



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:13 PM UTC

PDB ID : 6Z4X / pdb_00006z4x
Title : Structure of the CAK complex form Chaetomium thermophilum bound to ATP-gamma-S
Authors : Peissert, S.; Kuper, J.; Kisker, C.
Deposited on : 2020-05-26
Resolution : 2.98 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

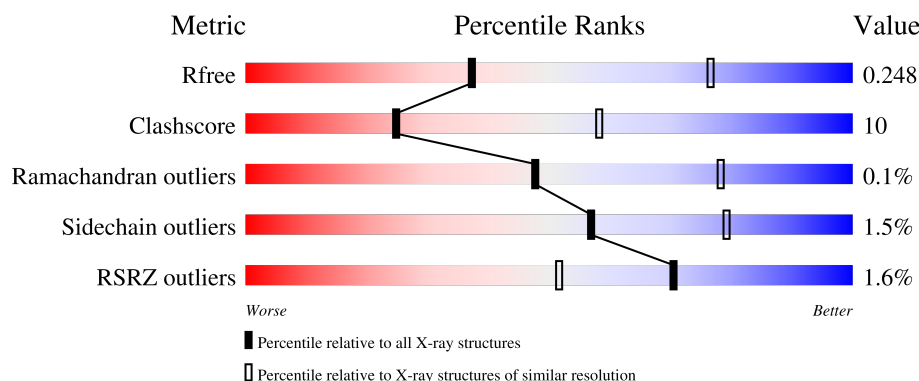
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	425	
1	D	425	
2	B	437	
2	E	437	
3	C	69	

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Mol	Chain	Length	Quality of chain
3	F	69	% 74% 22% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11470 atoms, of which 28 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 CYCLIN domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2522	1599	449	463	11			
1	D	314	Total	C	N	O	S	0	0	0
			2533	1605	451	466	11			

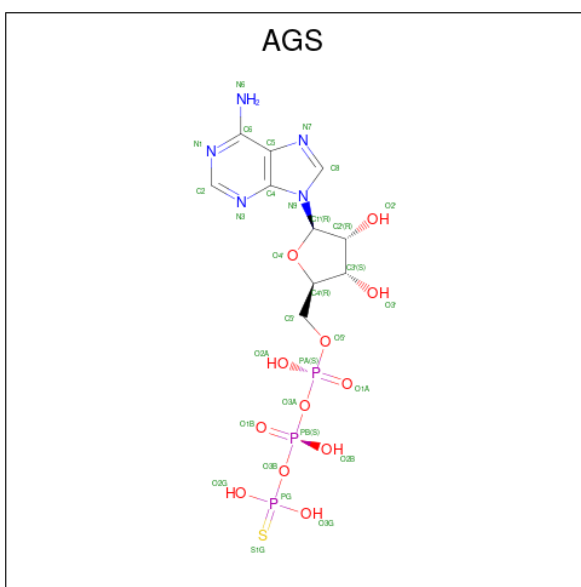
- Molecule 2 is a protein called Protein kinase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2613	1678	462	460	13			
2	E	323	Total	C	N	O	S	0	0	0
			2620	1682	463	462	13			

- Molecule 3 is a protein called RING-type domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	66	Total	C	N	O	S	0	0	0
			538	344	90	102	2			
3	F	67	Total	C	N	O	S	0	0	0
			550	353	91	104	2			

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	S	0	0
			45	10	14	5	12	3	1		
4	E	1	Total	C	H	N	O	P	S	0	0
			45	10	14	5	12	3	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

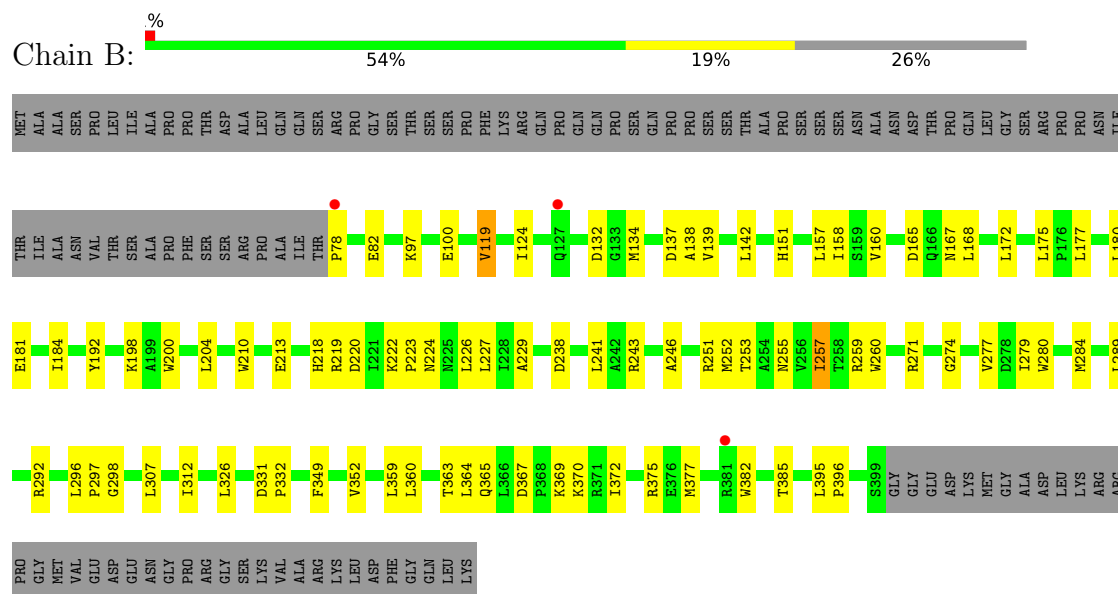
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

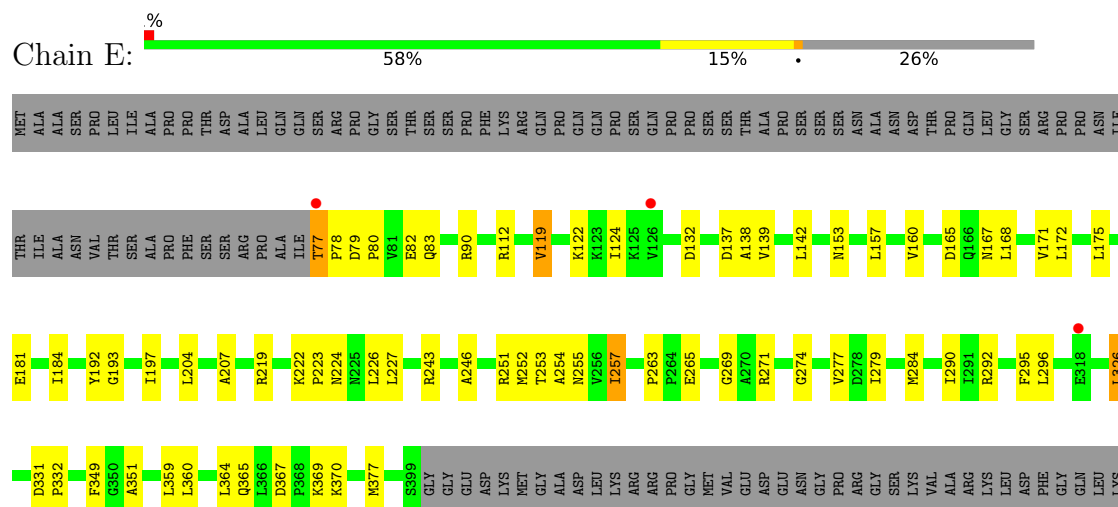
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		

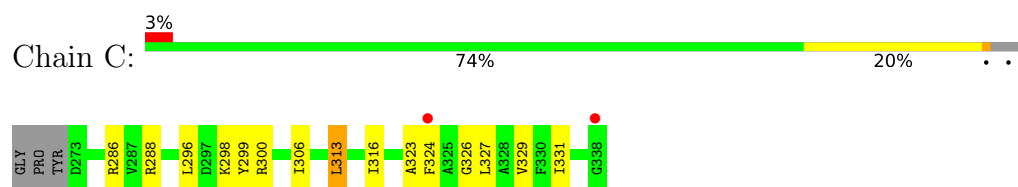
- Molecule 2: Protein kinase domain-containing protein



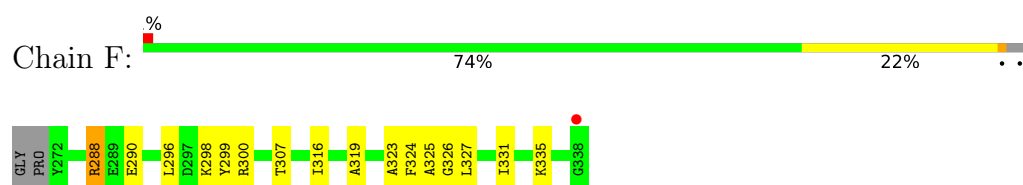
- Molecule 2: Protein kinase domain-containing protein



- Molecule 3: RING-type domain-containing protein



- Molecule 3: RING-type domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.97Å 84.90Å 154.48Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	46.65 – 2.98 46.65 – 2.98	Depositor EDS
% Data completeness (in resolution range)	61.1 (46.65-2.98) 61.1 (46.65-2.98)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.96Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.18rc4_3812	Depositor
R, R_{free}	0.203 , 0.246 0.208 , 0.248	Depositor DCC
R_{free} test set	1469 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11470	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: AGS, CL, MG

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	0/2574	0.30	0/3471
1	D	0.13	0/2585	0.32	0/3486
2	B	0.11	0/2684	0.30	0/3635
2	E	0.12	0/2691	0.32	0/3646
3	C	0.09	0/552	0.26	0/742
3	F	0.10	0/565	0.27	0/760
All	All	0.12	0/11651	0.31	0/15740

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	2522	0	2517	59	0
1	D	2533	0	2527	61	0
2	B	2613	0	2624	56	0
2	E	2620	0	2630	47	0
3	C	538	0	502	12	0
3	F	550	0	511	14	0
4	B	31	14	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	31	14	12	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
All	All	11442	28	11335	224	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 10.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:253:THR:HG22	2:E:255:ASN:H	1.28	0.96
2:B:253:THR:HG22	2:B:255:ASN:H	1.34	0.92
2:E:246:ALA:HB2	2:E:252:MET:HE3	1.55	0.88
1:A:381:ARG:HD3	1:A:385:ASP:HA	1.56	0.86
3:C:313:LEU:HD22	3:C:313:LEU:H	1.48	0.77
1:A:375:ARG:NH2	2:B:82:GLU:OE2	2.19	0.76
2:E:90:ARG:O	2:E:112:ARG:NH2	2.18	0.76
1:D:191:ALA:HB1	3:F:323:ALA:HA	1.68	0.74
2:B:243:ARG:HD3	2:B:252:MET:HE2	1.70	0.74
1:D:120:ARG:HA	1:D:123:ILE:HG22	1.73	0.69
2:E:367:ASP:HB3	2:E:370:LYS:HG2	1.75	0.69
2:E:279:ILE:HG13	2:E:377:MET:HE1	1.76	0.68
1:A:223:PHE:HB2	1:A:337:ARG:NH1	2.09	0.68
1:A:191:ALA:HB1	3:C:323:ALA:HA	1.74	0.68
1:D:210:LEU:HD23	1:D:251:LEU:HD13	1.76	0.68
1:A:82:THR:HG22	1:A:84:ALA:H	1.59	0.67
2:B:251:ARG:HH21	2:B:271:ARG:HG3	1.59	0.67
1:A:372:GLN:HG2	1:A:376:ARG:NH1	2.10	0.66
1:A:210:LEU:HD23	1:A:251:LEU:HD13	1.77	0.66
1:A:82:THR:HG23	1:A:83:PRO:HD2	1.78	0.66
1:A:120:ARG:HA	1:A:123:ILE:HG22	1.77	0.66
1:A:381:ARG:HD3	1:A:385:ASP:CA	2.26	0.65
2:B:365:GLN:OE1	2:B:370:LYS:NZ	2.29	0.65
1:A:91:THR:HG23	1:A:227:ILE:HG23	1.78	0.65
1:D:259:THR:HG21	3:F:324:PHE:HE1	1.62	0.65
2:B:279:ILE:HG13	2:B:377:MET:HE1	1.79	0.64
1:D:224:SER:O	1:D:228:THR:HG22	1.97	0.64
1:D:22:SER:O	3:F:335:LYS:HE3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:204:LEU:HD13	2:E:226:LEU:HD21	1.80	0.63
1:A:97:LEU:HB2	1:A:136:LEU:HG	1.81	0.63
1:D:91:THR:HG23	1:D:227:ILE:HG23	1.81	0.63
1:A:318:VAL:O	1:A:322:ILE:HG12	1.99	0.62
1:D:130:TYR:OH	1:D:365:ARG:NH2	2.32	0.62
2:B:284:MET:HE2	2:B:364:LEU:HD22	1.82	0.62
2:B:359:LEU:HD11	2:B:377:MET:HG3	1.81	0.61
2:E:246:ALA:CB	2:E:252:MET:HE3	2.28	0.61
3:C:296:LEU:O	3:C:300:ARG:HG3	1.99	0.61
2:B:246:ALA:HB2	2:B:252:MET:HE3	1.83	0.61
1:D:381:ARG:HD3	1:D:385:ASP:HA	1.83	0.60
1:D:152:SER:HA	2:E:132:ASP:OD2	2.01	0.60
2:B:142:LEU:HD11	2:B:160:VAL:HG11	1.84	0.60
2:E:165:ASP:OD2	2:E:167:ASN:ND2	2.33	0.60
2:B:222:LYS:HE3	2:B:224:ASN:HD21	1.67	0.60
2:B:218:HIS:NE2	2:B:238:ASP:O	2.35	0.59
2:E:243:ARG:HD3	2:E:252:MET:HE2	1.86	0.58
1:A:233:HIS:C	3:C:331:ILE:HD12	2.28	0.57
1:D:235:THR:HG21	3:F:326:GLY:HA3	1.85	0.57
2:E:253:THR:HG22	2:E:255:ASN:N	2.10	0.57
1:D:183:LEU:HD23	2:E:139:VAL:HG13	1.86	0.57
1:D:325:CYS:O	1:D:329:LEU:HD13	2.05	0.56
1:D:216:ARG:O	1:D:220:ILE:HG13	2.06	0.56
2:B:157:LEU:HA	2:B:172:LEU:HD23	1.87	0.56
2:B:274:GLY:O	2:B:277:VAL:HG22	2.05	0.56
2:E:359:LEU:HD11	2:E:377:MET:HG3	1.86	0.56
1:D:120:ARG:O	1:D:123:ILE:HG22	2.06	0.55
2:B:124:ILE:HD12	2:B:168:LEU:HD23	1.88	0.55
2:E:77:THR:N	2:E:78:PRO:HD3	2.22	0.55
1:A:216:ARG:O	1:A:220:ILE:HG13	2.06	0.55
1:A:120:ARG:O	1:A:123:ILE:HG22	2.07	0.55
3:F:296:LEU:O	3:F:300:ARG:HG3	2.07	0.55
2:B:365:GLN:HB3	2:B:370:LYS:HG3	1.90	0.54
1:D:97:LEU:HB2	1:D:136:LEU:HG	1.89	0.54
2:B:367:ASP:HB3	2:B:370:LYS:HG2	1.90	0.54
1:A:246:LEU:HG	1:A:326:ARG:HG3	1.90	0.54
1:D:207:PRO:O	1:D:211:VAL:HG23	2.08	0.54
1:A:135:MET:HE2	1:A:368:LEU:HD11	1.91	0.53
2:B:97:LYS:HE2	2:B:100:GLU:HG2	1.90	0.53
1:D:8:GLU:HB2	3:F:325:ALA:HA	1.89	0.53
1:A:163:GLU:CD	1:A:163:GLU:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ASP:OD1	1:D:204:ASP:N	2.42	0.53
1:A:325:CYS:O	1:A:329:LEU:HD13	2.09	0.53
2:B:198:LYS:NZ	2:B:385:THR:O	2.42	0.53
2:B:213:GLU:OE1	2:B:375:ARG:NH2	2.42	0.53
2:B:219:ARG:C	2:B:257:ILE:HG12	2.34	0.53
1:A:207:PRO:O	1:A:211:VAL:HG23	2.08	0.53
1:A:183:LEU:HD23	2:B:139:VAL:HG13	1.90	0.52
1:A:342:ASN:HD22	1:A:345:VAL:HG23	1.72	0.52
1:A:342:ASN:ND2	1:A:345:VAL:HG23	2.25	0.52
2:B:165:ASP:OD2	2:B:167:ASN:ND2	2.39	0.52
1:D:10:ALA:O	1:D:14:GLN:HG3	2.10	0.52
1:D:163:GLU:H	1:D:163:GLU:CD	2.17	0.51
1:D:164:ARG:HB2	1:D:167:GLU:OE1	2.10	0.51
1:D:372:GLN:HG2	1:D:376:ARG:HH21	1.75	0.51
2:E:157:LEU:HA	2:E:172:LEU:HD23	1.92	0.51
1:A:86:GLU:O	1:A:90:VAL:HG23	2.11	0.51
2:B:260:TRP:CD1	2:B:297:PRO:HA	2.46	0.51
1:D:97:LEU:C	1:D:97:LEU:HD23	2.36	0.51
1:A:206:GLU:HG3	1:A:207:PRO:HD2	1.94	0.50
1:D:81:LEU:HD23	1:D:356:LYS:HD3	1.92	0.50
1:D:196:ILE:HG21	1:D:214:GLU:OE2	2.12	0.50
2:E:331:ASP:OD1	2:E:332:PRO:HD2	2.11	0.50
1:A:235:THR:HG21	3:C:326:GLY:HA3	1.93	0.50
3:F:298:LYS:HE2	3:F:299:TYR:CE2	2.46	0.50
1:A:130:TYR:CE1	1:A:174:LEU:HD21	2.47	0.50
2:E:142:LEU:HD11	2:E:160:VAL:HG11	1.94	0.50
1:D:370:GLU:OE2	1:D:373:ARG:NH2	2.45	0.50
1:A:234:PHE:N	3:C:331:ILE:HD12	2.27	0.49
1:D:120:ARG:HA	1:D:123:ILE:CG2	2.41	0.49
2:E:222:LYS:HE3	2:E:224:ASN:HD21	1.77	0.49
1:A:224:SER:HB2	1:A:225:PRO:HD3	1.94	0.49
1:D:120:ARG:CA	1:D:123:ILE:HG22	2.42	0.49
1:D:202:LEU:HD23	1:D:254:ARG:CZ	2.43	0.49
1:A:249:ARG:HD3	1:A:253:GLU:OE2	2.12	0.49
2:B:181:GLU:HB2	2:B:223:PRO:HB2	1.94	0.49
2:B:204:LEU:HD13	2:B:226:LEU:HD21	1.93	0.49
1:A:19:GLU:HG3	1:A:20:LEU:HD13	1.95	0.49
1:D:381:ARG:HD3	1:D:384:PHE:C	2.38	0.49
2:B:372:ILE:HG23	2:B:377:MET:HE2	1.94	0.48
1:A:259:THR:HG21	3:C:324:PHE:HE2	1.77	0.48
1:D:122:TYR:CE1	1:D:127:ILE:HD13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLU:HG3	1:D:20:LEU:HD13	1.94	0.48
2:E:219:ARG:C	2:E:257:ILE:HG12	2.39	0.48
2:B:296:LEU:HD22	2:B:307:LEU:HB3	1.95	0.48
2:E:181:GLU:HB2	2:E:223:PRO:HB2	1.96	0.48
1:A:120:ARG:CA	1:A:123:ILE:HG22	2.43	0.47
1:A:120:ARG:HA	1:A:123:ILE:CG2	2.42	0.47
2:B:251:ARG:NH2	2:B:271:ARG:HG3	2.28	0.47
2:E:153:ASN:HB3	2:E:207:ALA:HB2	1.96	0.47
1:A:131:PRO:HB3	1:A:366:TRP:CE2	2.49	0.47
2:E:192:TYR:OH	2:E:292:ARG:HG2	2.14	0.47
2:E:274:GLY:O	2:E:277:VAL:HG22	2.14	0.47
2:E:80:PRO:HA	2:E:83:GLN:HG2	1.97	0.47
1:A:204:ASP:OD1	1:A:204:ASP:N	2.42	0.47
3:C:298:LYS:HE2	3:C:299:TYR:CE2	2.50	0.47
1:D:224:SER:HB2	1:D:225:PRO:HD3	1.98	0.46
1:D:381:ARG:HD3	1:D:385:ASP:CA	2.45	0.46
2:E:122:LYS:HE2	4:E:501:AGS:O1A	2.14	0.46
1:D:115:ALA:O	1:D:119:LYS:HG3	2.16	0.46
1:D:233:HIS:C	3:F:331:ILE:HD12	2.41	0.46
1:A:223:PHE:CE1	1:A:337:ARG:HG2	2.50	0.46
2:B:175:LEU:HD12	2:B:227:LEU:HD12	1.97	0.46
1:D:145:LYS:HG2	1:D:150:PHE:CD1	2.51	0.46
2:E:137:ASP:OD1	2:E:138:ALA:N	2.48	0.46
1:A:197:MET:HE1	3:C:316:ILE:HG23	1.97	0.46
2:B:259:ARG:HD2	2:B:298:GLY:O	2.16	0.46
1:D:332:GLU:OE2	1:D:336:ARG:NE	2.29	0.45
3:F:288:ARG:HG3	3:F:290:GLU:HG2	1.98	0.45
1:D:135:MET:HE1	1:D:174:LEU:HD23	1.98	0.45
2:E:284:MET:HE2	2:E:364:LEU:HD22	1.97	0.45
1:D:318:VAL:O	1:D:322:ILE:HG12	2.17	0.45
1:A:44:THR:O	1:A:48:LEU:HD22	2.17	0.45
1:A:152:SER:HA	2:B:132:ASP:OD2	2.16	0.45
2:E:251:ARG:HH12	2:E:271:ARG:HH11	1.64	0.45
1:A:110:ILE:HG12	1:A:147:GLU:HB2	1.99	0.45
2:B:246:ALA:CB	2:B:252:MET:HE3	2.46	0.45
2:B:192:TYR:HB3	2:B:396:PRO:HG2	1.98	0.44
1:D:86:GLU:O	1:D:90:VAL:HG23	2.17	0.44
2:B:151:HIS:HB2	2:B:210:TRP:CD1	2.52	0.44
1:A:164:ARG:HB2	1:A:167:GLU:OE1	2.17	0.44
1:D:255:LEU:O	1:D:259:THR:HG23	2.18	0.44
2:E:365:GLN:OE1	2:E:370:LYS:NZ	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ASP:OD1	2:B:138:ALA:N	2.49	0.44
2:B:184:ILE:HD11	2:B:289:LEU:HD23	1.99	0.44
2:B:220:ASP:HB2	2:B:241:LEU:HD12	1.99	0.44
2:B:331:ASP:OD1	2:B:332:PRO:HD2	2.17	0.44
2:B:369:LYS:HD3	3:C:306:ILE:O	2.18	0.44
2:B:359:LEU:HD11	2:B:377:MET:CG	2.48	0.44
1:D:130:TYR:CE1	1:D:174:LEU:HD21	2.53	0.44
2:E:90:ARG:C	2:E:112:ARG:HH22	2.26	0.44
2:E:263:PRO:HG3	2:E:277:VAL:HA	1.99	0.44
2:B:280:TRP:CH2	2:B:312:ILE:HD13	2.53	0.43
2:E:124:ILE:HD12	2:E:168:LEU:HD23	2.01	0.43
2:E:349:PHE:O	2:E:351:ALA:N	2.52	0.43
1:D:223:PHE:CE1	1:D:337:ARG:HG2	2.54	0.43
1:D:223:PHE:CZ	1:D:227:ILE:HG13	2.53	0.43
1:D:246:LEU:HG	1:D:326:ARG:HG3	2.01	0.43
1:D:259:THR:HG21	3:F:324:PHE:CE1	2.49	0.43
1:D:155:ASP:O	1:D:159:THR:HG23	2.19	0.43
2:E:254:ALA:HB1	2:E:269:GLY:HA2	2.00	0.43
2:E:326:LEU:HD11	3:F:307:THR:HG23	2.01	0.43
2:E:119:VAL:HG11	2:E:171:VAL:HG13	2.01	0.43
1:A:48:LEU:HD13	1:A:48:LEU:N	2.34	0.43
2:E:193:GLY:O	2:E:197:ILE:HG13	2.19	0.43
1:A:97:LEU:C	1:A:97:LEU:HD23	2.44	0.42
1:A:40:ARG:HG3	1:A:80:PHE:CG	2.55	0.42
1:A:120:ARG:C	1:A:123:ILE:HG22	2.44	0.42
2:B:198:LYS:HA	2:B:382:TRP:CH2	2.54	0.42
1:D:110:ILE:HG12	1:D:147:GLU:HB2	2.01	0.42
1:D:120:ARG:C	1:D:123:ILE:HG22	2.44	0.42
1:A:10:ALA:O	1:A:14:GLN:HG3	2.20	0.42
1:D:190:ARG:HG2	3:F:319:ALA:HA	2.02	0.42
2:B:180:LEU:HD12	2:B:180:LEU:HA	1.79	0.42
2:B:119:VAL:CG2	2:B:158:ILE:HD12	2.50	0.42
1:A:12:TYR:CE1	1:A:236:PRO:HD2	2.55	0.42
2:B:177:LEU:HD12	2:B:229:ALA:O	2.20	0.42
2:B:192:TYR:OH	2:B:292:ARG:HG2	2.20	0.42
1:A:28:LEU:HD21	1:A:32:ARG:CZ	2.49	0.42
2:B:349:PHE:O	2:B:352:VAL:HG22	2.20	0.42
2:E:175:LEU:HD13	2:E:227:LEU:HB2	2.01	0.42
2:B:184:ILE:HD11	2:B:289:LEU:CD2	2.50	0.42
2:E:290:ILE:HG21	2:E:349:PHE:HA	2.02	0.42
2:E:79:ASP:HB3	2:E:82:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:MET:HE3	2:B:134:MET:HB2	1.86	0.41
2:E:367:ASP:HB3	2:E:370:LYS:HE3	2.02	0.41
1:A:42:ARG:HD3	2:B:78:PRO:O	2.20	0.41
1:A:371:LEU:O	1:A:374:ILE:HG12	2.20	0.41
1:A:145:LYS:NZ	1:A:172:GLU:OE1	2.48	0.41
1:D:252:ALA:O	1:D:256:ILE:HG13	2.20	0.41
2:B:363:THR:HG22	2:B:377:MET:HE2	2.03	0.41
2:E:367:ASP:OD2	2:E:369:LYS:HE3	2.21	0.41
1:D:28:LEU:HD23	1:D:28:LEU:O	2.21	0.41
1:A:43:ILE:O	1:A:47:LEU:HG	2.20	0.41
1:A:330:SER:HA	1:A:333:LEU:HD21	2.03	0.41
2:B:119:VAL:HG22	2:B:172:LEU:O	2.20	0.41
1:D:382:LYS:HB2	1:D:384:PHE:CE2	2.56	0.41
2:E:263:PRO:HB2	2:E:265:GLU:OE2	2.20	0.41
1:A:223:PHE:CZ	1:A:227:ILE:HG13	2.55	0.41
1:D:136:LEU:HD23	1:D:136:LEU:C	2.45	0.41
2:E:251:ARG:NH2	2:E:271:ARG:HG3	2.36	0.41
2:E:295:PHE:O	2:E:296:LEU:HD23	2.21	0.41
1:A:82:THR:CG2	1:A:83:PRO:HD2	2.47	0.41
2:B:175:LEU:HD13	2:B:227:LEU:HB2	2.03	0.41
2:B:280:TRP:CZ2	2:B:284:MET:HE3	2.56	0.41
1:D:113:THR:HG23	1:D:185:VAL:HG11	2.02	0.41
1:A:255:LEU:O	1:A:259:THR:HG23	2.21	0.40
1:D:223:PHE:HB2	1:D:337:ARG:NH2	2.36	0.40
1:D:330:SER:HA	1:D:333:LEU:HD21	2.03	0.40
1:A:238:GLN:NE2	3:C:329:VAL:O	2.47	0.40
2:B:200:TRP:HE1	2:B:395:LEU:HD13	1.86	0.40
3:C:286:ARG:H	3:C:286:ARG:HD3	1.87	0.40
1:D:197:MET:HE1	3:F:316:ILE:HG23	2.03	0.40
1:D:234:PHE:N	3:F:331:ILE:HD12	2.37	0.40
2:E:184:ILE:HG23	2:E:292:ARG:HA	2.03	0.40
2:E:365:GLN:HB3	2:E:370:LYS:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/425 (72%)	297 (97%)	9 (3%)	0	100	100
1	D	308/425 (72%)	298 (97%)	10 (3%)	0	100	100
2	B	320/437 (73%)	311 (97%)	8 (2%)	1 (0%)	36	67
2	E	321/437 (74%)	312 (97%)	8 (2%)	1 (0%)	36	67
3	C	64/69 (93%)	64 (100%)	0	0	100	100
3	F	65/69 (94%)	65 (100%)	0	0	100	100
All	All	1384/1862 (74%)	1347 (97%)	35 (2%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	257	ILE
2	E	257	ILE

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	267/354 (75%)	264 (99%)	3 (1%)	65	82
1	D	268/354 (76%)	265 (99%)	3 (1%)	65	82
2	B	275/370 (74%)	272 (99%)	3 (1%)	65	82
2	E	276/370 (75%)	272 (99%)	4 (1%)	59	80
3	C	55/57 (96%)	52 (94%)	3 (6%)	19	51
3	F	56/57 (98%)	54 (96%)	2 (4%)	31	63
All	All	1197/1562 (77%)	1179 (98%)	18 (2%)	57	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	48	LEU
1	A	371	LEU
2	B	119	VAL
2	B	326	LEU
2	B	360	LEU
3	C	288	ARG
3	C	313	LEU
3	C	327	LEU
1	D	23	PHE
1	D	185	VAL
1	D	371	LEU
2	E	77	THR
2	E	119	VAL
2	E	326	LEU
2	E	360	LEU
3	F	288	ARG
3	F	327	LEU

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	177	GLN
1	A	215	GLN
1	A	257	GLN
2	B	85	ASN
2	B	116	ASN
2	B	166	GLN
2	B	169	ASN
1	D	215	GLN
2	E	105	ASN
2	E	116	ASN
2	E	166	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
4	AGS	E	501	-	32,33,33	2.09	8 (25%)	45,52,52	2.02	12 (26%)
4	AGS	B	501	5	32,33,33	2.08	7 (21%)	45,52,52	1.93	11 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	E	501	-	-	5/21/38/38	0/3/3/3
4	AGS	B	501	5	-	6/21/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	AGS	PG-S1G	8.12	2.08	1.90
4	E	501	AGS	PG-S1G	8.01	2.08	1.90
4	B	501	AGS	C5-C4	4.75	1.47	1.39
4	E	501	AGS	C5-C4	4.70	1.47	1.39
4	E	501	AGS	PA-O3A	2.61	1.62	1.59
4	E	501	AGS	C5-C6	2.61	1.48	1.41
4	B	501	AGS	C5-C6	2.59	1.48	1.41
4	E	501	AGS	C5-N7	-2.45	1.34	1.39
4	B	501	AGS	C8-N7	2.40	1.36	1.31
4	B	501	AGS	C5-N7	-2.36	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501	AGS	C8-N7	2.32	1.36	1.31
4	B	501	AGS	PA-O3A	2.29	1.62	1.59
4	E	501	AGS	PB-O3A	2.27	1.62	1.59
4	E	501	AGS	PG-O3G	2.11	1.61	1.54
4	B	501	AGS	PG-O3G	2.04	1.61	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	AGS	C5-C4-N3	-6.11	118.31	126.72
4	B	501	AGS	C5-C4-N3	-6.10	118.32	126.72
4	E	501	AGS	N3-C4-N9	5.09	135.82	127.17
4	B	501	AGS	N3-C4-N9	5.02	135.71	127.17
4	E	501	AGS	C2-N3-C4	4.07	121.76	111.83
4	E	501	AGS	N3-C2-N1	-4.03	122.49	128.58
4	B	501	AGS	C2-N3-C4	3.99	121.58	111.83
4	B	501	AGS	N3-C2-N1	-3.88	122.71	128.58
4	E	501	AGS	C2'-C3'-C4'	3.41	109.20	102.61
4	E	501	AGS	C4-C5-N7	-3.31	106.79	110.58
4	B	501	AGS	C4-C5-N7	-3.16	106.96	110.58
4	E	501	AGS	PB-O3B-PG	-2.91	122.52	133.17
4	E	501	AGS	C4-N9-C8	2.89	108.78	105.74
4	E	501	AGS	C5-N7-C8	2.79	107.83	103.45
4	B	501	AGS	C4-N9-C8	2.66	108.54	105.74
4	B	501	AGS	PB-O3B-PG	-2.62	123.59	133.17
4	B	501	AGS	C2'-C3'-C4'	2.58	107.60	102.61
4	B	501	AGS	C5-N7-C8	2.56	107.47	103.45
4	E	501	AGS	N9-C8-N7	-2.25	110.74	113.94
4	E	501	AGS	C2-N1-C6	2.14	122.25	118.73
4	E	501	AGS	C6-C5-N7	2.05	136.04	132.09
4	B	501	AGS	C2-N1-C6	2.04	122.09	118.73
4	B	501	AGS	N9-C8-N7	-2.03	111.06	113.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	AGS	PB-O3B-PG-O2G
4	B	501	AGS	O4'-C1'-N9-C8
4	B	501	AGS	O4'-C1'-N9-C4
4	E	501	AGS	PB-O3B-PG-O2G
4	E	501	AGS	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
4	E	501	AGS	O4'-C1'-N9-C8
4	E	501	AGS	O4'-C1'-N9-C4
4	B	501	AGS	PB-O3A-PA-O1A
4	B	501	AGS	PG-O3B-PB-O2B
4	B	501	AGS	PB-O3A-PA-O2A
4	E	501	AGS	PA-O3A-PB-O2B

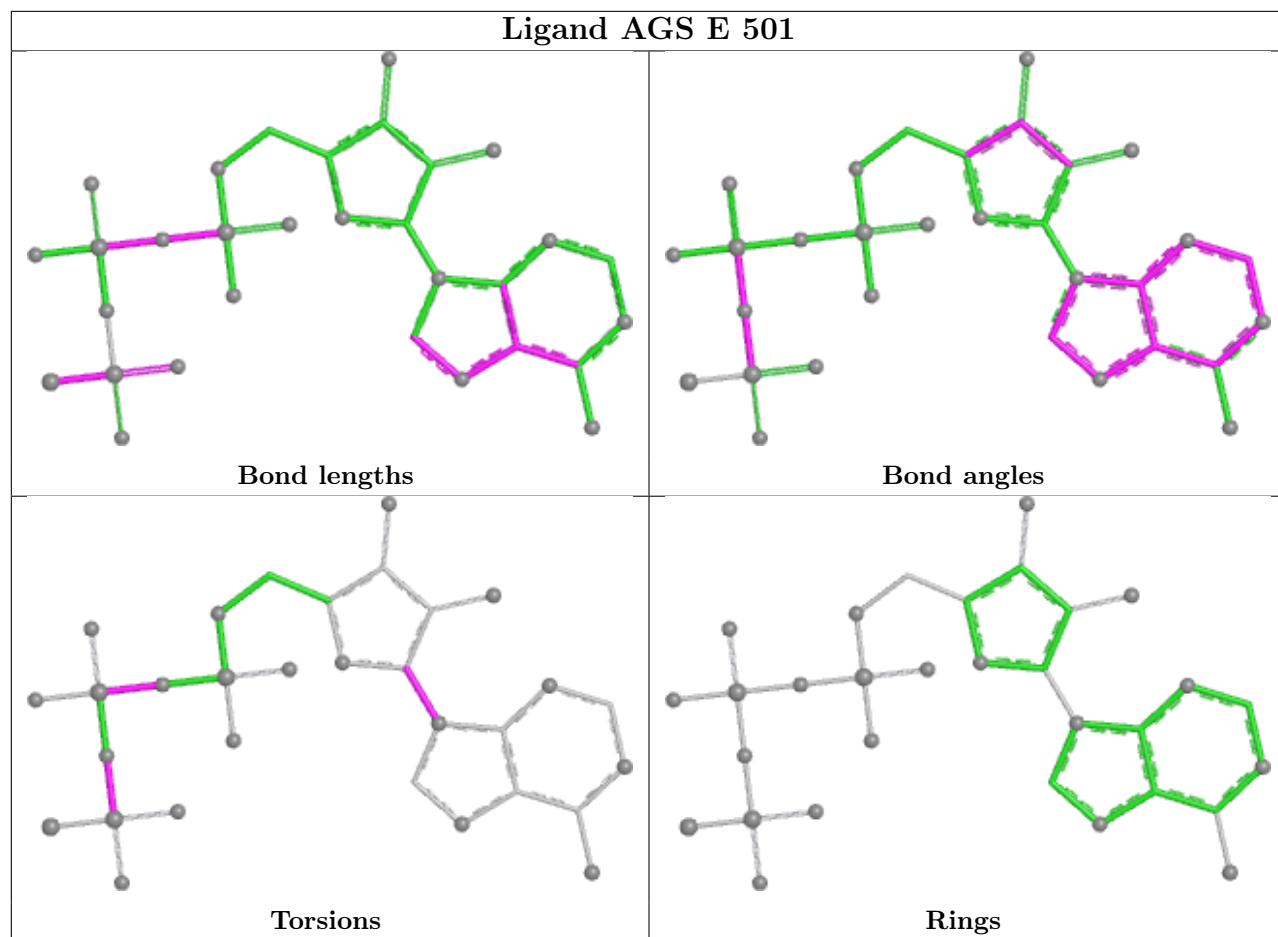
There are no ring outliers.

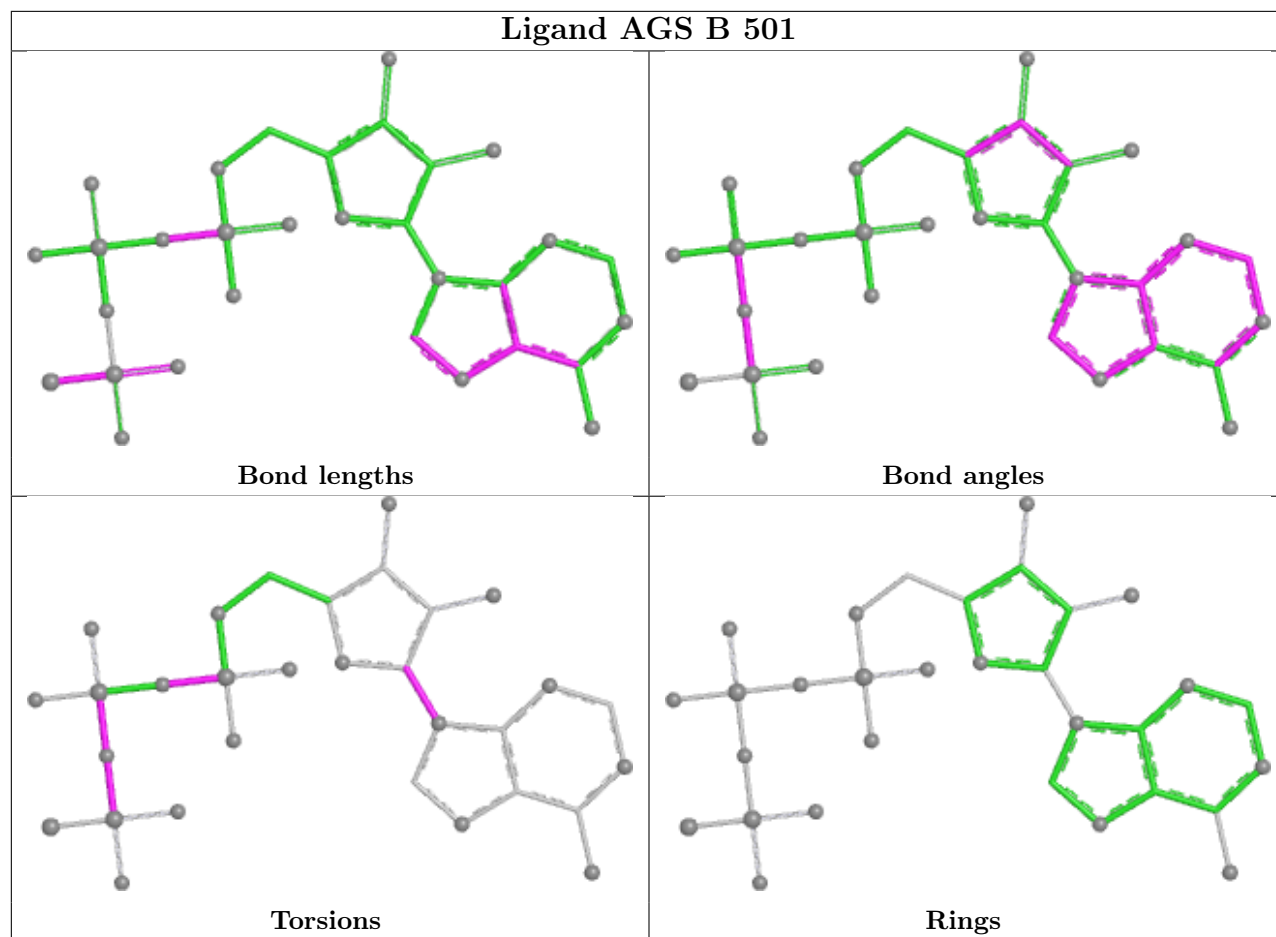
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	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.

Ligand AGS E 501





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	312/425 (73%)	0.30	8 (2%)	57 38	31, 65, 100, 127	0
1	D	314/425 (73%)	-0.08	6 (1%)	66 47	14, 40, 81, 124	0
2	B	322/437 (73%)	-0.14	3 (0%)	81 65	18, 40, 86, 110	0
2	E	323/437 (73%)	-0.29	3 (0%)	81 65	13, 30, 79, 124	0
3	C	66/69 (95%)	0.09	2 (3%)	52 34	38, 61, 84, 94	0
3	F	67/69 (97%)	-0.30	1 (1%)	72 53	17, 37, 67, 96	0
All	All	1404/1862 (75%)	-0.06	23 (1%)	70 51	13, 44, 88, 127	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	78	PRO	4.4
1	A	5	ILE	4.1
2	E	77	THR	3.8
1	A	384	PHE	3.7
1	D	384	PHE	3.7
1	D	262	TYR	3.5
1	A	382	LYS	3.4
1	A	75	PRO	3.3
2	B	381	ARG	3.2
3	C	338	GLY	3.1
1	D	261	HIS	2.7
1	D	382	LYS	2.7
1	A	312	SER	2.6
1	A	49	SER	2.5
1	A	390	GLY	2.4
1	D	386	SER	2.4
2	E	318	GLU	2.3
1	D	313	HIS	2.3
3	F	338	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	324	PHE	2.1
1	A	380	SER	2.1
2	B	127	GLN	2.1
2	E	126	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

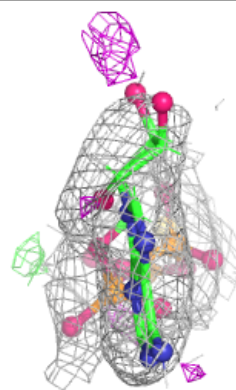
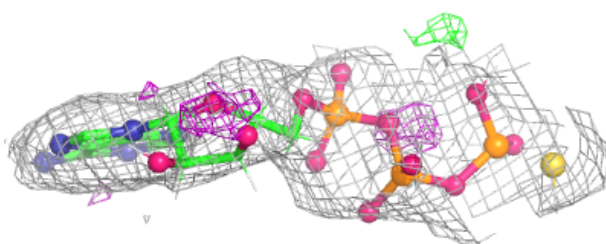
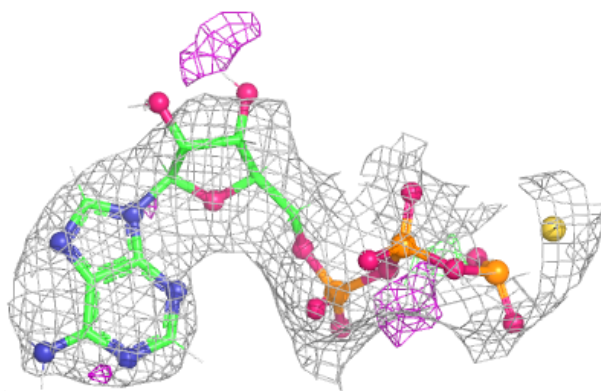
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AGS	E	501	31/31	0.85	0.12	35,77,136,146	0
5	MG	E	502	1/1	0.86	0.21	36,36,36,36	0
4	AGS	B	501	31/31	0.90	0.09	29,76,118,144	0
5	MG	B	502	1/1	0.92	0.11	19,19,19,19	0
6	CL	B	503	1/1	0.97	0.05	43,43,43,43	0

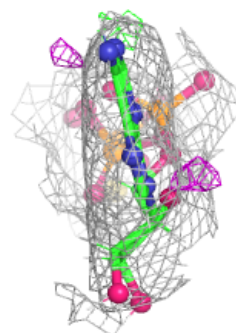
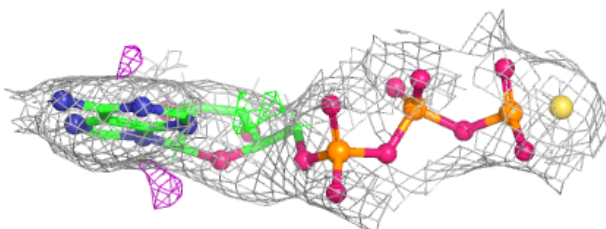
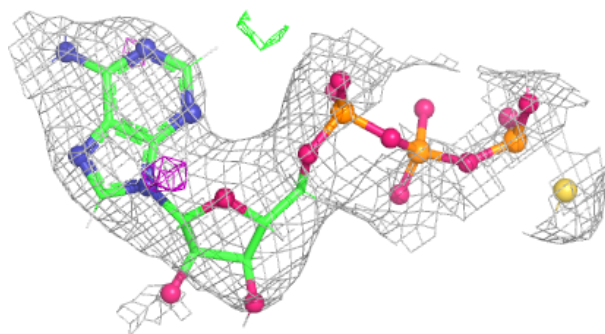
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS E 501:

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

**Electron density around AGS B 501:**

$2mF_o-DF_c$ (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.