



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 1WBP / pdb_00001wbp
Title : SRPK1 bound to 9mer docking motif peptide
Authors : Ngo, J.C.; Gullinsgrud, J.; Chakrabarti, S.; Nolen, B.; Aubol, B.E.; Fu, X.-D.;
Adams, J.A.; McCammon, J.A.; Ghosh, G.
Deposited on : 2004-11-04
Resolution : 2.40 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

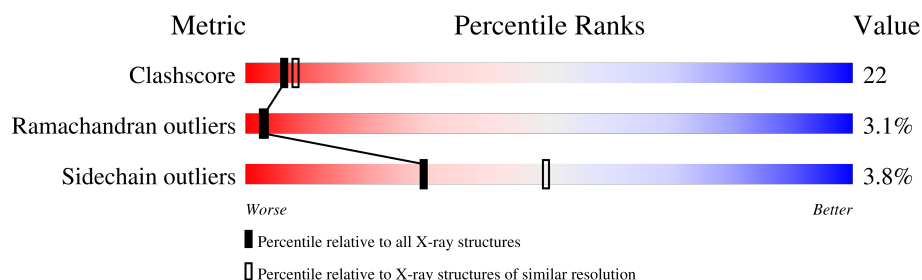
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	397	
2	B	9	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2941 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 SPRK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2848	1844	485	508	11			

- Molecule 2 is a protein called MEMBRANE-ASSOCIATED GUANYLATE KINASE, WW AND PDZ DOMAIN-CONTAINING PROTEIN 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			62	35	16	11			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



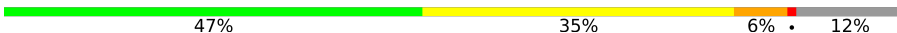
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

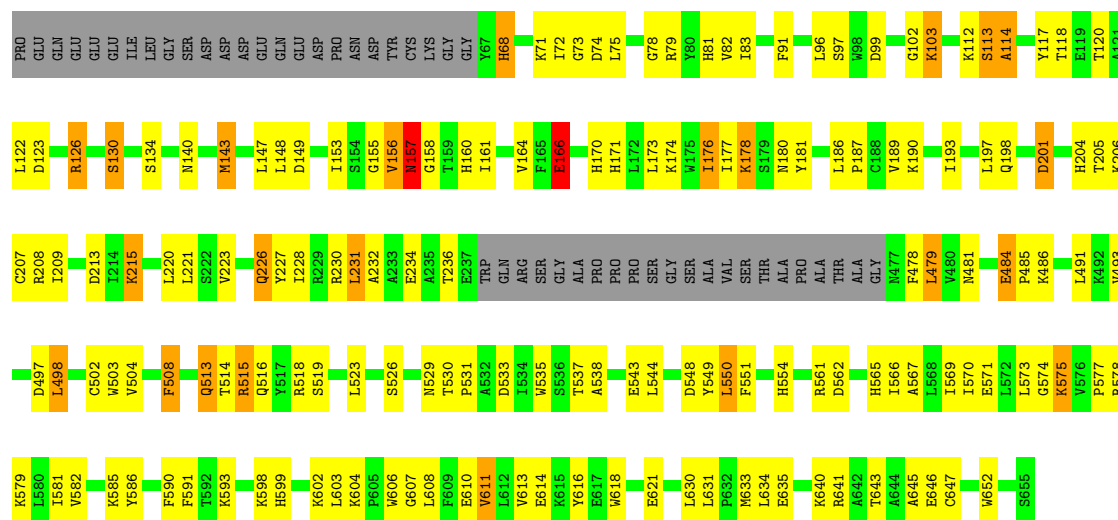
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: SERINE/THREONINE-PROTEIN KINASE SPRK1

Chain A: 



• Molecule 2: MEMBRANE-ASSOCIATED GUANYLATE KINASE, WW AND PDZ DOMAIN-CONTAINING PROTEIN 1

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.68Å 78.68Å 310.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.26 – 2.40	Depositor
% Data completeness (in resolution range)	67.1 (28.26-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2941	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.53	1/2919 (0.0%)	1.01	21/3952 (0.5%)
2	B	0.63	0/62	1.02	0/81
All	All	0.53	1/2981 (0.0%)	1.01	21/4033 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	GLY	C-N	-13.95	1.14	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	VAL	O-C-N	-7.53	113.16	122.57
1	A	113	SER	N-CA-C	7.48	120.32	111.71
1	A	155	GLY	CA-C-N	7.34	135.18	121.97
1	A	155	GLY	C-N-CA	7.34	135.18	121.97
1	A	126	ARG	N-CA-C	-6.40	104.22	111.07
1	A	176	ILE	N-CA-C	-6.13	104.36	110.62
1	A	630	LEU	N-CA-C	6.07	117.77	111.03
1	A	508	PHE	N-CA-C	-6.05	107.72	114.62
1	A	166	GLU	N-CA-C	-5.99	102.60	110.33
1	A	498	LEU	N-CA-C	-5.96	106.65	112.97
1	A	526	SER	N-CA-C	-5.82	105.49	112.59
1	A	550	LEU	N-CA-C	-5.57	105.29	111.36
1	A	613	VAL	N-CA-C	5.55	115.75	110.53
1	A	481	ASN	CA-C-N	5.40	125.09	119.64
1	A	481	ASN	C-N-CA	5.40	125.09	119.64
1	A	130	SER	N-CA-C	-5.31	105.39	111.07
1	A	611	VAL	CB-CA-C	-5.16	105.36	111.97
1	A	497	ASP	N-CA-C	5.16	116.94	110.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	GLU	CA-C-N	5.08	124.80	119.82
1	A	484	GLU	C-N-CA	5.08	124.80	119.82
1	A	201	ASP	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

There are no planarity outliers.

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	2848	0	2869	126	0
2	B	62	0	63	7	0
3	A	4	0	3	0	0
4	A	27	0	12	0	0
All	All	2941	0	2947	130	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 22.

All (130) 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:3:ARG:HG2	2:B:4:GLU:H	1.17	1.05
1:A:513:GLN:HE22	1:A:519:SER:H	1.14	0.88
2:B:3:ARG:HG2	2:B:4:GLU:N	1.91	0.85
1:A:513:GLN:NE2	1:A:519:SER:H	1.78	0.81
1:A:538:ALA:HB2	1:A:633:MET:HE2	1.62	0.81
1:A:176:ILE:HD11	1:A:544:LEU:HD23	1.64	0.79
1:A:567:ALA:O	1:A:571:GLU:HG3	1.83	0.78
2:B:3:ARG:CG	2:B:4:GLU:H	1.93	0.77
1:A:593:LYS:HD3	1:A:593:LYS:H	1.51	0.76
1:A:529:ASN:ND2	1:A:530:THR:H	1.85	0.74
1:A:504:VAL:HG13	1:A:529:ASN:HD21	1.56	0.71
1:A:565:HIS:O	1:A:569:ILE:HG13	1.91	0.69
1:A:504:VAL:HG13	1:A:529:ASN:ND2	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLU:HB3	1:A:614:GLU:OE1	1.92	0.69
1:A:484:GLU:OE1	1:A:486:LYS:HD2	1.93	0.69
1:A:170:HIS:CD2	1:A:174:LYS:HD2	2.28	0.68
1:A:71:LYS:O	1:A:82:VAL:HG21	1.94	0.68
1:A:516:GLN:NE2	1:A:516:GLN:H	1.91	0.67
1:A:75:LEU:HD21	1:A:78:GLY:HA2	1.76	0.67
1:A:197:LEU:HD11	1:A:537:THR:HG21	1.76	0.67
1:A:554:HIS:HA	1:A:561:ARG:NH2	2.11	0.66
1:A:635:GLU:HB2	1:A:641:ARG:HA	1.78	0.66
1:A:223:VAL:HG12	1:A:479:LEU:HD23	1.78	0.65
1:A:227:TYR:O	1:A:231:LEU:HB2	1.97	0.65
1:A:643:THR:OG1	1:A:646:GLU:HG3	1.97	0.64
1:A:82:VAL:HA	1:A:97:SER:HB3	1.80	0.64
1:A:607:GLY:O	1:A:611:VAL:HG23	1.99	0.62
1:A:204:HIS:HE1	1:A:533:ASP:OD2	1.83	0.62
1:A:204:HIS:CD2	1:A:530:THR:HB	2.34	0.61
1:A:516:GLN:HG2	1:A:549:TYR:CD2	2.35	0.61
1:A:230:ARG:O	1:A:234:GLU:HG3	2.00	0.61
1:A:577:PRO:O	1:A:581:ILE:HG13	2.01	0.61
1:A:498:LEU:HD12	1:A:498:LEU:N	2.15	0.61
1:A:593:LYS:HD3	1:A:593:LYS:N	2.16	0.60
1:A:143:MET:HG2	1:A:198:GLN:HB2	1.84	0.60
1:A:113:SER:HB3	1:A:160:HIS:CD2	2.37	0.59
1:A:207:CYS:HB3	1:A:209:ILE:HD12	1.84	0.59
1:A:221:LEU:HD23	1:A:493:VAL:HG12	1.85	0.59
1:A:118:THR:HG23	1:A:161:ILE:HG12	1.83	0.59
1:A:123:ASP:HA	1:A:126:ARG:HH11	1.67	0.59
1:A:114:ALA:HB3	1:A:117:TYR:CD2	2.37	0.58
1:A:143:MET:HE3	1:A:143:MET:HA	1.86	0.58
1:A:178:LYS:C	1:A:180:ASN:H	2.10	0.58
1:A:171:HIS:CD2	1:A:174:LYS:H	2.22	0.58
1:A:230:ARG:NH2	1:A:234:GLU:OE1	2.35	0.57
1:A:598:LYS:HG3	1:A:599:HIS:ND1	2.19	0.57
1:A:157:ASN:ND2	1:A:157:ASN:H	2.03	0.57
1:A:171:HIS:HD2	1:A:174:LYS:H	1.54	0.56
1:A:484:GLU:OE2	1:A:485:PRO:HD2	2.05	0.56
1:A:83:ILE:HG12	1:A:97:SER:HA	1.88	0.55
1:A:72:ILE:HA	1:A:82:VAL:HG23	1.89	0.55
1:A:573:LEU:HD11	1:A:634:LEU:HB3	1.89	0.54
1:A:523:LEU:HD11	1:A:565:HIS:CD2	2.43	0.54
1:A:118:THR:O	1:A:122:LEU:HG	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD23	1:A:647:CYS:HB2	1.91	0.53
1:A:226:GLN:O	1:A:230:ARG:HB2	2.08	0.53
1:A:197:LEU:CD1	1:A:537:THR:HG21	2.39	0.53
1:A:550:LEU:HD23	1:A:551:PHE:CE1	2.44	0.53
1:A:593:LYS:H	1:A:593:LYS:CD	2.20	0.53
1:A:513:GLN:NE2	1:A:518:ARG:HA	2.24	0.52
1:A:207:CYS:HB3	1:A:209:ILE:CD1	2.40	0.52
1:A:186:LEU:N	1:A:187:PRO:HD2	2.25	0.52
1:A:523:LEU:HD21	1:A:565:HIS:HD2	1.74	0.52
1:A:616:TYR:O	1:A:618:TRP:HD1	1.93	0.52
1:A:606:TRP:CE3	2:B:5:ARG:HD2	2.45	0.51
1:A:113:SER:HB3	1:A:160:HIS:NE2	2.25	0.51
1:A:581:ILE:HG23	1:A:591:PHE:CD2	2.45	0.51
1:A:513:GLN:O	1:A:518:ARG:NH2	2.41	0.51
1:A:578:ARG:O	1:A:582:VAL:HG13	2.11	0.51
1:A:606:TRP:HE3	2:B:5:ARG:HD2	1.75	0.51
1:A:529:ASN:ND2	1:A:530:THR:N	2.57	0.51
1:A:479:LEU:HD12	1:A:479:LEU:N	2.27	0.50
1:A:208:ARG:C	1:A:504:VAL:HG23	2.37	0.49
1:A:91:PHE:O	1:A:112:LYS:HG3	2.12	0.49
1:A:585:LYS:HD2	1:A:586:TYR:CZ	2.47	0.48
1:A:178:LYS:C	1:A:180:ASN:N	2.69	0.48
1:A:590:PHE:O	1:A:598:LYS:HG2	2.13	0.48
2:B:5:ARG:O	2:B:6:SER:C	2.56	0.48
1:A:570:ILE:HG23	1:A:575:LYS:N	2.28	0.48
1:A:79:ARG:NH1	1:A:99:ASP:OD1	2.46	0.47
1:A:608:LEU:HD23	1:A:631:LEU:HD21	1.96	0.47
1:A:171:HIS:HA	1:A:220:LEU:HD23	1.97	0.47
1:A:570:ILE:HG23	1:A:574:GLY:C	2.40	0.47
1:A:120:THR:HA	1:A:123:ASP:OD2	2.15	0.47
1:A:603:LEU:C	1:A:604:LYS:HD3	2.40	0.47
1:A:205:THR:HG22	1:A:206:LYS:N	2.30	0.46
1:A:608:LEU:HD23	1:A:631:LEU:CD2	2.45	0.46
1:A:562:ASP:O	1:A:566:ILE:HG13	2.16	0.46
1:A:602:LYS:O	1:A:604:LYS:HE3	2.16	0.46
1:A:180:ASN:O	1:A:181:TYR:HB2	2.16	0.46
1:A:148:LEU:HD12	1:A:164:VAL:HG12	1.98	0.45
1:A:96:LEU:HD21	1:A:232:ALA:HB2	1.97	0.45
1:A:204:HIS:CE1	1:A:533:ASP:OD2	2.67	0.45
1:A:228:ILE:O	1:A:231:LEU:HB3	2.17	0.45
1:A:543:GLU:HA	1:A:548:ASP:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:GLU:HB2	1:A:641:ARG:CA	2.46	0.45
1:A:73:GLY:HA2	1:A:81:HIS:CE1	2.52	0.45
1:A:190:LYS:HD3	1:A:652:TRP:O	2.17	0.44
1:A:71:LYS:O	1:A:82:VAL:CG2	2.65	0.44
1:A:201:ASP:OD1	1:A:645:ALA:HB2	2.18	0.44
1:A:554:HIS:HA	1:A:561:ARG:HH22	1.82	0.44
1:A:74:ASP:H	1:A:82:VAL:HG22	1.82	0.43
1:A:570:ILE:O	1:A:574:GLY:N	2.45	0.43
1:A:498:LEU:N	1:A:498:LEU:CD1	2.81	0.43
1:A:529:ASN:C	1:A:531:PRO:HD2	2.44	0.43
1:A:113:SER:O	1:A:114:ALA:C	2.62	0.42
1:A:535:TRP:CD1	1:A:535:TRP:C	2.97	0.42
1:A:514:THR:O	1:A:515:ARG:C	2.62	0.42
1:A:621:GLU:OE2	1:A:621:GLU:N	2.51	0.42
1:A:157:ASN:HB2	1:A:158:GLY:H	1.50	0.42
1:A:147:LEU:HD11	1:A:149:ASP:O	2.20	0.42
1:A:166:GLU:H	1:A:166:GLU:HG3	1.53	0.42
1:A:140:ASN:O	1:A:143:MET:HB2	2.20	0.42
1:A:502:CYS:CB	1:A:508:PHE:HD2	2.32	0.42
1:A:189:VAL:O	1:A:193:ILE:HG12	2.20	0.41
1:A:573:LEU:CD1	1:A:634:LEU:HB3	2.50	0.41
1:A:579:LYS:O	1:A:582:VAL:HG22	2.19	0.41
1:A:102:GLY:O	1:A:103:LYS:C	2.64	0.41
1:A:573:LEU:HD13	1:A:634:LEU:O	2.21	0.41
1:A:75:LEU:C	1:A:75:LEU:HD23	2.45	0.41
1:A:130:SER:HB2	1:A:503:TRP:HH2	1.84	0.41
1:A:529:ASN:HD22	1:A:530:THR:N	2.19	0.41
1:A:581:ILE:HG23	1:A:591:PHE:HD2	1.86	0.41
1:A:616:TYR:CD2	2:B:9:ARG:HD2	2.56	0.41
1:A:484:GLU:HA	1:A:485:PRO:HD2	1.91	0.41
1:A:173:LEU:O	1:A:177:ILE:HG13	2.20	0.40
1:A:208:ARG:O	1:A:504:VAL:HG23	2.21	0.40
1:A:213:ASP:OD1	1:A:215:LYS:HD3	2.21	0.40
1:A:153:ILE:O	1:A:153:ILE:HG13	2.21	0.40
1:A:643:THR:HG23	1:A:646:GLU:CD	2.46	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	346/397 (87%)	311 (90%)	25 (7%)	10 (3%)	3	3
2	B	5/9 (56%)	2 (40%)	2 (40%)	1 (20%)	0	0
All	All	351/406 (86%)	313 (89%)	27 (8%)	11 (3%)	3	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	157	ASN
1	A	575	LYS
1	A	103	LYS
1	A	134	SER
1	A	515	ARG
1	A	114	ALA
1	A	513	GLN
2	B	4	GLU
1	A	236	THR
1	A	491	LEU

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	310/346 (90%)	298 (96%)	12 (4%)	28	48
2	B	7/9 (78%)	7 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	317/355 (89%)	305 (96%)	12 (4%)	29 49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	143	MET
1	A	156	VAL
1	A	157	ASN
1	A	166	GLU
1	A	178	LYS
1	A	215	LYS
1	A	226	GLN
1	A	231	LEU
1	A	478	PHE
1	A	479	LEU
1	A	640	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	116	HIS
1	A	157	ASN
1	A	170	HIS
1	A	171	HIS
1	A	204	HIS
1	A	211	HIS
1	A	481	ASN
1	A	507	HIS
1	A	513	GLN
1	A	516	GLN
1	A	529	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	ACT	A	900	-	3,3,3	1.27	1 (33%)	3,3,3	0.71	0
4	ADP	A	950	-	28,29,29	1.44	4 (14%)	43,45,45	1.17	3 (6%)

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	ADP	A	950	-	-	7/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	950	ADP	C2-N1	3.68	1.40	1.33
4	A	950	ADP	C1'-N9	2.76	1.54	1.46
4	A	950	ADP	C5-C6	2.49	1.47	1.41
4	A	950	ADP	C8-N7	2.36	1.36	1.31
3	A	900	ACT	O-C	2.11	1.31	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	950	ADP	N3-C2-N1	-3.36	123.50	128.58
4	A	950	ADP	C2-N1-C6	3.08	123.79	118.73
4	A	950	ADP	O5'-C5'-C4'	2.33	116.94	108.99

There are no chirality outliers.

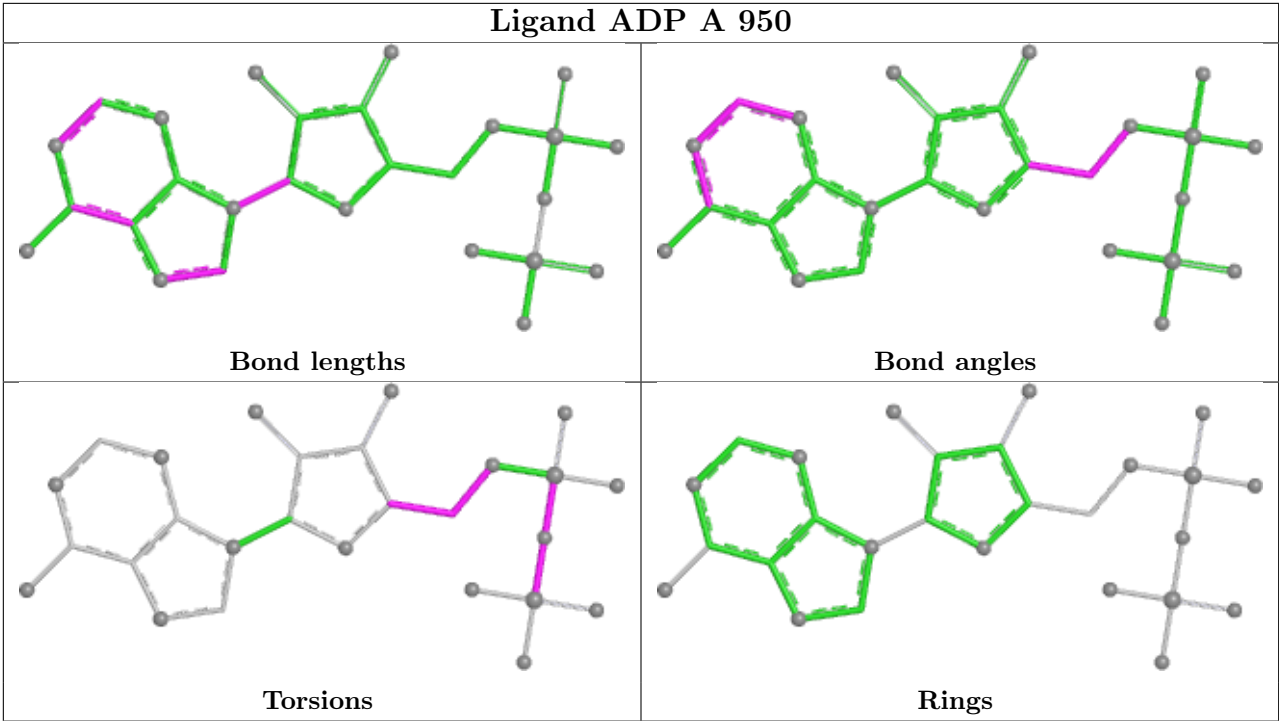
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	950	ADP	PA-O3A-PB-O3B
4	A	950	ADP	O4'-C4'-C5'-O5'
4	A	950	ADP	C3'-C4'-C5'-O5'
4	A	950	ADP	PB-O3A-PA-O1A
4	A	950	ADP	C4'-C5'-O5'-PA
4	A	950	ADP	PB-O3A-PA-O2A
4	A	950	ADP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	155:GLY	C	156:VAL	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.