



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:35 AM GMT

PDB ID : 3BEG  
Title : Crystal structure of SR protein kinase 1 complexed to its substrate ASF/SF2  
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Deposited on : 2007-11-18  
Resolution : 2.90 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

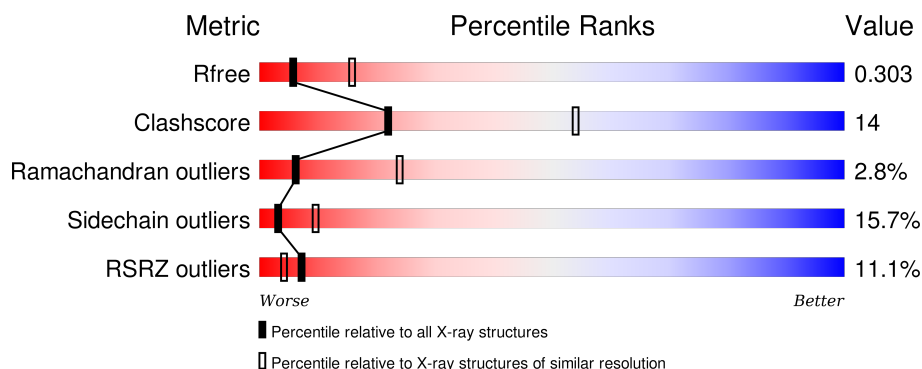
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	381	
2	B	115	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3446 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 SRPK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2744	1772	464	497	11			

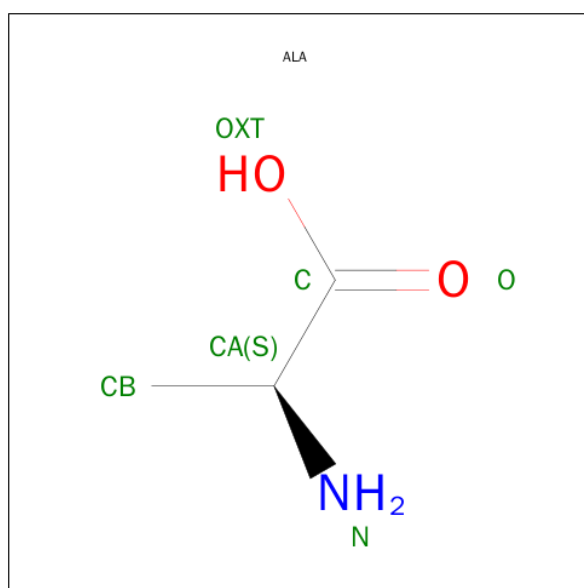
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	473	ALA	-	LINKER	? ?

- Molecule 2 is a protein called Splicing factor, arginine/serine-rich 1.

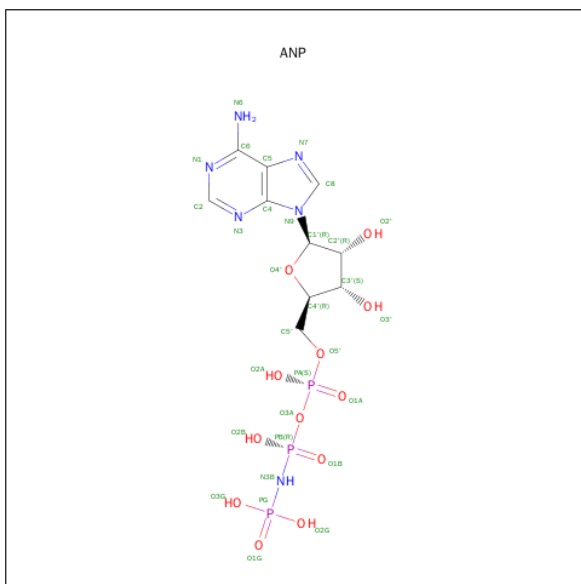
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			656	404	120	129	3			

- Molecule 3 is PHOSPHOSERINE (three-letter code: ALA, SEP) (formula:  $C_3H_7NO_2$ ,  $C_3H_8NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	2	Total	C	N	O	P	0	0
			15	6	2	6	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$ ).



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.41Å 117.53Å 193.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.40 – 2.90 38.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (38.40-2.90) 92.6 (38.40-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.237 , 0.298 0.233 , 0.303	Depositor DCC
$R_{free}$ test set	707 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	90.2	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 129.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 13862 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, SEP

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	0.54	0/2810	0.69	2/3819 (0.1%)
2	B	0.73	0/667	0.78	0/900
All	All	0.58	0/3477	0.71	2/4719 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	649	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	649	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	183	HIS	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	2744	0	2699	77	0
2	B	656	0	604	22	0
3	A	15	0	10	1	0
4	A	31	0	13	0	0
All	All	3446	0	3326	94	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 14.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:TRP:O	2:B:135:GLN:HB2	1.74	0.85
1:A:121:ALA:O	1:A:125:ILE:HG12	1.79	0.83
1:A:190:LYS:HE2	1:A:652:TRP:CE2	2.14	0.82
1:A:572:LEU:HD23	1:A:573:LEU:HD21	1.69	0.73
1:A:195:GLN:HE22	1:A:492:LYS:HG2	1.54	0.73
2:B:134:TRP:O	2:B:135:GLN:CB	2.40	0.68
1:A:73:GLY:H	1:A:82:VAL:HG23	1.58	0.68
1:A:604:LYS:HG3	1:A:604:LYS:O	1.94	0.66
1:A:601:THR:HG22	1:A:602:LYS:H	1.61	0.65
2:B:186:GLU:HG3	2:B:187:THR:H	1.62	0.65
1:A:193:ILE:O	1:A:197:LEU:HB2	1.98	0.63
2:B:129:PRO:HD3	2:B:156:GLY:O	1.99	0.62
1:A:215:LYS:HA	1:A:540:MET:HG3	1.81	0.62
2:B:182:SER:O	2:B:184:GLU:N	2.29	0.60
1:A:513:GLN:NE2	1:A:519:SER:H	1.98	0.60
2:B:186:GLU:CG	2:B:187:THR:H	2.15	0.59
1:A:560:THR:HG23	1:A:563:GLU:HB2	1.87	0.57
1:A:515:ARG:HE	1:A:565:HIS:HD2	1.53	0.56
1:A:118:THR:HG22	1:A:161:ILE:HG12	1.88	0.55
1:A:603:LEU:O	1:A:605:PRO:HD3	2.07	0.55
1:A:149:ASP:O	1:A:164:VAL:HG12	2.07	0.54
1:A:84:ARG:NH2	1:A:84:ARG:HB2	2.22	0.54
1:A:613:VAL:O	1:A:617:GLU:HA	2.08	0.54
1:A:477:ASN:O	1:A:479:LEU:N	2.41	0.53
2:B:155:ASP:OD1	2:B:157:THR:HG22	2.08	0.53
1:A:565:HIS:O	1:A:569:ILE:HG12	2.09	0.53
1:A:530:THR:N	1:A:531:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:HIS:HD2	1:A:174:LYS:H	1.55	0.52
1:A:143:MET:O	1:A:494:LYS:HA	2.09	0.52
1:A:145:VAL:HA	1:A:494:LYS:HE3	1.91	0.52
1:A:118:THR:O	1:A:122:LEU:HB2	2.10	0.52
1:A:185:PRO:HD3	1:A:483:LEU:HD12	1.93	0.51
1:A:79:ARG:HG3	1:A:99:ASP:HB2	1.92	0.51
1:A:148:LEU:HB2	1:A:164:VAL:HG13	1.92	0.51
1:A:207:CYS:O	1:A:209:ILE:HG13	2.12	0.49
1:A:516:GLN:NE2	1:A:516:GLN:H	2.11	0.49
2:B:166:GLU:HG2	2:B:167:ASP:N	2.28	0.49
1:A:84:ARG:HD2	1:A:235:ALA:HB3	1.93	0.49
2:B:153:TYR:HD2	2:B:157:THR:HG23	1.77	0.49
1:A:580:LEU:HB2	1:A:637:ILE:CD1	2.43	0.49
1:A:88:TRP:CH2	2:B:135:GLN:HA	2.49	0.48
2:B:166:GLU:HG2	2:B:167:ASP:H	1.78	0.48
1:A:190:LYS:HE2	1:A:652:TRP:CZ2	2.49	0.47
2:B:128:LEU:HA	2:B:156:GLY:O	2.14	0.47
1:A:134:SER:O	1:A:135:ASP:HB2	2.14	0.47
1:A:181:TYR:CE1	2:B:154:ARG:HD3	2.49	0.47
1:A:572:LEU:HD23	1:A:573:LEU:CD2	2.41	0.47
1:A:580:LEU:HB2	1:A:637:ILE:HD13	1.97	0.46
1:A:637:ILE:HB	1:A:640:LYS:HD2	1.97	0.46
2:B:129:PRO:CD	2:B:156:GLY:O	2.62	0.45
1:A:635:GLU:OE1	1:A:635:GLU:HA	2.16	0.45
1:A:191:LYS:HA	1:A:191:LYS:HE3	1.98	0.45
1:A:105:PHE:CD2	1:A:105:PHE:N	2.84	0.45
1:A:598:LYS:HB3	1:A:599:HIS:CD2	2.52	0.45
1:A:88:TRP:O	2:B:135:GLN:NE2	2.46	0.45
1:A:93:THR:HB	1:A:95:TRP:HE1	1.82	0.45
1:A:104:LYS:HD2	1:A:105:PHE:H	1.81	0.45
2:B:179:LYS:HA	2:B:188:ALA:O	2.16	0.44
1:A:84:ARG:HB2	1:A:84:ARG:HH21	1.81	0.44
1:A:609:PHE:HD1	1:A:623:ALA:O	2.00	0.44
1:A:533:ASP:O	1:A:536:SER:HB2	2.18	0.44
1:A:180:ASN:HD22	1:A:180:ASN:HA	1.63	0.44
1:A:629:PHE:O	1:A:632:PRO:HD2	2.17	0.44
1:A:606:TRP:HD1	1:A:610:GLU:HG3	1.83	0.43
2:B:127:GLY:N	2:B:191:ARG:O	2.48	0.43
1:A:128:LEU:HD13	1:A:147:LEU:HB2	2.00	0.43
1:A:110:VAL:HG22	1:A:162:CYS:SG	2.58	0.43
1:A:152:LYS:HG3	1:A:161:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:HD23	1:A:544:LEU:HA	1.94	0.43
2:B:137:LEU:HD23	2:B:137:LEU:HA	1.85	0.43
1:A:85:LYS:HB3	1:A:95:TRP:CZ3	2.55	0.42
1:A:549:TYR:CE2	2:B:154:ARG:NH1	2.88	0.42
1:A:130:SER:HB3	1:A:209:ILE:HD11	1.99	0.42
1:A:112:LYS:HA	1:A:112:LYS:HD2	1.85	0.42
1:A:515:ARG:HD2	1:A:515:ARG:HA	1.76	0.42
1:A:118:THR:O	1:A:161:ILE:HD11	2.20	0.42
1:A:121:ALA:HB3	1:A:161:ILE:HD11	2.02	0.42
1:A:227:TYR:O	1:A:231:LEU:HB2	2.20	0.41
1:A:590:PHE:HB2	1:A:591:PHE:CD2	2.55	0.41
1:A:75:LEU:HA	1:A:80:TYR:O	2.20	0.41
1:A:517:TYR:CD2	1:A:517:TYR:N	2.88	0.41
1:A:204:HIS:CG	1:A:530:THR:HB	2.56	0.41
1:A:604:LYS:HG2	2:B:205:SER:HB2	2.02	0.41
1:A:104:LYS:HG3	1:A:104:LYS:H	1.65	0.41
1:A:177:ILE:O	1:A:180:ASN:N	2.52	0.41
1:A:604:LYS:O	1:A:604:LYS:CG	2.67	0.41
1:A:106:VAL:HG11	1:A:148:LEU:CD1	2.51	0.41
1:A:147:LEU:HD13	1:A:163:MET:HB2	2.03	0.41
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.94	0.41
2:B:129:PRO:HD2	2:B:156:GLY:CA	2.51	0.40
1:A:576:VAL:HA	1:A:577:PRO:HD3	1.95	0.40
3:A:2:ALA:HB1	2:B:153:TYR:OH	2.20	0.40
1:A:220:LEU:O	1:A:494:LYS:N	2.45	0.40
1:A:607:GLY:O	1:A:611:VAL:HG23	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	344/381 (90%)	295 (86%)	42 (12%)	7 (2%)	9	33
2	B	82/115 (71%)	66 (80%)	11 (13%)	5 (6%)	2	5
All	All	426/496 (86%)	361 (85%)	53 (12%)	12 (3%)	6	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	478	PHE
2	B	131	SER
2	B	135	GLN
2	B	183	HIS
2	B	203	GLY
1	A	135	ASP
1	A	497	ASP
1	A	513	GLN
1	A	629	PHE
1	A	156	VAL
2	B	130	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/331 (88%)	243 (84%)	47 (16%)	3	9
2	B	67/98 (68%)	58 (87%)	9 (13%)	5	13
All	All	357/429 (83%)	301 (84%)	56 (16%)	3	9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	84	ARG
1	A	85	LYS
1	A	90	HIS

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Mol	Chain	Res	Type
1	A	93	THR
1	A	97	SER
1	A	104	LYS
1	A	105	PHE
1	A	106	VAL
1	A	115	GLU
1	A	130	SER
1	A	131	VAL
1	A	133	ASN
1	A	140	ASN
1	A	141	ARG
1	A	142	GLU
1	A	146	GLN
1	A	157	ASN
1	A	159	THR
1	A	168	LEU
1	A	172	LEU
1	A	180	ASN
1	A	191	LYS
1	A	208	ARG
1	A	221	LEU
1	A	223	VAL
1	A	495	ILE
1	A	510	GLU
1	A	513	GLN
1	A	514	THR
1	A	536	SER
1	A	537	THR
1	A	540	MET
1	A	555	SER
1	A	560	THR
1	A	569	ILE
1	A	576	VAL
1	A	594	LYS
1	A	597	LEU
1	A	598	LYS
1	A	603	LEU
1	A	608	LEU
1	A	617	GLU
1	A	631	LEU
1	A	634	LEU
1	A	635	GLU

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Mol	Chain	Res	Type
1	A	655	SER
2	B	124	VAL
2	B	137	LEU
2	B	147	VAL
2	B	155	ASP
2	B	169	THR
2	B	173	ARG
2	B	178	THR
2	B	181	ARG
2	B	187	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	160	HIS
1	A	171	HIS
1	A	180	ASN
1	A	218	ASN
1	A	481	ASN
1	A	505	HIS
1	A	513	GLN
1	A	516	GLN
1	A	565	HIS
1	A	620	GLN

### 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

3 ligands 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	$\# Z  > 2$
3	SEP	A	1	3	8,9,10	1.61	2 (25%)	8,12,14	1.79	1 (12%)
3	ALA	A	2	3	3,4,5	0.69	0	0,4,6	0.00	-
4	ANP	A	656	-	27,33,33	2.08	7 (25%)	30,52,52	2.53	7 (23%)

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	SEP	A	1	3	-	0/6/8/10	0/0/0/0
3	ALA	A	2	3	-	0/0/2/4	0/0/0/0
4	ANP	A	656	-	-	0/12/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	SEP	P-O2P	2.22	1.62	1.54
4	A	656	ANP	PB-O3A	2.33	1.62	1.59
4	A	656	ANP	C2-N3	2.35	1.36	1.32
3	A	1	SEP	P-O1P	3.09	1.61	1.51
4	A	656	ANP	C5-C4	3.56	1.48	1.40
4	A	656	ANP	PB-O1B	3.77	1.50	1.46
4	A	656	ANP	PB-N3B	3.88	1.73	1.63
4	A	656	ANP	PG-N3B	4.10	1.74	1.63
4	A	656	ANP	PG-O1G	5.22	1.52	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	656	ANP	O1G-PG-N3B	-7.79	99.96	111.90
4	A	656	ANP	N3-C2-N1	-6.63	123.82	128.89
4	A	656	ANP	O1B-PB-N3B	-4.95	104.31	111.90
4	A	656	ANP	C2'-C1'-N9	-3.47	108.98	114.29
4	A	656	ANP	PA-O3A-PB	-3.05	122.43	132.67
4	A	656	ANP	C4-C5-N7	-2.68	107.01	109.48
4	A	656	ANP	O2B-PB-O1B	3.85	118.04	110.00
3	A	1	SEP	OG-CB-CA	4.10	111.77	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	ALA	1	0

## 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	348/381 (91%)	0.88	41 (11%) 6 4	99, 117, 135, 141	0
2	B	86/115 (74%)	0.62	7 (8%) 15 9	101, 111, 125, 127	0
All	All	434/496 (87%)	0.83	48 (11%) 7 4	99, 116, 134, 141	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TRP	4.7
1	A	83	ILE	4.4
1	A	80	TYR	4.3
1	A	559	TYR	4.1
1	A	150	ASP	3.9
2	B	183	HIS	3.9
1	A	96	LEU	3.8
1	A	72	ILE	3.7
1	A	76	PHE	3.5
1	A	97	SER	3.5
1	A	555	SER	3.4
1	A	591	PHE	3.3
1	A	86	LEU	3.3
1	A	592	THR	3.2
1	A	497	ASP	3.2
1	A	100	ILE	3.2
1	A	162	CYS	3.1
1	A	500	ASN	3.0
1	A	157	ASN	3.0
1	A	218	ASN	3.0
1	A	101	GLN	3.0
1	A	105	PHE	2.9
2	B	190	ILE	2.9
1	A	75	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	558	GLU	2.8
2	B	128	LEU	2.8
1	A	231	LEU	2.7
1	A	106	VAL	2.7
1	A	135	ASP	2.7
1	A	158	GLY	2.6
1	A	161	ILE	2.6
2	B	195	ASP	2.5
1	A	147	LEU	2.5
1	A	209	ILE	2.5
1	A	214	ILE	2.5
2	B	162	PHE	2.3
1	A	480	VAL	2.3
1	A	636	LEU	2.3
1	A	215	LYS	2.2
1	A	95	TRP	2.2
1	A	485	PRO	2.2
2	B	138	LYS	2.2
1	A	499	GLY	2.1
1	A	163	MET	2.1
1	A	630	LEU	2.0
2	B	187	THR	2.0
1	A	537	THR	2.0
1	A	210	ILE	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( $\text{\AA}^2$ )	Q<0.9
4	ANP	A	656	31/31	0.86	0.20	-0.75	115,118,121,121	0
3	ALA	A	2	5/6	0.69	0.66	-	137,137,137,137	0
3	SEP	A	1	10/11	0.59	0.31	-	136,137,138,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.