



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:35 PM BST

PDB ID : 4JAV  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

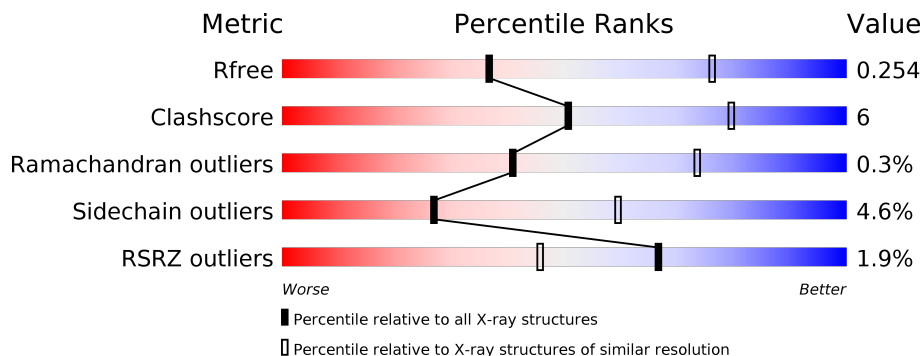
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

# 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 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	258	
2	C	122	
2	D	122	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	503	-	-	X	-

## 2 Entry composition [i](#)

There are 7 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
			Total	C	N	O	S			
1	A	246	Total 1968	C 1253	N 333	O 379	S 3	0	0	0
1	B	244	Total 1953	C 1243	N 333	O 374	S 3	0	1	0

- Molecule 2 is a protein called Response regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace	
			Total	Be	C	F	N	O				S
2	C	121	Total 965	Be 1	C 620	F 3	N 155	O 181	S 5	0	0	0
2	D	120	Total 961	Be 1	C 619	F 3	N 154	O 179	S 5	0	2	0

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 (three-letter code: SO4) (formula: O<sub>4</sub>S).

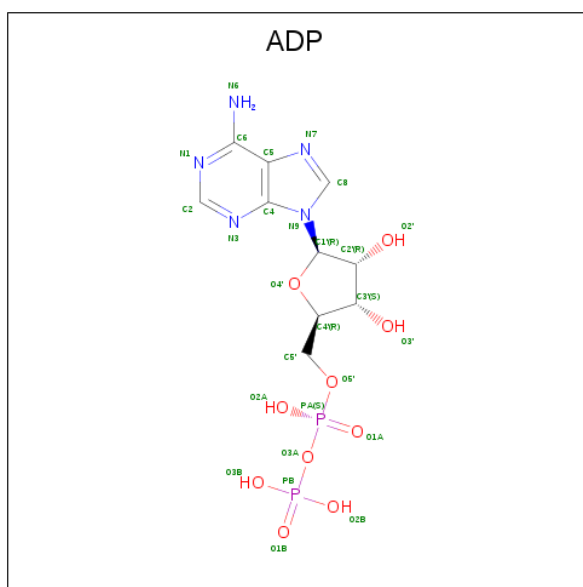


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is water.

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.32Å 143.93Å 138.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.55 – 3.10 44.51 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.55-3.10) 99.8 (44.51-3.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 3.12Å)	Xtrriage
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 (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: MG, BFD, SO4, ADP, CL

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	0.27	0/2000	0.46	0/2705
1	B	0.29	0/1988	0.59	5/2688 (0.2%)
2	C	0.27	0/966	0.48	0/1294
2	D	0.28	0/968	0.46	0/1298
All	All	0.28	0/5922	0.51	5/7985 (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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	412	ASN	N-CA-C	-10.35	83.04	111.00
1	B	412	ASN	CB-CA-C	7.96	126.32	110.40
1	B	359	CYS	C-N-CD	-6.73	105.80	120.60
1	B	413	GLY	N-CA-C	-5.44	99.51	113.10
1	B	360	PRO	N-CA-CB	5.18	109.51	103.30

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

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	21	0
1	B	1953	0	1976	36	0
2	C	965	0	1010	7	0
2	D	961	0	1014	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	A	8	0	0	0	0
7	B	1	0	0	0	0
7	C	4	0	0	0	0
All	All	5944	0	6013	68	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.

All (68) 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:HE3	1:B:435:LEU:HD11	1.43	0.99
1:B:387:LYS:NZ	1:B:435:LEU:HD21	1.81	0.95
1:B:387:LYS:HE2	1:B:435:LEU:HD11	1.47	0.94
1:B:387:LYS:HZ3	1:B:435:LEU:HD21	1.35	0.88
1:B:441:GLY:HA2	3:B:503:SO4:O1	1.74	0.86
2:C:21:VAL:HG12	2:C:113:ILE:HD11	1.60	0.82
1:B:265:PRO:HA	1:B:298:GLN:HE21	1.51	0.75
1:B:387:LYS:NZ	1:B:435:LEU:CD2	2.54	0.71
1:B:387:LYS:CE	1:B:435:LEU:CD1	2.61	0.67
1:B:387:LYS:HZ1	1:B:435:LEU:HG	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LYS:HZ1	1:B:435:LEU:CG	2.08	0.66
1:A:386:LYS:NZ	1:A:467:GLY:O	2.24	0.66
1:B:387:LYS:CE	1:B:435:LEU:HD21	2.29	0.63
1:B:435:LEU:C	1:B:435:LEU:HD12	2.19	0.63
1:B:387:LYS:HE2	1:B:435:LEU:CD1	2.24	0.61
1:B:441:GLY:CA	3:B:503:SO4:O1	2.46	0.60
1:B:410:GLU:HG3	1:B:471:ARG:HG2	1.83	0.59
2:C:25:GLU:HG3	2:C:113:ILE:HD12	1.84	0.59
1:A:404:GLY:HA2	1:A:478:LYS:HG2	1.84	0.57
1:A:265:PRO:HG3	1:A:301:HIS:HD2	1.69	0.57
1:B:265:PRO:HG3	1:B:301:HIS:CD2	2.40	0.57
1:B:265:PRO:HG3	1:B:301:HIS:HD2	1.70	0.57
2:D:68:LEU:HD23	2:D:74:TRP:HB3	1.86	0.56
1:A:266:LEU:HD13	1:B:302:LEU:HD22	1.86	0.56
1:A:410:GLU:HG3	1:A:471:ARG:HG2	1.88	0.56
1:A:418:ASP:HA	1:A:421:LYS:HD3	1.90	0.54
2:D:101:LYS:HD2	2:D:115:GLU:HG2	1.89	0.53
1:A:265:PRO:HA	1:A:298:GLN:HE21	1.75	0.52
1:A:310:LEU:HD22	1:B:263:ARG:HH11	1.76	0.51
1:B:327:VAL:HG11	1:B:367:PRO:HB3	1.92	0.50
1:B:435:LEU:O	1:B:435:LEU:HD12	2.12	0.50
1:B:435:LEU:CG	1:B:435:LEU:O	2.60	0.50
1:B:322:ILE:HG12	1:B:456:HIS:CE1	2.47	0.50
2:C:3:LYS:HG2	2:C:120:LEU:HD22	1.95	0.49
1:B:283:LEU:HD11	1:B:288:LEU:HD13	1.95	0.49
1:B:329:LEU:HD13	1:B:405:VAL:HG11	1.95	0.48
1:A:277:TYR:HA	1:A:280:LEU:HD23	1.94	0.48
1:B:387:LYS:HE2	1:B:435:LEU:HD21	1.95	0.48
1:B:387:LYS:NZ	1:B:435:LEU:CG	2.74	0.47
1:A:428:PHE:CE1	1:A:444:LEU:HD11	2.50	0.47
1:A:397:ILE:HB	1:A:408:ILE:HB	1.97	0.47
2:C:82:LEU:HD22	2:C:105:LYS:HG3	1.98	0.46
1:B:435:LEU:O	1:B:435:LEU:HG	2.17	0.45
1:A:404:GLY:HA3	1:A:477:PRO:HA	1.98	0.45
1:A:276:ILE:HD11	1:A:291:PHE:HB3	1.99	0.45
1:B:243:ARG:O	1:B:247:ILE:HD12	2.17	0.45
1:A:276:ILE:HA	1:A:283:LEU:HD11	1.99	0.45
1:A:356:ASN:OD1	1:A:399:ASP:HA	2.17	0.45
1:B:435:LEU:HB3	1:B:439:VAL:HG22	1.99	0.45
1:A:265:PRO:HG3	1:A:301:HIS:CD2	2.50	0.44
1:A:264:THR:HB	1:A:265:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:HG13	1:A:449:THR:HG23	2.00	0.43
2:C:4:LYS:HG2	2:C:28:GLU:HB2	2.00	0.43
2:D:89:GLU:H	2:D:89:GLU:CD	2.22	0.43
1:A:329:LEU:HD11	1:A:476:ILE:HD11	2.01	0.43
1:B:329:LEU:O	1:B:333:VAL:HG22	2.18	0.43
2:D:113:ILE:HD13	2:D:113:ILE:HA	1.87	0.42
1:B:431:VAL:HG13	1:B:434:SER:H	1.84	0.42
2:D:84:ALA:HB2	2:D:105:LYS:HD2	2.01	0.42
1:A:416:ILE:HA	1:A:417:PRO:HD2	1.90	0.42
1:A:329:LEU:HD13	1:A:398:LEU:HD11	2.02	0.41
2:C:21:VAL:CG1	2:C:113:ILE:HD11	2.38	0.41
1:B:365:ILE:HG22	1:B:456:HIS:HD2	1.86	0.40
2:D:5:VAL:HG13	2:D:49:LEU:HB3	2.04	0.40
2:C:77:ILE:HA	2:C:78:PRO:HD3	1.97	0.40
1:B:251:LYS:O	1:B:255:ILE:HG12	2.22	0.40
1:B:264:THR:HB	1:B:265:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/258 (95%)	237 (97%)	7 (3%)	0	100	100
1	B	243/258 (94%)	233 (96%)	8 (3%)	2 (1%)	19	54
2	C	118/122 (97%)	117 (99%)	1 (1%)	0	100	100
2	D	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
All	All	724/760 (95%)	703 (97%)	19 (3%)	2 (0%)	41	73

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%)	213 (96%)	8 (4%)	35	67
1	B	219/232 (94%)	207 (94%)	12 (6%)	21	53
2	C	108/109 (99%)	104 (96%)	4 (4%)	34	66
2	D	109/109 (100%)	103 (94%)	6 (6%)	21	53
All	All	657/682 (96%)	627 (95%)	30 (5%)	27	59

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ILE
1	A	248	ASP
1	A	280	LEU
1	A	329	LEU
1	A	402	ASP
1	A	422	ASP
1	A	436	THR
1	A	450	LYS
1	B	236	THR
1	B	248	ASP
1	B	279	SER
1	B	284	ASP
1	B	292	LEU
1	B	322	ILE
1	B	329	LEU
1	B	331	ASP
1	B	359	CYS
1	B	391	ASP
1	B	432	ASP
1	B	435	LEU

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Mol	Chain	Res	Type
2	C	7	LEU
2	C	42	LEU
2	C	82	LEU
2	C	104	ARG
2	D	7	LEU
2	D	42	LEU
2	D	82	LEU
2	D	107	PHE
2	D	108	SER
2	D	113	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	ASN
1	A	298	GLN
1	A	300	ASN
1	A	301	HIS
1	A	323	ASN
1	B	298	GLN
1	B	300	ASN
1	B	301	HIS
1	B	356	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	2,4	8,11,12	1.12	0	3,15,17	1.83	1 (33%)
2	BFD	D	53	2,4	8,11,12	1.13	0	3,15,17	1.77	1 (33%)

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	2,4	-	2/5/11/13	-
2	BFD	D	53	2,4	-	2/5/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	53	BFD	OD2-CG-CB	-3.09	117.91	124.73
2	D	53	BFD	OD2-CG-CB	-3.03	118.05	124.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	53	BFD	CA-CB-CG-OD2
2	C	53	BFD	CA-CB-CG-OD1
2	D	53	BFD	CA-CB-CG-OD1
2	D	53	BFD	CA-CB-CG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	24,29,29	1.04	3 (12%)	29,45,45	1.31	4 (13%)
3	SO4	B	501	-	4,4,4	0.32	0	6,6,6	0.10	0
3	SO4	A	501	-	4,4,4	0.31	0	6,6,6	0.10	0
5	ADP	B	505	4	24,29,29	1.02	2 (8%)	29,45,45	1.38	5 (17%)
3	SO4	A	502	4	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	B	503	-	4,4,4	0.31	0	6,6,6	0.05	0
3	SO4	B	502	-	4,4,4	0.31	0	6,6,6	0.08	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
5	ADP	A	504	4	-	1/12/32/32	0/3/3/3
5	ADP	B	505	4	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	ADP	C5-C4	2.59	1.47	1.40
5	A	504	ADP	C5-C4	2.58	1.47	1.40
5	A	504	ADP	O4'-C1'	2.06	1.44	1.41
5	A	504	ADP	C2-N3	2.02	1.35	1.32
5	B	505	ADP	C2-N3	2.00	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	ADP	N3-C2-N1	-3.32	123.49	128.68
5	B	505	ADP	PA-O3A-PB	-3.29	121.54	132.83
5	A	504	ADP	N3-C2-N1	-3.23	123.64	128.68
5	A	504	ADP	C3'-C2'-C1'	2.88	105.31	100.98
5	B	505	ADP	C3'-C2'-C1'	2.84	105.26	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	ADP	C4-C5-N7	-2.73	106.55	109.40
5	A	504	ADP	C4-C5-N7	-2.60	106.69	109.40
5	A	504	ADP	PA-O3A-PB	-2.33	124.82	132.83
5	B	505	ADP	O3B-PB-O2B	2.07	115.54	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

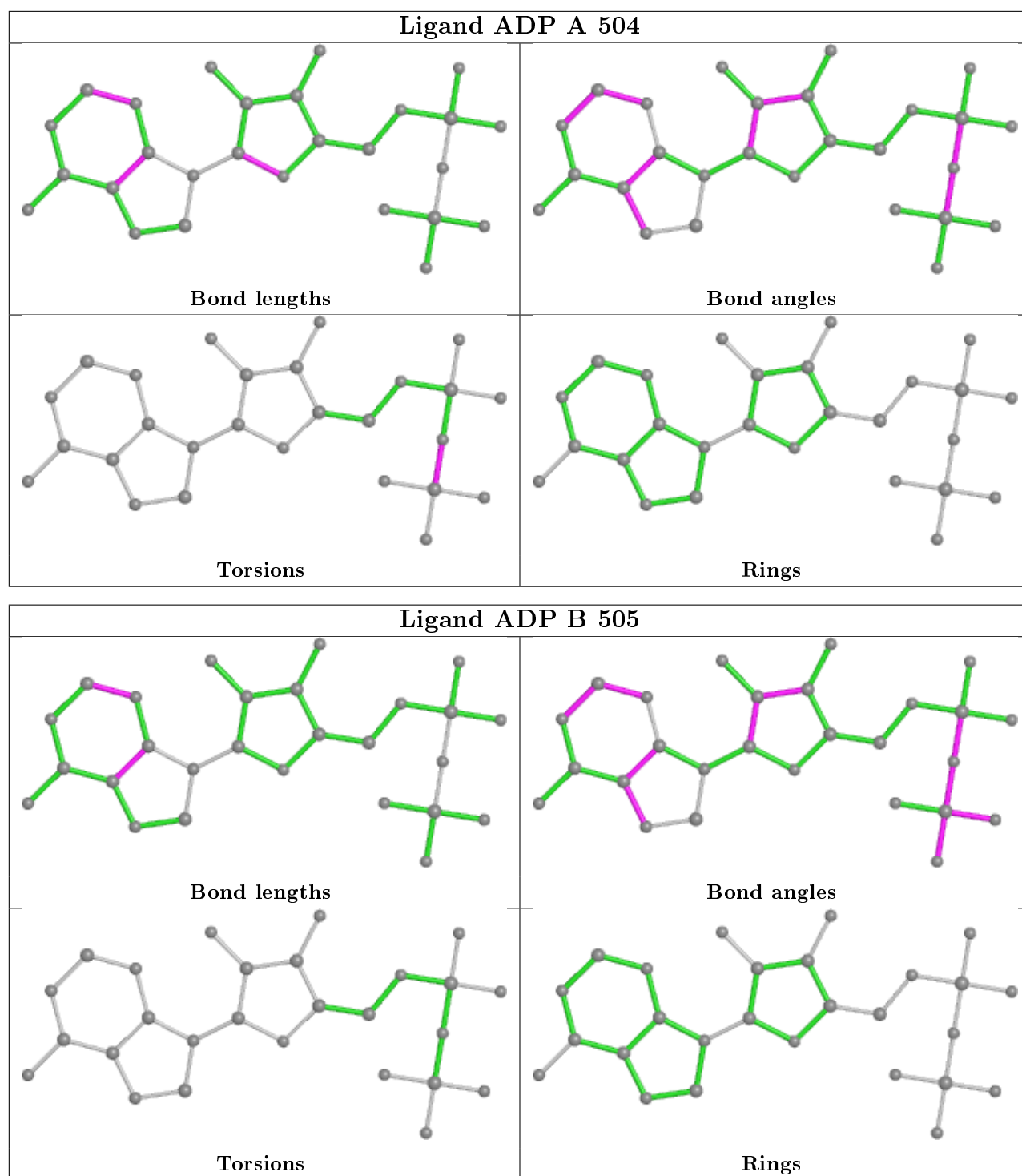
Mol	Chain	Res	Type	Atoms
5	A	504	ADP	PA-O3A-PB-O3B

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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	246/258 (95%)	-0.12	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	44, 63, 87, 99	0
1	B	244/258 (94%)	0.14	3 (1%) <span style="border: 1px solid blue; padding: 2px;">79</span> <span style="border: 1px solid blue; padding: 2px;">61</span>	47, 75, 110, 160	0
2	C	120/122 (98%)	-0.01	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	45, 58, 81, 91	0
2	D	119/122 (97%)	0.61	11 (9%) <span style="border: 1px solid red; padding: 2px;">9</span> <span style="border: 1px solid red; padding: 2px;">3</span>	49, 82, 120, 128	0
All	All	729/760 (95%)	0.10	14 (1%) <span style="border: 1px solid blue; padding: 2px;">66</span> <span style="border: 1px solid blue; padding: 2px;">46</span>	44, 68, 106, 160	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	69	GLN	4.3
2	D	97	LEU	3.4
1	B	436	THR	3.2
2	D	68	LEU	2.8
2	D	121	ASN	2.6
2	D	95	LEU	2.5
1	B	403	GLY	2.5
2	D	86	GLY	2.5
2	D	65	LEU	2.5
2	D	96	SER	2.4
1	B	477	PRO	2.3
2	D	76	ARG	2.2
2	D	75	LYS	2.2
2	D	87	GLY	2.1

### 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, 95<sup>th</sup> 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	BFD	D	53	12/13	0.95	0.17	55,58,64,65	0
2	BFD	C	53	12/13	0.98	0.17	47,49,54,54	0

### 6.3 Carbohydrates [i](#)

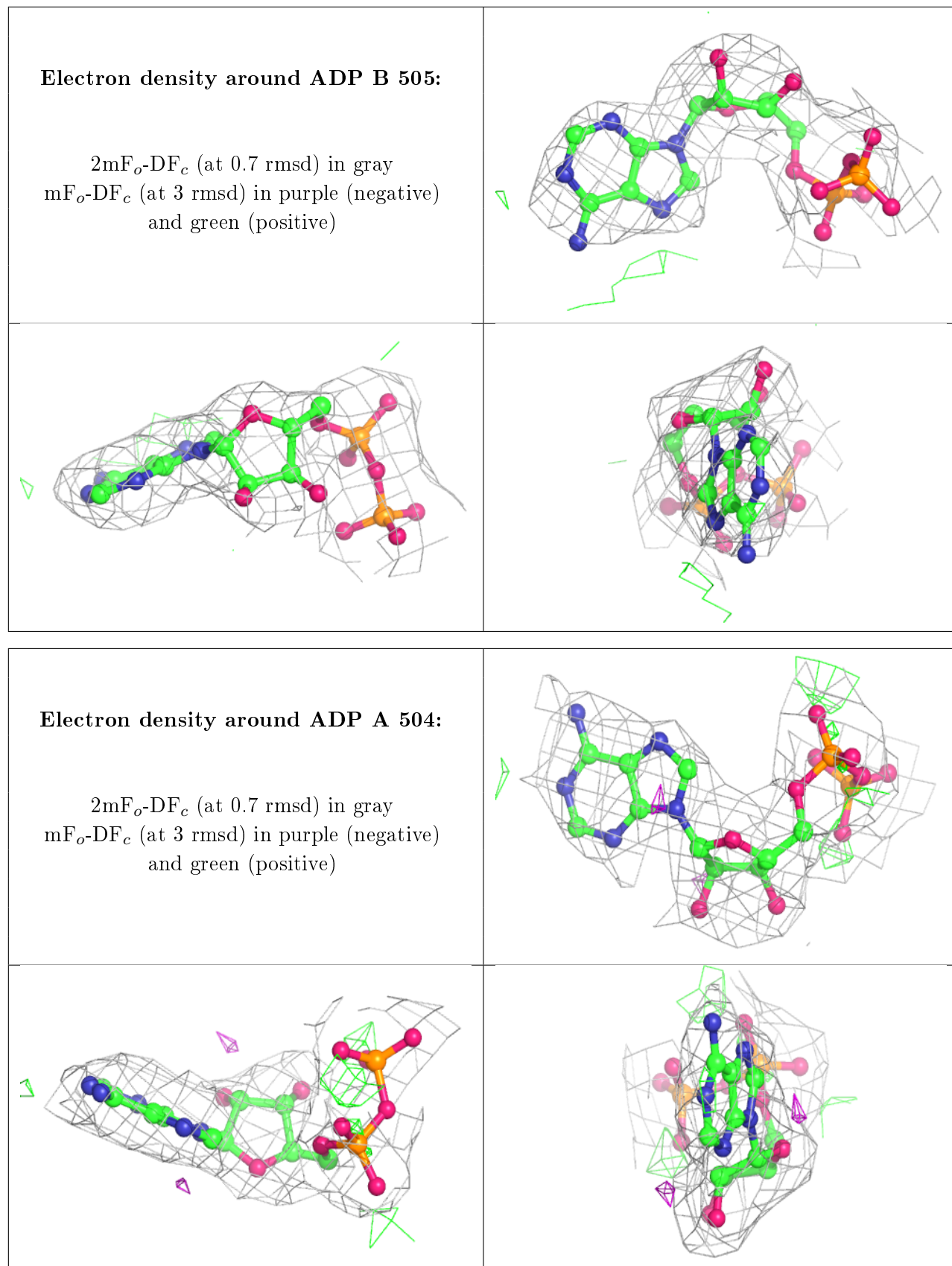
There are no monosaccharides in this entry.

### 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<sup>th</sup> 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
3	SO4	B	503	5/5	0.83	0.21	161,162,163,165	0
6	CL	B	506	1/1	0.86	0.28	79,79,79,79	0
3	SO4	A	502	5/5	0.89	0.18	110,112,112,113	0
3	SO4	B	502	5/5	0.91	0.23	141,142,143,143	0
4	MG	B	504	1/1	0.92	0.16	60,60,60,60	0
4	MG	A	503	1/1	0.94	0.29	40,40,40,40	0
4	MG	D	201	1/1	0.95	0.15	45,45,45,45	0
3	SO4	B	501	5/5	0.96	0.13	83,84,86,86	0
4	MG	C	201	1/1	0.97	0.18	40,40,40,40	0
3	SO4	A	501	5/5	0.97	0.13	79,81,82,82	0
5	ADP	B	505	27/27	0.98	0.20	70,73,75,76	0
5	ADP	A	504	27/27	0.98	0.21	48,52,53,54	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.



## 6.5 Other polymers

There are no such residues in this entry.