WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2014 – 11:13 PM EDT

PDB ID : 3BEG
Title : Crystal structure of SR protein kinase 1 complexed to its substrate ASF/SF2
Authors : Ngo, J.C.; Giang, K.; Chakrabarti, S.; Ma, C.-T.; Huynh, N.; Hagopian, J.; Dorrestein, P.C.; Fu, X.-D.; Adams, J.A.; Ghosh, G.
Deposited on : 2007-11-18
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
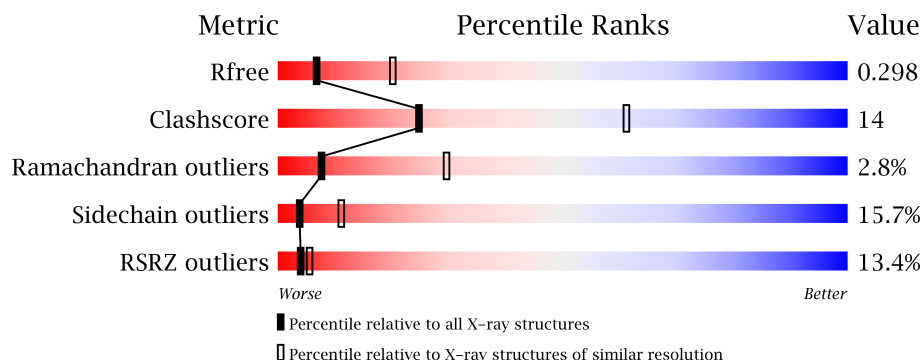A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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

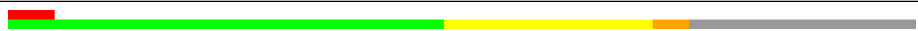|		
MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23489

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.298
Clashscore		14
Ramachandran outliers		2.8%
Sidechain outliers		15.7%
RSRZ outliers		13.4%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	381	
2	B	115	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3446 atoms, of which 0 are hydrogen and 0 are deuterium.

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-proteinkinase 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: $C_3H_7NO_2$, $C_3H_8NO_6P$).
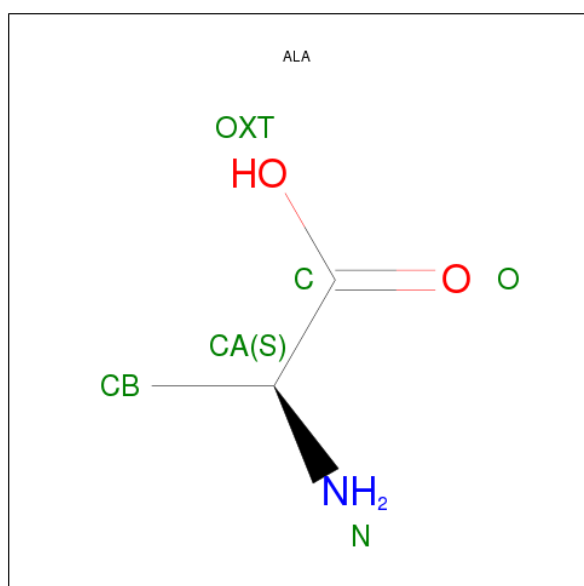
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	2	Total	C	N	O	P	0	0
			15	6	2	6	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).
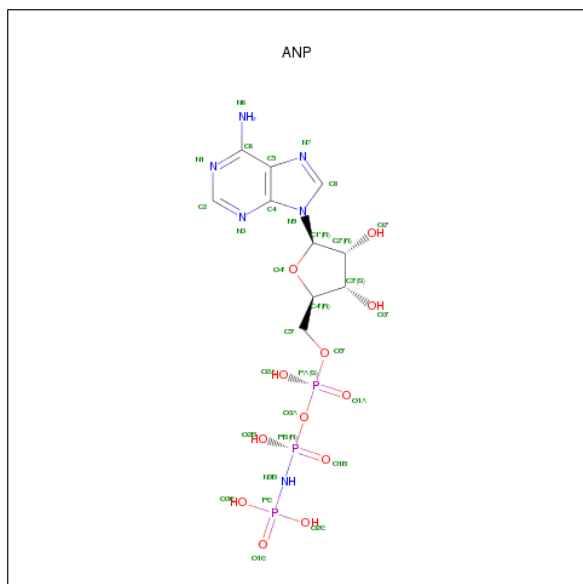
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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-proteinkinase SRPK1

Chain A:
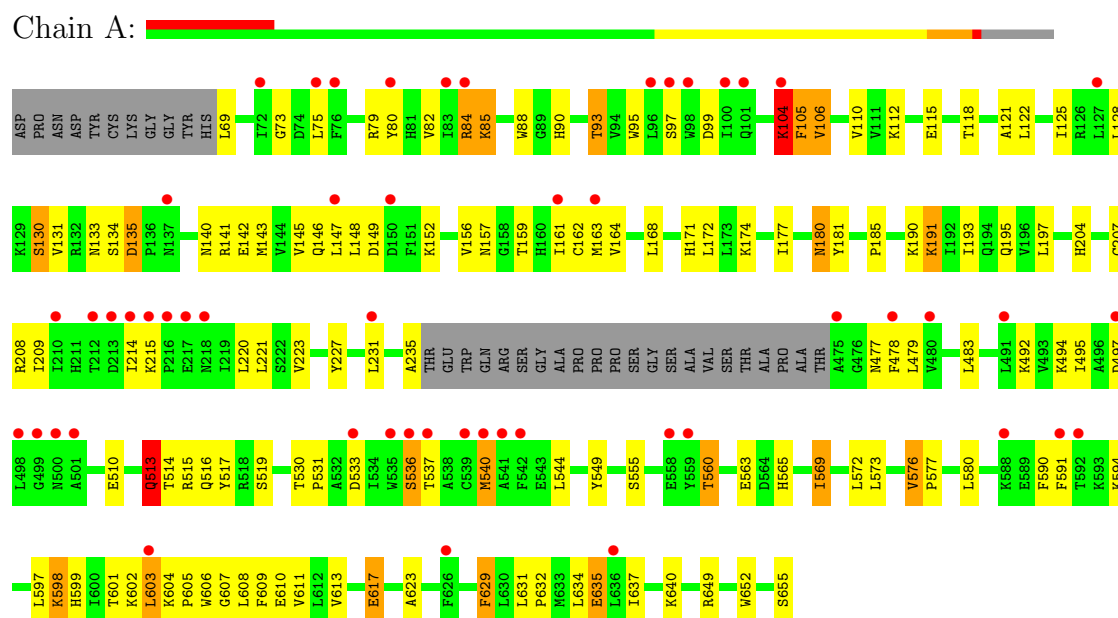
• Molecule 2: Splicing factor, arginine/serine-rich 1

Chain B:
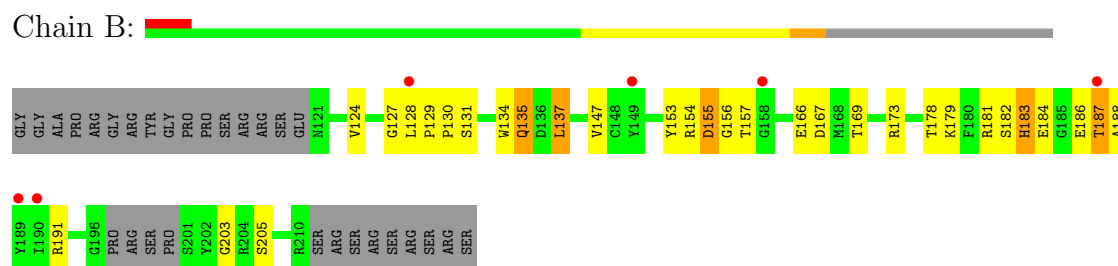
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.08 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.237 , 0.298 0.235 , 0.298	Depositor DCC
R_{free} test set	707 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	90.2	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 80.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \vert L \vert > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	1 of 13862 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3446	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.

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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(^{o})	Ideal(^{o})
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 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (94) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:215:LYS:HA	1:A:540:MET:HG3	1.81	0.62
2:B:129:PRO:HD3	2:B:156:GLY:O	1.99	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:530:THR:N	1:A:531:PRO:HD2	2.24	0.53
1:A:565:HIS:O	1:A:569:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:580:LEU:HB2	1:A:637:ILE:CD1	2.43	0.49
2:B:153:TYR:HD2	2:B:157:THR:HG23	1.77	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
1:A:134:SER:O	1:A:135:ASP:HB2	2.14	0.47
2:B:128:LEU:HA	2:B:156:GLY:O	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:191:LYS:HA	1:A:191:LYS:HE3	1.98	0.45
1:A:635:GLU:OE1	1:A:635:GLU:HA	2.16	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
1:A:544:LEU:HD23	1:A:544:LEU:HA	1.94	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:112:LYS:HA	1:A:112:LYS:HD2	1.85	0.42
1:A:130:SER:HB3	1:A:209:ILE:HD11	1.99	0.42
1:A:515:ARG:HA	1:A:515:ARG:HD2	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:517:TYR:CD2	1:A:517:TYR:N	2.88	0.41
1:A:75:LEU:HA	1:A:80:TYR:O	2.20	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: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
1:A:604:LYS:O	1:A:604:LYS:CG	2.67	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
1:A:220:LEU:O	1:A:494:LYS:N	2.45	0.40
3:A:2:ALA:HB1	2:B:153:TYR:OH	2.20	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

5.3.1 Protein backbone ⓘ

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%)	11	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	82/115 (71%)	66 (80%)	11 (13%)	5 (6%)	2	7
All	All	426/496 (86%)	361 (85%)	53 (12%)	12 (3%)	8	29

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	10
2	B	67/98 (68%)	58 (87%)	9 (13%)	6	15
All	All	357/429 (83%)	301 (84%)	56 (16%)	4	11

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
1	A	93	THR
1	A	97	SER

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Mol	Chain	Res	Type
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
1	A	655	SER
2	B	124	VAL

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Mol	Chain	Res	Type
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 chains 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	9,9,10	6.26	4 (44%)	10,12,14	1.44	2 (20%)
3	ALA	A	2	3	4,4,5	9.79	2 (50%)	3,4,6	8.92	2 (66%)
4	ANP	A	656	-	33,33,33	3.18	7 (21%)	48,52,52	2.85	11 (22%)

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	-	-	0/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	ALA	O-C	19.45	1.24	1.11
3	A	1	SEP	O-C	18.11	1.23	1.11
4	A	656	ANP	PG-N3B	11.35	1.74	1.64
4	A	656	ANP	PB-N3B	10.68	1.73	1.64
4	A	656	ANP	PG-O1G	5.20	1.52	1.46
4	A	656	ANP	PB-O1B	3.75	1.50	1.46
4	A	656	ANP	C5-C4	3.56	1.48	1.40
3	A	1	SEP	P-O1P	3.06	1.61	1.51
4	A	656	ANP	C2-N3	2.41	1.36	1.32
3	A	1	SEP	CA-C	2.34	1.54	1.49
4	A	656	ANP	PB-O3A	2.33	1.62	1.59
3	A	1	SEP	P-O2P	2.20	1.62	1.54
3	A	2	ALA	CA-C	2.10	1.53	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2	ALA	C-CA-N	-14.70	111.60	113.27
4	A	656	ANP	PB-N3B-PG	-9.78	113.61	130.07
4	A	656	ANP	C5-C4-N3	-8.26	117.92	125.98
4	A	656	ANP	O1G-PG-N3B	-7.86	99.96	111.83
4	A	656	ANP	N3-C4-N9	6.06	135.79	125.39
4	A	656	ANP	N3-C2-N1	-5.77	123.82	128.89
4	A	656	ANP	O1B-PB-N3B	-4.98	104.31	111.83
3	A	2	ALA	CB-CA-C	4.76	110.58	108.46
4	A	656	ANP	O2B-PB-O1B	3.85	118.04	109.90
4	A	656	ANP	PA-O3A-PB	-2.80	122.43	132.05
4	A	656	ANP	C2-N3-C4	2.74	121.17	113.27
4	A	656	ANP	C3'-C2'-C1'	2.50	104.85	100.92
3	A	1	SEP	P-OG-CB	-2.50	112.24	118.63
4	A	656	ANP	C4-C5-N7	-2.48	107.01	109.41
3	A	1	SEP	OG-CB-CA	2.31	111.77	108.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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, 95th 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	348/381 (91%)	0.93	52 (14%)	3	4	99, 117, 135, 141	0
2	B	86/115 (74%)	0.43	6 (6%)	16	19	101, 111, 125, 127	0
All	All	434/496 (87%)	0.83	58 (13%)	4	5	99, 116, 134, 141	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ILE	4.7
1	A	497	ASP	4.5
1	A	592	THR	4.3
1	A	98	TRP	4.2
1	A	559	TYR	4.0
1	A	500	ASN	3.8
1	A	76	PHE	3.5
1	A	75	LEU	3.5
1	A	72	ILE	3.5
1	A	218	ASN	3.4
1	A	215	LYS	3.3
1	A	480	VAL	3.3
1	A	214	ILE	3.2
1	A	231	LEU	3.2
1	A	475	ALA	3.1
1	A	499	GLY	3.0
1	A	163	MET	3.0
1	A	591	PHE	2.9
1	A	83	ILE	2.9
1	A	137	ASN	2.9
1	A	80	TYR	2.9
1	A	636	LEU	2.9
1	A	478	PHE	2.8
1	A	213	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	491	LEU	2.8
1	A	537	THR	2.8
2	B	190	ILE	2.8
1	A	212	THR	2.7
2	B	128	LEU	2.6
1	A	216	PRO	2.6
1	A	97	SER	2.6
2	B	189	TYR	2.5
1	A	147	LEU	2.5
1	A	539	CYS	2.5
2	B	187	THR	2.4
1	A	603	LEU	2.4
1	A	217	GLU	2.4
1	A	558	GLU	2.4
1	A	96	LEU	2.3
1	A	540	MET	2.3
1	A	501	ALA	2.3
1	A	104	LYS	2.2
1	A	626	PHE	2.2
2	B	158	GLY	2.2
1	A	84	ARG	2.2
1	A	542	PHE	2.1
1	A	210	ILE	2.1
1	A	536	SER	2.1
1	A	127	LEU	2.1
1	A	498	LEU	2.1
1	A	541	ALA	2.1
2	B	149	TYR	2.1
1	A	588	LYS	2.1
1	A	533	ASP	2.1
1	A	101	GLN	2.1
1	A	150	ASP	2.0
1	A	535	TRP	2.0
1	A	161	ILE	2.0

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 (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, 95th 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SEP	A	1	10/11	0.29	0.26	136,137,138,138	0
4	ANP	A	656	31/31	0.24	-0.15	115,118,121,121	0
3	ALA	A	2	5/6	0.18	-0.84	137,137,137,137	0

6.5   Other polymers (i)

There are no such residues in this entry.