



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:05 AM UTC

PDB ID : 6QV4 / pdb_00006qv4
Title : Crystal structure of the Ski2 RNA-helicase Brr2 from Chaetomium thermophilum bound to ATP-gamma-S
Authors : Absmeier, E.; Santos, K.F.; Wahl, M.C.
Deposited on : 2019-03-01
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

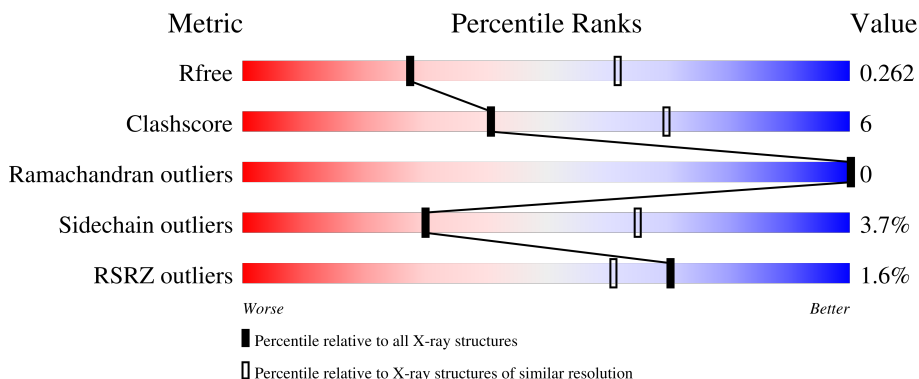
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

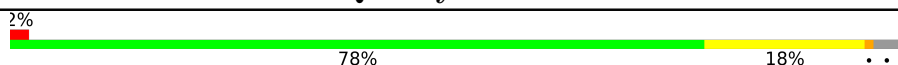
The reported resolution of this entry is 2.80 Å.

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	1725	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13506 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 Pre-mRNA splicing helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1666	Total	C	N	O	S	0	0	0
			13362	8544	2273	2481	64			

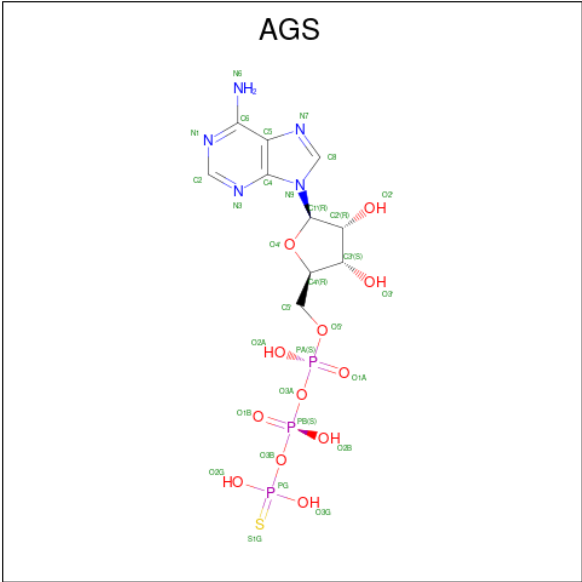
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	GLY	-	expression tag	UNP G0S0B9
A	470	ALA	-	expression tag	UNP G0S0B9
A	471	GLU	-	expression tag	UNP G0S0B9
A	472	PHE	-	expression tag	UNP G0S0B9

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

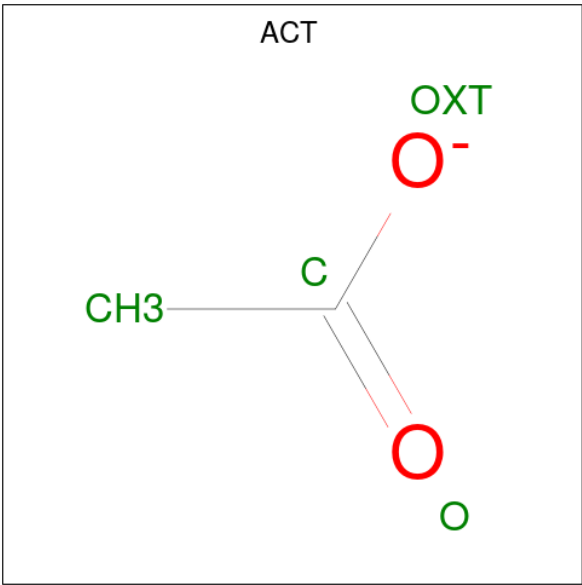
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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

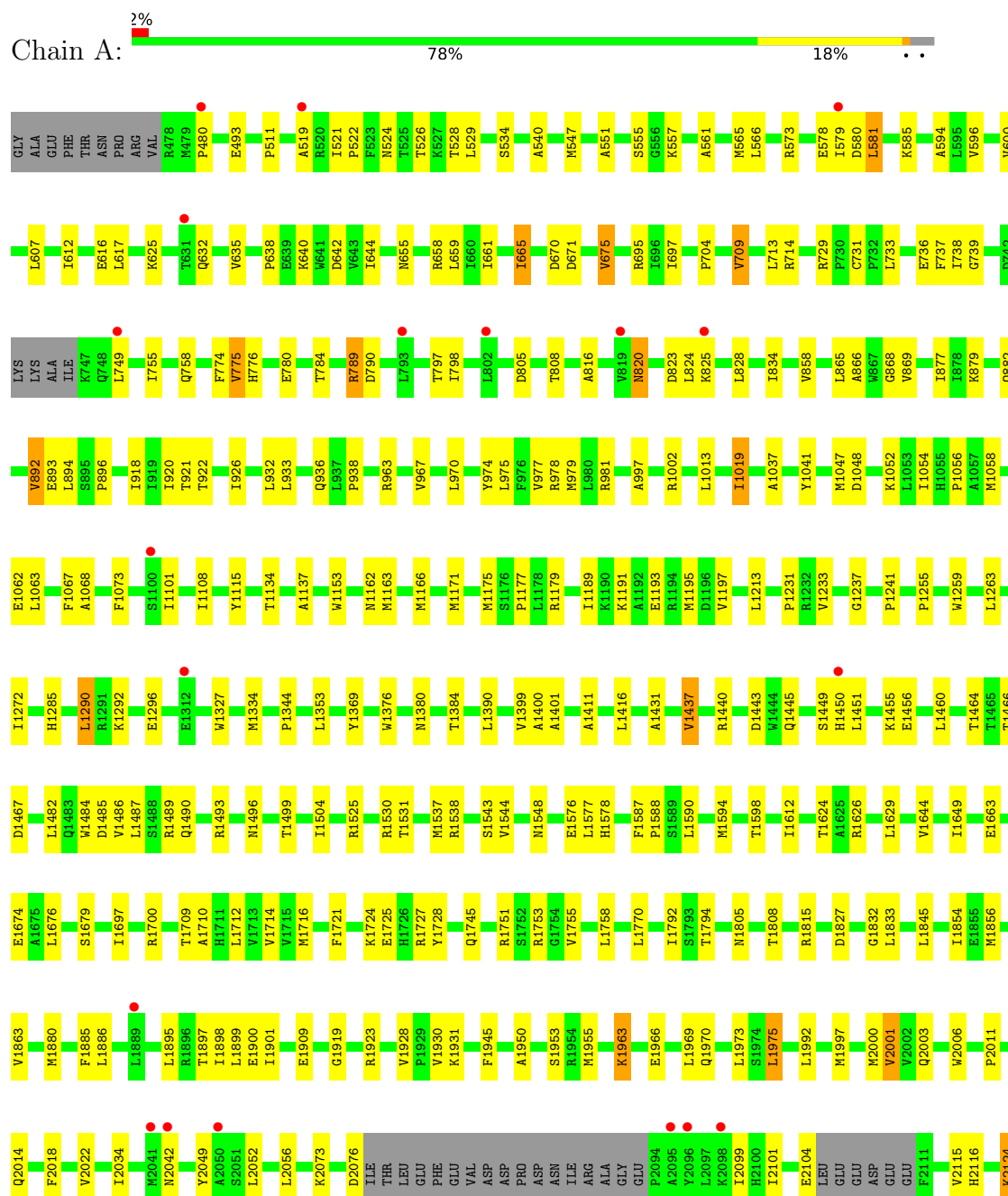
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		

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: Pre-mRNA splicing helicase-like protein



W2129	L2130	V2131	V2132	L2141	A2142	I2143	K2144	R2145	V2146	T2147	V2148	GLY	LYS	E2151	L2152	N2153	V2154	K2155	L2156	E2157	F2158	V2159	VAL	PRO	SER	PRO	GLY	LYS	HIS	ASP	LEU	LYS	LEU	F2171	L2172	N2173	S2174	D2175	S2176	Y2177	V2178	G2179	V2180	D2181	Q2182	D2183	PRO	SER	PHE	SER	VAL	ASN	VAL	ALA	GLU	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.82Å 124.82Å 127.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.53 – 2.80 44.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.53-2.80) 99.3 (44.53-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.209 , 0.260 0.212 , 0.262	Depositor DCC
R_{free} test set	3009 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.033 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, ACT, 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	0.12	0/13656	0.31	0/18520

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 [i](#)

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	13362	0	13423	173	0
2	A	3	0	0	0	0
3	A	93	0	36	1	0
4	A	8	0	6	0	0
5	A	40	0	0	0	0
All	All	13506	0	13465	174	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 (174) 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:1255:PRO:HG3	1:A:1290:LEU:HD11	1.61	0.81
1:A:1460:LEU:HD22	1:A:1467:ASP:HB2	1.64	0.78
1:A:1431:ALA:HB3	1:A:1437:VAL:HG12	1.70	0.74
1:A:1485:ASP:OD1	1:A:1525:ARG:NH2	2.22	0.72
1:A:2130:LEU:HD11	1:A:2146:VAL:HB	1.74	0.69
1:A:1578:HIS:HB2	1:A:1755:VAL:HG12	1.73	0.69
1:A:1530:ARG:HD3	1:A:1537:MET:HE2	1.77	0.66
1:A:2124:LYS:NZ	1:A:2175:ASP:OD2	2.29	0.65
1:A:1440:ARG:NH1	1:A:1443:ASP:OD2	2.29	0.65
1:A:816:ALA:O	1:A:820:ASN:ND2	2.29	0.65
1:A:1179:ARG:NH1	1:A:1193:GLU:OE1	2.30	0.64
1:A:1489:ARG:HB3	1:A:1794:THR:HG21	1.80	0.64
1:A:1037:ALA:HB2	1:A:1047:MET:HG3	1.81	0.63
1:A:1899:LEU:HG	1:A:1997:MET:HE1	1.79	0.63
1:A:581:LEU:HD13	1:A:632:GLN:HE21	1.64	0.62
1:A:784:THR:HG21	1:A:879:LYS:HE2	1.81	0.62
1:A:1709:THR:HG22	1:A:1745:GLN:HG3	1.83	0.61
1:A:2129:TRP:HB3	1:A:2143:ILE:HD11	1.82	0.60
1:A:573:ARG:HG2	1:A:579:ILE:H	1.67	0.59
1:A:2174:SER:H	1:A:2180:VAL:HG23	1.67	0.59
1:A:738:ILE:HD11	1:A:920:ILE:HG12	1.84	0.59
1:A:1068:ALA:O	1:A:1108:ILE:HD11	2.03	0.58
1:A:1197:VAL:HG11	1:A:1213:LEU:HD11	1.86	0.58
1:A:1058:MET:HG3	1:A:1062:GLU:HB2	1.84	0.58
1:A:1805:ASN:O	1:A:1808:THR:OG1	2.22	0.58
1:A:1590:LEU:HG	1:A:1594:MET:HE2	1.87	0.57
1:A:1792:ILE:HG21	1:A:1854:ILE:HD11	1.85	0.56
1:A:1598:THR:HG21	1:A:1716:MET:HE2	1.86	0.56
1:A:1950:ALA:HA	1:A:1955:MET:HE3	1.86	0.56
1:A:776:HIS:CE1	1:A:894:LEU:HD21	2.41	0.55
1:A:511:PRO:HD3	1:A:534:SER:HB2	1.88	0.55
1:A:661:ILE:HD13	1:A:697:ILE:HB	1.88	0.55
1:A:617:LEU:HD21	1:A:644:ILE:HG13	1.88	0.55
1:A:825:LYS:HE2	1:A:828:LEU:HD11	1.90	0.54
1:A:1455:LYS:HG3	1:A:1456:GLU:H	1.73	0.54
1:A:1624:THR:HG22	1:A:1697:ILE:HD13	1.89	0.54
1:A:729:ARG:HH22	1:A:733:LEU:HD13	1.73	0.53
1:A:1259:TRP:HZ3	1:A:1290:LEU:HD23	1.72	0.53
1:A:970:LEU:HD23	1:A:1002:ARG:HG2	1.91	0.53
1:A:877:ILE:HG12	1:A:918:ILE:HB	1.91	0.53
1:A:1450:HIS:O	1:A:1450:HIS:ND1	2.41	0.53
1:A:1390:LEU:HA	1:A:1538:ARG:HH22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1966:GLU:O	1:A:1970:GLN:HG2	2.08	0.52
1:A:1445:GLN:O	1:A:1449:SER:OG	2.20	0.52
1:A:1598:THR:HG22	1:A:1714:VAL:HG11	1.90	0.52
1:A:1827:ASP:HB3	1:A:1832:GLY:HA3	1.90	0.52
1:A:805:ASP:OD1	1:A:808:THR:OG1	2.26	0.51
1:A:1577:LEU:HD11	1:A:1770:LEU:HD13	1.92	0.51
1:A:1272:ILE:O	1:A:1285:HIS:HA	2.10	0.51
1:A:1380:ASN:O	1:A:1384:THR:HG23	2.11	0.51
1:A:521:ILE:O	1:A:524:ASN:ND2	2.44	0.51
1:A:2076:ASP:HB3	1:A:2104:GLU:HB3	1.92	0.50
1:A:1900:GLU:HG2	1:A:1945:PHE:CE1	2.47	0.50
1:A:561:ALA:O	1:A:565:MET:HG3	2.11	0.50
1:A:1612:ILE:HG13	1:A:1710:ALA:HB2	1.93	0.50
1:A:522:PRO:HG2	1:A:566:LEU:HD21	1.93	0.50
1:A:551:ALA:HB3	1:A:557:LYS:HD2	1.94	0.50
1:A:642:ASP:OD2	1:A:1041:TYR:OH	2.25	0.50
1:A:738:ILE:HD12	1:A:755:ILE:HG21	1.93	0.50
1:A:1231:PRO:HG2	1:A:1327:TRP:CD1	2.47	0.49
1:A:975:LEU:HD11	1:A:979:MET:HE3	1.94	0.49
1:A:493:GLU:HG2	1:A:738:ILE:HG22	1.94	0.49
1:A:1056:PRO:HG3	1:A:1153:TRP:CE2	2.47	0.49
1:A:659:LEU:HD21	1:A:697:ILE:HG12	1.94	0.49
1:A:579:ILE:HG12	1:A:580:ASP:H	1.76	0.49
1:A:1724:LYS:HE2	1:A:1909:GLU:HB3	1.95	0.49
1:A:997:ALA:O	1:A:1002:ARG:NH2	2.46	0.48
1:A:573:ARG:HD3	1:A:578:GLU:HG3	1.96	0.48
1:A:585:LYS:HG2	1:A:632:GLN:HA	1.96	0.48
1:A:709:VAL:HG12	1:A:974:TYR:CE1	2.49	0.48
1:A:511:PRO:HD2	1:A:529:LEU:HB2	1.94	0.48
1:A:1115:TYR:CG	1:A:1134:THR:HG21	2.49	0.48
1:A:2147:THR:HB	1:A:2148:VAL:HG22	1.96	0.48
1:A:2144:LYS:HD2	1:A:2154:VAL:HG11	1.95	0.48
1:A:739:GLY:HA3	1:A:926:ILE:HD11	1.96	0.47
1:A:2000:MET:HE3	1:A:2006:TRP:HA	1.95	0.47
1:A:2115:VAL:HG11	1:A:2176:SER:HB2	1.96	0.47
1:A:736:GLU:HB3	1:A:918:ILE:HG13	1.95	0.47
1:A:659:LEU:HG	1:A:695:ARG:HB3	1.96	0.47
1:A:1171:MET:HA	1:A:1175:MET:HE2	1.97	0.47
1:A:2042:ASN:HB2	1:A:2049:TYR:HB2	1.96	0.47
1:A:2129:TRP:HB2	1:A:2173:MET:HB2	1.96	0.47
1:A:1845:LEU:HD22	1:A:1863:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:ASN:O	1:A:1166:MET:HG3	2.14	0.46
3:A:2205:AGS:O3G	3:A:2205:AGS:O2B	2.33	0.46
1:A:1237:GLY:N	1:A:1334:MET:HE1	2.29	0.46
1:A:1496:ASN:HA	1:A:1499:THR:HG22	1.97	0.46
1:A:480:PRO:HG3	1:A:936:GLN:HG2	1.97	0.46
1:A:596:VAL:HG13	1:A:635:VAL:HG12	1.97	0.46
1:A:638:PRO:HB2	1:A:675:VAL:HG23	1.98	0.46
1:A:1067:PHE:HE1	1:A:1137:ALA:HA	1.81	0.46
1:A:1644:VAL:HB	1:A:1649:ILE:HD11	1.98	0.46
1:A:1895:LEU:O	1:A:1898:ILE:HG12	2.15	0.46
1:A:1058:MET:HE2	1:A:1062:GLU:HB3	1.98	0.45
1:A:1969:LEU:HD22	1:A:2001:VAL:HG23	1.98	0.45
1:A:774:PHE:CZ	1:A:866:ALA:HB2	2.52	0.45
1:A:896:PRO:HA	1:A:932:LEU:HD11	1.98	0.45
1:A:2052:LEU:O	1:A:2056:LEU:HG	2.16	0.45
1:A:1674:GLU:O	1:A:1963:LYS:NZ	2.48	0.45
1:A:2182:GLN:N	1:A:2182:GLN:OE1	2.50	0.45
1:A:921:THR:OG1	1:A:922:THR:N	2.49	0.45
1:A:978:ARG:HH21	1:A:981:ARG:HB2	1.82	0.45
1:A:1885:PHE:CE2	1:A:1975:LEU:HD12	2.52	0.45
1:A:1931:LYS:HE2	1:A:1931:LYS:HB3	1.81	0.45
1:A:789:ARG:NH1	1:A:790:ASP:OD1	2.50	0.44
1:A:1897:THR:O	1:A:1901:ILE:HG12	2.18	0.44
1:A:882:GLN:NE2	1:A:893:GLU:OE2	2.50	0.44
1:A:1400:ALA:HA	1:A:1543:SER:O	2.17	0.44
1:A:1626:ARG:HA	1:A:1626:ARG:HE	1.81	0.44
1:A:2011:PRO:HB2	1:A:2034:ILE:HG13	1.98	0.44
1:A:1576:GLU:HG3	1:A:1751:ARG:HD3	1.97	0.44
1:A:1712:LEU:HA	1:A:1753:ARG:O	2.17	0.44
1:A:581:LEU:H	1:A:581:LEU:HG	1.53	0.44
1:A:704:PRO:HG2	1:A:938:PRO:HA	1.98	0.44
1:A:1973:LEU:HD13	1:A:2124:LYS:HE3	1.99	0.44
1:A:519:ALA:HA	1:A:566:LEU:HD22	1.99	0.44
1:A:655:ASN:O	1:A:658:ARG:NH1	2.51	0.44
1:A:729:ARG:HG3	1:A:731:CYS:H	1.82	0.44
1:A:823:ASP:OD1	1:A:824:LEU:N	2.48	0.44
1:A:1390:LEU:HA	1:A:1538:ARG:NH2	2.32	0.44
1:A:1919:GLY:O	1:A:1923:ARG:N	2.38	0.44
1:A:977:VAL:O	1:A:981:ARG:HG2	2.17	0.44
1:A:1411:ALA:HB1	1:A:1504:ILE:HD13	2.00	0.44
1:A:526:THR:HG22	1:A:528:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ALA:HB1	1:A:566:LEU:HD13	2.01	0.43
1:A:1721:PHE:HB2	1:A:1728:TYR:CE1	2.53	0.43
1:A:1054:ILE:HG22	1:A:1153:TRP:HZ3	1.83	0.43
1:A:2003:GLN:HG3	1:A:2014:GLN:HE21	1.82	0.43
1:A:2022:VAL:HG13	1:A:2056:LEU:HD22	1.99	0.43
1:A:1048:ASP:OD2	1:A:1052:LYS:NZ	2.42	0.43
1:A:1369:TYR:CE2	1:A:1416:LEU:HB3	2.54	0.43
1:A:1401:ALA:O	1:A:1544:VAL:HA	2.19	0.43
1:A:1594:MET:O	1:A:1598:THR:HG23	2.18	0.43
1:A:1482:LEU:O	1:A:1486:VAL:HG23	2.20	0.42
1:A:607:LEU:HD13	1:A:612:ILE:HD11	2.00	0.42
1:A:775:VAL:HG11	1:A:780:GLU:HG3	2.01	0.42
1:A:737:PHE:CZ	1:A:933:LEU:HD12	2.55	0.42
1:A:892:VAL:HG12	1:A:893:GLU:H	1.84	0.42
1:A:1484:TRP:CE3	1:A:1487:LEU:HD11	2.54	0.42
1:A:665:ILE:H	1:A:665:ILE:HG13	1.57	0.42
1:A:1013:LEU:HB3	1:A:1019:ILE:HB	2.01	0.42
1:A:511:PRO:HD3	1:A:534:SER:CB	2.50	0.42
1:A:2099:ILE:HG12	1:A:2154:VAL:H	1.84	0.42
1:A:1490:GLN:HB3	1:A:1493:ARG:HG2	2.00	0.42
1:A:493:GLU:HA	1:A:738:ILE:HG22	2.01	0.42
1:A:1171:MET:HE1	1:A:1177:PRO:HA	2.02	0.41
1:A:1263:LEU:HD12	1:A:1327:TRP:HH2	1.85	0.41
1:A:1587:PHE:HB3	1:A:1588:PRO:HD3	2.02	0.41
1:A:1953:SER:HB2	1:A:1955:MET:HE2	2.02	0.41
1:A:967:VAL:HG22	1:A:1002:ARG:HB3	2.02	0.41
1:A:1241:PRO:HB2	1:A:1344:PRO:HD3	2.02	0.41
1:A:670:ASP:OD1	1:A:671:ASP:N	2.49	0.41
1:A:1063:LEU:HB3	1:A:1163:MET:HE1	2.03	0.41
1:A:1292:LYS:O	1:A:1296:GLU:HG2	2.19	0.41
1:A:1449:SER:HA	1:A:1455:LYS:HB3	2.01	0.41
1:A:1449:SER:HB3	1:A:1455:LYS:HD3	2.02	0.41
1:A:2073:LYS:HG3	1:A:2116:HIS:HB2	2.03	0.41
1:A:600:VAL:HG21	1:A:616:GLU:HB2	2.02	0.41
1:A:640:LYS:HD2	1:A:640:LYS:HA	1.88	0.41
1:A:1191:LYS:O	1:A:1195:MET:HG3	2.20	0.41
1:A:1548:ASN:HD22	1:A:1815:ARG:NH2	2.19	0.41
1:A:1073:PHE:CD2	1:A:1108:ILE:HD12	2.55	0.41
1:A:1856:MET:HB2	1:A:1863:VAL:HG12	2.02	0.41
1:A:2130:LEU:CD1	1:A:2146:VAL:HB	2.47	0.41
1:A:594:ALA:HB1	1:A:868:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:VAL:HG12	1:A:776:HIS:H	1.86	0.41
1:A:1101:ILE:HD12	1:A:1101:ILE:H	1.86	0.41
1:A:865:LEU:O	1:A:869:VAL:HG22	2.20	0.40
1:A:1451:LEU:HD23	1:A:1451:LEU:HA	1.81	0.40
1:A:2141:LEU:HD21	1:A:2158:PHE:HD1	1.87	0.40
1:A:1725:GLU:HB2	1:A:1727:ARG:HG2	2.04	0.40
1:A:540:ALA:HA	1:A:547:MET:HE1	2.03	0.40
1:A:1714:VAL:HG13	1:A:1755:VAL:HG23	2.02	0.40
1:A:625:LYS:HD2	1:A:644:ILE:HD11	2.02	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	1654/1725 (96%)	1606 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1473/1523 (97%)	1418 (96%)	55 (4%)	30	65

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	555	SER
1	A	581	LEU
1	A	665	ILE
1	A	675	VAL
1	A	709	VAL
1	A	713	LEU
1	A	714	ARG
1	A	749	LEU
1	A	758	GLN
1	A	775	VAL
1	A	789	ARG
1	A	797	THR
1	A	798	ILE
1	A	820	ASN
1	A	834	ILE
1	A	858	VAL
1	A	892	VAL
1	A	963	ARG
1	A	1019	ILE
1	A	1189	ILE
1	A	1233	VAL
1	A	1290	LEU
1	A	1353	LEU
1	A	1376	TRP
1	A	1399	VAL
1	A	1437	VAL
1	A	1464	THR
1	A	1466	THR
1	A	1531	THR
1	A	1629	LEU
1	A	1663	GLU
1	A	1676	LEU
1	A	1679	SER
1	A	1700	ARG
1	A	1758	LEU
1	A	1833	LEU
1	A	1880	MET
1	A	1886	LEU
1	A	1928	VAL
1	A	1930	VAL
1	A	1963	LYS
1	A	1975	LEU

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Mol	Chain	Res	Type
1	A	1992	LEU
1	A	2001	VAL
1	A	2018	PHE
1	A	2101	ILE
1	A	2124	LYS
1	A	2132	VAL
1	A	2141	LEU
1	A	2145	ARG
1	A	2147	THR
1	A	2148	VAL
1	A	2152	LEU
1	A	2156	LEU
1	A	2180	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	572	ASN
1	A	666	HIS
1	A	735	GLN
1	A	770	GLN
1	A	835	HIS
1	A	882	GLN
1	A	952	ASN
1	A	1258	GLN
1	A	1388	ASN
1	A	1392	ASN
1	A	1532	GLN

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

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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
3	AGS	A	2204	2	32,33,33	0.46	1 (3%)	45,52,52	0.60	1 (2%)
4	ACT	A	2207	-	3,3,3	1.38	0	3,3,3	1.36	0
3	AGS	A	2205	-	32,33,33	0.46	1 (3%)	45,52,52	0.64	1 (2%)
3	AGS	A	2206	2	32,33,33	0.50	1 (3%)	45,52,52	0.70	1 (2%)
4	ACT	A	2208	-	3,3,3	1.31	0	3,3,3	1.35	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
3	AGS	A	2204	2	-	2/21/38/38	0/3/3/3
3	AGS	A	2205	-	-	5/21/38/38	0/3/3/3
3	AGS	A	2206	2	-	8/21/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2204	AGS	PG-S1G	2.16	1.95	1.90
3	A	2206	AGS	PG-S1G	2.16	1.95	1.90
3	A	2205	AGS	PG-S1G	2.10	1.95	1.90

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2206	AGS	PB-O3B-PG	-3.65	119.82	133.17
3	A	2205	AGS	PB-O3B-PG	-3.30	121.10	133.17
3	A	2204	AGS	PB-O3B-PG	-2.98	122.25	133.17

There are no chirality outliers.

All (15) torsion outliers are listed below:

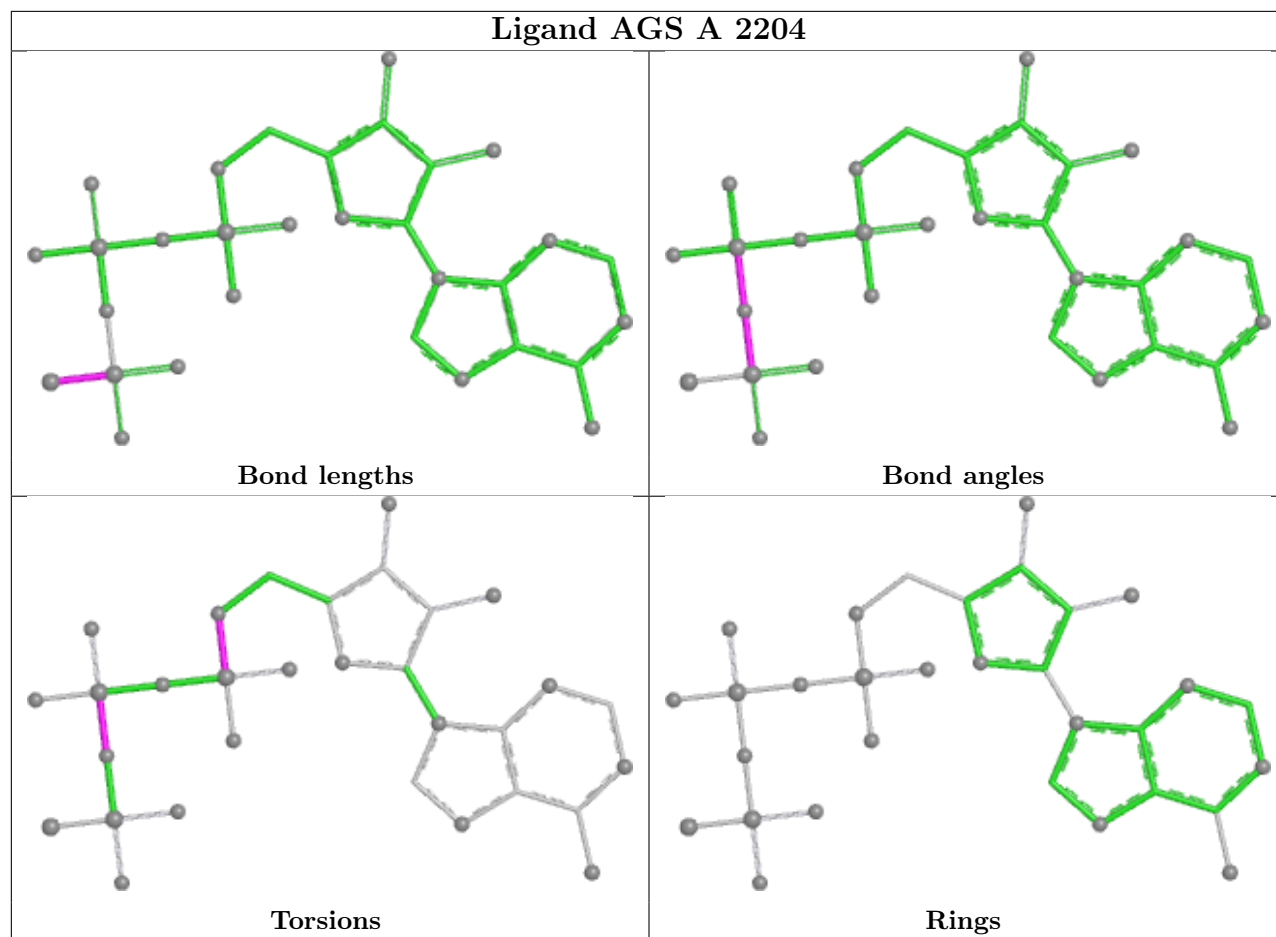
Mol	Chain	Res	Type	Atoms
3	A	2205	AGS	C5'-O5'-PA-O1A
3	A	2205	AGS	C5'-O5'-PA-O2A
3	A	2205	AGS	C5'-O5'-PA-O3A
3	A	2206	AGS	C5'-O5'-PA-O1A
3	A	2206	AGS	C5'-O5'-PA-O2A
3	A	2206	AGS	C5'-O5'-PA-O3A
3	A	2206	AGS	O4'-C4'-C5'-O5'
3	A	2205	AGS	PB-O3A-PA-O5'
3	A	2206	AGS	C2'-C1'-N9-C8
3	A	2204	AGS	C5'-O5'-PA-O3A
3	A	2205	AGS	PG-O3B-PB-O2B
3	A	2206	AGS	C3'-C4'-C5'-O5'
3	A	2204	AGS	PG-O3B-PB-O2B
3	A	2206	AGS	O4'-C1'-N9-C8
3	A	2206	AGS	PB-O3A-PA-O2A

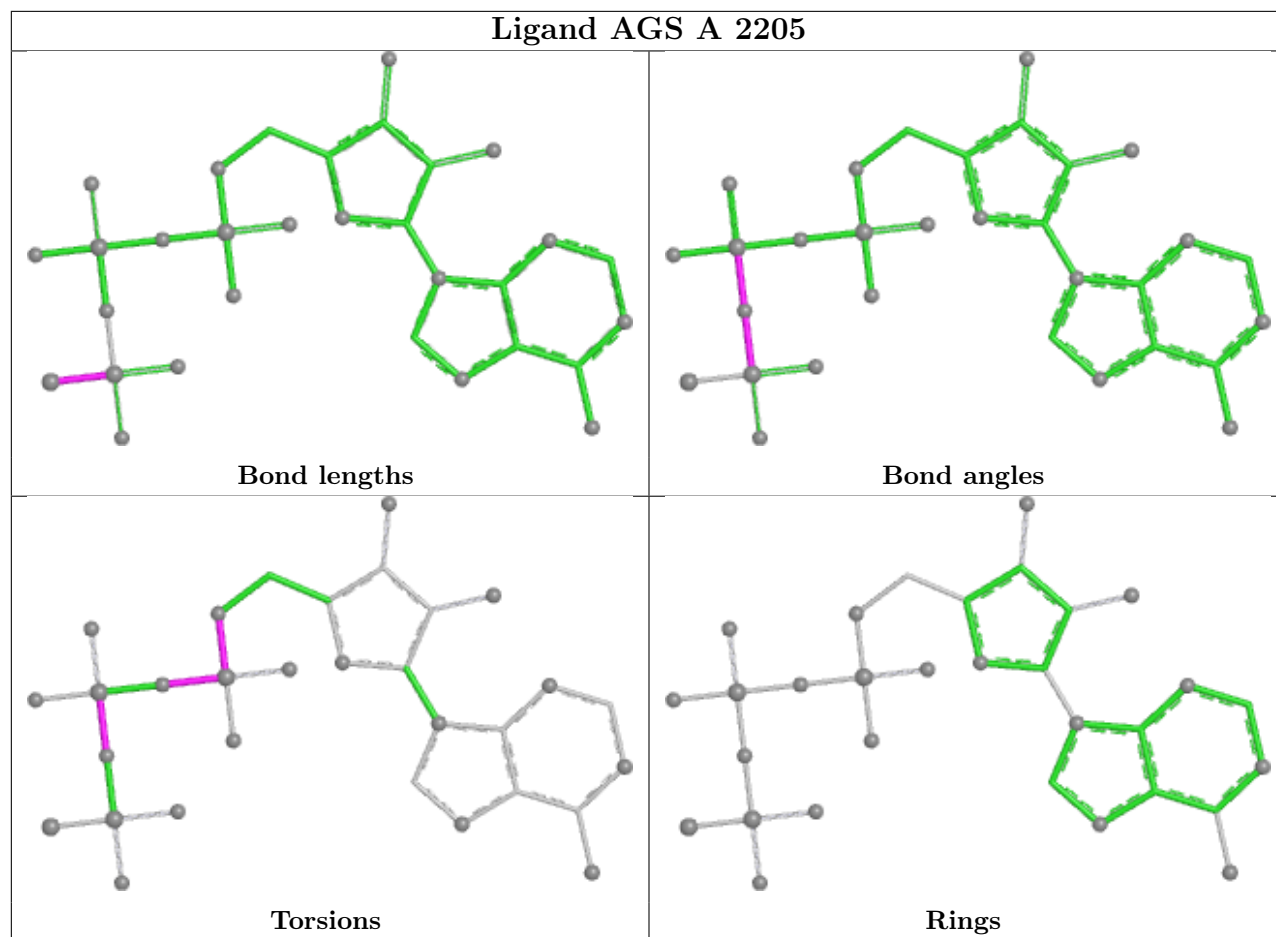
There are no ring outliers.

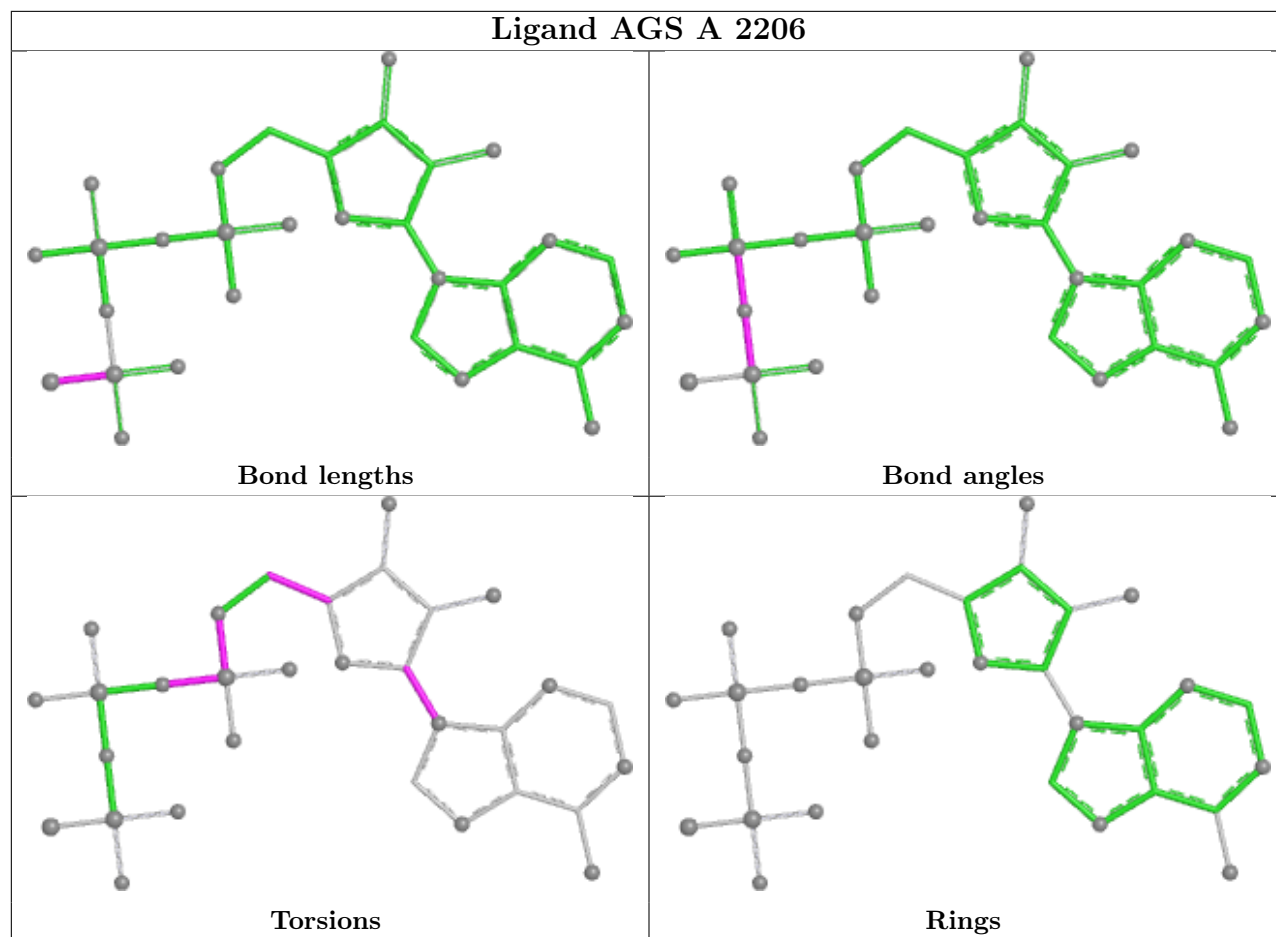
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2205	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 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	1666/1725 (96%)	-0.03	26 (1%) 70 61	41, 84, 158, 219	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	749	LEU	3.3
1	A	2172	LEU	3.2
1	A	2132	VAL	2.9
1	A	2158	PHE	2.9
1	A	519	ALA	2.4
1	A	2178	VAL	2.4
1	A	579	ILE	2.4
1	A	2148	VAL	2.4
1	A	2147	THR	2.4
1	A	1889	LEU	2.3
1	A	2042	ASN	2.3
1	A	2095	ALA	2.3
1	A	2096	TYR	2.3
1	A	631	THR	2.2
1	A	2180	VAL	2.2
1	A	2041	MET	2.2
1	A	1100	SER	2.2
1	A	2098	LYS	2.2
1	A	480	PRO	2.2
1	A	819	VAL	2.2
1	A	1450	HIS	2.1
1	A	825	LYS	2.1
1	A	1312	GLU	2.1
1	A	793	LEU	2.0
1	A	2050	ALA	2.0
1	A	802	LEU	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](#)

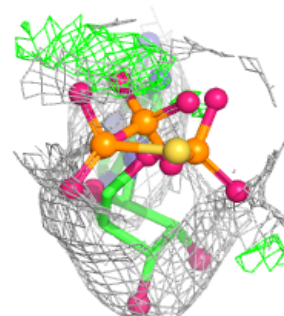
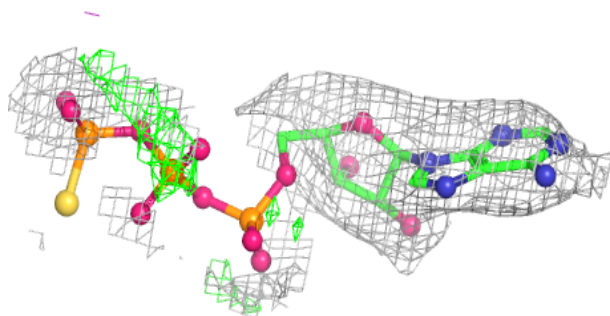
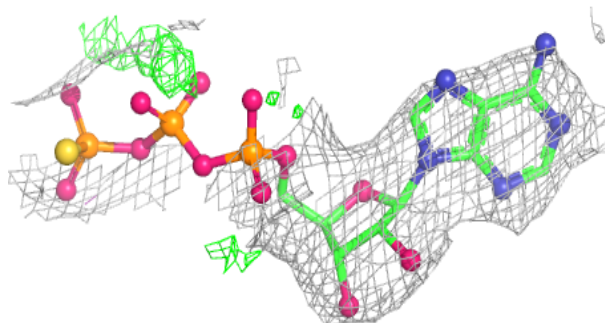
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	2208	4/4	0.63	0.20	80,91,98,112	0
4	ACT	A	2207	4/4	0.70	0.21	112,113,113,113	0
3	AGS	A	2204	31/31	0.83	0.10	114,125,153,161	0
3	AGS	A	2206	31/31	0.91	0.09	51,69,107,124	0
3	AGS	A	2205	31/31	0.94	0.07	42,66,85,109	0
2	MN	A	2203	1/1	0.94	0.07	106,106,106,106	0
2	MN	A	2201	1/1	0.96	0.05	108,108,108,108	0
2	MN	A	2202	1/1	0.97	0.05	113,113,113,113	0

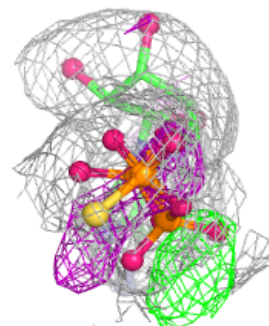
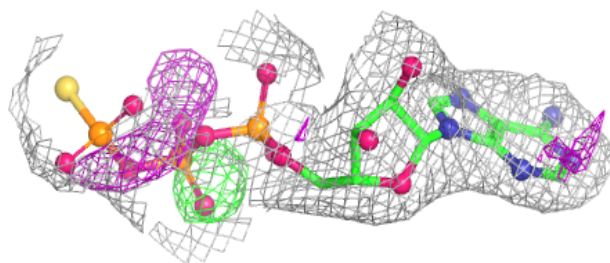
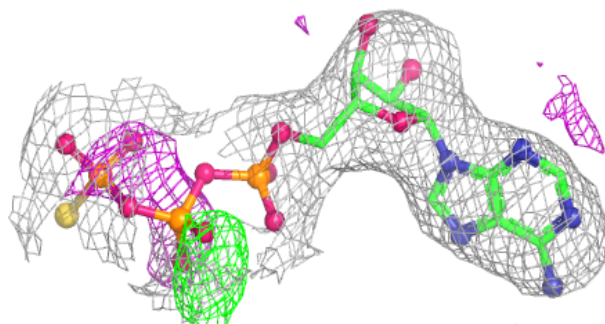
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS A 2204:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

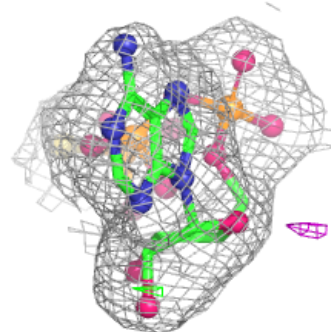
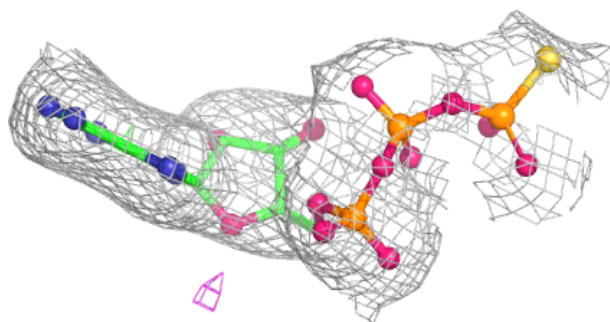
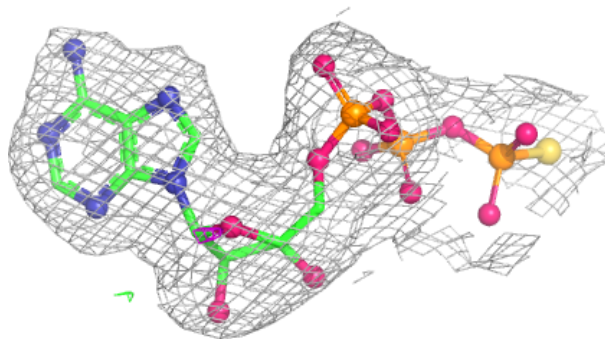
**Electron density around AGS A 2206:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AGS A 2205:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.