Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 07:37 PM EDT

PDB ID	:	3DQW
Title	:	c-Src kinase domain Thr338Ile mutant in complex with ATPgS
Authors	:	Azam, M.; Seeliger, M.A.; Gray, N.; Kuriyan, J.; Daley, G.Q.
Deposited on	:	2008-07-09
Resolution	:	2.02 Å(reported)

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

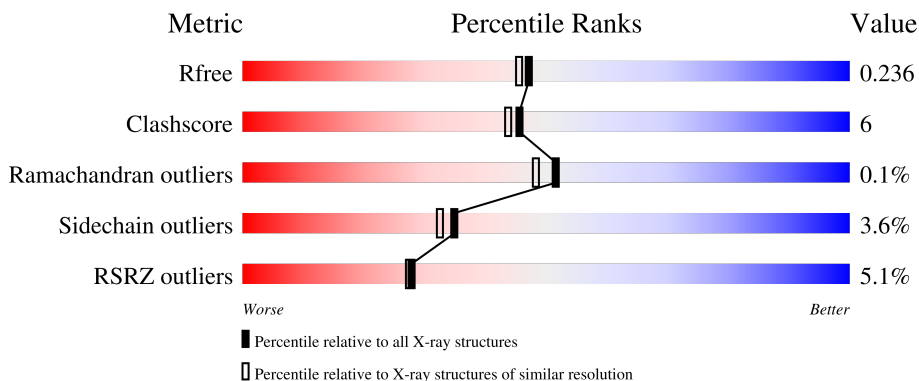|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.02 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		0.236
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		3.6%
RSRZ outliers		5.1%

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$_{free}$	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	286	2% / 85% / 11% / ••
1	B	286	2% / 83% / 14% / ••
1	C	286	5% / 77% / 18% / ••
1	D	286	11% / 80% / 16% / ••

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9717 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 Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	P	S	0	0	0
			2249	1439	377	415	1	17			
1	B	279	Total	C	N	O	P	S	0	0	0
			2249	1439	377	415	1	17			
1	C	276	Total	C	N	O	P	S	0	0	0
			2227	1424	373	412	1	17			
1	D	277	Total	C	N	O	P	S	0	0	0
			2236	1430	375	413	1	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
A	338	ILE	THR	engineered mutation	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523
B	338	ILE	THR	engineered mutation	UNP P00523
C	248	GLY	-	expression tag	UNP P00523
C	249	HIS	-	expression tag	UNP P00523
C	250	MET	-	expression tag	UNP P00523
C	338	ILE	THR	engineered mutation	UNP P00523
D	248	GLY	-	expression tag	UNP P00523
D	249	HIS	-	expression tag	UNP P00523
D	250	MET	-	expression tag	UNP P00523
D	338	ILE	THR	engineered mutation	UNP P00523

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

AGS
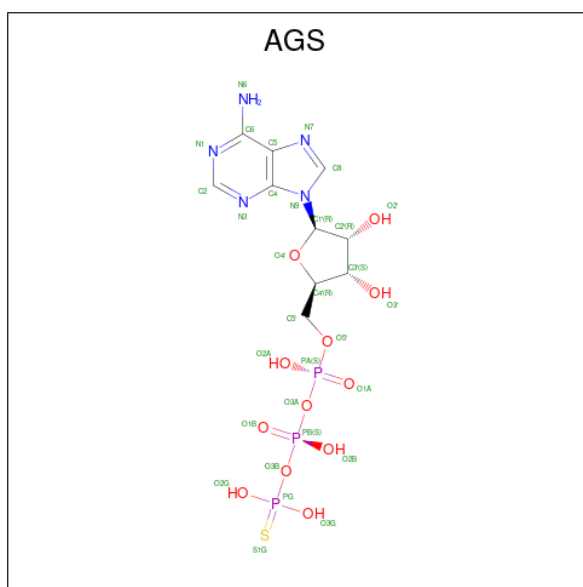
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	190	Total 190	O 190	0	0
4	C	133	Total 133	O 133	0	0
4	D	104	Total 104	O 104	0	0

# 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 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.
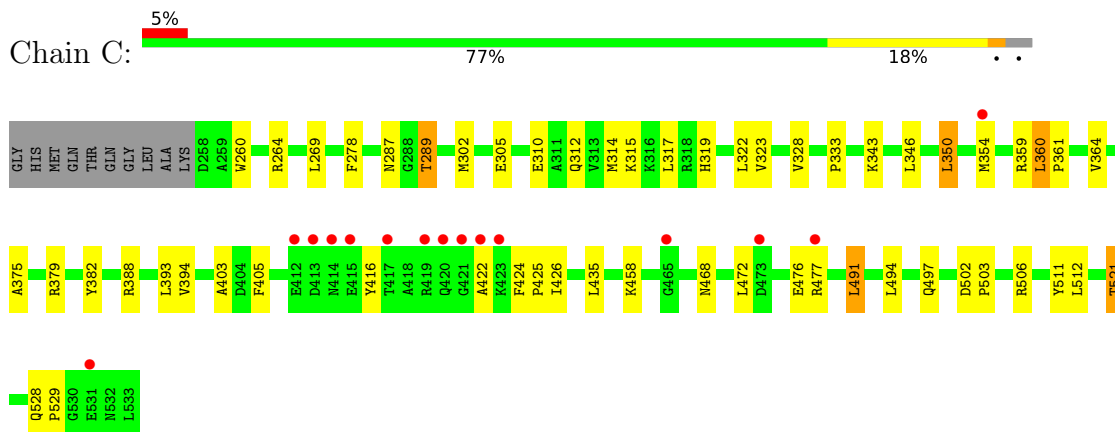
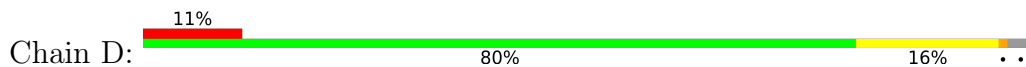- Molecule 1: Proto-oncogene tyrosine-protein kinase Src
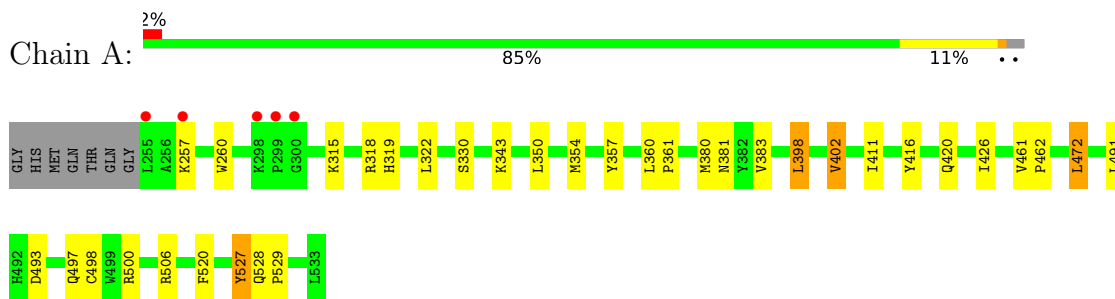
Chain A:

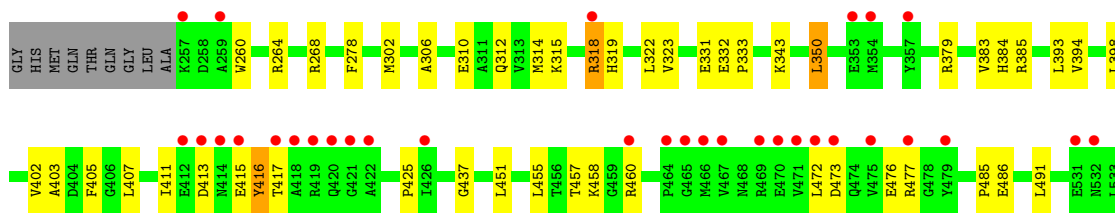- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain B:
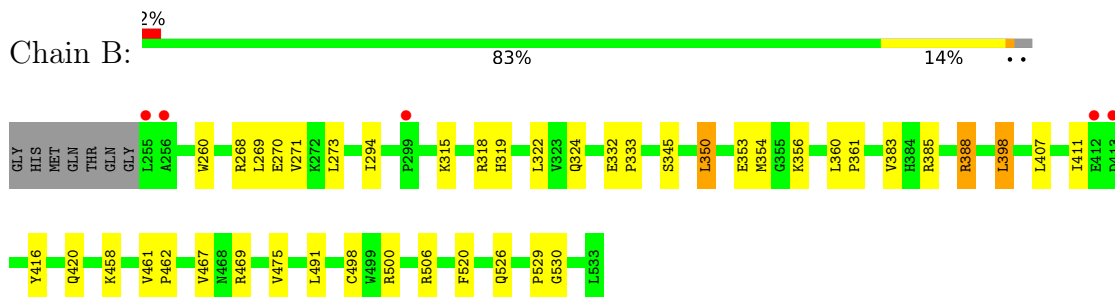
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain C:

- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.42Å 103.65Å 83.69Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	43.69 – 2.02	Depositor
	43.69 – 2.02	EDS
% Data completeness	91.3 (43.69-2.02)	Depositor
(in resolution range)	91.4 (43.69-2.02)	EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.205 , 0.245	Depositor
	0.200 , 0.236	DCC
R_{free} test set	4411 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.4	EDS
L-test for twinning[2]	$< |L| > = 0.58, < L^2 > = 0.42$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9717	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6334e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PTR, MG, AGS

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	0.31	0/2285	0.50	0/3091
1	B	0.32	0/2285	0.51	0/3091
1	C	0.29	0/2263	0.49	0/3062
1	D	0.27	0/2272	0.45	0/3073
All	All	0.30	0/9105	0.49	0/12317

There are no bond length outliers.

There are no bond angle outliers.

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	2249	0	2233	22	0
1	B	2249	0	2233	27	0
1	C	2227	0	2204	35	0
1	D	2236	0	2217	35	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	201	0	0	4	0
4	B	190	0	0	6	0
4	C	133	0	0	2	0
4	D	104	0	0	3	0
All	All	9717	0	8935	116	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 6.

All (116) 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:A:354:MET:SD	1:B:354:MET:SD	2.81	0.77
1:A:322:LEU:HD22	1:A:402:VAL:HG22	1.69	0.74
1:C:379:ARG:HD3	4:C:614:HOH:O	1.97	0.64
1:D:383:VAL:HG23	1:D:411:ILE:HG12	1.80	0.64
1:C:422:ALA:HB1	1:C:424:PHE:CE1	2.34	0.62
1:C:422:ALA:HB1	1:C:424:PHE:HE1	1.65	0.62
1:D:323:VAL:HG21	1:D:393:LEU:HD12	1.80	0.61
1:C:375:ALA:O	1:C:379:ARG:HG3	2.00	0.61
1:D:332:GLU:HG2	4:D:604:HOH:O	2.01	0.60
1:B:385:ARG:HD3	1:B:407:LEU:O	2.02	0.60
1:A:420:GLN:HB3	4:A:598:HOH:O	2.03	0.59
1:C:278:PHE:HB3	1:C:302:MET:HE2	1.85	0.59
1:B:529:PRO:HB3	4:B:689:HOH:O	2.02	0.59
1:D:310:GLU:O	1:D:314:MET:HG3	2.02	0.58
1:D:385:ARG:HD3	1:D:407:LEU:O	2.03	0.58
1:A:529:PRO:HB3	4:A:582:HOH:O	2.03	0.58
1:C:343:LYS:HB2	1:C:394:VAL:O	2.04	0.57
1:C:388:ARG:HG2	4:C:553:HOH:O	2.03	0.57
1:D:350:LEU:HG	1:D:458:LYS:HA	1.85	0.57
1:C:310:GLU:O	1:C:314:MET:HG3	2.05	0.56
1:D:473:ASP:O	1:D:477:ARG:HG3	2.05	0.56
1:C:472:LEU:O	1:C:476:GLU:HG3	2.05	0.56
1:A:322:LEU:HD22	1:A:402:VAL:CG2	2.38	0.54
1:C:260:TRP:HB3	1:C:328:VAL:HG12	1.89	0.54
1:B:475:VAL:HG21	4:B:672:HOH:O	2.07	0.54
1:B:388:ARG:HD3	4:B:543:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:HE3	1:B:353:GLU:OE2	2.08	0.53
1:A:318:ARG:NE	4:A:695:HOH:O	2.40	0.53
1:D:264:ARG:NH1	1:D:333:PRO:HG2	2.23	0.53
1:B:383:VAL:HB	1:B:411:ILE:HD11	1.90	0.52
1:D:302:MET:HG2	1:D:306:ALA:HB3	1.91	0.52
1:B:269:LEU:HD23	1:B:269:LEU:N	2.25	0.52
1:C:323:VAL:HG21	1:C:393:LEU:HD12	1.90	0.51
1:D:264:ARG:HH11	1:D:264:ARG:HG2	1.76	0.51
1:A:383:VAL:HB	1:A:411:ILE:HD11	1.92	0.51
1:A:500:ARG:O	1:A:506:ARG:HD2	2.11	0.51
1:D:318:ARG:O	1:D:318:ARG:HD3	2.11	0.50
1:C:426:ILE:HD12	1:C:468:ASN:HB3	1.94	0.50
1:A:498:CYS:O	1:A:506:ARG:HG2	2.12	0.50
1:D:264:ARG:HD2	4:D:571:HOH:O	2.11	0.49
1:C:359:ARG:HB3	1:C:361:PRO:HD2	1.94	0.49
1:A:260:TRP:CD1	1:A:315:LYS:HE2	2.48	0.49
1:C:319:HIS:HB3	1:C:322:LEU:HG	1.95	0.49
1:C:322:LEU:HD13	1:C:405:PHE:CZ	2.48	0.49
1:A:357:TYR:CE2	1:B:398:LEU:HD13	2.47	0.49
1:B:260:TRP:CD1	1:B:315:LYS:HE2	2.47	0.49
4:A:690:HOH:O	1:C:521:THR:HG21	2.11	0.49
1:D:322:LEU:HD13	1:D:405:PHE:CZ	2.49	0.48
1:D:260:TRP:CD1	1:D:315:LYS:HE2	2.49	0.48
1:D:383:VAL:HG23	1:D:411:ILE:CG1	2.44	0.48
1:D:485:PRO:O	1:D:486:GLU:HB2	2.13	0.48
1:B:269:LEU:HD22	1:B:294:ILE:HD13	1.96	0.48
1:D:318:ARG:HD3	1:D:318:ARG:C	2.35	0.48
1:D:457:THR:HB	1:D:460:ARG:HD2	1.96	0.47
1:D:343:LYS:HB2	1:D:394:VAL:O	2.14	0.47
1:B:530:GLY:HA3	4:B:648:HOH:O	2.14	0.47
1:A:319:HIS:HB3	1:A:322:LEU:HG	1.95	0.47
1:C:346:LEU:HG	1:C:350:LEU:HD22	1.97	0.47
1:D:278:PHE:CG	1:D:302:MET:HE2	2.50	0.46
1:A:461:VAL:HG12	1:A:462:PRO:O	2.16	0.46
1:D:264:ARG:HH12	1:D:333:PRO:HG2	1.81	0.46
2:D:534:AGS:H8	2:D:534:AGS:O5'	2.15	0.46
1:A:380:MET:O	1:A:381:ASN:HB2	2.14	0.46
1:C:317:LEU:HD21	1:C:382:TYR:CD2	2.51	0.46
1:D:451:LEU:HD23	1:D:451:LEU:O	2.16	0.45
1:C:278:PHE:CB	1:C:302:MET:HE2	2.46	0.45
1:D:417:THR:HA	1:D:437:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:GLU:HG2	1:D:416:PTR:N	2.32	0.45
1:A:527:TYR:CD1	1:A:527:TYR:C	2.90	0.45
1:C:350:LEU:HG	1:C:458:LYS:HA	1.98	0.45
1:C:269:LEU:HD23	1:C:269:LEU:N	2.31	0.45
1:D:379:ARG:HD3	4:D:614:HOH:O	2.17	0.44
1:D:350:LEU:HD21	1:D:455:LEU:HA	1.99	0.44
1:D:384:HIS:O	1:D:385:ARG:HB2	2.17	0.44
1:D:322:LEU:HD22	1:D:402:VAL:HB	2.00	0.44
1:A:497:GLN:HG2	1:A:500:ARG:NH2	2.33	0.44
1:D:319:HIS:HB3	1:D:322:LEU:HG	2.00	0.43
1:D:264:ARG:NH1	1:D:264:ARG:HG2	2.33	0.43
1:B:353:GLU:O	1:B:356:LYS:HG2	2.19	0.43
1:A:257:LYS:HE2	1:A:330:SER:HB2	2.00	0.43
1:C:287:ASN:O	1:C:289:THR:HG22	2.19	0.43
1:C:323:VAL:HG21	1:C:403:ALA:HB2	2.01	0.43
1:B:271:VAL:O	1:B:273:LEU:HD13	2.18	0.43
1:B:498:CYS:O	1:B:506:ARG:HG2	2.19	0.43
1:B:500:ARG:O	1:B:506:ARG:HD2	2.19	0.43
1:C:424:PHE:HA	1:C:425:PRO:HD3	1.95	0.43
1:D:472:LEU:O	1:D:476:GLU:HG3	2.18	0.42
1:C:494:LEU:HD11	1:C:512:LEU:HD23	2.00	0.42
1:D:491:LEU:HD23	1:D:491:LEU:HA	1.75	0.42
1:A:426:ILE:CG2	1:A:472:LEU:HD13	2.49	0.42
1:B:268:ARG:HD2	1:B:270:GLU:HG2	2.01	0.42
1:B:350:LEU:HG	1:B:458:LYS:HA	2.01	0.42
1:B:361:PRO:HA	1:B:520:PHE:CE2	2.54	0.42
1:C:435:LEU:HD21	1:C:472:LEU:HD21	2.00	0.42
1:C:502:ASP:HA	1:C:503:PRO:HD3	1.87	0.42
1:D:278:PHE:HB3	1:D:302:MET:HE3	2.01	0.42
1:B:461:VAL:HG12	1:B:462:PRO:O	2.19	0.42
1:C:528:GLN:HA	1:C:529:PRO:HD3	1.91	0.41
1:C:264:ARG:NH1	1:C:333:PRO:HG2	2.35	0.41
1:C:360:LEU:HD22	1:C:364:VAL:HG23	2.02	0.41
1:B:356:LYS:HE3	1:B:356:LYS:HB3	1.81	0.41
1:B:411:ILE:HD13	4:B:610:HOH:O	2.20	0.41
1:C:260:TRP:CD1	1:C:315:LYS:HE2	2.55	0.41
1:D:350:LEU:HD12	1:D:350:LEU:HA	1.87	0.41
1:B:332:GLU:HA	1:B:333:PRO:HA	1.91	0.41
1:C:360:LEU:HD23	1:C:360:LEU:HA	1.92	0.41
1:A:461:VAL:HG21	1:C:511:TYR:HA	2.03	0.41
1:B:420:GLN:HG3	4:B:646:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PRO:HA	1:A:520:PHE:CE2	2.56	0.41
1:B:353:GLU:HA	1:B:356:LYS:HD2	2.01	0.41
1:C:491:LEU:HD23	1:C:491:LEU:HA	1.86	0.41
1:C:497:GLN:O	1:C:506:ARG:HG3	2.20	0.41
1:B:318:ARG:HH22	1:B:324:GLN:HE21	1.70	0.40
1:D:323:VAL:HG21	1:D:403:ALA:HB2	2.04	0.40
1:A:398:LEU:HD12	1:A:398:LEU:HA	1.88	0.40
1:B:319:HIS:HB3	1:B:322:LEU:HG	2.04	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	276/286 (96%)	270 (98%)	6 (2%)	0	100	100
1	B	276/286 (96%)	271 (98%)	5 (2%)	0	100	100
1	C	273/286 (96%)	265 (97%)	8 (3%)	0	100	100
1	D	274/286 (96%)	261 (95%)	12 (4%)	1 (0%)	34	28
All	All	1099/1144 (96%)	1067 (97%)	31 (3%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	425	PRO

5.3.2 Protein sidechains (i)

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	239/244 (98%)	230 (96%)	9 (4%)	33	30
1	B	239/244 (98%)	230 (96%)	9 (4%)	33	30
1	C	237/244 (97%)	228 (96%)	9 (4%)	33	30
1	D	238/244 (98%)	231 (97%)	7 (3%)	42	41
All	All	953/976 (98%)	919 (96%)	34 (4%)	35	32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	LEU
1	A	360	LEU
1	A	398	LEU
1	A	402	VAL
1	A	472	LEU
1	A	491	LEU
1	A	493	ASP
1	A	527	TYR
1	A	528	GLN
1	B	345	SER
1	B	350	LEU
1	B	360	LEU
1	B	388	ARG
1	B	398	LEU
1	B	467	VAL
1	B	469	ARG
1	B	491	LEU
1	B	526	GLN
1	C	289	THR
1	C	305	GLU
1	C	312	GLN
1	C	350	LEU
1	C	354	MET
1	C	360	LEU
1	C	477	ARG
1	C	491	LEU
1	C	521	THR
1	D	268	ARG
1	D	312	GLN
1	D	318	ARG

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Mol	Chain	Res	Type
1	D	331	GLU
1	D	350	LEU
1	D	398	LEU
1	D	413	ASP

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	287	ASN
1	A	309	GLN
1	A	391	ASN
1	A	526	GLN
1	B	324	GLN
1	B	526	GLN
1	C	309	GLN
1	C	468	ASN
1	D	309	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	PTR	A	416	1	15,16,17	1.94	1 (6%)	19,22,24	0.67	0
1	PTR	C	416	1	15,16,17	2.01	1 (6%)	19,22,24	0.50	0
1	PTR	D	416	1	15,16,17	1.95	1 (6%)	19,22,24	0.65	0
1	PTR	B	416	1	15,16,17	1.97	2 (13%)	19,22,24	0.62	0

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
1	PTR	A	416	1	-	0/10/11/13	0/1/1/1
1	PTR	C	416	1	-	0/10/11/13	0/1/1/1
1	PTR	D	416	1	-	1/10/11/13	0/1/1/1
1	PTR	B	416	1	-	2/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	416	PTR	OH-CZ	-7.22	1.24	1.40
1	C	416	PTR	OH-CZ	-7.20	1.24	1.40
1	A	416	PTR	OH-CZ	-7.09	1.24	1.40
1	B	416	PTR	OH-CZ	-6.93	1.24	1.40
1	B	416	PTR	P-OH	2.08	1.62	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	416	PTR	CE2-CZ-OH-P
1	B	416	PTR	CE1-CZ-OH-P
1	D	416	PTR	CE1-CZ-OH-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	416	PTR	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	AGS	B	534	-	26,33,33	1.78	7 (26%)	26,52,52	1.58	5 (19%)
2	AGS	C	534	-	26,33,33	1.77	4 (15%)	26,52,52	1.33	3 (11%)
2	AGS	A	534	-	26,33,33	1.69	5 (19%)	26,52,52	1.47	5 (19%)
2	AGS	D	534	-	26,33,33	1.66	6 (23%)	26,52,52	1.43	4 (15%)

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	AGS	B	534	-	-	4/17/38/38	0/3/3/3
2	AGS	C	534	-	-	0/17/38/38	0/3/3/3
2	AGS	A	534	-	-	6/17/38/38	0/3/3/3
2	AGS	D	534	-	-	6/17/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	534	AGS	PG-S1G	5.59	2.02	1.90
2	A	534	AGS	PG-S1G	5.57	2.02	1.90
2	D	534	AGS	PG-S1G	5.53	2.02	1.90
2	B	534	AGS	PG-S1G	5.32	2.02	1.90
2	C	534	AGS	C2'-C1'	2.75	1.57	1.53
2	B	534	AGS	C2'-C1'	2.47	1.57	1.53
2	A	534	AGS	C2'-C1'	2.46	1.57	1.53
2	D	534	AGS	C2'-C1'	2.42	1.57	1.53
2	A	534	AGS	C2-N3	2.33	1.35	1.32
2	B	534	AGS	C2-N3	2.32	1.35	1.32
2	D	534	AGS	C2-N3	2.29	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	534	AGS	PG-O3G	-2.23	1.47	1.54
2	B	534	AGS	C5'-C4'	2.21	1.58	1.51
2	B	534	AGS	PG-O3G	-2.21	1.47	1.54
2	C	534	AGS	PG-O3G	-2.18	1.47	1.54
2	C	534	AGS	C2-N3	2.17	1.35	1.32
2	D	534	AGS	PG-O3G	-2.12	1.48	1.54
2	A	534	AGS	C5'-C4'	2.09	1.58	1.51
2	D	534	AGS	O3'-C3'	-2.08	1.38	1.43
2	B	534	AGS	O3'-C3'	-2.08	1.38	1.43
2	D	534	AGS	C5'-C4'	2.03	1.57	1.51
2	B	534	AGS	PA-O1A	2.03	1.58	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	534	AGS	C3'-C2'-C1'	-4.50	94.21	100.98
2	A	534	AGS	C3'-C2'-C1'	-3.78	95.29	100.98
2	D	534	AGS	C3'-C2'-C1'	-3.54	95.65	100.98
2	D	534	AGS	O3G-PG-O3B	3.23	115.41	104.64
2	C	534	AGS	O3G-PG-O3B	2.84	114.13	104.64
2	A	534	AGS	O3G-PG-O3B	2.83	114.07	104.64
2	C	534	AGS	C5-C6-N6	2.75	124.53	120.35
2	B	534	AGS	O3G-PG-O3B	2.60	113.31	104.64
2	C	534	AGS	C3'-C2'-C1'	-2.59	97.08	100.98
2	D	534	AGS	C5-C6-N6	2.51	124.17	120.35
2	B	534	AGS	O4'-C4'-C3'	-2.50	100.16	105.11
2	B	534	AGS	C5-C6-N6	2.49	124.13	120.35
2	D	534	AGS	O4'-C4'-C3'	-2.36	100.44	105.11
2	B	534	AGS	O2G-PG-O3B	2.29	112.27	104.64
2	A	534	AGS	O5'-PA-O1A	2.27	117.92	109.07
2	A	534	AGS	PA-O3A-PB	2.10	140.04	132.83
2	A	534	AGS	O4'-C4'-C3'	-2.03	101.11	105.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	534	AGS	PB-O3B-PG-O2G
2	A	534	AGS	C5'-O5'-PA-O3A
2	B	534	AGS	C5'-O5'-PA-O1A
2	B	534	AGS	C5'-O5'-PA-O3A
2	D	534	AGS	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
2	D	534	AGS	PB-O3B-PG-O3G
2	A	534	AGS	C3'-C4'-C5'-O5'
2	A	534	AGS	C5'-O5'-PA-O1A
2	A	534	AGS	C5'-O5'-PA-O2A
2	B	534	AGS	C5'-O5'-PA-O2A
2	D	534	AGS	PG-O3B-PB-O2B
2	D	534	AGS	PB-O3A-PA-O2A
2	D	534	AGS	PB-O3A-PA-O1A
2	A	534	AGS	O4'-C4'-C5'-O5'
2	D	534	AGS	PA-O3A-PB-O1B
2	B	534	AGS	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	534	AGS	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 then 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.

Ligand AGS B 534

Bond lengths

Bond angles

Torsions

Rings

Ligand AGS C 534

Bond lengths

Bond angles

Torsions

Rings

Ligand AGS A 534

Bond lengths

Bond angles

Torsions

Rings

Ligand AGS D 534

Bond lengths

Bond angles

Torsions

Rings
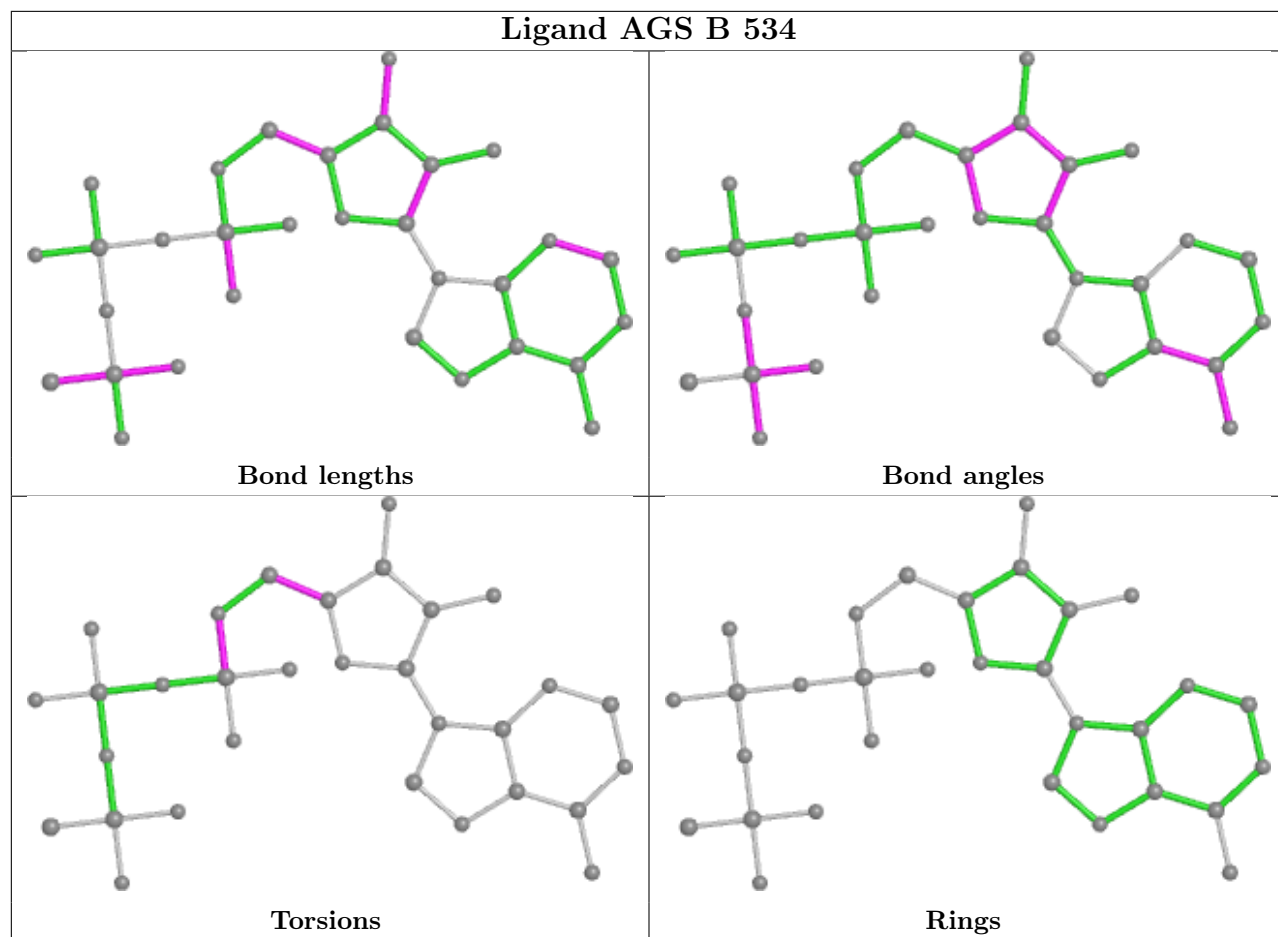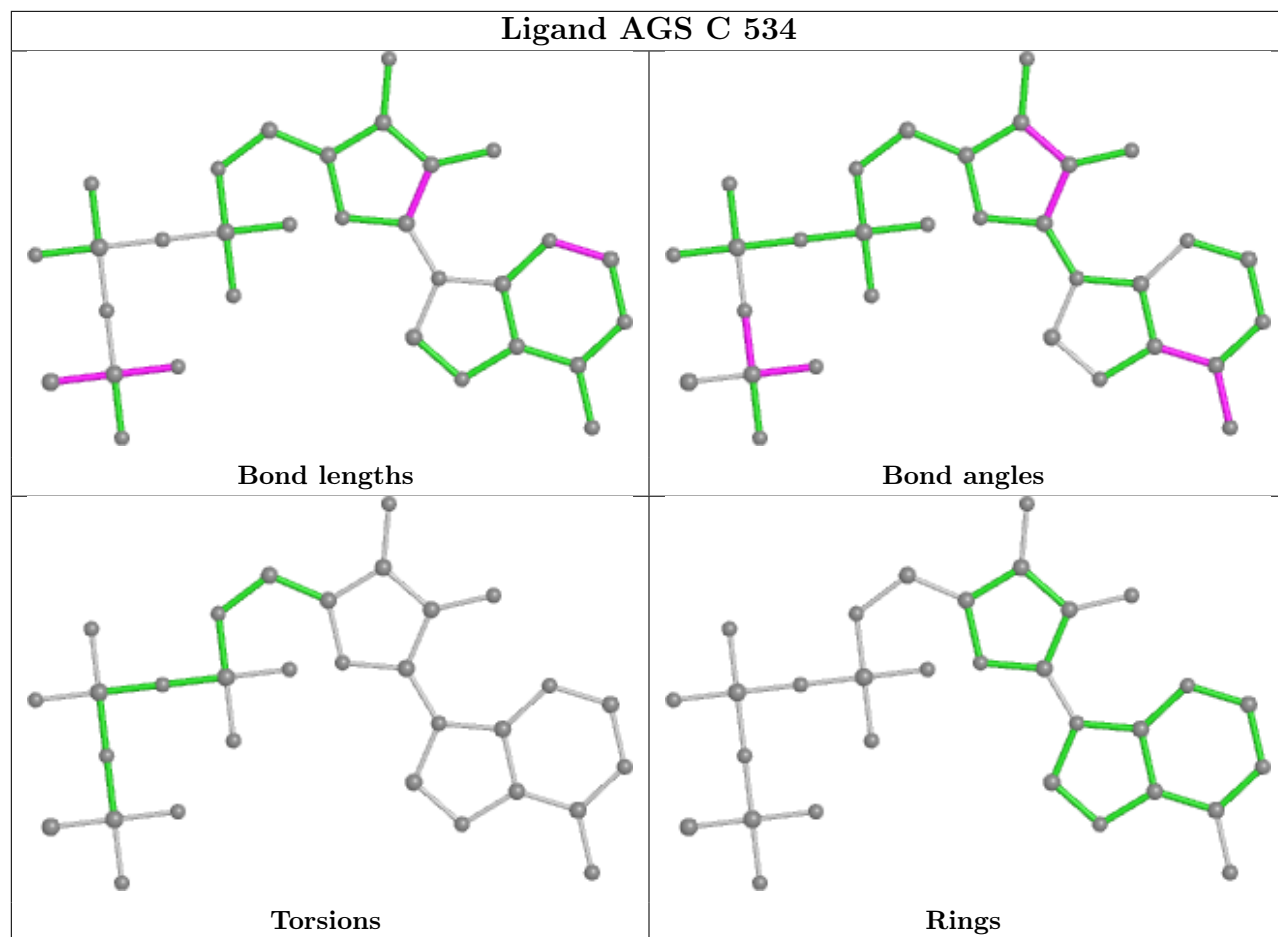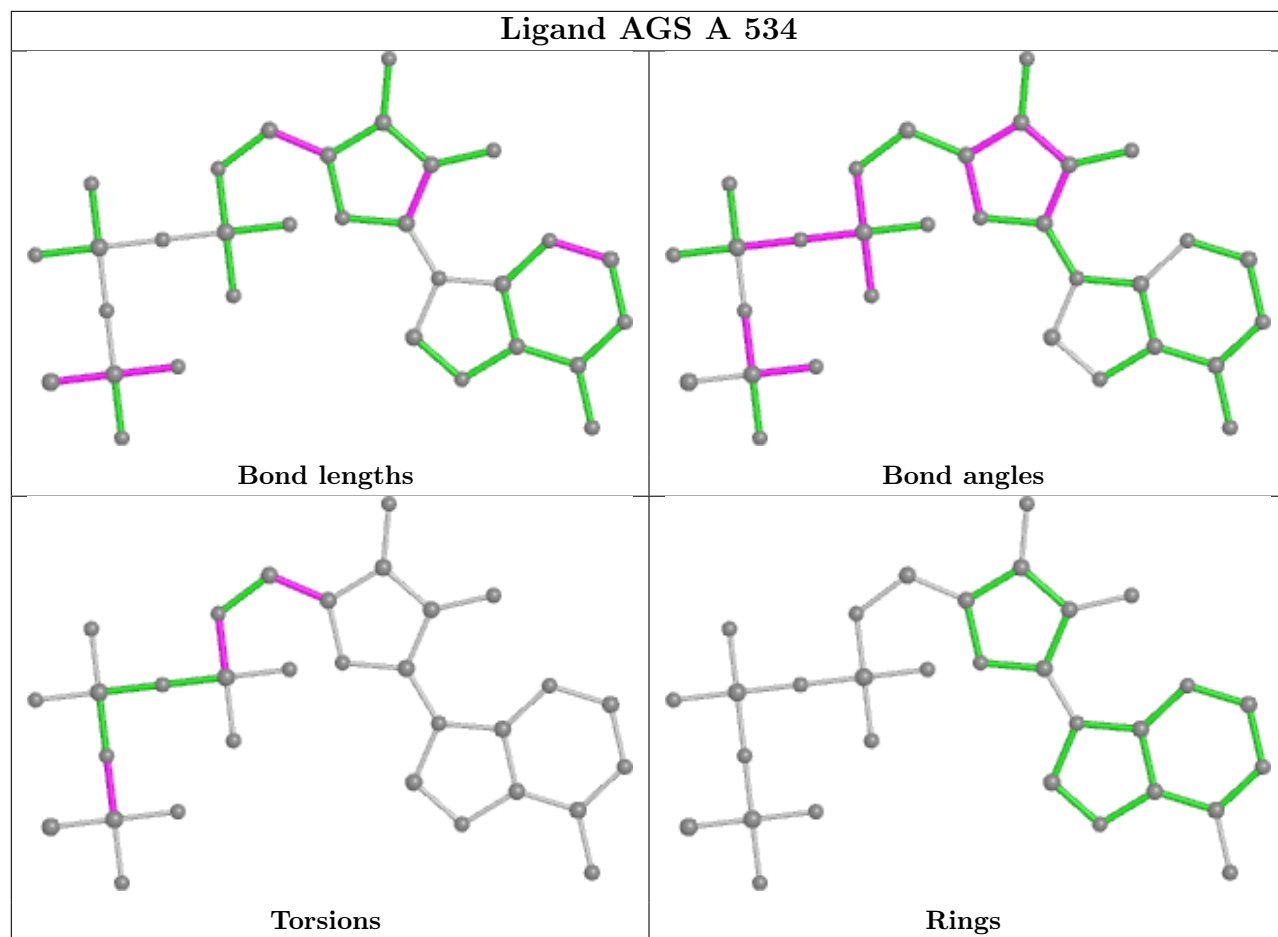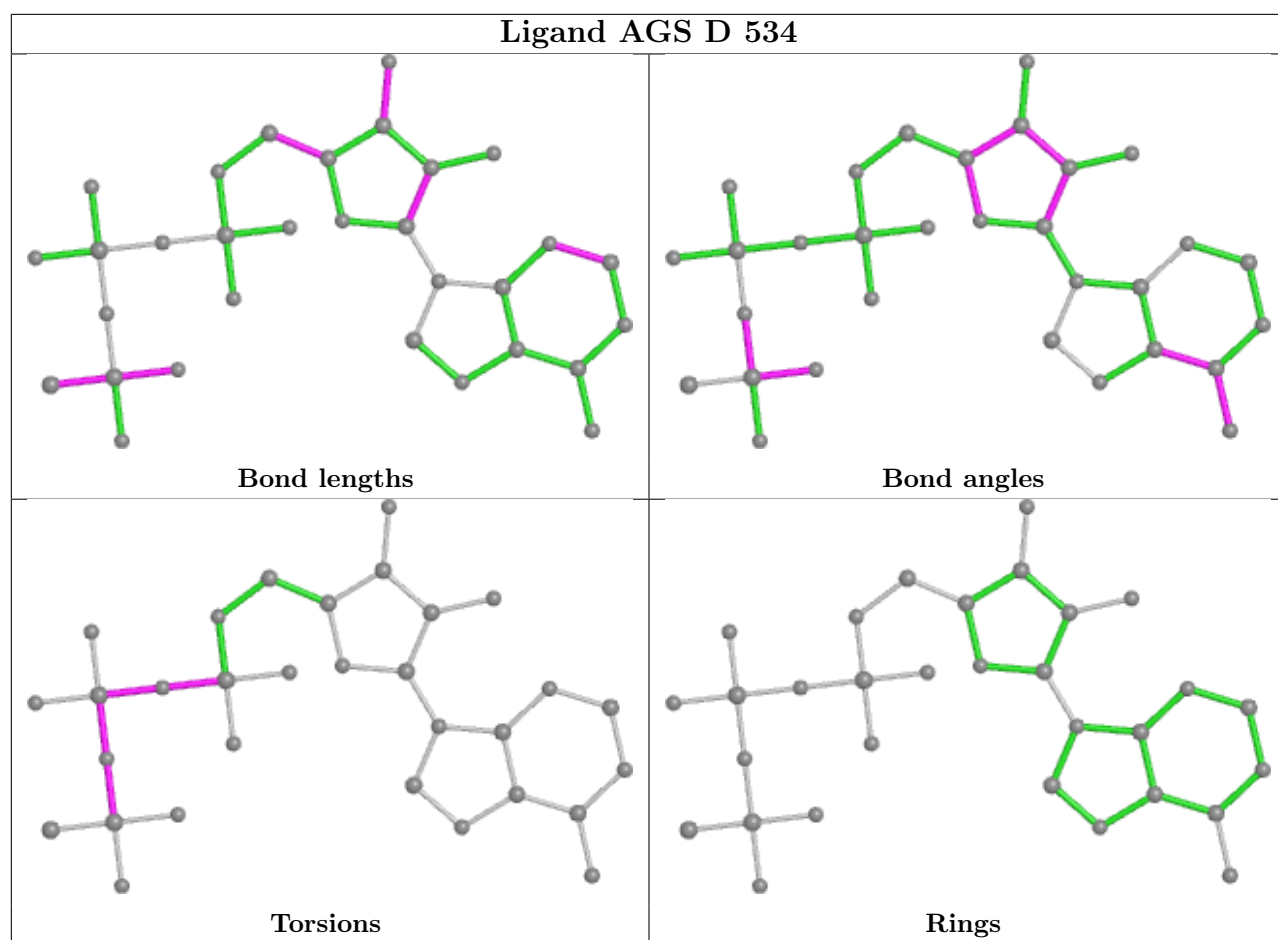
5.7 Other polymers ⓘ

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	278/286 (97%)	-0.09	5 (1%)	68	67	19, 30, 51, 70	0
1	B	278/286 (97%)	-0.14	5 (1%)	68	67	20, 29, 54, 72	0
1	C	275/286 (96%)	0.27	15 (5%)	25	24	19, 37, 62, 90	0
1	D	276/286 (96%)	0.47	32 (11%)	4	4	26, 43, 70, 91	0
All	All	1107/1144 (96%)	0.13	57 (5%)	28	27	19, 35, 60, 91	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	419	ARG	7.5
1	D	412	GLU	6.8
1	D	420	GLN	6.4
1	B	255	LEU	6.3
1	D	421	GLY	4.9
1	D	414	ASN	4.8
1	C	414	ASN	4.7
1	C	421	GLY	4.5
1	C	412	GLU	4.4
1	C	415	GLU	4.4
1	A	255	LEU	4.4
1	C	413	ASP	4.3
1	C	419	ARG	3.8
1	D	413	ASP	3.6
1	C	420	GLN	3.5
1	D	465	GLY	3.5
1	D	531	GLU	3.4
1	A	299	PRO	3.4
1	D	532	ASN	3.3
1	D	477	ARG	3.2
1	D	471	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	426	ILE	3.1
1	C	417	THR	3.0
1	D	460	ARG	3.0
1	C	423	LYS	2.9
1	C	465	GLY	2.8
1	D	357	TYR	2.8
1	D	472	LEU	2.7
1	D	353	GLU	2.7
1	D	418	ALA	2.7
1	D	415	GLU	2.6
1	D	257	LYS	2.6
1	D	469	ARG	2.6
1	D	466	MET	2.6
1	B	412	GLU	2.5
1	D	475	VAL	2.5
1	C	422	ALA	2.5
1	C	531	GLU	2.5
1	C	477	ARG	2.5
1	A	257	LYS	2.5
1	D	473	ASP	2.4
1	D	467	VAL	2.4
1	B	299	PRO	2.4
1	D	422	ALA	2.4
1	D	417	THR	2.3
1	D	464	PRO	2.3
1	D	318	ARG	2.2
1	A	300	GLY	2.1
1	C	473	ASP	2.1
1	B	256	ALA	2.1
1	D	259	ALA	2.1
1	D	470	GLU	2.0
1	D	479	TYR	2.0
1	B	413	ASP	2.0
1	A	298	LYS	2.0
1	C	354	MET	2.0
1	D	354	MET	2.0

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

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
1	PTR	C	416	16/17	0.79	0.26	61,66,78,81	0
1	PTR	D	416	16/17	0.81	0.25	63,68,80,84	0
1	PTR	A	416	16/17	0.94	0.10	28,32,50,50	0
1	PTR	B	416	16/17	0.94	0.09	28,34,50,51	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	MG	B	2	1/1	0.67	0.14	53,53,53,53	0
3	MG	A	1	1/1	0.72	0.25	57,57,57,57	0
3	MG	C	3	1/1	0.80	0.21	63,63,63,63	0
2	AGS	D	534	31/31	0.81	0.18	32,43,80,90	0
2	AGS	C	534	31/31	0.83	0.19	26,40,81,88	0
2	AGS	B	534	31/31	0.86	0.16	28,42,72,75	0
2	AGS	A	534	31/31	0.87	0.16	27,40,74,89	0
3	MG	D	4	1/1	0.92	0.08	66,66,66,66	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Electron density around AGS D 534:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
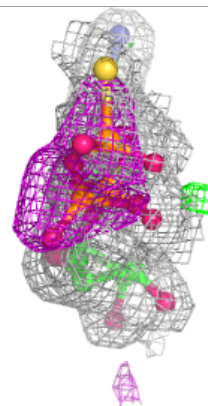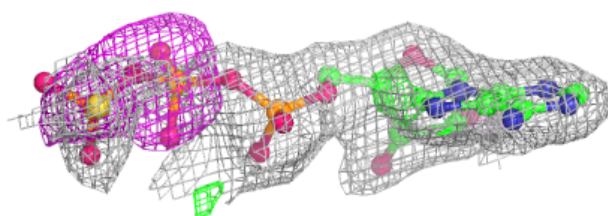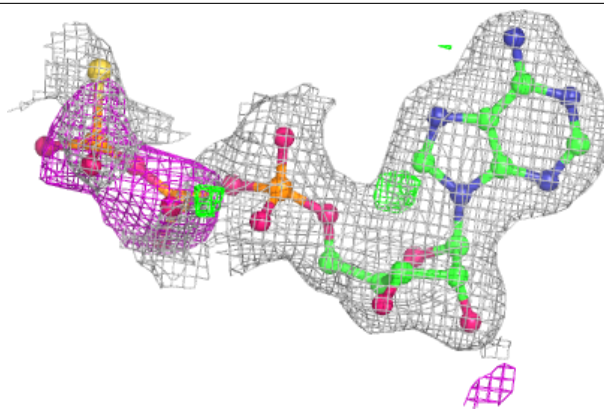
Electron density around AGS C 534:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
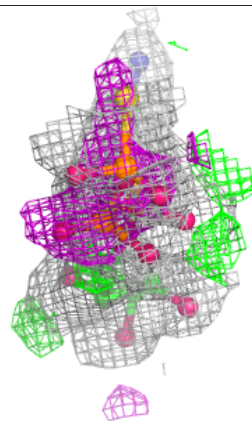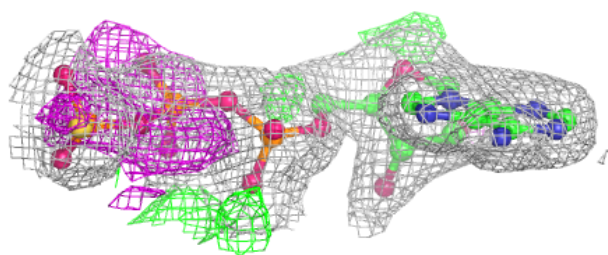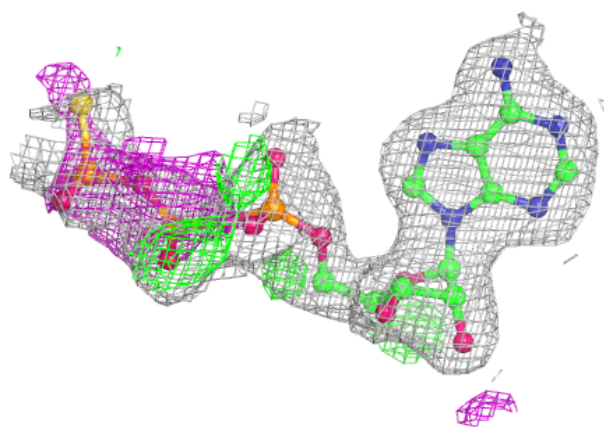$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
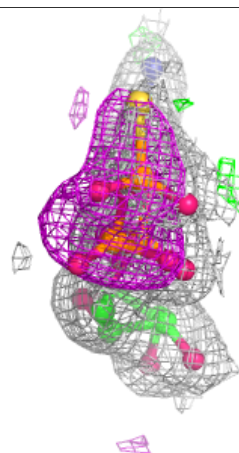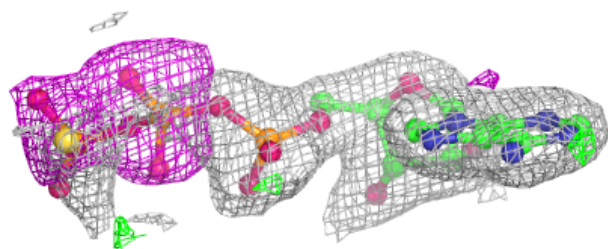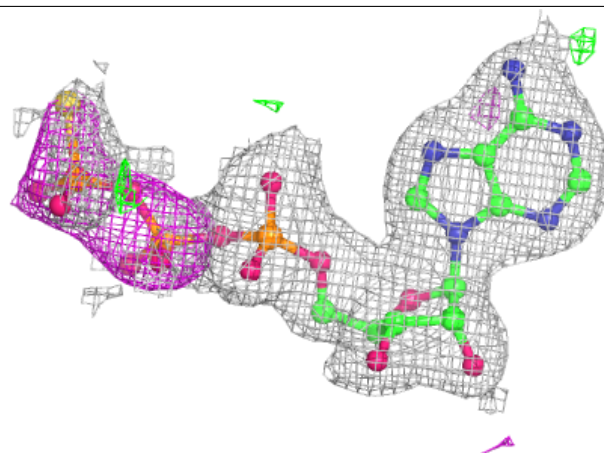
Electron density around AGS B 534:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
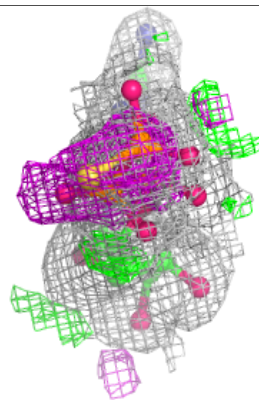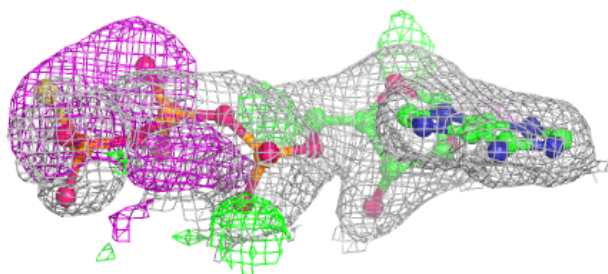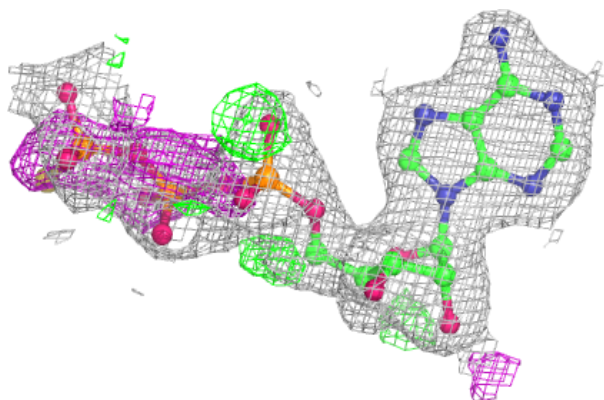mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AGS A 534:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.