



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:58 AM UTC

PDB ID : 3BEG / pdb_00003beg
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

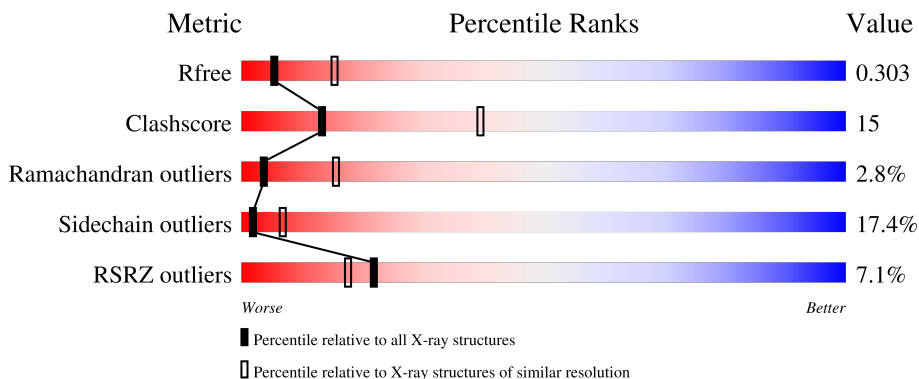
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 5 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			

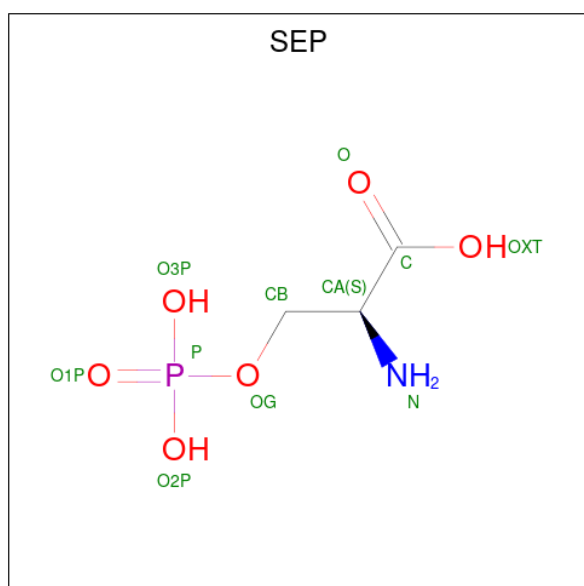
There is a discrepancy between the modelled and reference sequences:

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

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

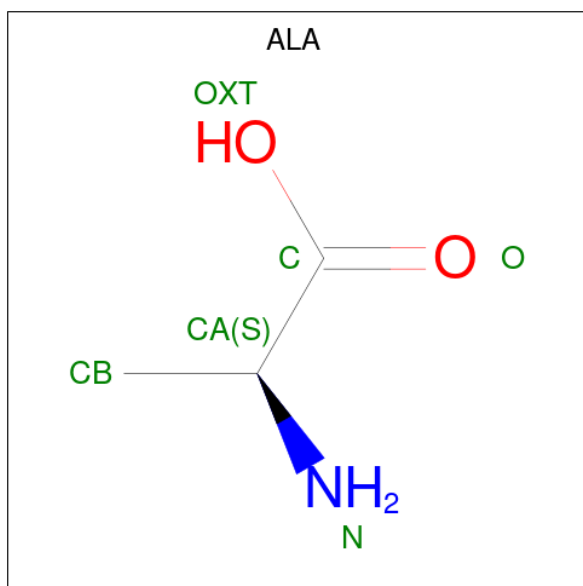
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			656	404	120	129	3			

- Molecule 3 is PHOSPHOSERINE (CCD ID: SEP) (formula: C₃H₈NO₆P).



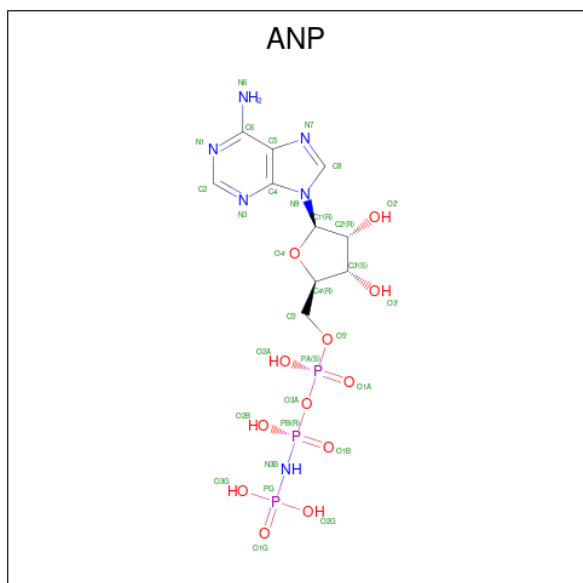
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

- Molecule 4 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

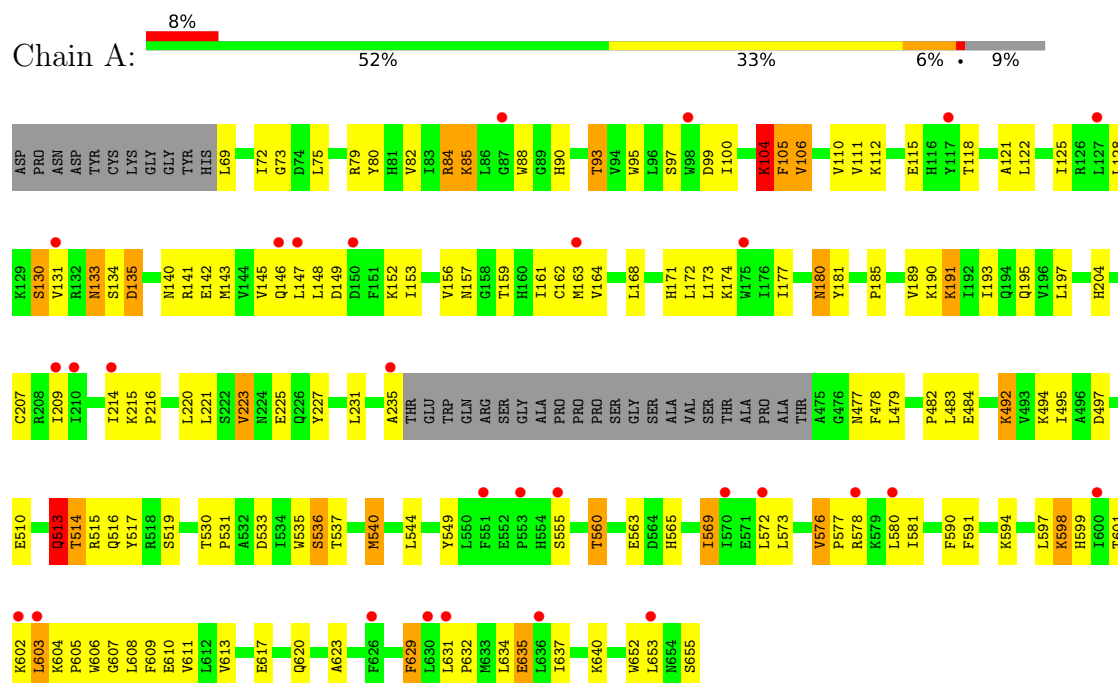


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

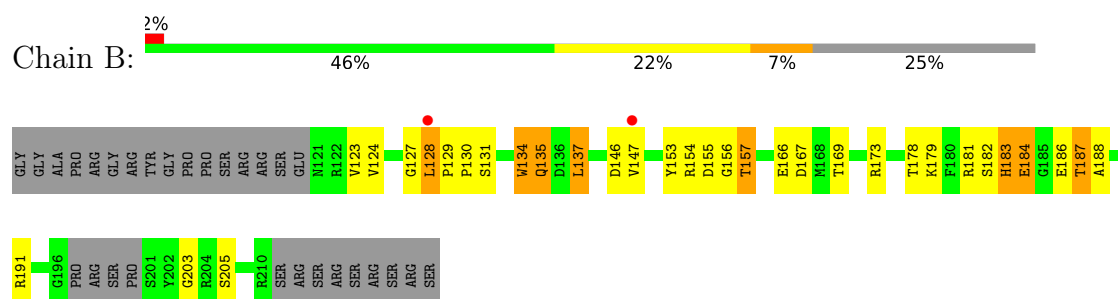
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Serine/threonine-protein kinase SRPK1



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



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
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.298 0.233 , 0.303	Depositor DCC
R_{free} test set	707 reflections (4.72%)	wwPDB-VP
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 , 133.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, 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	0.69	0/2810	1.03	5/3819 (0.1%)
2	B	0.88	1/667 (0.1%)	1.07	4/900 (0.4%)
All	All	0.73	1/3477 (0.0%)	1.04	9/4719 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	123	VAL	CA-CB	5.11	1.61	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	184	GLU	N-CA-C	-7.13	104.20	114.12
1	A	653	LEU	N-CA-C	7.09	118.66	111.07
2	B	134	TRP	N-CA-C	-6.48	101.54	110.35
1	A	133	ASN	N-CA-C	6.47	118.00	107.32
1	A	223	VAL	N-CA-C	6.12	117.29	108.48
2	B	157	THR	N-CA-C	-5.71	102.01	110.46
1	A	72	ILE	N-CA-C	5.53	116.40	108.93
2	B	128	LEU	N-CA-C	5.27	121.46	109.81
1	A	225	GLU	N-CA-C	5.11	116.85	111.28

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	82	0
2	B	656	0	604	23	0
3	A	10	0	5	0	0
4	A	5	0	5	1	0
5	A	31	0	13	0	0
All	All	3446	0	3326	100	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 15.

All (100) 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:O	1:A:604:LYS:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:PRO:HA	1:A:540:MET:HE3	1.87	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
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
2:B:182:SER:C	2:B:184:GLU:H	2.21	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:HE3	1:A:191:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:482:PRO:C	1:A:484:GLU:H	2.28	0.42
1:A:514:THR:O	1:A:515:ARG:C	2.62	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:535:TRP:CD1	1:A:535:TRP:C	2.98	0.41
1:A:204:HIS:CG	1:A:530:THR:HB	2.56	0.41
1:A:577:PRO:O	1:A:578:ARG:C	2.64	0.41
1:A:104:LYS:H	1:A:104:LYS:HG3	1.65	0.41
1:A:177:ILE:O	1:A:180:ASN:N	2.52	0.41
1:A:604:LYS:HG2	2:B:205:SER:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:O	1:A:494:LYS:N	2.45	0.40
4: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 [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%)	6	22
2	B	82/115 (71%)	66 (80%)	11 (13%)	5 (6%)	1	4
All	All	426/496 (86%)	361 (85%)	53 (12%)	12 (3%)	4	15

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%)	237 (82%)	53 (18%)	2	6
2	B	67/98 (68%)	58 (87%)	9 (13%)	4	12
All	All	357/429 (83%)	295 (83%)	62 (17%)	2	7

All (62) 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
1	A	100	ILE
1	A	104	LYS
1	A	105	PHE
1	A	106	VAL
1	A	111	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	153	ILE
1	A	157	ASN
1	A	159	THR
1	A	168	LEU
1	A	172	LEU
1	A	173	LEU
1	A	180	ASN
1	A	189	VAL

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Mol	Chain	Res	Type
1	A	191	LYS
1	A	221	LEU
1	A	223	VAL
1	A	492	LYS
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	581	ILE
1	A	594	LYS
1	A	597	LEU
1	A	598	LYS
1	A	603	LEU
1	A	608	LEU
1	A	620	GLN
1	A	631	LEU
1	A	634	LEU
1	A	635	GLU
1	A	655	SER
2	B	124	VAL
2	B	137	LEU
2	B	146	ASP
2	B	147	VAL
2	B	169	THR
2	B	173	ARG
2	B	178	THR
2	B	181	ARG
2	B	187	THR

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

Mol	Chain	Res	Type
1	A	77	ASN
1	A	157	ASN
1	A	171	HIS

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Mol	Chain	Res	Type
1	A	180	ASN
1	A	218	ASN
1	A	505	HIS
1	A	513	GLN
1	A	516	GLN
1	A	565	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 oligosaccharides 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	$\# Z > 2$
4	ALA	A	2	3	3,4,5	0.80	0	2,4,6	0.82	0
3	SEP	A	1	4	8,9,10	1.70	2 (25%)	7,12,14	1.67	1 (14%)
5	ANP	A	656	-	33,33,33	2.02	9 (27%)	45,52,52	2.36	9 (20%)

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
4	ALA	A	2	3	-	0/1/2/4	-
3	SEP	A	1	4	-	0/6/8/10	-
5	ANP	A	656	-	-	3/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	656	ANP	C5-C4	5.29	1.48	1.39
5	A	656	ANP	PG-N3B	4.15	1.74	1.63
5	A	656	ANP	PB-N3B	3.93	1.73	1.63
5	A	656	ANP	PG-O1G	3.91	1.52	1.46
3	A	1	SEP	P-O1P	3.49	1.61	1.50
5	A	656	ANP	C5-C6	2.84	1.48	1.41
5	A	656	ANP	PB-O1B	2.80	1.50	1.46
5	A	656	ANP	C8-N7	2.53	1.36	1.31
5	A	656	ANP	PB-O3A	2.35	1.62	1.59
5	A	656	ANP	C5-N7	-2.34	1.34	1.39
3	A	1	SEP	P-O2P	2.12	1.62	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	656	ANP	O1G-PG-N3B	-8.02	99.96	111.77
5	A	656	ANP	C5-C4-N3	-6.39	117.92	126.72
5	A	656	ANP	N3-C4-N9	5.07	135.79	127.17
5	A	656	ANP	O1B-PB-N3B	-5.07	104.31	111.77
5	A	656	ANP	C2-N3-C4	3.82	121.17	111.83
5	A	656	ANP	O2B-PB-O1B	3.81	118.04	109.87
3	A	1	SEP	OG-CB-CA	3.72	111.77	108.14
5	A	656	ANP	N3-C2-N1	-3.15	123.82	128.58
5	A	656	ANP	C4-C5-N7	-3.12	107.01	110.58
5	A	656	ANP	C5-N7-C8	2.19	106.90	103.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

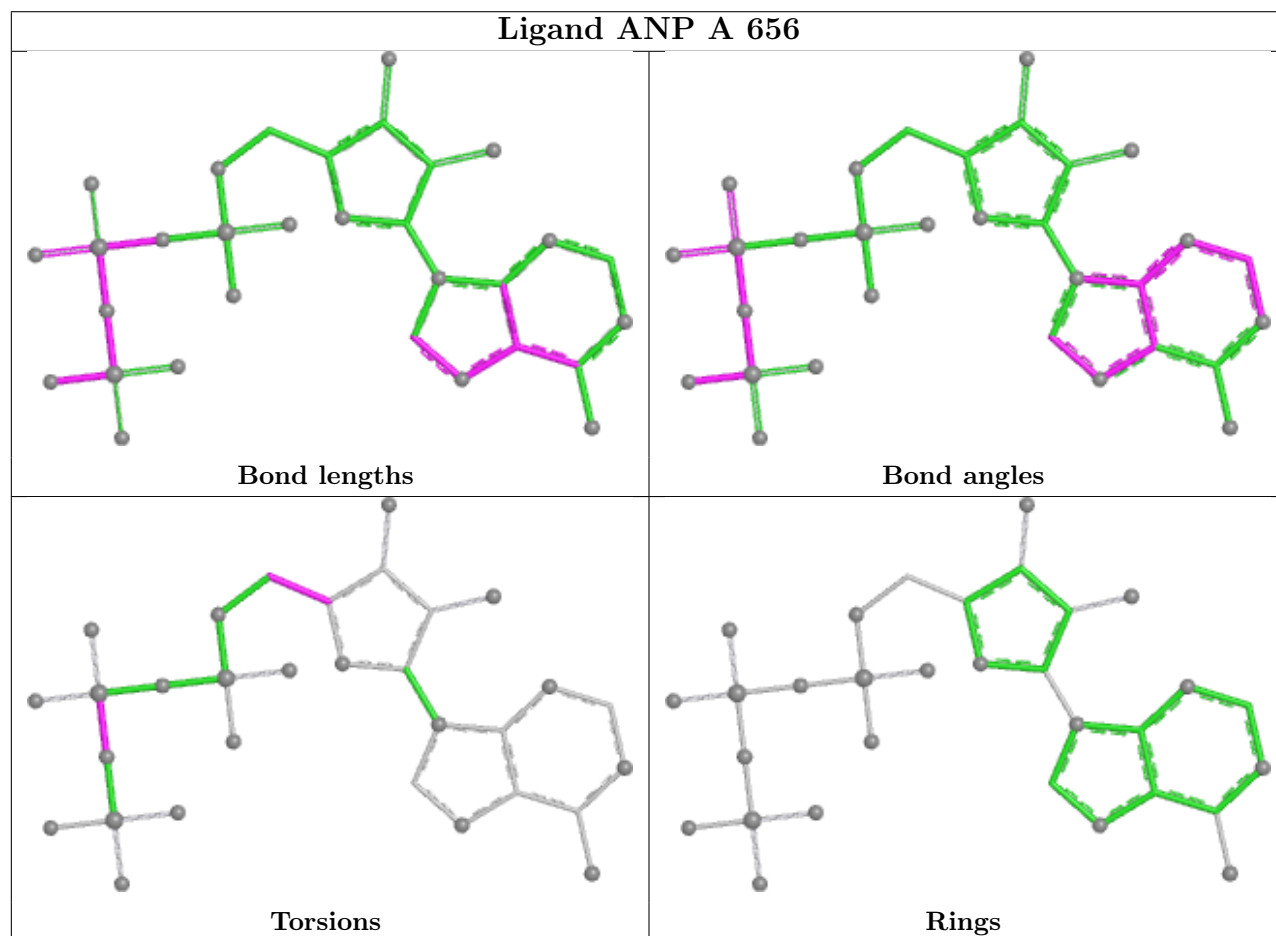
Mol	Chain	Res	Type	Atoms
5	A	656	ANP	PG-N3B-PB-O1B
5	A	656	ANP	O4'-C4'-C5'-O5'
5	A	656	ANP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	ALA	1	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 [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, 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%)	0.73	29 (8%) 17 14	99, 117, 135, 141	0
2	B	86/115 (74%)	0.61	2 (2%) 61 52	101, 111, 125, 127	0
All	All	434/496 (87%)	0.71	31 (7%) 22 17	99, 116, 134, 141	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	3.9
1	A	636	LEU	3.6
1	A	603	LEU	3.5
1	A	147	LEU	3.2
1	A	578	ARG	3.1
1	A	209	ILE	3.1
1	A	175	TRP	3.0
1	A	555	SER	2.8
1	A	553	PRO	2.8
1	A	626	PHE	2.7
1	A	653	LEU	2.7
1	A	631	LEU	2.7
1	A	580	LEU	2.7
1	A	98	TRP	2.6
1	A	117	TYR	2.5
1	A	210	ILE	2.5
1	A	572	LEU	2.4
2	B	128	LEU	2.4
2	B	147	VAL	2.4
1	A	570	ILE	2.3
1	A	602	LYS	2.3
1	A	600	ILE	2.3
1	A	551	PHE	2.3
1	A	235	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	2.2
1	A	131	VAL	2.2
1	A	630	LEU	2.1
1	A	214	ILE	2.1
1	A	146	GLN	2.0
1	A	150	ASP	2.0
1	A	163	MET	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](#)

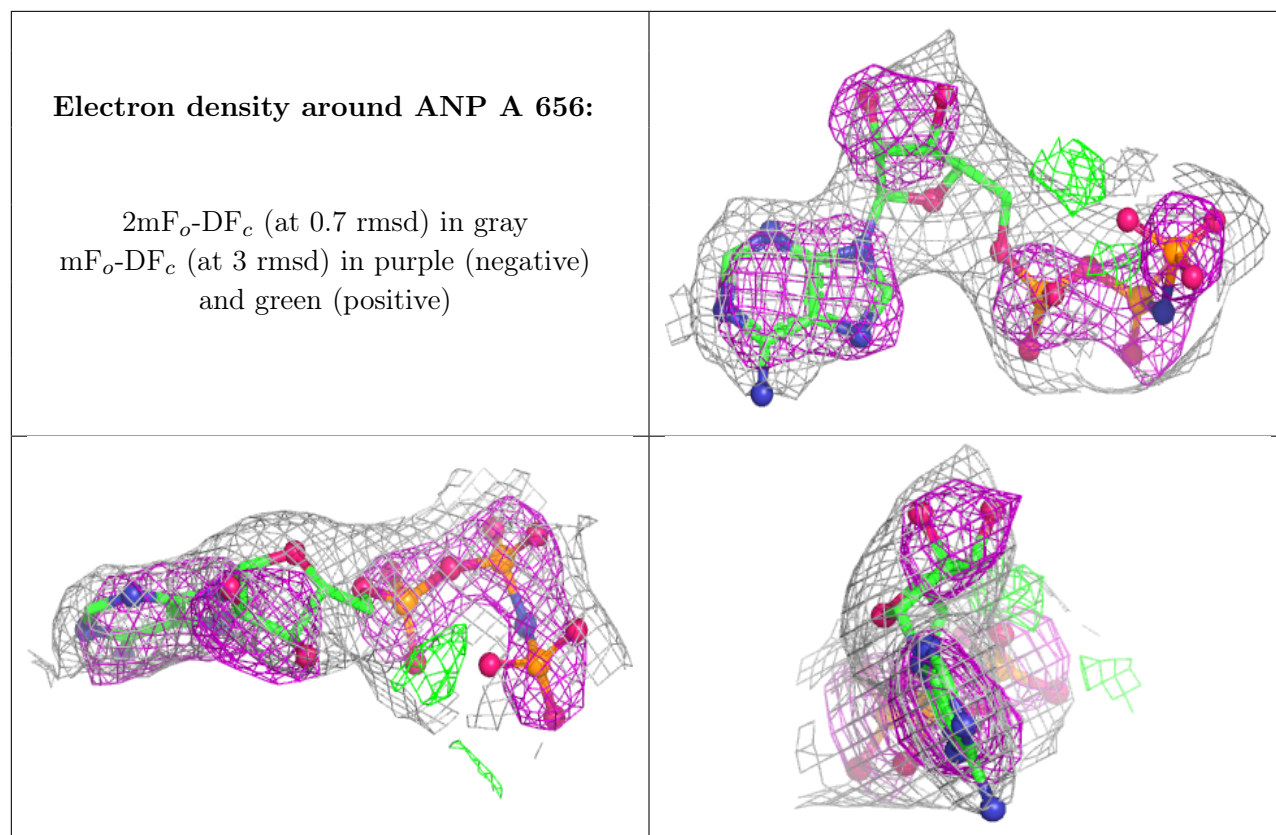
There are no oligosaccharides in this entry.

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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ALA	A	2	5/6	0.44	0.21	137,137,137,137	0
3	SEP	A	1	10/11	0.59	0.17	136,137,138,138	0
5	ANP	A	656	31/31	0.81	0.15	115,118,121,121	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 [i](#)

There are no such residues in this entry.