



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:06 AM GMT

PDB ID : 2VWI  
Title : Structure of the OSR1 kinase, a hypertension drug target  
Authors : Villa, F.; Deak, M.; Alessi, D.R.; vanAalten, D.M.F.  
Deposited on : 2008-06-25  
Resolution : 2.15 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

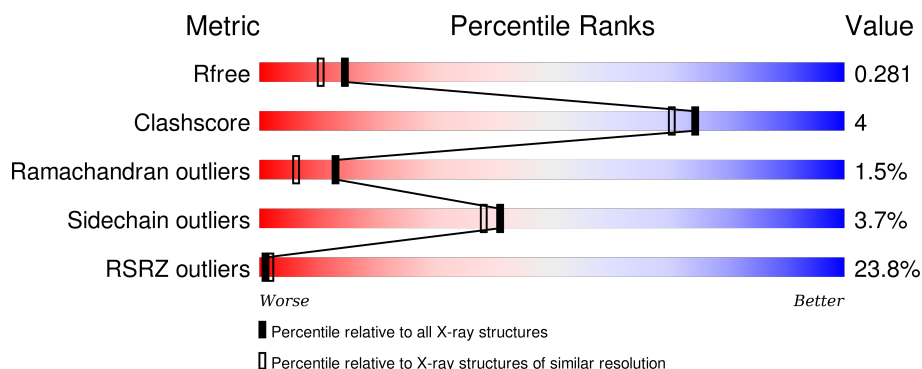
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	303	 22% 68% 9% • 22%
1	B	303	 22% 75% 11% • 13%
1	C	303	 17% 81% 7% • 11%
1	D	303	 22% 85% 8% • 6%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8508 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 SERINE/THREONINE-PROTEIN KINASE OSR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	1
			1792	1155	302	325	10			
1	B	264	Total	C	N	O	S	0	1	0
			2040	1306	343	378	13			
1	C	271	Total	C	N	O	S	0	0	1
			2106	1346	358	389	13			
1	D	284	Total	C	N	O	S	0	0	0
			2204	1406	374	410	14			

- Molecule 2 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Au	0	0
			4	4		
2	A	3	Total	Au	0	0
			3	3		
2	D	2	Total	Au	0	0
			2	2		
2	C	2	Total	Au	0	0
			2	2		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	D	1	Total 31	C 10	N 6	O 12	P 3	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	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	B	32	Total O 32 32	0	0

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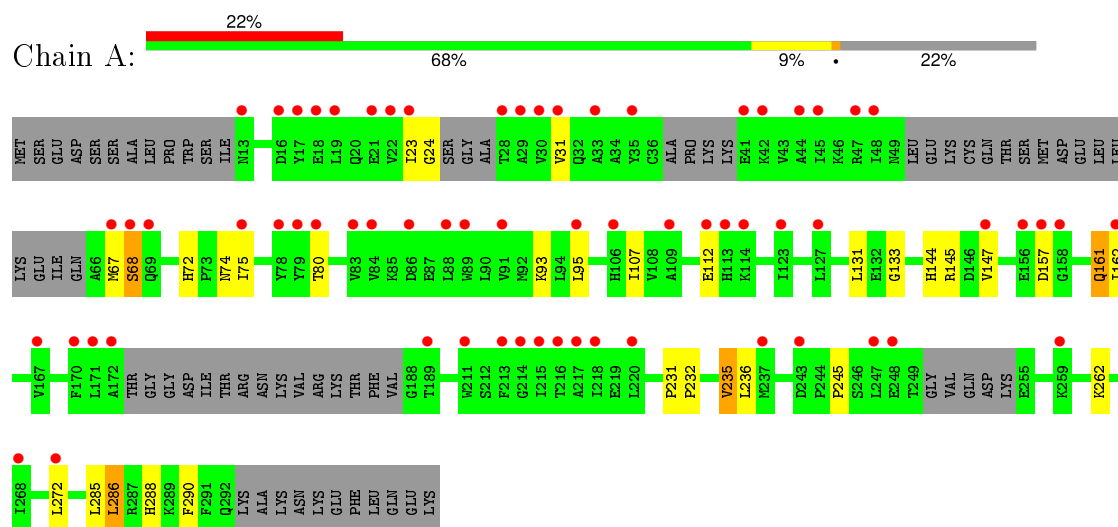
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	55	Total	O	0	0
			55	55		
5	D	91	Total	O	0	0
			91	91		

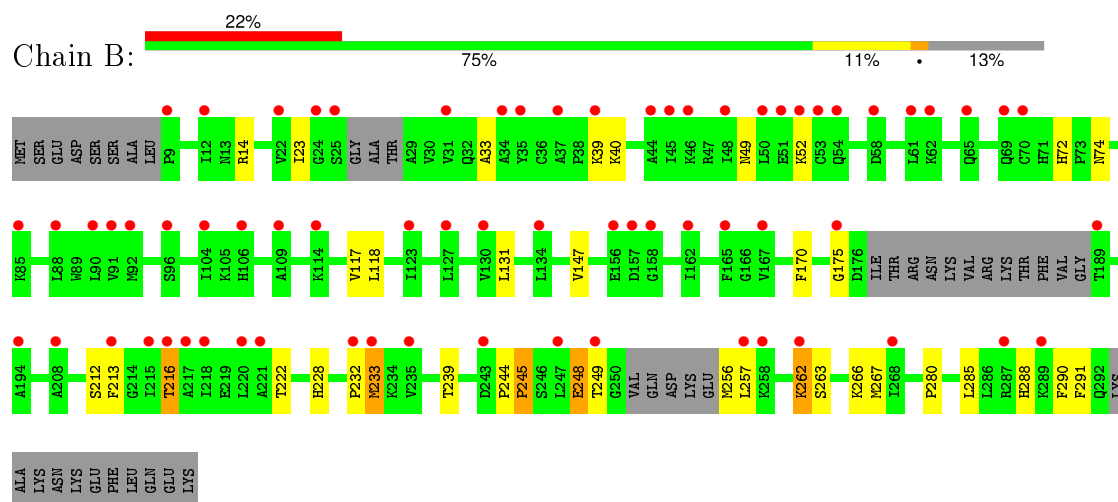
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

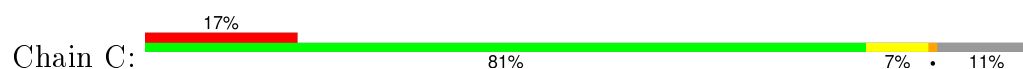
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE OSR1

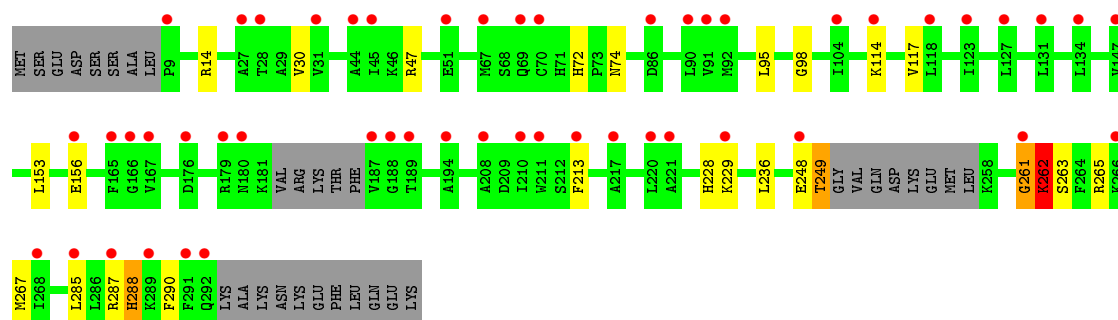


- Molecule 1: SERINE/THREONINE-PROTEIN KINASE OSR1

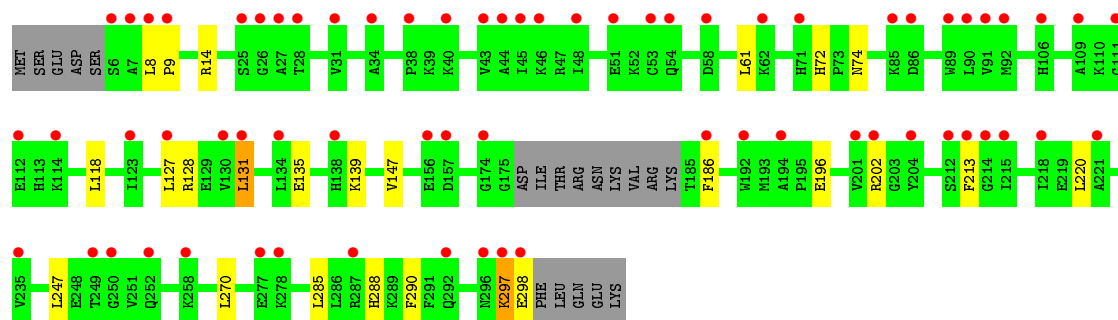
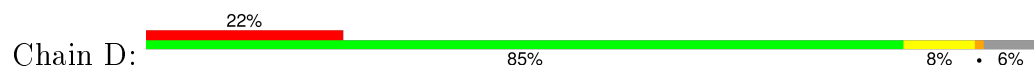


- Molecule 1: SERINE/THREONINE-PROTEIN KINASE OSR1





- Molecule 1: SERINE/THREONINE-PROTEIN KINASE OSR1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.13Å 99.90Å 158.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.15 19.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.94-2.15) 98.6 (19.94-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.253 , 0.287 0.252 , 0.281	Depositor DCC
$R_{free}$ test set	637 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63796 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AU, MG, ANP

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	0/1826	0.51	0/2469
1	B	0.33	0/2083	0.48	0/2812
1	C	0.34	0/2148	0.49	0/2900
1	D	0.34	0/2247	0.48	0/3028
All	All	0.34	0/8304	0.49	0/11209

There are no bond length outliers.

There are no bond angle outliers.

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	1792	0	1761	19	0
1	B	2040	0	2031	21	0
1	C	2106	0	2124	12	0
1	D	2204	0	2225	9	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	13	0	0
3	D	31	0	13	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	50	0	0	0	0
5	B	32	0	0	1	0
5	C	55	0	0	0	0
5	D	91	0	0	0	0
All	All	8508	0	8192	60	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 4.

All (60) 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:67:MET:HA	1:A:68:SER:HB2	1.30	1.13
1:A:131:LEU:HD21	1:A:285:LEU:HB3	1.65	0.78
1:B:245:PRO:HD2	1:B:248:GLU:HB2	1.67	0.77
1:B:131:LEU:HD21	1:B:285:LEU:HB3	1.73	0.70
1:A:72:HIS:HB3	1:A:75:ILE:HD12	1.76	0.67
1:A:67:MET:HA	1:A:68:SER:CB	2.13	0.67
1:D:297:LYS:O	1:D:298:GLU:HB2	1.95	0.66
1:A:107:ILE:HG23	1:A:112:GLU:HG3	1.79	0.65
1:D:135:GLU:O	1:D:139:LYS:HG2	2.02	0.58
1:C:30:VAL:HG13	1:C:47:ARG:HB2	1.85	0.57
1:C:213:PHE:HE2	1:C:267:MET:HE3	1.69	0.57
1:A:288:HIS:HD2	1:A:290:PHE:H	1.50	0.57
1:B:267:MET:HE2	1:B:285:LEU:HD22	1.87	0.56
1:C:261:GLY:HA2	1:C:265:ARG:HE	1.69	0.56
1:A:72:HIS:HD2	1:A:74:ASN:H	1.55	0.55
1:D:72:HIS:CD2	1:D:74:ASN:H	2.25	0.54
1:A:23:ILE:N	1:A:24:GLY:HA3	2.23	0.53
1:B:267:MET:HE3	1:B:291:PHE:HE2	1.74	0.52
1:B:212:SER:O	1:B:216:THR:HG23	2.09	0.52
1:D:288:HIS:HD2	1:D:290:PHE:H	1.57	0.52
1:C:248:GLU:O	1:C:249:THR:HB	2.10	0.51
1:B:49:ASN:HD22	1:B:52:LYS:H	1.60	0.49
1:B:262:LYS:HG3	1:B:263:SER:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:HIS:NE2	1:B:249:THR:HG23	2.27	0.49
1:D:72:HIS:HD2	1:D:74:ASN:H	1.59	0.49
1:D:288:HIS:CD2	1:D:290:PHE:H	2.31	0.48
1:A:72:HIS:CD2	1:A:74:ASN:H	2.32	0.48
1:C:95:LEU:HD22	1:C:153:LEU:HB3	1.96	0.48
1:D:131:LEU:HD21	1:D:285:LEU:HB3	1.95	0.47
1:B:72:HIS:CD2	1:B:74:ASN:H	2.31	0.47
1:C:72:HIS:CD2	1:C:74:ASN:H	2.33	0.47
1:B:288:HIS:CD2	1:B:290:PHE:H	2.33	0.47
1:B:213:PHE:HE1	1:B:267:MET:CE	2.28	0.47
1:C:288:HIS:HD2	1:C:290:PHE:H	1.62	0.46
1:C:267:MET:HE2	1:C:285:LEU:HD11	1.98	0.46
1:A:67:MET:CA	1:A:68:SER:HB2	2.22	0.46
1:D:118:LEU:HD12	1:D:220:LEU:HB3	1.98	0.46
1:B:213:PHE:HE1	1:B:267:MET:HE3	1.81	0.46
1:A:75:ILE:HD11	1:A:133:GLY:O	2.16	0.45
1:B:280:PRO:HG2	1:B:285:LEU:HG	1.98	0.45
1:A:288:HIS:CD2	1:A:290:PHE:H	2.33	0.45
1:A:131:LEU:HD23	1:A:286:LEU:HD13	2.00	0.44
1:B:239:THR:HA	5:B:2026:HOH:O	2.18	0.44
1:A:245:PRO:HB2	1:A:272:LEU:HD13	2.00	0.43
1:B:23:ILE:HD11	1:B:33:ALA:HB2	2.00	0.43
1:B:170:PHE:CZ	1:B:175:GLY:HA2	2.54	0.43
1:B:222:THR:HB	1:B:249:THR:HG21	2.00	0.43
1:C:72:HIS:HD2	1:C:74:ASN:H	1.66	0.43
1:C:228:HIS:CE1	1:C:229:LYS:HG3	2.53	0.43
1:B:267:MET:HE3	1:B:291:PHE:CE2	2.54	0.42
1:A:231:PRO:HG3	1:C:98:GLY:HA3	2.02	0.42
1:A:144:HIS:O	1:A:145:ARG:HB2	2.19	0.42
1:A:23:ILE:HD12	1:A:31:VAL:HG12	2.02	0.41
1:B:232:PRO:O	1:B:233:MET:CB	2.67	0.41
1:D:127:LEU:HB3	1:D:213:PHE:CZ	2.55	0.41
1:A:95:LEU:HD21	1:A:161:GLN:CD	2.40	0.41
1:B:117:VAL:HG12	1:B:118:LEU:HD12	2.03	0.41
1:C:262:LYS:HB3	1:C:263:SER:H	1.66	0.41
1:B:244:PRO:HA	1:B:245:PRO:HD3	1.81	0.41
1:A:232:PRO:O	1:A:235:VAL:HG13	2.21	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	225/303 (74%)	211 (94%)	13 (6%)	1 (0%)	39	34
1	B	256/303 (84%)	236 (92%)	15 (6%)	5 (2%)	9	3
1	C	265/303 (88%)	251 (95%)	9 (3%)	5 (2%)	10	3
1	D	280/303 (92%)	266 (95%)	10 (4%)	4 (1%)	14	7
All	All	1026/1212 (85%)	964 (94%)	47 (5%)	15 (2%)	13	6

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	LYS
1	B	40	LYS
1	D	8	LEU
1	B	233	MET
1	C	261	GLY
1	C	287	ARG
1	B	262	LYS
1	C	288	HIS
1	A	68	SER
1	C	262	LYS
1	B	245	PRO
1	D	186	PHE
1	D	297	LYS
1	C	117	VAL
1	D	9	PRO

### 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	183/260 (70%)	173 (94%)	10 (6%)	27	21
1	B	218/260 (84%)	211 (97%)	7 (3%)	46	45
1	C	227/260 (87%)	221 (97%)	6 (3%)	54	55
1	D	237/260 (91%)	228 (96%)	9 (4%)	40	37
All	All	865/1040 (83%)	833 (96%)	32 (4%)	41	38

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	93	LYS
1	A	147	VAL
1	A	157	ASP
1	A	161	GLN
1	A	162	ILE
1	A	235	VAL
1	A	236	LEU
1	A	262	LYS
1	A	286	LEU
1	B	14	ARG
1	B	147	VAL
1	B	216	THR
1	B	248	GLU
1	B	256	MET
1	B	257	LEU
1	B	266	LYS
1	C	14	ARG
1	C	114	LYS
1	C	156	GLU
1	C	236	LEU
1	C	249	THR
1	C	262	LYS
1	D	14	ARG
1	D	61	LEU
1	D	128	ARG
1	D	131	LEU
1	D	147	VAL
1	D	196	GLU
1	D	202	ARG
1	D	247	LEU

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Mol	Chain	Res	Type
1	D	270	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	74	ASN
1	A	288	HIS
1	B	32	GLN
1	B	49	ASN
1	B	69	GLN
1	B	72	HIS
1	B	273	GLN
1	B	288	HIS
1	C	69	GLN
1	C	72	HIS
1	C	140	ASN
1	C	151	ASN
1	C	228	HIS
1	C	288	HIS
1	D	69	GLN
1	D	72	HIS
1	D	228	HIS
1	D	288	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 14 are monoatomic - leaving 4 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
3	ANP	A	1294	-	27,33,33	3.06	6 (22%)	30,52,52	2.37	7 (23%)
3	ANP	B	1295	4	27,33,33	3.07	5 (18%)	30,52,52	2.34	8 (26%)
3	ANP	C	1294	4	27,33,33	3.12	6 (22%)	30,52,52	2.36	6 (20%)
3	ANP	D	1300	4	27,33,33	3.09	7 (25%)	30,52,52	2.36	5 (16%)

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	ANP	A	1294	-	-	0/12/38/38	0/3/3/3
3	ANP	B	1295	4	-	0/12/38/38	0/3/3/3
3	ANP	C	1294	4	-	0/12/38/38	0/3/3/3
3	ANP	D	1300	4	-	0/12/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1294	ANP	PB-O2B	-2.99	1.48	1.56
3	A	1294	ANP	PB-O2B	-2.98	1.48	1.56
3	B	1295	ANP	PB-O2B	-2.91	1.48	1.56
3	D	1300	ANP	PB-O2B	-2.88	1.48	1.56
3	B	1295	ANP	PG-O3G	-2.80	1.48	1.56
3	D	1300	ANP	PG-O3G	-2.74	1.49	1.56
3	A	1294	ANP	PG-O3G	-2.73	1.49	1.56
3	C	1294	ANP	PG-O3G	-2.63	1.49	1.56
3	D	1300	ANP	PG-O2G	2.09	1.62	1.56
3	D	1300	ANP	PB-O3A	2.14	1.61	1.59
3	A	1294	ANP	PG-O2G	2.17	1.62	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1294	ANP	PB-O1B	2.23	1.48	1.46
3	D	1300	ANP	PB-O1B	2.30	1.48	1.46
3	C	1294	ANP	PG-O2G	2.30	1.63	1.56
3	D	1300	ANP	O4'-C1'	2.48	1.44	1.41
3	A	1294	ANP	PB-O3A	2.54	1.62	1.59
3	B	1295	ANP	O4'-C1'	2.73	1.44	1.41
3	A	1294	ANP	O4'-C1'	2.89	1.44	1.41
3	B	1295	ANP	PB-O3A	2.89	1.62	1.59
3	C	1294	ANP	O4'-C1'	3.08	1.45	1.41
3	A	1294	ANP	PG-O1G	14.28	1.62	1.46
3	B	1295	ANP	PG-O1G	14.36	1.62	1.46
3	D	1300	ANP	PG-O1G	14.57	1.62	1.46
3	C	1294	ANP	PG-O1G	14.57	1.62	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1300	ANP	N3-C2-N1	-9.82	121.38	128.89
3	C	1294	ANP	N3-C2-N1	-9.75	121.43	128.89
3	B	1295	ANP	N3-C2-N1	-9.59	121.55	128.89
3	A	1294	ANP	N3-C2-N1	-9.43	121.67	128.89
3	B	1295	ANP	O2G-PG-O1G	-3.43	104.36	113.49
3	D	1300	ANP	O2G-PG-O1G	-3.41	104.44	113.49
3	A	1294	ANP	O2G-PG-O1G	-3.29	104.74	113.49
3	A	1294	ANP	O1G-PG-N3B	-3.23	106.94	111.90
3	A	1294	ANP	O1B-PB-N3B	-3.19	107.00	111.90
3	C	1294	ANP	O2G-PG-O1G	-3.10	105.24	113.49
3	A	1294	ANP	PA-O3A-PB	-3.06	122.40	132.67
3	C	1294	ANP	O1G-PG-N3B	-2.94	107.39	111.90
3	B	1295	ANP	O1B-PB-N3B	-2.85	107.53	111.90
3	C	1294	ANP	O1B-PB-N3B	-2.75	107.69	111.90
3	C	1294	ANP	PA-O3A-PB	-2.73	123.52	132.67
3	D	1300	ANP	PA-O3A-PB	-2.71	123.58	132.67
3	D	1300	ANP	O1G-PG-N3B	-2.56	107.97	111.90
3	B	1295	ANP	O1G-PG-N3B	-2.54	108.00	111.90
3	B	1295	ANP	PA-O3A-PB	-2.35	124.78	132.67
3	B	1295	ANP	C4-C5-N7	-2.17	107.48	109.48
3	A	1294	ANP	C4-C5-N7	-2.06	107.58	109.48
3	B	1295	ANP	C4'-O4'-C1'	-2.04	107.48	109.72
3	A	1294	ANP	O2B-PB-O1B	4.24	118.84	110.00
3	D	1300	ANP	O2B-PB-O1B	4.36	119.09	110.00
3	B	1295	ANP	O2B-PB-O1B	4.43	119.24	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1294	ANP	O2B-PB-O1B	4.56	119.51	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	237/303 (78%)	1.41	66 (27%) ⓘ ⓘ	38, 50, 65, 67	0
1	B	264/303 (87%)	1.39	68 (25%) ⓘ ⓘ	43, 53, 66, 78	0
1	C	271/303 (89%)	1.11	50 (18%) ⓘ ⓘ	39, 49, 56, 58	0
1	D	284/303 (93%)	1.29	67 (23%) ⓘ ⓘ	37, 50, 61, 66	0
All	All	1056/1212 (87%)	1.30	251 (23%) ⓘ ⓘ	37, 51, 64, 78	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	THR	10.2
1	D	27	ALA	9.8
1	A	172	ALA	9.4
1	C	187	VAL	7.3
1	B	39	LYS	6.6
1	C	292	GLN	6.2
1	A	170	PHE	6.0
1	D	25	SER	5.8
1	B	45	ILE	5.8
1	A	89	TRP	5.6
1	A	22	VAL	5.5
1	B	54	GLN	5.4
1	C	261	GLY	5.4
1	B	51	GLU	5.3
1	D	45	ILE	5.3
1	A	30	VAL	5.1
1	C	220	LEU	5.1
1	D	44	ALA	5.0
1	C	114	LYS	5.0
1	D	6	SER	5.0
1	D	8	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	19	LEU	4.8
1	D	7	ALA	4.7
1	B	233	MET	4.7
1	B	220	LEU	4.7
1	B	44	ALA	4.6
1	C	45	ILE	4.4
1	A	215	ILE	4.4
1	B	12	ILE	4.4
1	D	186	PHE	4.4
1	D	296	ASN	4.4
1	D	28	THR	4.4
1	A	156	GLU	4.3
1	D	218	ILE	4.3
1	B	249	THR	4.2
1	C	188	GLY	4.2
1	A	86	ASP	4.1
1	D	134	LEU	4.1
1	B	90	LEU	4.1
1	A	23	ILE	4.1
1	A	41	GLU	4.0
1	C	27	ALA	4.0
1	B	156	GLU	4.0
1	A	13	ASN	4.0
1	A	42	LYS	3.9
1	C	180	ASN	3.9
1	D	194	ALA	3.9
1	A	189	THR	3.9
1	C	91	VAL	3.9
1	B	213	PHE	3.9
1	B	175	GLY	3.8
1	D	86	ASP	3.8
1	D	90	LEU	3.8
1	D	26	GLY	3.8
1	A	75	ILE	3.7
1	B	85	LYS	3.7
1	A	113	HIS	3.6
1	B	232	PRO	3.6
1	B	37	ALA	3.6
1	C	44	ALA	3.6
1	D	277	GLU	3.5
1	B	127	LEU	3.5
1	D	298	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	48	ILE	3.5
1	D	130	VAL	3.4
1	A	29	ALA	3.4
1	B	221	ALA	3.4
1	A	114	LYS	3.4
1	C	229	LYS	3.4
1	B	91	VAL	3.4
1	D	292	GLN	3.4
1	C	217	ALA	3.4
1	A	48	ILE	3.3
1	A	112	GLU	3.3
1	A	158	GLY	3.3
1	C	213	PHE	3.3
1	C	176	ASP	3.2
1	A	216	THR	3.2
1	C	28	THR	3.2
1	B	9	PRO	3.2
1	C	287	ARG	3.2
1	A	259	LYS	3.2
1	B	130	VAL	3.1
1	C	118	LEU	3.1
1	D	85	LYS	3.1
1	A	109	ALA	3.0
1	B	88	LEU	3.0
1	C	90	LEU	3.0
1	B	134	LEU	3.0
1	A	80	THR	3.0
1	D	249	THR	3.0
1	D	297	LYS	3.0
1	B	109	ALA	3.0
1	D	109	ALA	3.0
1	C	289	LYS	3.0
1	D	91	VAL	3.0
1	B	217	ALA	3.0
1	A	45	ILE	2.9
1	D	131	LEU	2.9
1	D	106	HIS	2.9
1	B	123	ILE	2.9
1	D	213	PHE	2.9
1	C	51	GLU	2.9
1	A	171	LEU	2.9
1	B	58	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	216	THR	2.9
1	D	287	ARG	2.9
1	B	243[A]	ASP	2.9
1	B	258	LYS	2.8
1	A	248	GLU	2.8
1	D	127	LEU	2.8
1	C	127	LEU	2.8
1	A	243	ASP	2.8
1	A	237	MET	2.8
1	B	46	LYS	2.8
1	D	46	LYS	2.8
1	A	220	LEU	2.8
1	B	247	LEU	2.8
1	C	221	ALA	2.7
1	B	50	LEU	2.7
1	B	157	ASP	2.7
1	B	167	VAL	2.7
1	A	84	VAL	2.7
1	A	167	VAL	2.7
1	A	211	TRP	2.7
1	A	88	LEU	2.6
1	B	257	LEU	2.6
1	C	134	LEU	2.6
1	D	31	VAL	2.6
1	A	79	TYR	2.6
1	B	165	PHE	2.6
1	D	114	LYS	2.6
1	C	123	ILE	2.6
1	B	235	VAL	2.6
1	B	31	VAL	2.6
1	B	96	SER	2.6
1	A	157	ASP	2.6
1	B	158	GLY	2.6
1	B	52	LYS	2.6
1	A	127	LEU	2.6
1	B	65	GLN	2.6
1	A	17	TYR	2.5
1	A	247	LEU	2.5
1	D	53	CYS	2.5
1	A	147	VAL	2.5
1	C	31	VAL	2.5
1	D	48	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	262	LYS	2.5
1	B	215	ILE	2.5
1	A	213	PHE	2.5
1	C	70	CYS	2.5
1	D	58	ASP	2.4
1	D	40	LYS	2.4
1	D	71	HIS	2.4
1	B	62	LYS	2.4
1	C	9	PRO	2.4
1	A	83	VAL	2.4
1	A	268	ILE	2.4
1	C	86	ASP	2.4
1	B	25	SER	2.4
1	B	194	ALA	2.4
1	A	95	LEU	2.4
1	D	112	GLU	2.4
1	A	33	ALA	2.3
1	B	22	VAL	2.3
1	D	43	VAL	2.3
1	C	210	ILE	2.3
1	D	215	ILE	2.3
1	A	67	MET	2.3
1	B	70	CYS	2.3
1	C	131	LEU	2.3
1	D	221	ALA	2.3
1	C	156	GLU	2.3
1	D	252	GLN	2.3
1	A	44	ALA	2.3
1	C	291	PHE	2.3
1	A	16	ASP	2.3
1	B	218	ILE	2.3
1	B	189	THR	2.3
1	A	272	LEU	2.3
1	B	61	LEU	2.3
1	C	208	ALA	2.3
1	D	54	GLN	2.3
1	C	189	THR	2.3
1	C	69	GLN	2.3
1	C	165	PHE	2.2
1	B	104	ILE	2.2
1	C	194	ALA	2.2
1	D	174	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	62	LYS	2.2
1	D	92	MET	2.2
1	A	218	ILE	2.2
1	D	123	ILE	2.2
1	B	24	GLY	2.2
1	C	248	GLU	2.2
1	B	114	LYS	2.2
1	C	285	LEU	2.2
1	D	202	ARG	2.2
1	D	156	GLU	2.2
1	A	106	HIS	2.2
1	B	268	ILE	2.2
1	D	34	ALA	2.2
1	B	289	LYS	2.2
1	B	106	HIS	2.2
1	A	21	GLU	2.2
1	B	53	CYS	2.2
1	C	67	MET	2.2
1	A	35	TYR	2.2
1	A	18	GLU	2.2
1	C	147	VAL	2.2
1	A	91	VAL	2.1
1	D	235	VAL	2.1
1	C	92	MET	2.1
1	C	104	ILE	2.1
1	D	212	SER	2.1
1	B	69	GLN	2.1
1	D	89	TRP	2.1
1	B	35	TYR	2.1
1	C	167	VAL	2.1
1	D	138	HIS	2.1
1	B	162	ILE	2.1
1	D	111	GLY	2.1
1	C	179	ARG	2.1
1	D	258	LYS	2.1
1	A	78	TYR	2.1
1	C	211	TRP	2.1
1	D	192	TRP	2.1
1	D	201	VAL	2.1
1	B	287	ARG	2.1
1	A	217	ALA	2.1
1	B	34	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	SER	2.1
1	B	92	MET	2.1
1	D	9	PRO	2.1
1	A	214	GLY	2.1
1	D	204	TYR	2.1
1	D	51	GLU	2.0
1	A	162	ILE	2.0
1	C	268	ILE	2.0
1	D	250	GLY	2.0
1	B	208	ALA	2.0
1	A	31	VAL	2.0
1	A	47	ARG	2.0
1	D	278	LYS	2.0
1	D	38	PRO	2.0
1	A	123	ILE	2.0
1	D	214	GLY	2.0
1	C	266	LYS	2.0
1	A	69	GLN	2.0
1	C	166	GLY	2.0
1	D	157	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	AU	B	1297	1/1	0.95	0.23	0.67	78,78,78,78	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ANP	A	1294	31/31	0.73	0.23	0.59	63,64,70,70	0
3	ANP	B	1295	31/31	0.82	0.23	0.57	55,57,65,65	0
3	ANP	C	1294	31/31	0.88	0.17	-0.08	26,29,45,46	0
3	ANP	D	1300	31/31	0.76	0.21	-0.20	39,41,57,58	0
2	AU	A	1296	1/1	0.97	0.12	-0.98	47,47,47,47	1
2	AU	A	1295	1/1	0.99	0.10	-2.11	56,56,56,56	1
2	AU	D	1301	1/1	0.99	0.10	-2.97	36,36,36,36	1
2	AU	A	1293	1/1	0.99	0.06	-3.76	35,35,35,35	1
2	AU	B	1294	1/1	0.99	0.10	-	39,39,39,39	1
2	AU	C	1296	1/1	0.98	0.27	-	57,57,57,57	1
2	AU	B	1298	1/1	0.97	0.12	-	69,69,69,69	1
4	MG	B	1293	1/1	0.75	0.12	-	58,58,58,58	0
2	AU	D	1302	1/1	0.99	0.14	-	53,53,53,53	1
2	AU	B	1296	1/1	0.99	0.25	-	55,55,55,55	1
2	AU	C	1295	1/1	0.95	0.14	-	65,65,65,65	1
4	MG	C	1293	1/1	0.94	0.14	-	40,40,40,40	0
4	MG	D	1299	1/1	0.95	0.07	-	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.