



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:18 AM EDT

PDB ID : 2FGH / pdb_00002fgh
Title : ATP bound gelsolin
Authors : Ma, Q.; Robinson, R.C.; Burtnick, L.D.; Urosev, D.
Deposited on : 2005-12-22
Resolution : 2.80 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

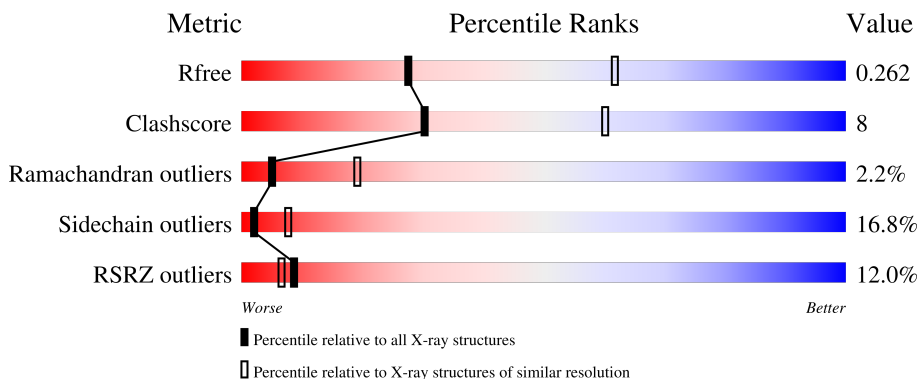
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	731	10% 73% 20% 5%
1	B	731	14% 72% 22% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11378 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.

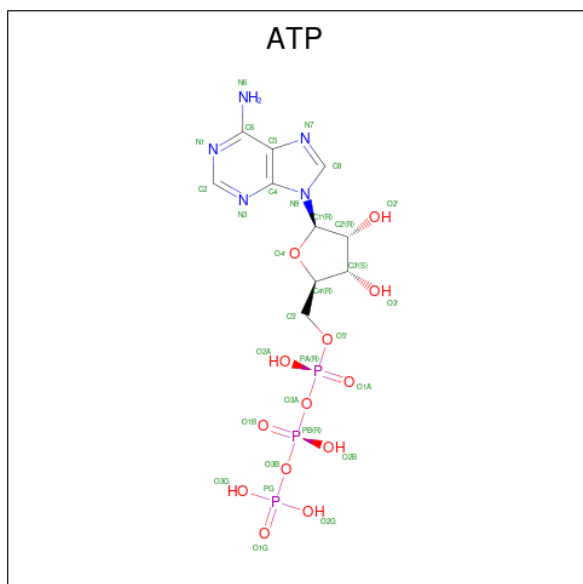
- Molecule 1 is a protein called gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5633	3564	981	1072	16			
1	B	721	Total	C	N	O	S	0	0	0
			5633	3564	981	1072	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	insertion	UNP Q28372
B	25	MET	-	insertion	UNP Q28372

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

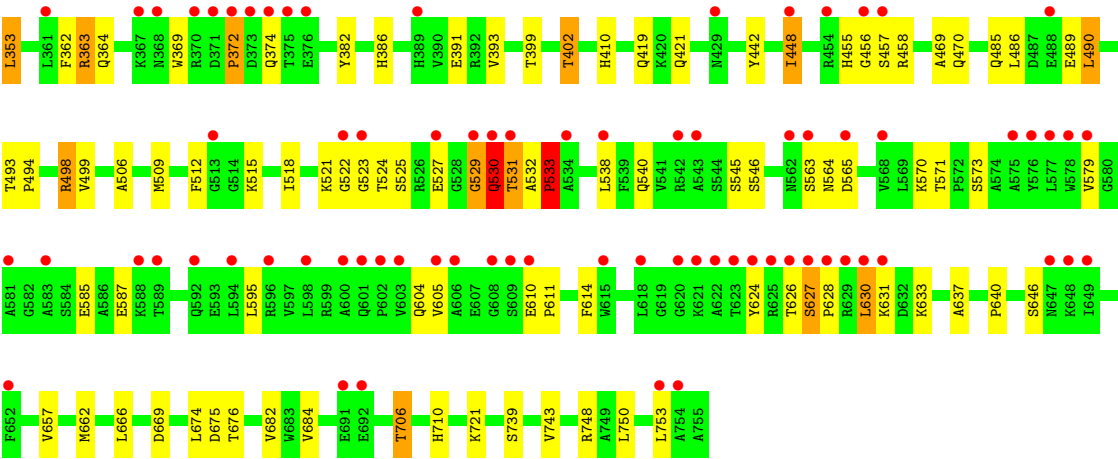


Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	23	Total	O	0	0
			23	23		



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.34Å 167.34Å 149.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.80) 98.5 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.242 , 0.265 0.241 , 0.262	Depositor DCC
R_{free} test set	2650 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11378	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: ATP

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	0.68	2/5766 (0.0%)	0.94	5/7812 (0.1%)
1	B	0.69	0/5766	0.94	5/7812 (0.1%)
All	All	0.69	2/11532 (0.0%)	0.94	10/15624 (0.1%)

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
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	HIS	CA-C	-5.91	1.45	1.52
1	A	151	HIS	CA-C	-5.03	1.47	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	HIS	CB-CA-C	-9.67	98.25	111.88
1	A	86	HIS	CA-CB-CG	-7.27	106.53	113.80
1	B	224	GLU	N-CA-C	-7.20	101.24	110.53
1	A	224	GLU	N-CA-C	-7.13	100.25	110.59
1	A	529	GLY	N-CA-C	-5.84	105.54	113.37
1	A	278	ASN	N-CA-C	5.34	116.92	108.96
1	B	529	GLY	N-CA-C	-5.34	106.21	113.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ASN	N-CA-C	5.15	116.63	108.96
1	A	533	PRO	N-CA-C	5.13	123.03	112.47
1	B	533	PRO	N-CA-C	5.08	122.94	112.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	TYR	Peptide
1	A	86	HIS	Sidechain
1	B	624	TYR	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	5633	0	5493	101	1
1	B	5633	0	5493	88	1
2	A	31	0	12	1	0
2	B	31	0	12	1	0
3	A	27	0	0	22	0
3	B	23	0	0	9	0
All	All	11378	0	11010	188	1

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 8.

All (188) 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:B:152:VAL:O	1:B:153:VAL:HG13	1.66	0.94
1:A:152:VAL:O	1:A:153:VAL:HG13	1.70	0.92
1:B:75:GLN:HG3	3:B:9387:HOH:O	1.69	0.92
1:B:627:SER:HA	3:B:9398:HOH:O	1.72	0.90
1:A:624:TYR:HA	3:A:5397:HOH:O	1.71	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:HIS:CE1	3:B:9394:HOH:O	2.28	0.86
1:B:153:VAL:HB	1:B:157:VAL:HG21	1.57	0.85
1:A:86:HIS:CE1	3:A:5381:HOH:O	2.30	0.84
1:A:267:ASN:O	1:A:267:ASN:ND2	2.11	0.84
1:A:153:VAL:HB	1:A:157:VAL:HG21	1.60	0.82
1:B:267:ASN:O	1:B:267:ASN:ND2	2.14	0.81
1:B:154:PRO:O	1:B:157:VAL:HG22	1.83	0.79
1:A:151:HIS:CE1	3:A:5383:HOH:O	2.36	0.77
1:A:154:PRO:O	1:A:157:VAL:HG22	1.85	0.77
1:A:86:HIS:CE1	1:A:119:HIS:HD2	2.03	0.76
1:A:86:HIS:ND1	3:A:5381:HOH:O	2.17	0.75
1:A:151:HIS:ND1	3:A:5383:HOH:O	2.20	0.73
1:B:86:HIS:CE1	1:B:133:TYR:CE2	2.77	0.73
1:A:498:ARG:HH11	1:A:498:ARG:HG2	1.54	0.71
1:A:86:HIS:CG	3:A:5381:HOH:O	2.44	0.70
1:A:151:HIS:C	3:A:5391:HOH:O	2.35	0.70
1:B:86:HIS:CE1	1:B:133:TYR:HE2	2.10	0.70
1:B:86:HIS:CE1	3:B:9402:HOH:O	2.44	0.70
1:B:292:ASN:H	1:B:292:ASN:HD22	1.38	0.69
1:B:498:ARG:HG2	1:B:498:ARG:HH11	1.56	0.69
1:A:117:VAL:HG12	1:A:119:HIS:CE1	2.28	0.69
1:A:63:PHE:CD1	1:A:151:HIS:HE1	2.11	0.68
1:B:86:HIS:ND1	3:B:9402:HOH:O	2.27	0.67
1:A:626:THR:O	1:A:628:PRO:HD3	1.94	0.67
1:A:155:ASN:O	1:A:156:GLU:HB2	1.93	0.67
1:A:485:GLN:O	1:A:489:GLU:HG3	1.93	0.67
1:A:676:THR:HG21	3:A:5401:HOH:O	1.95	0.67
1:B:626:THR:O	1:B:628:PRO:HD3	1.95	0.66
1:A:152:VAL:O	1:A:153:VAL:CG1	2.44	0.66
1:B:155:ASN:O	1:B:156:GLU:HB2	1.95	0.66
1:B:152:VAL:O	1:B:153:VAL:CG1	2.41	0.66
1:A:86:HIS:ND1	1:A:119:HIS:HD2	1.94	0.65
1:B:485:GLN:O	1:B:489:GLU:HG3	1.95	0.65
1:A:292:ASN:HD22	1:A:292:ASN:H	1.43	0.65
1:B:86:HIS:CD2	1:B:86:HIS:N	2.66	0.64
1:B:151:HIS:ND1	3:B:9394:HOH:O	2.28	0.63
1:A:84:ASP:HB3	1:A:86:HIS:HE1	1.66	0.60
1:B:675:ASP:OD1	1:B:676:THR:O	2.19	0.60
1:A:86:HIS:CE1	1:A:119:HIS:CD2	2.89	0.60
1:A:209:GLU:HG2	3:A:5398:HOH:O	2.02	0.60
1:A:93:CYS:HA	3:A:5389:HOH:O	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:N	1:B:353:LEU:HD23	2.15	0.59
1:A:63:PHE:CE1	1:A:151:HIS:CE1	2.91	0.59
1:A:119:HIS:CG	3:A:5390:HOH:O	2.55	0.59
1:B:86:HIS:ND1	1:B:130:PHE:HD1	2.00	0.59
1:A:754:ALA:HB2	3:A:5387:HOH:O	2.02	0.58
1:A:119:HIS:CE1	3:A:5390:HOH:O	2.55	0.58
1:A:109:ASP:CG	1:A:118:GLN:HE21	2.12	0.58
1:A:702:ARG:HD3	3:A:5400:HOH:O	2.02	0.58
1:A:353:LEU:N	1:A:353:LEU:HD23	2.18	0.57
1:B:27:VAL:O	1:B:28:GLU:HG2	2.04	0.57
1:B:532:ALA:HB1	1:B:533:PRO:HD2	1.86	0.57
1:A:151:HIS:CG	3:A:5383:HOH:O	2.58	0.57
1:A:152:VAL:N	3:A:5391:HOH:O	2.38	0.56
1:A:86:HIS:ND1	1:A:119:HIS:CD2	2.73	0.56
1:B:155:ASN:O	1:B:156:GLU:CB	2.53	0.56
1:A:448:ILE:HD11	1:A:486:LEU:HD22	1.86	0.56
1:A:90:GLY:O	1:A:93:CYS:HB2	2.05	0.56
1:A:155:ASN:O	1:A:156:GLU:CB	2.53	0.55
1:B:448:ILE:HD11	1:B:486:LEU:HD22	1.88	0.55
1:A:63:PHE:HD1	1:A:151:HIS:HE1	1.55	0.55
1:A:57:ASN:HB3	3:A:5395:HOH:O	2.07	0.55
1:B:109:ASP:CG	1:B:118:GLN:HE21	2.15	0.54
1:A:45:ARG:HD2	1:A:151:HIS:NE2	2.21	0.54
1:A:630:LEU:HD22	2:A:5380:ATP:C8	2.43	0.54
1:A:532:ALA:HB1	1:A:533:PRO:HD2	1.88	0.54
1:B:86:HIS:NE2	1:B:133:TYR:HE2	2.05	0.54
1:A:155:ASN:HB3	3:A:5407:HOH:O	2.08	0.53
1:A:191:LEU:HG	1:A:193:LEU:HD13	1.91	0.53
1:A:675:ASP:OD1	1:A:676:THR:O	2.25	0.53
1:B:154:PRO:O	1:B:157:VAL:CG2	2.55	0.53
1:B:675:ASP:C	1:B:676:THR:O	2.50	0.53
1:A:154:PRO:O	1:A:157:VAL:CG2	2.57	0.52
1:B:270:LEU:HA	1:B:292:ASN:HD21	1.75	0.52
1:B:191:LEU:HG	1:B:193:LEU:HD13	1.91	0.52
1:B:319:LYS:HD2	1:B:328:ARG:HG2	1.92	0.52
1:A:27:VAL:O	1:A:28:GLU:HG2	2.10	0.52
1:A:320:GLY:O	1:A:323:ALA:HB2	2.10	0.52
1:B:117:VAL:HG13	1:B:353:LEU:HD22	1.92	0.51
1:B:630:LEU:HD22	2:B:9380:ATP:C8	2.44	0.51
1:A:323:ALA:O	1:A:324:ASN:CB	2.57	0.51
1:B:485:GLN:HB3	3:B:9403:HOH:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:TYR:CD2	1:B:525:SER:HB3	2.45	0.51
1:A:57:ASN:CB	3:A:5395:HOH:O	2.57	0.51
1:A:63:PHE:CD1	1:A:151:HIS:CE1	2.95	0.51
1:B:201:CYS:SG	1:B:210:ARG:HG2	2.51	0.51
1:A:154:PRO:O	1:A:155:ASN:C	2.55	0.50
1:A:442:TYR:CD2	1:A:525:SER:HB3	2.47	0.50
1:A:679:GLN:HB3	3:A:5401:HOH:O	2.11	0.49
1:A:269:LYS:HE2	1:A:710:HIS:CE1	2.47	0.49
1:B:54:VAL:HG22	1:B:151:HIS:NE2	2.26	0.49
1:B:323:ALA:O	1:B:324:ASN:CB	2.60	0.49
1:B:442:TYR:HB3	1:B:523:GLY:O	2.12	0.49
1:B:455:HIS:O	1:B:457:SER:N	2.46	0.49
1:B:109:ASP:CB	1:B:118:GLN:HE21	2.25	0.49
1:B:90:GLY:O	1:B:93:CYS:HB2	2.12	0.49
1:B:183:PHE:HA	1:B:189:PHE:CZ	2.48	0.49
1:A:84:ASP:HB3	1:A:86:HIS:CE1	2.47	0.48
1:A:278:ASN:HB3	1:A:283:MET:HA	1.96	0.48
1:A:486:LEU:O	1:A:490:LEU:HB2	2.13	0.48
1:A:270:LEU:HA	1:A:292:ASN:HD21	1.78	0.48
1:B:352:VAL:C	1:B:353:LEU:HD23	2.38	0.48
1:A:181:GLU:OE1	1:B:181:GLU:OE1	2.31	0.48
1:B:278:ASN:HB3	1:B:283:MET:HA	1.95	0.48
1:B:386:HIS:HE1	1:B:640:PRO:O	1.96	0.48
1:A:319:LYS:HD2	1:A:328:ARG:HG2	1.95	0.48
1:B:200:TRP:CD1	1:B:243:MET:HE1	2.48	0.48
1:B:469:ALA:HB2	3:B:9396:HOH:O	2.14	0.48
1:B:363:ARG:HG2	1:B:369:TRP:CD2	2.49	0.48
1:A:626:THR:O	1:A:628:PRO:CD	2.61	0.47
1:A:138:LEU:HD12	1:A:138:LEU:N	2.30	0.47
1:B:64:THR:HG22	1:B:92:GLU:HG2	1.97	0.47
1:A:64:THR:HG22	1:A:92:GLU:HG2	1.95	0.47
1:B:118:GLN:O	1:B:351:SER:HA	2.16	0.46
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.50	0.46
1:A:200:TRP:CD1	1:A:243:MET:HE1	2.50	0.46
1:A:363:ARG:HG2	1:A:369:TRP:CD2	2.50	0.46
1:A:524:THR:CG2	1:A:529:GLY:HA3	2.46	0.46
1:B:154:PRO:O	1:B:155:ASN:C	2.58	0.46
1:B:293:PRO:HG3	1:B:710:HIS:HB2	1.97	0.46
1:B:540:GLN:NE2	1:B:565:ASP:OD1	2.47	0.46
1:B:630:LEU:HD21	1:B:637:ALA:HB2	1.97	0.46
1:B:564:ASN:HD21	1:B:628:PRO:HA	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:THR:O	1:B:628:PRO:CD	2.62	0.45
1:A:506:ALA:HA	1:A:509:MET:HE3	1.99	0.45
1:B:138:LEU:N	1:B:138:LEU:HD12	2.31	0.45
1:B:161:ARG:HG3	1:B:192:ASP:HB3	1.99	0.45
1:A:161:ARG:HG3	1:A:192:ASP:HB3	1.99	0.45
1:B:80:ILE:HB	3:B:9391:HOH:O	2.16	0.45
1:A:442:TYR:HB3	1:A:523:GLY:O	2.17	0.45
1:A:352:VAL:C	1:A:353:LEU:HD23	2.42	0.44
1:A:307:LEU:HD12	1:A:307:LEU:C	2.42	0.44
1:B:153:VAL:HA	1:B:154:PRO:HD2	1.86	0.44
1:B:269:LYS:HB2	1:B:706:THR:O	2.18	0.44
1:A:353:LEU:HD11	1:A:362:PHE:HB2	2.00	0.44
1:B:168:ARG:NH2	1:B:669:ASP:OD1	2.50	0.44
1:A:386:HIS:HE1	1:A:640:PRO:O	2.01	0.43
1:A:410:HIS:ND1	1:A:545:SER:HB3	2.32	0.43
1:B:271:ALA:H	1:B:292:ASN:ND2	2.15	0.43
1:A:455:HIS:O	1:A:457:SER:N	2.50	0.43
1:A:526:ARG:O	1:A:527:GLU:C	2.61	0.43
1:A:630:LEU:HD21	1:A:637:ALA:HB2	1.99	0.43
1:B:66:ASP:OD2	1:B:145:VAL:HG23	2.17	0.43
1:A:153:VAL:HA	1:A:154:PRO:HD2	1.87	0.43
1:A:292:ASN:HA	1:A:293:PRO:C	2.43	0.43
1:B:176:VAL:HB	1:B:177:PRO:HD2	2.01	0.43
1:B:211:LEU:O	1:B:214:THR:HB	2.17	0.43
1:B:82:GLN:OE1	1:B:382:TYR:HA	2.19	0.43
1:B:493:THR:N	1:B:494:PRO:CD	2.82	0.43
1:B:320:GLY:O	1:B:323:ALA:HB2	2.19	0.43
1:B:530:GLN:CG	1:B:531:THR:H	2.32	0.43
1:A:271:ALA:H	1:A:292:ASN:ND2	2.16	0.43
1:B:410:HIS:ND1	1:B:545:SER:HB3	2.34	0.43
1:B:512:PHE:O	1:B:515:LYS:HB2	2.19	0.43
1:B:506:ALA:HA	1:B:509:MET:HE3	2.01	0.42
1:A:119:HIS:CD2	3:A:5390:HOH:O	2.71	0.42
1:A:176:VAL:HB	1:A:177:PRO:HD2	2.00	0.42
1:A:493:THR:N	1:A:494:PRO:CD	2.82	0.42
1:A:526:ARG:O	1:A:527:GLU:O	2.38	0.42
1:B:353:LEU:HD11	1:B:362:PHE:HB2	2.02	0.42
1:A:126:GLU:HG2	1:A:131:LEU:HD21	2.02	0.42
1:A:162:LEU:HD11	1:A:183:PHE:CE2	2.55	0.41
1:B:162:LEU:HD11	1:B:183:PHE:CE2	2.55	0.41
1:B:486:LEU:O	1:B:490:LEU:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:HE1	1:A:151:HIS:CE1	2.37	0.41
1:A:509:MET:HE1	3:A:5406:HOH:O	2.20	0.41
1:B:28:GLU:O	1:B:29:HIS:HB2	2.21	0.41
1:B:524:THR:CG2	1:B:529:GLY:HA3	2.51	0.41
1:A:201:CYS:SG	1:A:210:ARG:HG2	2.60	0.41
1:A:45:ARG:HD3	1:A:47:GLU:OE2	2.20	0.41
1:A:109:ASP:CB	1:A:118:GLN:HE21	2.33	0.41
1:A:585:GLU:O	1:A:589:THR:HG22	2.21	0.41
1:A:448:ILE:HD11	1:A:486:LEU:CD2	2.51	0.41
1:A:87:TYR:OH	1:A:120:ARG:HD2	2.21	0.41
1:A:524:THR:HG23	1:A:529:GLY:HA3	2.03	0.41
1:B:399:THR:O	1:B:402:THR:HG22	2.21	0.41
1:A:29:HIS:ND1	1:A:30:PRO:HD2	2.36	0.40
1:A:675:ASP:C	1:A:676:THR:O	2.59	0.40
1:B:86:HIS:NE2	1:B:133:TYR:CE2	2.84	0.40
1:B:122:VAL:O	1:B:123:GLN:C	2.64	0.40
1:B:611:PRO:O	1:B:614:PHE:HB3	2.21	0.40
1:B:126:GLU:HG2	1:B:131:LEU:HD21	2.03	0.40
1:B:292:ASN:HA	1:B:293:PRO:C	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASP:OD2	1:B:419:GLN:OE1[5_545]	2.18	0.02

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	717/731 (98%)	664 (93%)	37 (5%)	16 (2%)	5 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	717/731 (98%)	664 (93%)	38 (5%)	15 (2%)	5	20
All	All	1434/1462 (98%)	1328 (93%)	75 (5%)	31 (2%)	5	19

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	280	ALA
1	A	324	ASN
1	A	456	GLY
1	A	527	GLU
1	A	533	PRO
1	B	29	HIS
1	B	156	GLU
1	B	280	ALA
1	B	324	ASN
1	B	456	GLY
1	B	527	GLU
1	B	533	PRO
1	A	156	GLU
1	A	323	ALA
1	A	573	SER
1	B	323	ALA
1	B	573	SER
1	A	627	SER
1	B	530	GLN
1	B	627	SER
1	A	154	PRO
1	A	530	GLN
1	A	531	THR
1	B	154	PRO
1	B	531	THR
1	B	372	PRO
1	A	372	PRO
1	B	522	GLY
1	A	522	GLY
1	A	605	VAL

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	591/599 (99%)	492 (83%)	99 (17%)	2	8
1	B	591/599 (99%)	492 (83%)	99 (17%)	2	8
All	All	1182/1198 (99%)	984 (83%)	198 (17%)	2	8

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	49	PHE
1	A	64	THR
1	A	86	HIS
1	A	92	GLU
1	A	94	SER
1	A	96	ASP
1	A	108	LEU
1	A	115	ARG
1	A	147	SER
1	A	150	LYS
1	A	152	VAL
1	A	154	PRO
1	A	157	VAL
1	A	159	VAL
1	A	162	LEU
1	A	166	LYS
1	A	168	ARG
1	A	169	ARG
1	A	170	VAL
1	A	171	VAL
1	A	193	LEU
1	A	204	LYS
1	A	206	ASN
1	A	209	GLU
1	A	218	LYS
1	A	228	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	SER
1	A	233	VAL
1	A	235	GLU
1	A	239	GLU
1	A	244	LEU
1	A	246	VAL
1	A	267	ASN
1	A	268	ARG
1	A	269	LYS
1	A	272	LYS
1	A	286	SER
1	A	292	ASN
1	A	299	LEU
1	A	306	ILE
1	A	307	LEU
1	A	322	GLN
1	A	328	ARG
1	A	329	LYS
1	A	332	LEU
1	A	333	LYS
1	A	336	SER
1	A	343	ASP
1	A	347	GLN
1	A	352	VAL
1	A	353	LEU
1	A	363	ARG
1	A	364	GLN
1	A	372	PRO
1	A	374	GLN
1	A	391	GLU
1	A	393	VAL
1	A	402	THR
1	A	421	GLN
1	A	448	ILE
1	A	458	ARG
1	A	470	GLN
1	A	490	LEU
1	A	498	ARG
1	A	499	VAL
1	A	518	ILE
1	A	521	LYS
1	A	530	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	533	PRO
1	A	538	LEU
1	A	546	SER
1	A	563	SER
1	A	570	LYS
1	A	571	THR
1	A	579	VAL
1	A	585	GLU
1	A	587	GLU
1	A	595	LEU
1	A	604	GLN
1	A	605	VAL
1	A	610	GLU
1	A	630	LEU
1	A	631	LYS
1	A	633	LYS
1	A	646	SER
1	A	657	VAL
1	A	662	MET
1	A	666	LEU
1	A	674	LEU
1	A	682	VAL
1	A	684	VAL
1	A	706	THR
1	A	721	LYS
1	A	739	SER
1	A	743	VAL
1	A	748	ARG
1	A	750	LEU
1	A	753	LEU
1	B	27	VAL
1	B	49	PHE
1	B	64	THR
1	B	75	GLN
1	B	86	HIS
1	B	92	GLU
1	B	94	SER
1	B	96	ASP
1	B	108	LEU
1	B	115	ARG
1	B	142	LYS
1	B	147	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	150	LYS
1	B	152	VAL
1	B	154	PRO
1	B	157	VAL
1	B	159	VAL
1	B	162	LEU
1	B	166	LYS
1	B	168	ARG
1	B	169	ARG
1	B	170	VAL
1	B	171	VAL
1	B	193	LEU
1	B	204	LYS
1	B	206	ASN
1	B	218	LYS
1	B	228	ARG
1	B	232	SER
1	B	233	VAL
1	B	235	GLU
1	B	239	GLU
1	B	244	LEU
1	B	246	VAL
1	B	267	ASN
1	B	268	ARG
1	B	269	LYS
1	B	272	LYS
1	B	286	SER
1	B	292	ASN
1	B	299	LEU
1	B	306	ILE
1	B	307	LEU
1	B	322	GLN
1	B	329	LYS
1	B	332	LEU
1	B	333	LYS
1	B	336	SER
1	B	343	ASP
1	B	347	GLN
1	B	352	VAL
1	B	353	LEU
1	B	363	ARG
1	B	364	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	372	PRO
1	B	374	GLN
1	B	391	GLU
1	B	393	VAL
1	B	402	THR
1	B	421	GLN
1	B	448	ILE
1	B	458	ARG
1	B	470	GLN
1	B	490	LEU
1	B	498	ARG
1	B	499	VAL
1	B	518	ILE
1	B	521	LYS
1	B	530	GLN
1	B	533	PRO
1	B	538	LEU
1	B	546	SER
1	B	563	SER
1	B	570	LYS
1	B	571	THR
1	B	579	VAL
1	B	585	GLU
1	B	587	GLU
1	B	595	LEU
1	B	604	GLN
1	B	605	VAL
1	B	610	GLU
1	B	630	LEU
1	B	631	LYS
1	B	633	LYS
1	B	646	SER
1	B	657	VAL
1	B	662	MET
1	B	666	LEU
1	B	674	LEU
1	B	682	VAL
1	B	684	VAL
1	B	706	THR
1	B	721	LYS
1	B	739	SER
1	B	743	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	748	ARG
1	B	750	LEU
1	B	753	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	118	GLN
1	A	119	HIS
1	A	151	HIS
1	A	160	GLN
1	A	195	ASN
1	A	215	GLN
1	A	292	ASN
1	A	324	ASN
1	A	374	GLN
1	A	386	HIS
1	A	459	GLN
1	A	467	GLN
1	A	470	GLN
1	A	496	GLN
1	A	507	HIS
1	A	564	ASN
1	A	647	ASN
1	A	710	HIS
1	B	91	ASN
1	B	118	GLN
1	B	164	GLN
1	B	195	ASN
1	B	215	GLN
1	B	278	ASN
1	B	292	ASN
1	B	324	ASN
1	B	374	GLN
1	B	386	HIS
1	B	459	GLN
1	B	467	GLN
1	B	496	GLN
1	B	507	HIS
1	B	564	ASN
1	B	647	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	710	HIS

5.3.3 RNA [i](#)

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$
2	ATP	B	9380	-	32,33,33	1.21	4 (12%)	48,52,52	1.86	11 (22%)
2	ATP	A	5380	-	32,33,33	1.35	4 (12%)	48,52,52	1.93	12 (25%)

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
2	ATP	B	9380	-	-	6/22/38/38	0/3/3/3
2	ATP	A	5380	-	-	6/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5380	ATP	PA-O3A	4.93	1.64	1.59
2	B	9380	ATP	C8-N7	2.98	1.37	1.31
2	B	9380	ATP	C2-N1	2.96	1.39	1.33
2	B	9380	ATP	PB-O3B	2.94	1.62	1.59
2	A	5380	ATP	C8-N7	2.50	1.36	1.31
2	A	5380	ATP	PB-O3B	2.40	1.62	1.59
2	A	5380	ATP	C2-N1	2.33	1.38	1.33
2	B	9380	ATP	C2-N3	2.28	1.38	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5380	ATP	O4'-C1'-N9	5.40	118.47	108.09
2	A	5380	ATP	N3-C2-N1	-5.09	120.88	128.58
2	B	9380	ATP	O4'-C1'-N9	5.09	117.86	108.09
2	B	9380	ATP	N3-C2-N1	-4.78	121.35	128.58
2	A	5380	ATP	N9-C8-N7	-3.85	108.47	113.94
2	B	9380	ATP	N9-C8-N7	-3.63	108.79	113.94
2	A	5380	ATP	C2'-C1'-N9	-3.55	104.49	113.30
2	B	9380	ATP	C2'-C1'-N9	-3.40	104.86	113.30
2	B	9380	ATP	C5-C4-N3	-3.30	122.17	126.72
2	A	5380	ATP	C4-N9-C1'	-3.21	119.12	126.63
2	A	5380	ATP	C5-N7-C8	3.04	108.23	103.45
2	A	5380	ATP	C5-C4-N3	-2.90	122.72	126.72
2	B	9380	ATP	O2B-PB-O3B	2.71	114.61	107.27
2	A	5380	ATP	C1'-N9-C8	2.64	132.96	127.09
2	B	9380	ATP	C2-N3-C4	2.62	118.24	111.83
2	A	5380	ATP	C2-N3-C4	2.57	118.10	111.83
2	B	9380	ATP	C5-N7-C8	2.49	107.36	103.45
2	B	9380	ATP	C4-N9-C1'	-2.49	120.82	126.63
2	A	5380	ATP	O2B-PB-O3A	-2.36	100.90	107.27
2	B	9380	ATP	C5-C6-N6	-2.31	117.57	123.29
2	B	9380	ATP	O2A-PA-O3A	2.29	113.45	107.27
2	A	5380	ATP	C4-C5-N7	-2.21	108.05	110.58
2	A	5380	ATP	O2A-PA-O3A	2.06	112.83	107.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	9380	ATP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

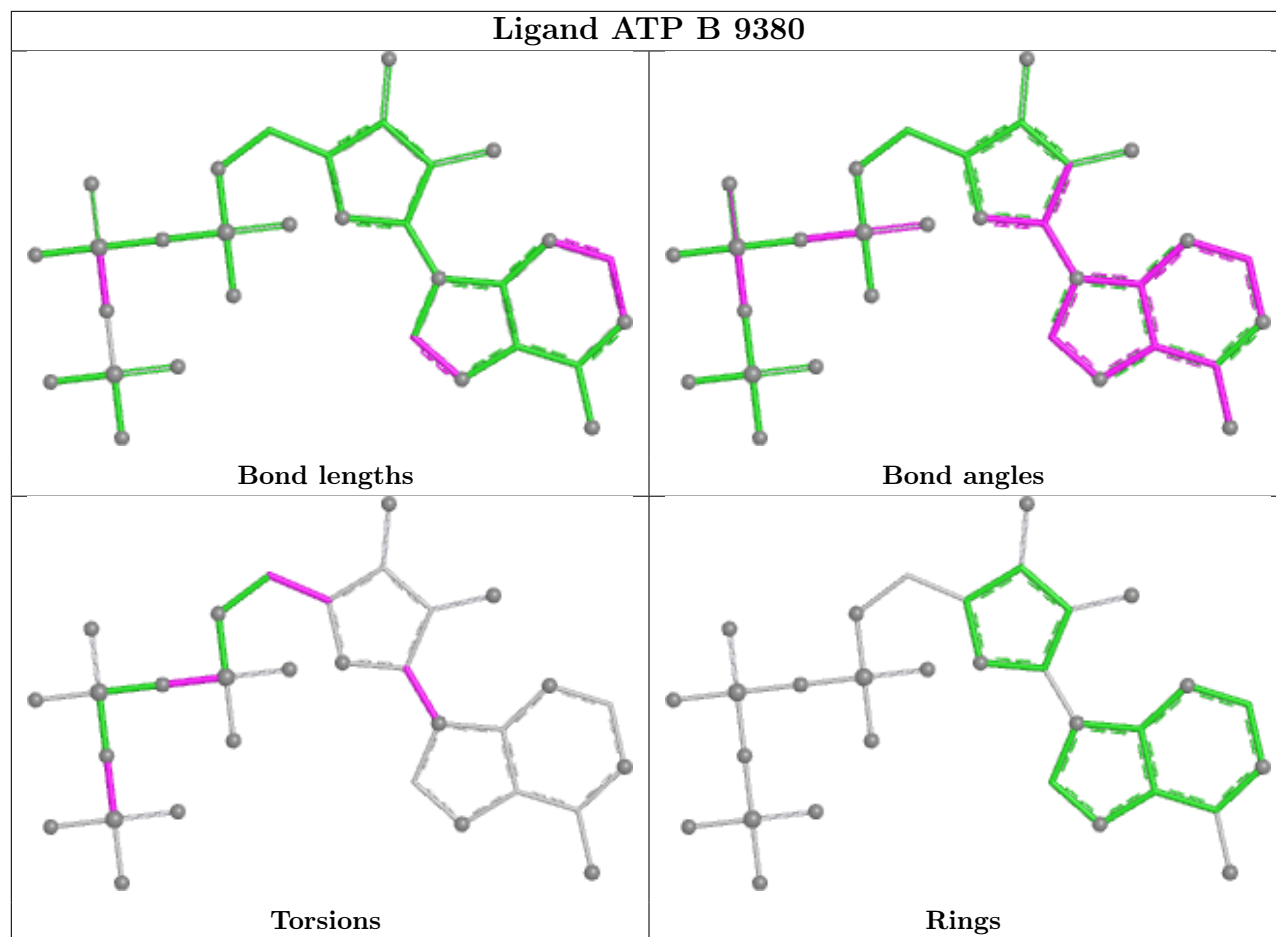
Mol	Chain	Res	Type	Atoms
2	A	5380	ATP	O4'-C4'-C5'-O5'
2	A	5380	ATP	C3'-C4'-C5'-O5'
2	B	9380	ATP	O4'-C4'-C5'-O5'
2	A	5380	ATP	PB-O3B-PG-O1G
2	B	9380	ATP	PB-O3B-PG-O1G
2	B	9380	ATP	PB-O3B-PG-O3G
2	A	5380	ATP	C2'-C1'-N9-C8
2	B	9380	ATP	C2'-C1'-N9-C8
2	A	5380	ATP	PB-O3A-PA-O1A
2	B	9380	ATP	PB-O3A-PA-O1A
2	A	5380	ATP	O4'-C1'-N9-C8

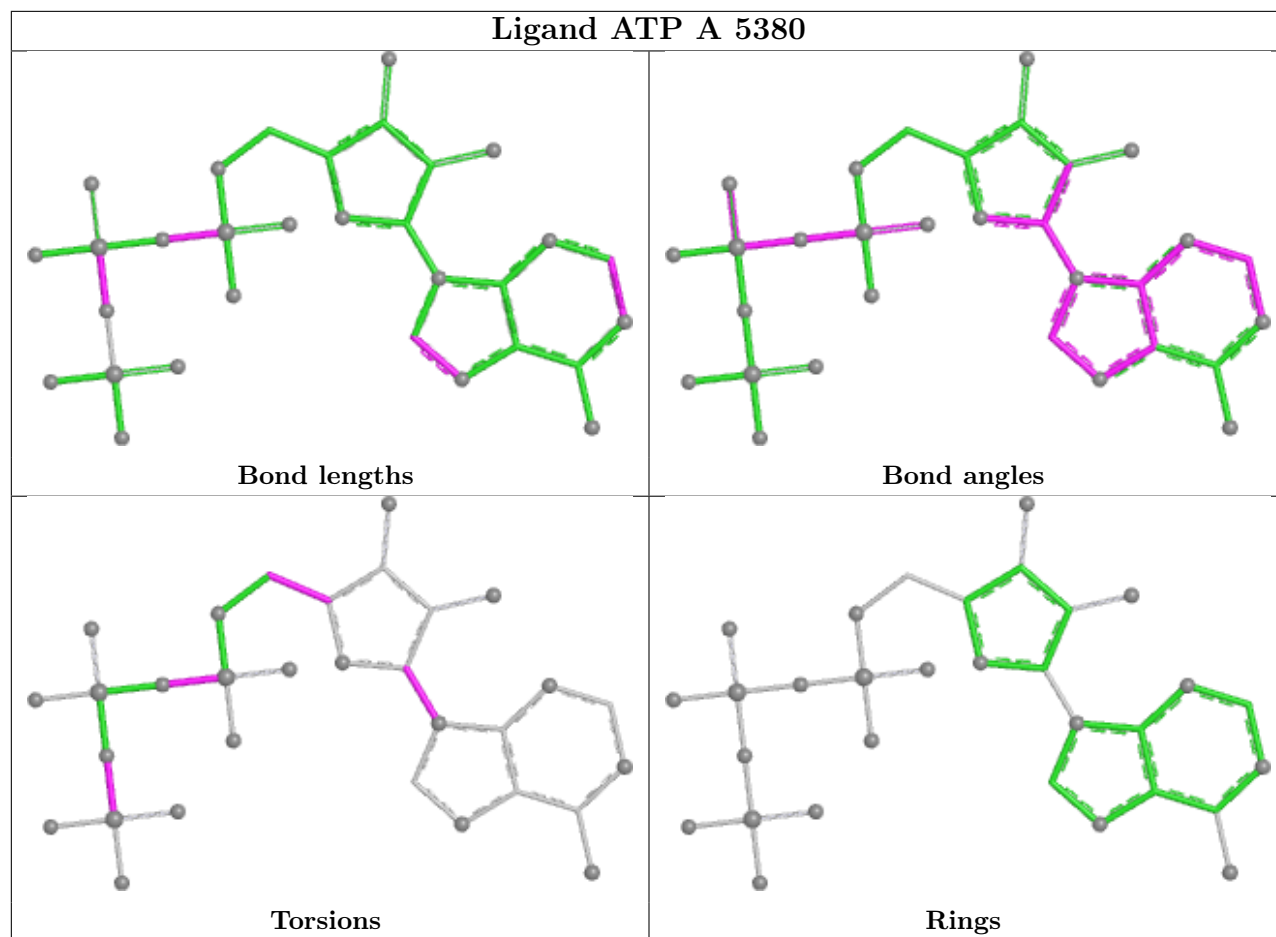
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9380	ATP	1	0
2	A	5380	ATP	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	721/731 (98%)	0.45	72 (9%) 12 9	28, 54, 110, 114	0
1	B	721/731 (98%)	0.62	101 (14%) 6 5	28, 54, 110, 114	0
All	All	1442/1462 (98%)	0.53	173 (11%) 9 6	28, 54, 110, 114	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	627	SER	7.3
1	B	27	VAL	5.9
1	A	755	ALA	5.2
1	B	630	LEU	5.2
1	A	627	SER	5.2
1	B	374	GLN	5.0
1	A	528	GLY	5.0
1	B	628	PRO	4.9
1	A	649	ILE	4.9
1	B	629	ARG	4.8
1	B	625	ARG	4.8
1	B	280	ALA	4.7
1	B	375	THR	4.7
1	A	529	GLY	4.6
1	B	649	ILE	4.6
1	A	280	ALA	4.5
1	B	278	ASN	4.3
1	A	457	SER	4.2
1	B	615	TRP	4.1
1	B	601	GLN	4.1
1	A	630	LEU	4.1
1	B	600	ALA	4.1
1	B	279	GLY	4.1
1	B	624	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	527	GLU	4.0
1	B	153	VAL	3.9
1	B	457	SER	3.9
1	A	151	HIS	3.9
1	B	522	GLY	3.8
1	B	608	GLY	3.8
1	B	157	VAL	3.8
1	B	754	ALA	3.7
1	A	152	VAL	3.6
1	A	628	PRO	3.6
1	B	577	LEU	3.6
1	B	605	VAL	3.6
1	B	647	ASN	3.6
1	B	609	SER	3.6
1	B	626	THR	3.6
1	B	281	GLY	3.5
1	B	621	LYS	3.5
1	B	631	LYS	3.5
1	B	562	ASN	3.5
1	A	527	GLU	3.5
1	A	279	GLY	3.5
1	B	529	GLY	3.5
1	B	603	VAL	3.5
1	A	454	ARG	3.5
1	A	282	PRO	3.4
1	B	588	LYS	3.4
1	A	389	HIS	3.4
1	B	623	THR	3.3
1	B	282	PRO	3.2
1	A	86	HIS	3.2
1	B	542	ARG	3.2
1	B	326	GLU	3.2
1	A	531	THR	3.2
1	A	268	ARG	3.1
1	B	620	GLY	3.1
1	A	373	ASP	3.1
1	A	456	GLY	3.0
1	B	371	ASP	3.0
1	A	458	ARG	3.0
1	B	753	LEU	3.0
1	A	562	ASN	3.0
1	B	602	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	326	GLU	2.9
1	B	691	GLU	2.9
1	A	618	LEU	2.9
1	B	576	TYR	2.9
1	B	154	PRO	2.9
1	A	632	ASP	2.9
1	B	531	THR	2.9
1	A	530	GLN	2.9
1	A	626	THR	2.9
1	A	611	PRO	2.9
1	B	367	LYS	2.9
1	B	579	VAL	2.8
1	A	629	ARG	2.8
1	A	753	LEU	2.8
1	A	574	ALA	2.8
1	A	343	ASP	2.8
1	A	277	SER	2.8
1	B	323	ALA	2.8
1	A	623	THR	2.8
1	B	513	GLY	2.8
1	A	372	PRO	2.8
1	A	323	ALA	2.7
1	B	583	ALA	2.7
1	B	589	THR	2.7
1	A	605	VAL	2.7
1	B	454	ARG	2.7
1	B	618	LEU	2.7
1	A	325	MET	2.7
1	A	27	VAL	2.7
1	A	370	ARG	2.6
1	B	268	ARG	2.6
1	B	538	LEU	2.6
1	A	94	SER	2.6
1	B	596	ARG	2.6
1	B	523	GLY	2.6
1	A	622	ALA	2.6
1	B	86	HIS	2.6
1	B	648	LYS	2.6
1	A	337	ASP	2.6
1	B	368	ASN	2.6
1	A	303	ASP	2.6
1	B	598	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	328	ARG	2.5
1	B	610	GLU	2.5
1	B	575	ALA	2.5
1	B	97	GLU	2.5
1	A	572	PRO	2.5
1	B	530	GLN	2.5
1	A	153	VAL	2.4
1	A	651	ARG	2.4
1	A	619	GLY	2.4
1	B	389	HIS	2.4
1	A	57	ASN	2.4
1	A	603	VAL	2.4
1	A	648	LYS	2.4
1	B	448	ILE	2.4
1	A	588	LYS	2.3
1	B	155	ASN	2.3
1	B	543	ALA	2.3
1	B	652	PHE	2.3
1	B	622	ALA	2.3
1	B	284	VAL	2.3
1	A	580	GLY	2.3
1	A	583	ALA	2.3
1	B	28	GLU	2.3
1	B	488	GLU	2.3
1	B	594	LEU	2.3
1	A	157	VAL	2.3
1	B	152	VAL	2.3
1	B	277	SER	2.3
1	B	276	VAL	2.3
1	A	614	PHE	2.2
1	A	28	GLU	2.2
1	B	267	ASN	2.2
1	B	151	HIS	2.2
1	B	456	GLY	2.2
1	A	156	GLU	2.2
1	A	419	GLN	2.2
1	A	371	ASP	2.2
1	A	276	VAL	2.2
1	B	565	ASP	2.2
1	B	372	PRO	2.2
1	B	592	GLN	2.2
1	A	534	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	156	GLU	2.2
1	A	647	ASN	2.1
1	B	429	ASN	2.1
1	A	579	VAL	2.1
1	B	373	ASP	2.1
1	A	631	LYS	2.1
1	B	361	LEU	2.1
1	A	624	TYR	2.1
1	B	370	ARG	2.1
1	B	376	GLU	2.1
1	B	692	GLU	2.1
1	B	568	VAL	2.1
1	B	578	TRP	2.1
1	A	97	GLU	2.1
1	A	596	ARG	2.1
1	B	563	SER	2.1
1	A	473	GLN	2.1
1	B	115	ARG	2.1
1	B	581	ALA	2.1
1	A	606	ALA	2.0
1	B	534	ALA	2.0
1	B	606	ALA	2.0
1	A	625	ARG	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](#)

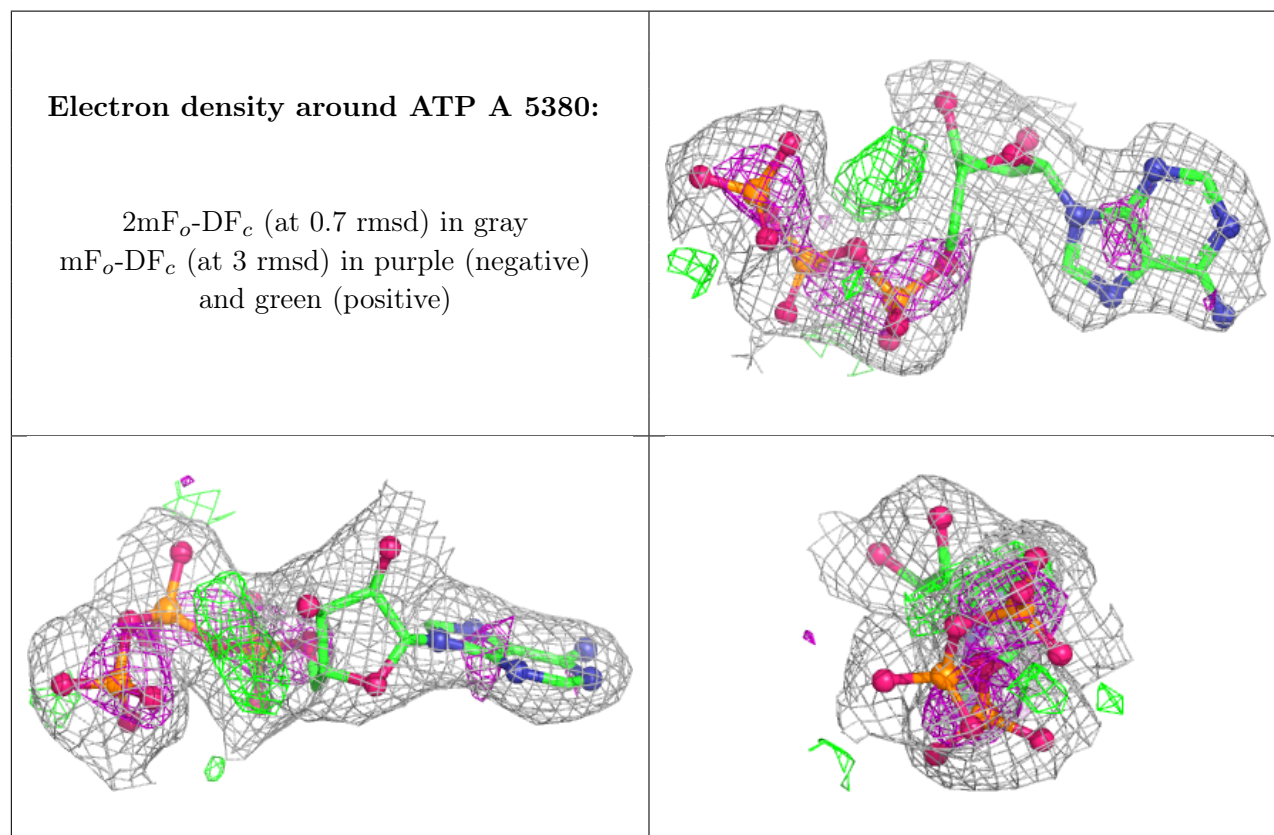
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

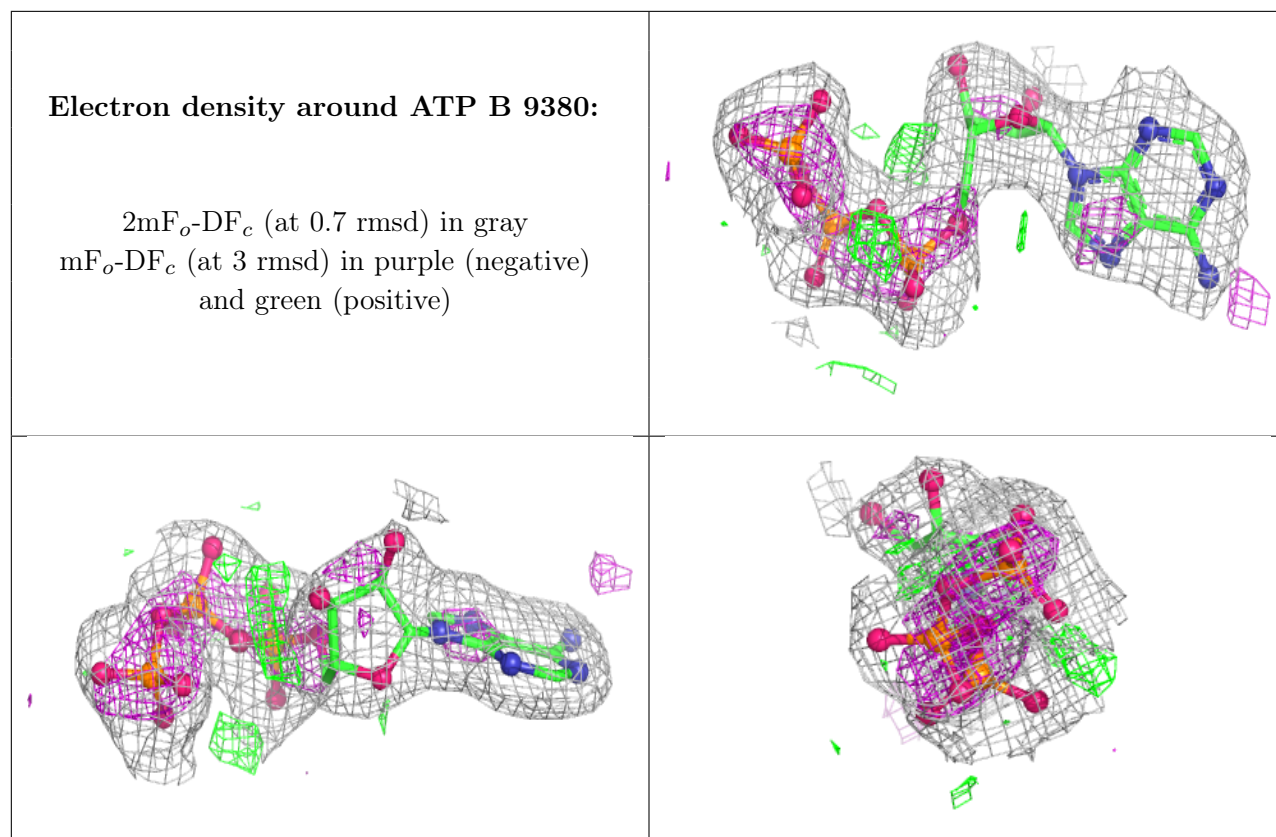
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	A	5380	31/31	0.95	0.08	20,26,33,34	0
2	ATP	B	9380	31/31	0.95	0.08	20,26,33,34	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 ⓘ

There are no such residues in this entry.