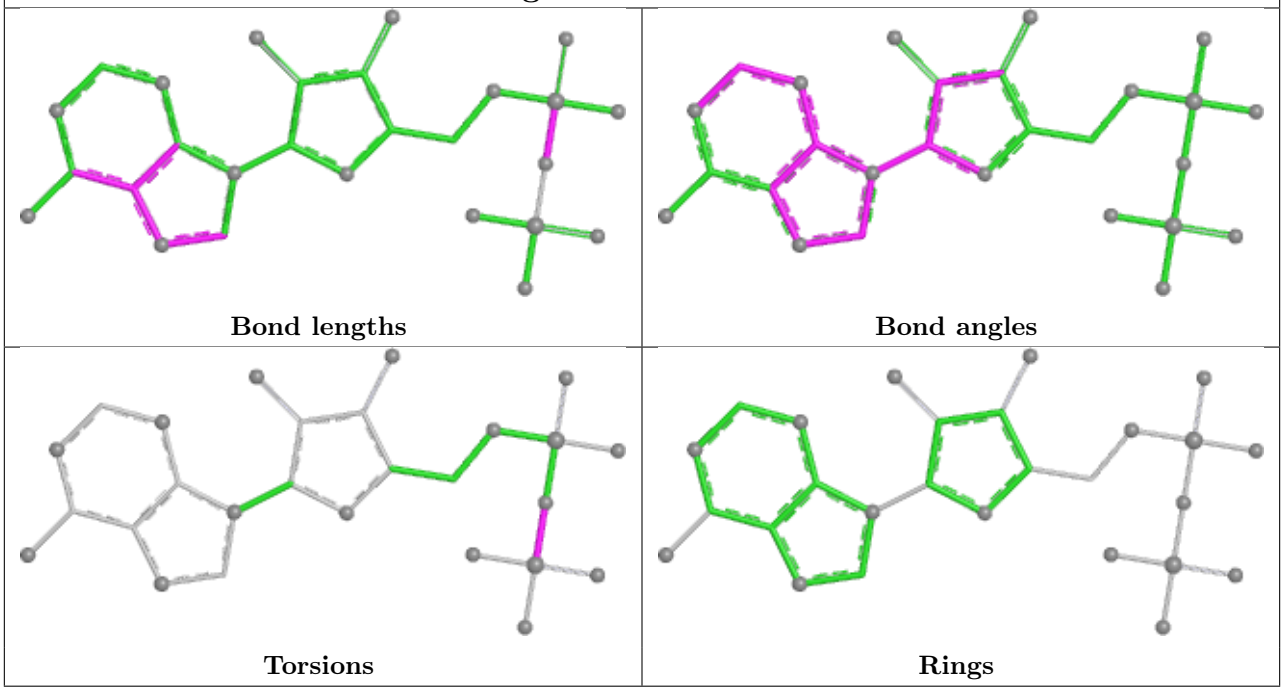
There are no ring outliers.

1 monomer is involved in 2 short contacts:

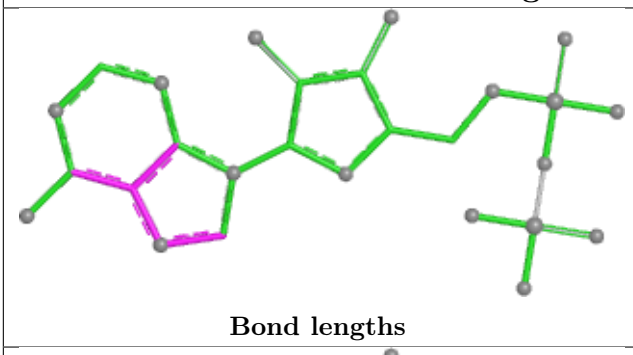
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	SO4	2	0

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

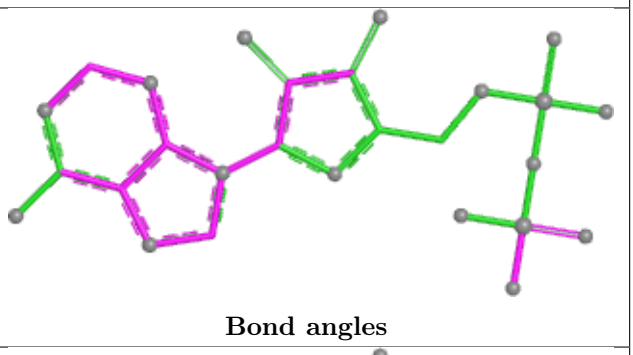
Ligand ADP A 504



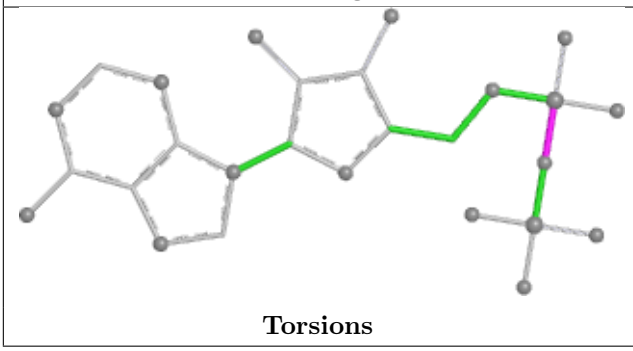
Ligand ADP B 505



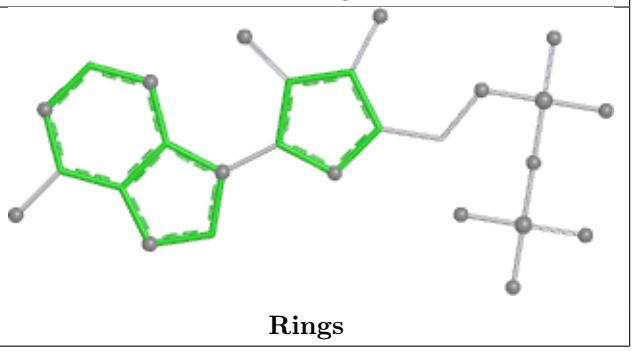
Bond lengths



Bond angles



Torsions



Rings

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, 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	246/258 (95%)	-0.22	1 (0%) 88 76	44, 63, 87, 99	0
1	B	244/258 (94%)	0.01	7 (2%) 53 32	35, 75, 110, 160	1 (0%)
2	C	121/122 (99%)	-0.48	0 100 100	45, 58, 80, 91	0
2	D	120/122 (98%)	-0.05	2 (1%) 69 48	37, 82, 120, 128	2 (1%)
All	All	731/760 (96%)	-0.16	10 (1%) 73 53	35, 68, 106, 160	3 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	ASN	4.5
1	B	479	ASP	3.6
1	B	435	LEU	3.0
1	B	466	VAL	2.6
2	D	69	GLN	2.5

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

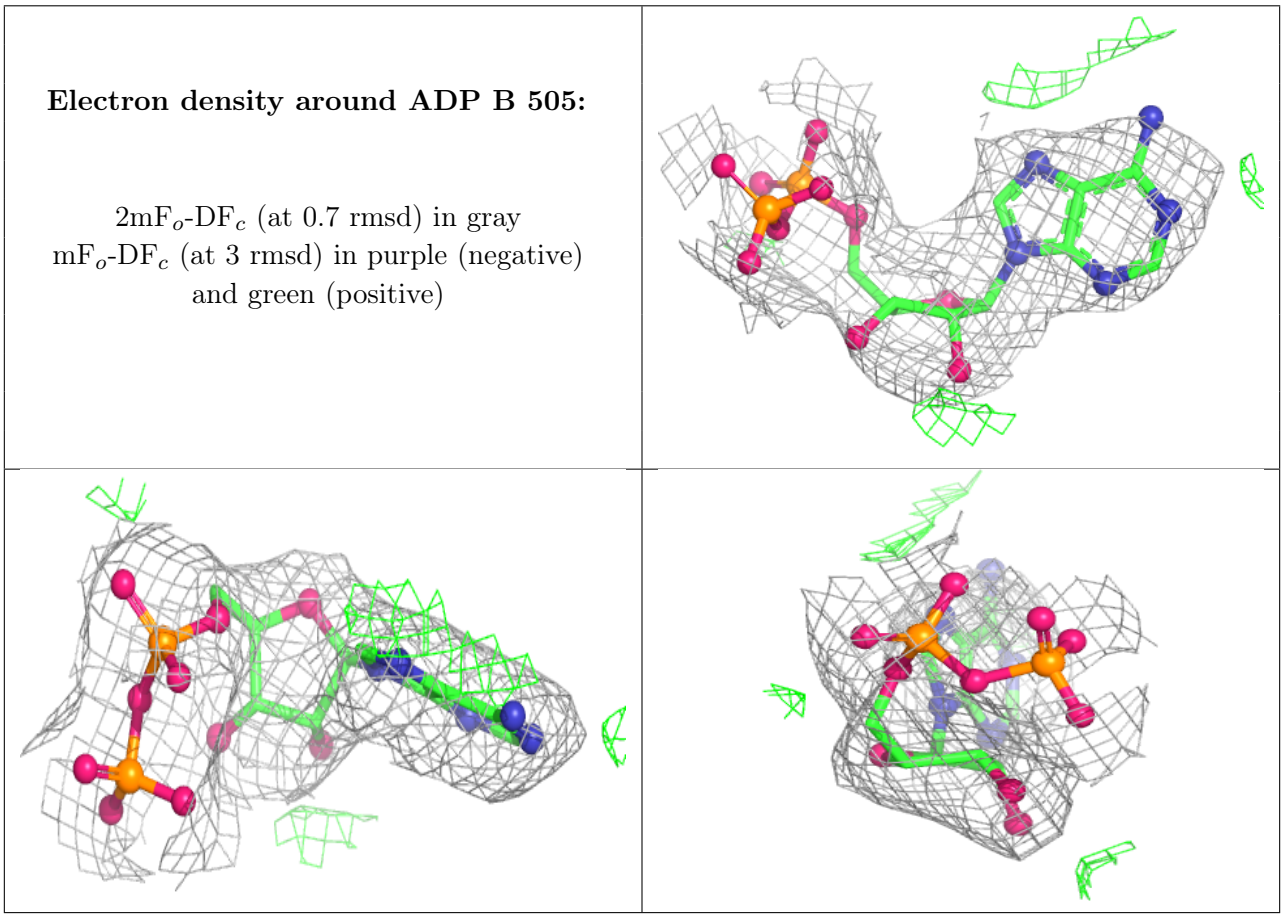
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	SO4	A	502	5/5	0.74	0.13	110,112,112,113	0
3	SO4	B	503	5/5	0.74	0.12	161,162,163,165	0
4	MG	B	504	1/1	0.89	0.16	60,60,60,60	0
3	SO4	B	502	5/5	0.90	0.13	141,142,143,143	0
6	CL	B	506	1/1	0.93	0.12	79,79,79,79	0
3	SO4	A	501	5/5	0.94	0.09	79,81,82,82	0
3	SO4	B	501	5/5	0.94	0.09	83,84,86,86	0
5	ADP	B	505	27/27	0.96	0.07	70,73,75,76	0
4	MG	D	201	1/1	0.96	0.06	45,45,45,45	0
4	MG	A	503	1/1	0.97	0.13	40,40,40,40	0
5	ADP	A	504	27/27	0.97	0.07	48,52,53,54	0
4	MG	C	201	1/1	0.98	0.08	40,40,40,40	0
7	BEF	C	202	4/4	0.98	0.04	51,53,54,54	0
7	BEF	D	202	4/4	0.98	0.04	63,64,64,65	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.

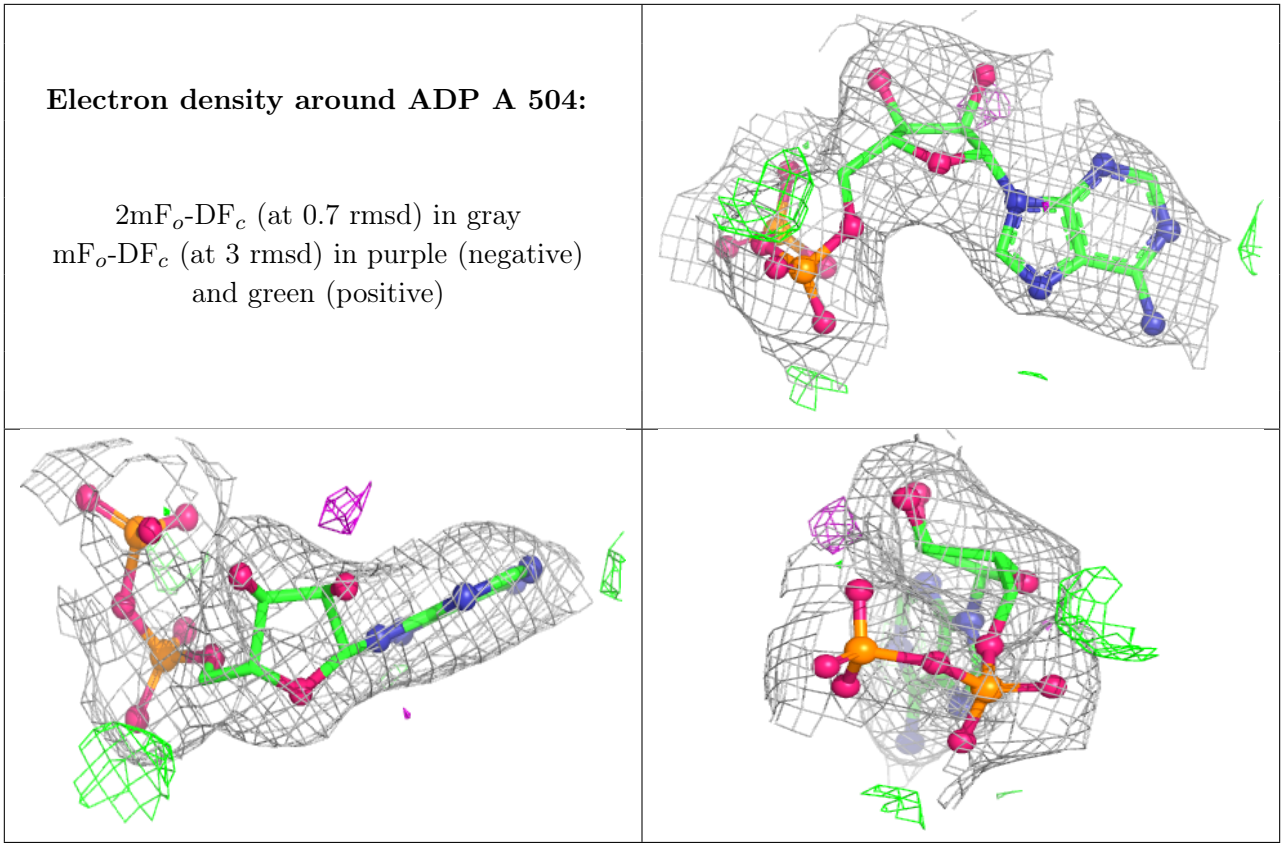
Electron density around ADP B 505:

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



Electron density around ADP A 504:

$2mF_o$-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.