



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:17 pm BST

PDB ID : 3HU2
Title : Structure of p97 N-D1 R86A mutant in complex with ATPgS
Authors : Tang, W.-K.
Deposited on : 2009-06-12
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

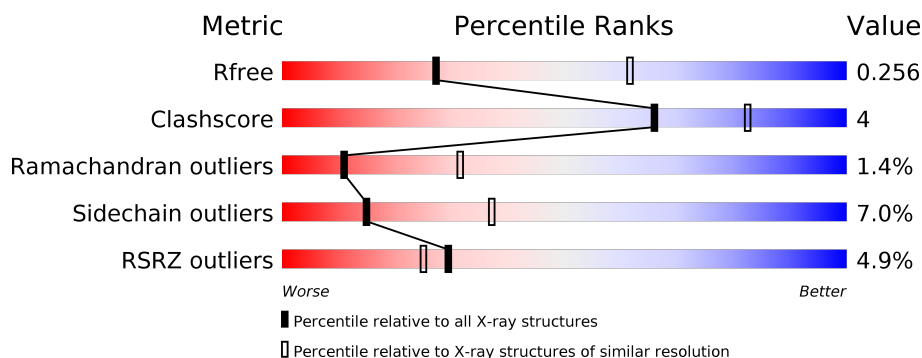
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	489	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	B	489	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 8%</div> </div> </div>
1	C	489	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 8%</div> </div> </div>
1	D	489	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 8%</div> </div> </div>
1	E	489	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 8%</div> </div> </div>
1	F	489	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21453 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3528	2215	624	671	18			
1	B	452	Total	C	N	O	S	0	0	0
			3528	2215	624	671	18			
1	C	452	Total	C	N	O	S	0	0	0
			3528	2215	624	671	18			
1	D	452	Total	C	N	O	S	0	0	0
			3528	2215	624	671	18			
1	E	452	Total	C	N	O	S	0	0	0
			3528	2215	624	671	18			
1	F	452	Total	C	N	O	S	0	0	0
			3528	2215	624	671	18			

There are 54 discrepancies between the modelled and reference sequences:

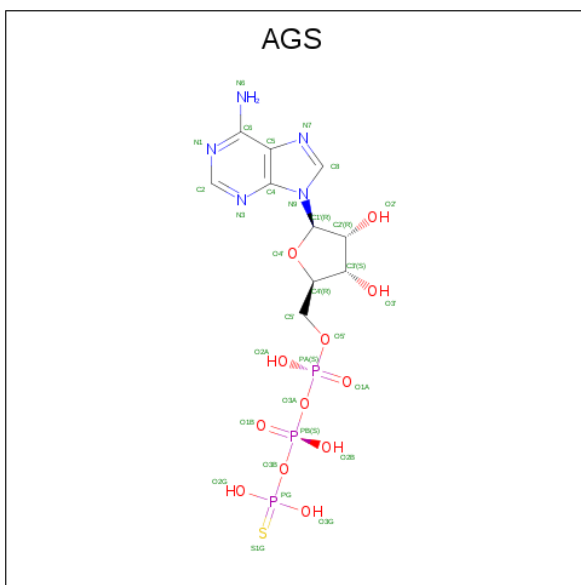
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ALA	ARG	engineered mutation	UNP P55072
A	482	ARG	-	expression tag	UNP P55072
A	483	SER	-	expression tag	UNP P55072
A	484	HIS	-	expression tag	UNP P55072
A	485	HIS	-	expression tag	UNP P55072
A	486	HIS	-	expression tag	UNP P55072
A	487	HIS	-	expression tag	UNP P55072
A	488	HIS	-	expression tag	UNP P55072
A	489	HIS	-	expression tag	UNP P55072
B	86	ALA	ARG	engineered mutation	UNP P55072
B	482	ARG	-	expression tag	UNP P55072
B	483	SER	-	expression tag	UNP P55072
B	484	HIS	-	expression tag	UNP P55072
B	485	HIS	-	expression tag	UNP P55072
B	486	HIS	-	expression tag	UNP P55072
B	487	HIS	-	expression tag	UNP P55072
B	488	HIS	-	expression tag	UNP P55072

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	489	HIS	-	expression tag	UNP P55072
C	86	ALA	ARG	engineered mutation	UNP P55072
C	482	ARG	-	expression tag	UNP P55072
C	483	SER	-	expression tag	UNP P55072
C	484	HIS	-	expression tag	UNP P55072
C	485	HIS	-	expression tag	UNP P55072
C	486	HIS	-	expression tag	UNP P55072
C	487	HIS	-	expression tag	UNP P55072
C	488	HIS	-	expression tag	UNP P55072
C	489	HIS	-	expression tag	UNP P55072
D	86	ALA	ARG	engineered mutation	UNP P55072
D	482	ARG	-	expression tag	UNP P55072
D	483	SER	-	expression tag	UNP P55072
D	484	HIS	-	expression tag	UNP P55072
D	485	HIS	-	expression tag	UNP P55072
D	486	HIS	-	expression tag	UNP P55072
D	487	HIS	-	expression tag	UNP P55072
D	488	HIS	-	expression tag	UNP P55072
D	489	HIS	-	expression tag	UNP P55072
E	86	ALA	ARG	engineered mutation	UNP P55072
E	482	ARG	-	expression tag	UNP P55072
E	483	SER	-	expression tag	UNP P55072
E	484	HIS	-	expression tag	UNP P55072
E	485	HIS	-	expression tag	UNP P55072
E	486	HIS	-	expression tag	UNP P55072
E	487	HIS	-	expression tag	UNP P55072
E	488	HIS	-	expression tag	UNP P55072
E	489	HIS	-	expression tag	UNP P55072
F	86	ALA	ARG	engineered mutation	UNP P55072
F	482	ARG	-	expression tag	UNP P55072
F	483	SER	-	expression tag	UNP P55072
F	484	HIS	-	expression tag	UNP P55072
F	485	HIS	-	expression tag	UNP P55072
F	486	HIS	-	expression tag	UNP P55072
F	487	HIS	-	expression tag	UNP P55072
F	488	HIS	-	expression tag	UNP P55072
F	489	HIS	-	expression tag	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

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

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

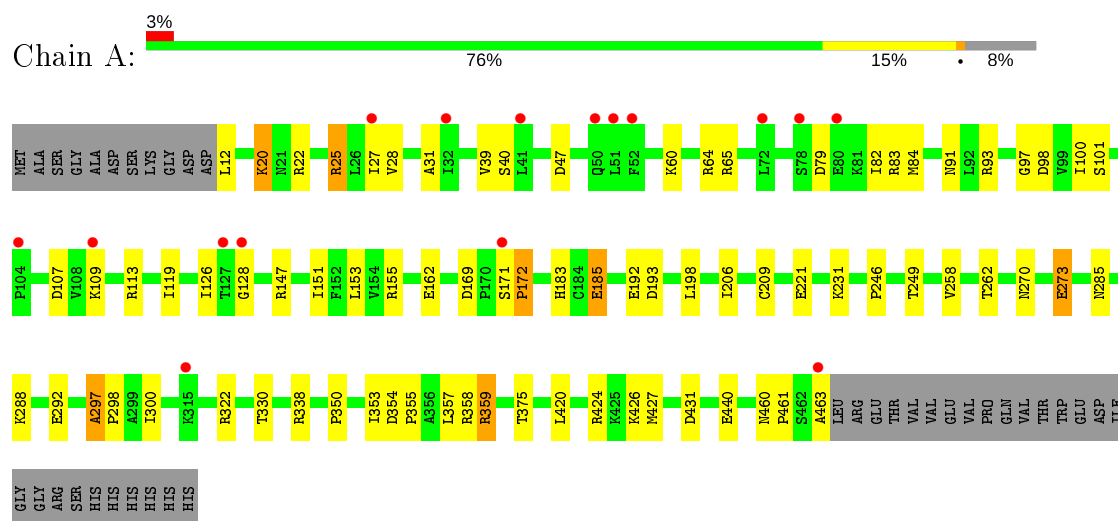
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	B	16	Total 16	O 16	0	0
4	C	15	Total 15	O 15	0	0
4	D	13	Total 13	O 13	0	0
4	E	13	Total 13	O 13	0	0
4	F	16	Total 16	O 16	0	0

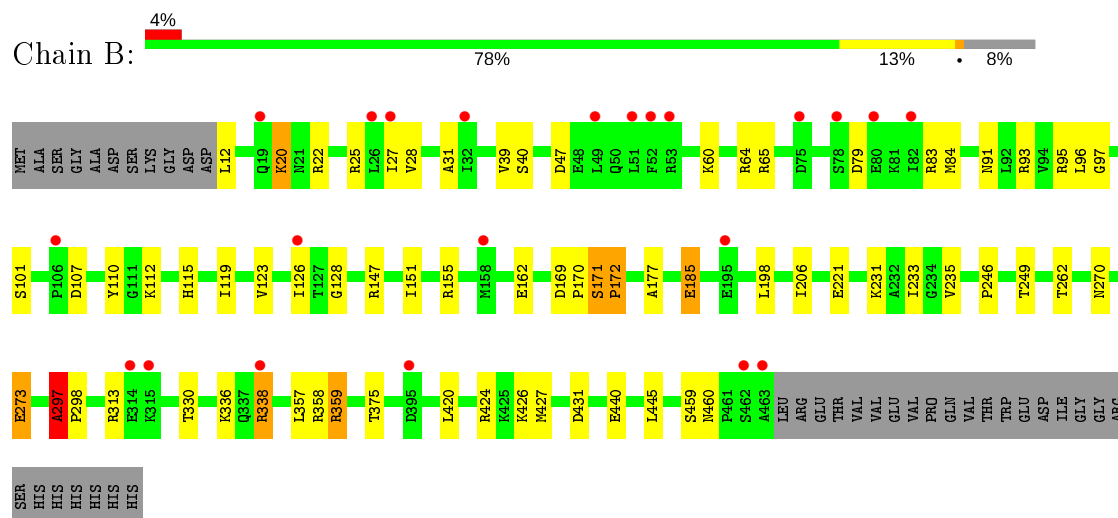
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

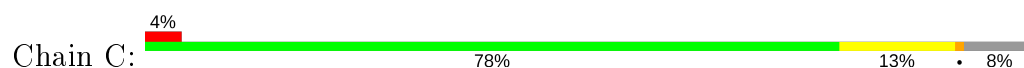
- Molecule 1: Transitional endoplasmic reticulum ATPase

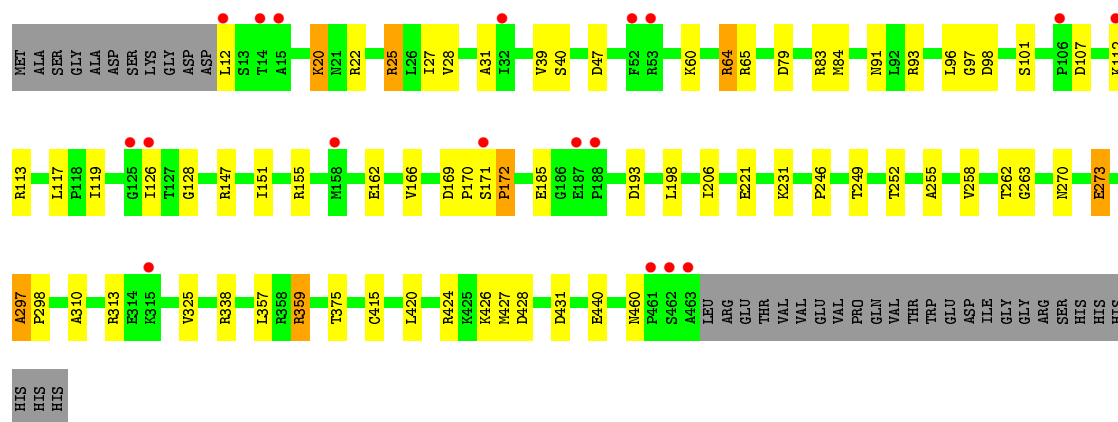


- Molecule 1: Transitional endoplasmic reticulum ATPase

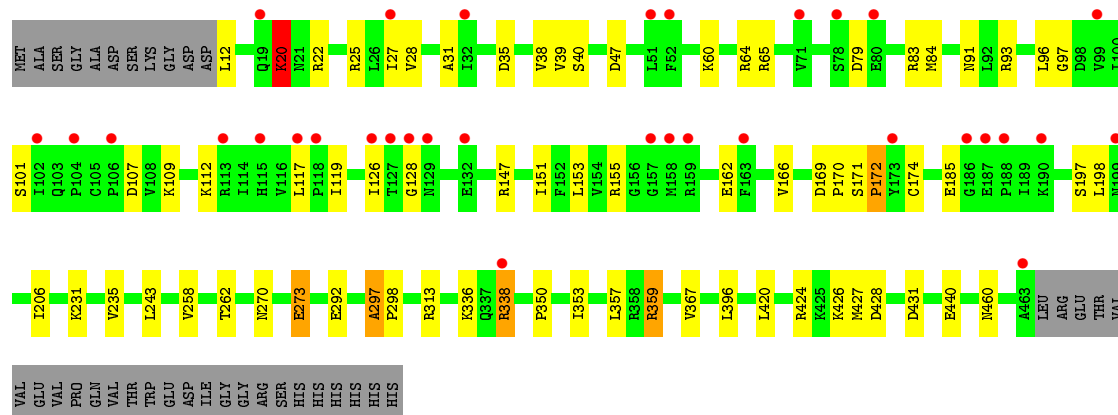
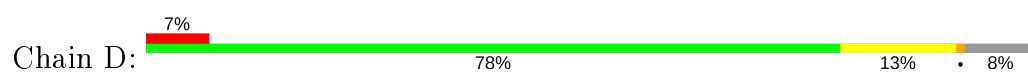


- Molecule 1: Transitional endoplasmic reticulum ATPase

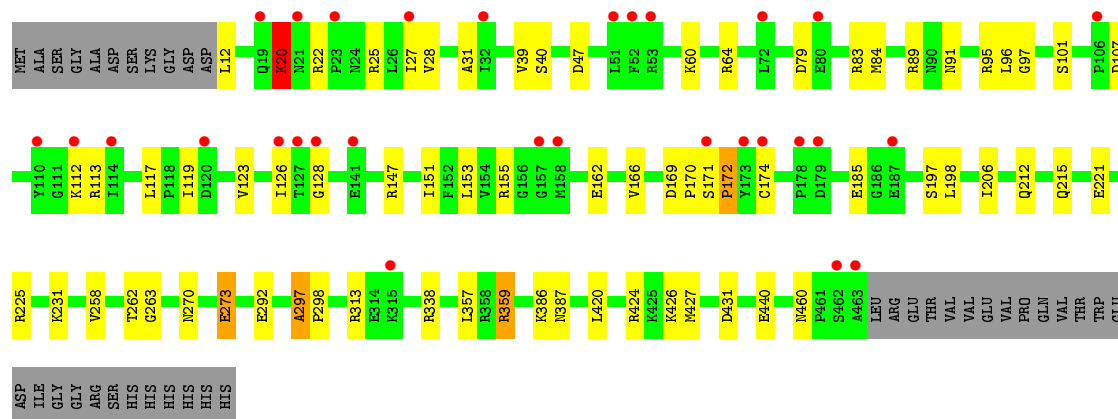
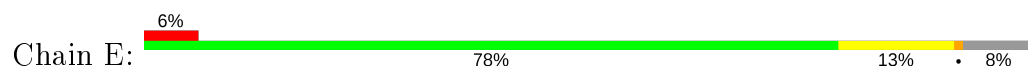




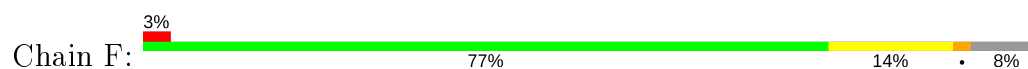
• Molecule 1: Transitional endoplasmic reticulum ATPase

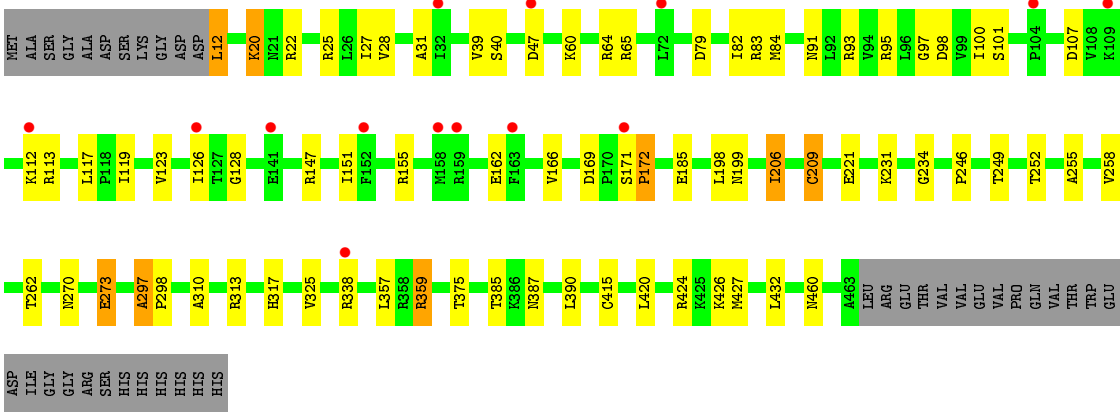


• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.89Å 102.64Å 107.18Å 97.52° 90.63° 91.45°	Depositor
Resolution (Å)	40.00 – 2.85 33.91 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.0 (40.00-2.85) 93.0 (33.91-2.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.258 , 0.290 0.226 , 0.256	Depositor DCC
R_{free} test set	4194 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l 0.010 for -h,l,k 0.007 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21453	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: 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	0.95	1/3582 (0.0%)	0.75	0/4841
1	B	0.97	2/3582 (0.1%)	0.75	0/4841
1	C	0.96	1/3582 (0.0%)	0.74	0/4841
1	D	0.94	0/3582	0.73	0/4841
1	E	0.97	0/3582	0.75	0/4841
1	F	0.95	2/3582 (0.1%)	0.75	1/4841 (0.0%)
All	All	0.96	6/21492 (0.0%)	0.75	1/29046 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	415	CYS	CB-SG	-7.82	1.69	1.82
1	F	415	CYS	CB-SG	-6.47	1.71	1.82
1	A	209	CYS	CB-SG	-5.72	1.72	1.81
1	F	209	CYS	CB-SG	-5.63	1.72	1.81
1	B	297	ALA	CA-CB	5.12	1.63	1.52
1	B	185	GLU	CB-CG	5.11	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	12	LEU	CA-CB-CG	5.30	127.50	115.30

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	3528	0	3590	38	0
1	B	3528	0	3590	29	0
1	C	3528	0	3590	33	0
1	D	3528	0	3590	30	0
1	E	3528	0	3590	26	0
1	F	3528	0	3590	30	0
2	A	31	0	12	1	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	20	0	0	0	0
4	B	16	0	0	1	0
4	C	15	0	0	0	0
4	D	13	0	0	0	0
4	E	13	0	0	0	0
4	F	16	0	0	0	0
All	All	21453	0	21612	172	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 4.

All (172) 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:E:91:ASN:HD21	1:E:151:ILE:H	1.28	0.80
1:A:193:ASP:HA	1:B:338:ARG:NH1	2.02	0.75
1:B:171:SER:HB2	1:B:172:PRO:HD3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.75	0.68
1:D:91:ASN:HD21	1:D:151:ILE:H	1.41	0.68
1:E:270:ASN:HB2	1:E:273:GLU:HB2	1.76	0.68
1:F:270:ASN:HB2	1:F:273:GLU:HB2	1.76	0.68
1:D:270:ASN:HB2	1:D:273:GLU:HB2	1.77	0.67
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.76	0.67
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.75	0.67
1:B:91:ASN:HD21	1:B:151:ILE:H	1.42	0.66
1:C:193:ASP:HA	1:D:338:ARG:HH12	1.60	0.66
1:E:424:ARG:HA	1:E:427:MET:HG2	1.78	0.66
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.78	0.66
2:E:800:AGS:S1G	1:F:359:ARG:HG2	2.35	0.65
1:B:424:ARG:HA	1:B:427:MET:HG2	1.79	0.65
1:C:270:ASN:HB2	1:C:273:GLU:HB2	1.79	0.65
1:A:193:ASP:HA	1:B:338:ARG:HH12	1.61	0.64
1:A:461:PRO:HG2	1:A:463:ALA:HB2	1.80	0.64
1:A:359:ARG:HG2	2:F:800:AGS:S1G	2.38	0.64
2:B:800:AGS:S1G	1:C:359:ARG:HG2	2.38	0.64
1:E:91:ASN:ND2	1:E:151:ILE:H	1.96	0.63
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.80	0.63
1:D:297:ALA:HB3	1:D:298:PRO:HD3	1.81	0.63
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.80	0.62
2:A:800:AGS:S1G	1:B:359:ARG:HG2	2.39	0.62
1:C:297:ALA:HB3	1:C:298:PRO:HD3	1.82	0.62
1:A:171:SER:HB2	1:A:172:PRO:HD3	1.81	0.61
1:B:119:ILE:HD12	1:B:162:GLU:HB3	1.82	0.61
1:A:221:GLU:OE2	1:A:262:THR:HG22	2.01	0.61
1:A:91:ASN:HD21	1:A:151:ILE:H	1.49	0.61
1:B:270:ASN:HB2	1:B:273:GLU:HB2	1.81	0.60
1:C:171:SER:HB2	1:C:172:PRO:HD3	1.84	0.60
1:A:297:ALA:HB3	1:A:298:PRO:HD3	1.85	0.58
1:C:424:ARG:HA	1:C:427:MET:HG2	1.86	0.58
1:B:171:SER:CB	1:B:172:PRO:HD3	2.34	0.58
1:C:193:ASP:OD2	1:D:338:ARG:NH1	2.36	0.58
1:B:221:GLU:OE2	1:B:262:THR:HG22	2.04	0.57
1:D:424:ARG:HA	1:D:427:MET:HG2	1.85	0.57
1:E:171:SER:HB2	1:E:172:PRO:HD3	1.86	0.57
1:D:171:SER:HB2	1:D:172:PRO:HD3	1.85	0.57
2:C:800:AGS:S1G	1:D:359:ARG:HG2	2.45	0.57
1:D:91:ASN:ND2	1:D:151:ILE:H	2.02	0.57
1:E:39:VAL:HG12	1:E:84:MET:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:HB2	1:A:273:GLU:HB2	1.87	0.56
2:D:800:AGS:S1G	1:E:359:ARG:HG2	2.46	0.56
1:F:91:ASN:HD21	1:F:151:ILE:H	1.52	0.56
1:A:27:ILE:HG23	1:A:97:GLY:HA2	1.87	0.56
1:A:193:ASP:OD2	1:B:338:ARG:NH1	2.39	0.56
1:F:27:ILE:HG23	1:F:97:GLY:HA2	1.86	0.56
1:D:39:VAL:HG12	1:D:84:MET:HB3	1.88	0.55
1:A:424:ARG:HA	1:A:427:MET:HG2	1.88	0.55
1:A:39:VAL:HG12	1:A:84:MET:HB3	1.89	0.55
1:F:171:SER:HB2	1:F:172:PRO:HD3	1.87	0.55
1:B:27:ILE:HG23	1:B:97:GLY:HA2	1.89	0.55
1:C:91:ASN:HD21	1:C:151:ILE:H	1.55	0.54
1:C:221:GLU:OE2	1:C:262:THR:HG22	2.06	0.54
1:E:297:ALA:HB3	1:E:298:PRO:HD3	1.87	0.54
1:E:31:ALA:HA	1:E:83:ARG:HB3	1.90	0.54
1:F:297:ALA:HB3	1:F:298:PRO:HD3	1.88	0.54
1:B:31:ALA:HA	1:B:83:ARG:HB3	1.88	0.54
1:D:27:ILE:HG23	1:D:97:GLY:HA2	1.89	0.54
1:D:119:ILE:HD12	1:D:162:GLU:HB3	1.90	0.53
1:C:27:ILE:HG23	1:C:97:GLY:HA2	1.88	0.53
1:F:39:VAL:HG12	1:F:84:MET:HB3	1.89	0.53
1:D:258:VAL:O	1:D:262:THR:HG23	2.09	0.53
1:F:119:ILE:HD12	1:F:162:GLU:HB3	1.91	0.53
1:A:31:ALA:HA	1:A:83:ARG:HB3	1.91	0.52
1:F:221:GLU:OE2	1:F:262:THR:HG22	2.09	0.52
1:A:119:ILE:HD12	1:A:162:GLU:HB3	1.91	0.52
1:E:221:GLU:OE2	1:E:262:THR:HG22	2.10	0.52
1:A:273:GLU:HG2	1:B:330:THR:HG23	1.92	0.52
1:B:39:VAL:HG12	1:B:84:MET:HB3	1.91	0.52
1:C:119:ILE:HD12	1:C:162:GLU:HB3	1.92	0.52
1:D:31:ALA:HA	1:D:83:ARG:HB3	1.92	0.52
1:F:424:ARG:HA	1:F:427:MET:HG2	1.92	0.51
1:C:39:VAL:HG12	1:C:84:MET:HB3	1.91	0.51
1:E:60:LYS:HB2	1:E:101:SER:HB2	1.93	0.50
1:B:115:HIS:HB2	4:B:817:HOH:O	2.11	0.50
1:C:258:VAL:O	1:C:262:THR:HG23	2.10	0.50
1:A:91:ASN:ND2	1:A:151:ILE:H	2.10	0.49
1:C:31:ALA:HA	1:C:83:ARG:HB3	1.93	0.49
1:E:27:ILE:HG23	1:E:97:GLY:HA2	1.93	0.49
1:F:91:ASN:ND2	1:F:151:ILE:H	2.09	0.49
1:B:246:PRO:HD2	1:B:249:THR:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:HB3	1:B:338:ARG:HB3	1.94	0.48
1:B:297:ALA:HB3	1:B:298:PRO:HD3	1.94	0.48
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.94	0.48
1:B:65:ARG:HG3	1:B:93:ARG:HG3	1.95	0.47
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.96	0.47
1:C:113:ARG:H	1:C:169:ASP:HB2	1.79	0.47
1:C:65:ARG:HG3	1:C:93:ARG:HG3	1.95	0.47
1:F:258:VAL:O	1:F:262:THR:HG23	2.14	0.47
1:D:428:ASP:HA	1:E:20:LYS:HD2	1.96	0.47
1:B:91:ASN:ND2	1:B:151:ILE:H	2.10	0.47
1:A:285:ASN:HD22	1:A:288:LYS:HE3	1.80	0.47
1:A:65:ARG:HG3	1:A:93:ARG:HG3	1.96	0.46
1:E:258:VAL:O	1:E:262:THR:HG23	2.14	0.46
1:A:246:PRO:HD2	1:A:249:THR:HG21	1.96	0.46
1:E:95:ARG:HH22	1:E:386:LYS:HD2	1.80	0.46
1:E:113:ARG:H	1:E:169:ASP:HB2	1.81	0.45
1:F:206:ILE:HD11	1:F:209:CYS:SG	2.56	0.45
1:F:385:THR:HB	1:F:390:LEU:HD11	1.98	0.45
1:E:119:ILE:HD12	1:E:162:GLU:HB3	1.98	0.45
1:D:297:ALA:CB	1:D:298:PRO:HD3	2.46	0.45
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.99	0.45
1:D:35:ASP:HB3	1:D:38:VAL:HG12	1.98	0.45
1:C:193:ASP:HA	1:D:338:ARG:NH1	2.29	0.45
1:C:428:ASP:HA	1:D:20:LYS:HD2	1.99	0.45
1:D:65:ARG:HG3	1:D:93:ARG:HG3	1.99	0.45
1:F:60:LYS:HB2	1:F:101:SER:HB2	1.97	0.45
1:D:60:LYS:HB2	1:D:101:SER:HB2	1.97	0.44
1:A:322:ARG:HH12	1:F:317:HIS:H	1.65	0.44
1:A:60:LYS:HB2	1:A:101:SER:HB2	1.98	0.44
1:C:91:ASN:ND2	1:C:151:ILE:H	2.16	0.44
1:C:65:ARG:HG3	1:C:93:ARG:CG	2.48	0.44
1:C:252:THR:O	1:C:255:ALA:HB3	2.17	0.44
1:A:258:VAL:O	1:A:262:THR:HG23	2.18	0.43
1:F:246:PRO:HD2	1:F:249:THR:HG21	2.00	0.43
1:F:252:THR:O	1:F:255:ALA:HB3	2.18	0.43
1:D:336:LYS:HD2	1:D:338:ARG:HH21	1.82	0.43
1:E:170:PRO:HD2	1:E:174:CYS:HB3	1.99	0.43
1:E:225:ARG:HD3	1:E:263:GLY:HA3	1.99	0.43
1:A:297:ALA:CB	1:A:298:PRO:HD3	2.49	0.43
1:C:246:PRO:HD2	1:C:249:THR:HG21	2.01	0.43
1:D:117:LEU:HD12	1:D:166:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:ALA:HA	1:F:83:ARG:HB3	1.98	0.43
1:A:221:GLU:HG2	1:F:432:LEU:HD21	2.00	0.43
1:A:25:ARG:HH11	1:A:25:ARG:HB2	1.83	0.43
1:A:82:ILE:HD13	1:A:100:ILE:HD11	2.00	0.43
1:C:64:ARG:CZ	1:C:263:GLY:HA2	2.49	0.43
1:D:28:VAL:HG23	1:D:96:LEU:HA	2.01	0.43
1:A:153:LEU:HD13	1:A:162:GLU:HG3	2.01	0.43
1:B:336:LYS:HD2	1:B:338:ARG:HH21	1.84	0.43
1:F:117:LEU:HD12	1:F:166:VAL:HG21	2.00	0.43
1:A:330:THR:HG23	1:F:273:GLU:HG2	2.01	0.43
1:A:183:HIS:HB3	1:A:185:GLU:OE1	2.19	0.42
1:C:28:VAL:HG23	1:C:96:LEU:HA	2.00	0.42
1:A:354:ASP:HA	1:A:355:PRO:HD3	1.95	0.42
1:D:350:PRO:HA	1:D:353:ILE:HD12	2.01	0.42
1:F:28:VAL:HG22	1:F:98:ASP:H	1.84	0.42
1:D:153:LEU:HD13	1:D:162:GLU:HG3	2.01	0.42
1:E:212:GLN:HA	1:E:215:GLN:HE21	1.84	0.42
1:F:65:ARG:HG3	1:F:93:ARG:HG3	2.02	0.42
1:A:113:ARG:H	1:A:169:ASP:HB2	1.84	0.42
1:E:153:LEU:HD13	1:E:162:GLU:HG3	2.01	0.42
1:C:310:ALA:HA	1:C:325:VAL:HG22	2.00	0.42
1:E:117:LEU:HD12	1:E:166:VAL:HG21	2.02	0.42
1:A:28:VAL:HG22	1:A:98:ASP:H	1.85	0.41
1:F:199:ASN:HD21	1:F:387:ASN:HD21	1.67	0.41
1:B:60:LYS:HB2	1:B:101:SER:HB2	2.03	0.41
1:B:233:ILE:HG23	1:B:235:VAL:HB	2.02	0.41
1:A:350:PRO:HA	1:A:353:ILE:HD12	2.02	0.41
1:E:387:ASN:O	1:F:234:GLY:HA3	2.21	0.41
1:E:84:MET:HG3	1:E:89:ARG:HG3	2.02	0.41
1:D:243:LEU:HD22	1:D:367:VAL:HB	2.03	0.41
1:C:117:LEU:HD12	1:C:166:VAL:HG21	2.01	0.41
1:D:169:ASP:HB3	1:D:170:PRO:HD3	2.02	0.41
1:D:170:PRO:HD2	1:D:174:CYS:HB3	2.02	0.41
1:A:262:THR:HG21	1:A:300:ILE:CD1	2.50	0.41
1:A:171:SER:CB	1:A:172:PRO:HD3	2.51	0.41
1:E:28:VAL:HG23	1:E:96:LEU:HA	2.03	0.41
1:F:310:ALA:HA	1:F:325:VAL:HG22	2.03	0.41
1:F:113:ARG:H	1:F:169:ASP:HB2	1.86	0.40
1:C:60:LYS:HB2	1:C:101:SER:HB2	2.03	0.40
1:C:28:VAL:HG22	1:C:98:ASP:H	1.87	0.40
1:C:25:ARG:HH11	1:C:25:ARG:HB2	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ALA:CB	1:C:298:PRO:HD3	2.50	0.40
1:B:110:TYR:CD2	1:B:177:ALA:HB2	2.57	0.40
1:B:65:ARG:HG3	1:B:93:ARG:CG	2.51	0.40
1:C:171:SER:CB	1:C:172:PRO:HD3	2.50	0.40
1:F:82:ILE:HD13	1:F:100:ILE:HD11	2.03	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	450/489 (92%)	421 (94%)	24 (5%)	5 (1%)	14	38
1	B	450/489 (92%)	423 (94%)	19 (4%)	8 (2%)	8	25
1	C	450/489 (92%)	418 (93%)	26 (6%)	6 (1%)	12	33
1	D	450/489 (92%)	420 (93%)	24 (5%)	6 (1%)	12	33
1	E	450/489 (92%)	423 (94%)	20 (4%)	7 (2%)	9	28
1	F	450/489 (92%)	421 (94%)	23 (5%)	6 (1%)	12	33
All	All	2700/2934 (92%)	2526 (94%)	136 (5%)	38 (1%)	11	31

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ILE
1	A	297	ALA
1	B	126	ILE
1	B	297	ALA
1	C	126	ILE
1	C	297	ALA
1	D	126	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	297	ALA
1	E	126	ILE
1	E	297	ALA
1	F	126	ILE
1	F	297	ALA
1	A	128	GLY
1	B	20	LYS
1	B	128	GLY
1	B	313	ARG
1	E	128	GLY
1	E	313	ARG
1	F	128	GLY
1	F	313	ARG
1	A	172	PRO
1	C	128	GLY
1	C	172	PRO
1	D	172	PRO
1	F	172	PRO
1	A	20	LYS
1	B	172	PRO
1	B	445	LEU
1	C	20	LYS
1	C	313	ARG
1	D	20	LYS
1	D	128	GLY
1	D	313	ARG
1	E	20	LYS
1	E	172	PRO
1	F	20	LYS
1	B	171	SER
1	E	123	VAL

5.3.2 Protein sidechains ⓘ

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/417 (93%)	359 (93%)	27 (7%)	15	37
1	B	386/417 (93%)	357 (92%)	29 (8%)	13	34
1	C	386/417 (93%)	361 (94%)	25 (6%)	17	41
1	D	386/417 (93%)	357 (92%)	29 (8%)	13	34
1	E	386/417 (93%)	360 (93%)	26 (7%)	16	39
1	F	386/417 (93%)	361 (94%)	25 (6%)	17	41
All	All	2316/2502 (93%)	2155 (93%)	161 (7%)	15	37

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	20	LYS
1	A	22	ARG
1	A	25	ARG
1	A	47	ASP
1	A	64	ARG
1	A	79	ASP
1	A	107	ASP
1	A	109	LYS
1	A	147	ARG
1	A	155	ARG
1	A	185	GLU
1	A	198	LEU
1	A	206	ILE
1	A	231	LYS
1	A	273	GLU
1	A	292	GLU
1	A	338	ARG
1	A	357	LEU
1	A	358	ARG
1	A	359	ARG
1	A	375	THR
1	A	420	LEU
1	A	426	LYS
1	A	431	ASP
1	A	440	GLU
1	A	460	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	12	LEU
1	B	20	LYS
1	B	22	ARG
1	B	25	ARG
1	B	47	ASP
1	B	64	ARG
1	B	79	ASP
1	B	95	ARG
1	B	107	ASP
1	B	112	LYS
1	B	123	VAL
1	B	147	ARG
1	B	155	ARG
1	B	185	GLU
1	B	198	LEU
1	B	206	ILE
1	B	231	LYS
1	B	273	GLU
1	B	338	ARG
1	B	357	LEU
1	B	358	ARG
1	B	359	ARG
1	B	375	THR
1	B	420	LEU
1	B	426	LYS
1	B	431	ASP
1	B	440	GLU
1	B	459	SER
1	B	460	ASN
1	C	12	LEU
1	C	20	LYS
1	C	22	ARG
1	C	25	ARG
1	C	47	ASP
1	C	64	ARG
1	C	79	ASP
1	C	107	ASP
1	C	112	LYS
1	C	147	ARG
1	C	155	ARG
1	C	185	GLU
1	C	198	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	206	ILE
1	C	231	LYS
1	C	273	GLU
1	C	338	ARG
1	C	357	LEU
1	C	359	ARG
1	C	375	THR
1	C	420	LEU
1	C	426	LYS
1	C	431	ASP
1	C	440	GLU
1	C	460	ASN
1	D	12	LEU
1	D	20	LYS
1	D	22	ARG
1	D	25	ARG
1	D	47	ASP
1	D	64	ARG
1	D	79	ASP
1	D	107	ASP
1	D	109	LYS
1	D	112	LYS
1	D	147	ARG
1	D	155	ARG
1	D	185	GLU
1	D	197	SER
1	D	198	LEU
1	D	206	ILE
1	D	231	LYS
1	D	235	VAL
1	D	273	GLU
1	D	292	GLU
1	D	338	ARG
1	D	357	LEU
1	D	359	ARG
1	D	396	LEU
1	D	420	LEU
1	D	426	LYS
1	D	431	ASP
1	D	440	GLU
1	D	460	ASN
1	E	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	20	LYS
1	E	22	ARG
1	E	25	ARG
1	E	47	ASP
1	E	64	ARG
1	E	79	ASP
1	E	107	ASP
1	E	112	LYS
1	E	147	ARG
1	E	155	ARG
1	E	185	GLU
1	E	197	SER
1	E	198	LEU
1	E	206	ILE
1	E	231	LYS
1	E	273	GLU
1	E	292	GLU
1	E	338	ARG
1	E	357	LEU
1	E	359	ARG
1	E	420	LEU
1	E	426	LYS
1	E	431	ASP
1	E	440	GLU
1	E	460	ASN
1	F	12	LEU
1	F	20	LYS
1	F	22	ARG
1	F	25	ARG
1	F	47	ASP
1	F	64	ARG
1	F	79	ASP
1	F	95	ARG
1	F	107	ASP
1	F	112	LYS
1	F	123	VAL
1	F	147	ARG
1	F	155	ARG
1	F	185	GLU
1	F	198	LEU
1	F	206	ILE
1	F	231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	273	GLU
1	F	338	ARG
1	F	357	LEU
1	F	359	ARG
1	F	375	THR
1	F	420	LEU
1	F	426	LYS
1	F	460	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	199	ASN
1	A	260	ASN
1	A	285	ASN
1	B	91	ASN
1	B	215	GLN
1	B	260	ASN
1	B	285	ASN
1	C	85	ASN
1	C	91	ASN
1	C	215	GLN
1	C	260	ASN
1	C	285	ASN
1	C	327	GLN
1	D	43	GLN
1	D	91	ASN
1	D	199	ASN
1	D	215	GLN
1	D	260	ASN
1	D	285	ASN
1	E	91	ASN
1	E	215	GLN
1	E	285	ASN
1	E	296	ASN
1	E	387	ASN
1	F	43	GLN
1	F	91	ASN
1	F	199	ASN
1	F	260	ASN
1	F	285	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	800	3	26,33,33	1.52	3 (11%)	26,52,52	1.37	4 (15%)
2	AGS	A	800	3	26,33,33	1.47	2 (7%)	26,52,52	1.40	5 (19%)
2	AGS	F	800	3	26,33,33	1.53	2 (7%)	26,52,52	1.42	4 (15%)
2	AGS	E	800	3	26,33,33	1.37	2 (7%)	26,52,52	1.40	3 (11%)
2	AGS	D	800	3	26,33,33	1.37	3 (11%)	26,52,52	1.45	4 (15%)
2	AGS	C	800	3	26,33,33	1.54	3 (11%)	26,52,52	1.45	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	800	3	-	4/17/38/38	0/3/3/3
2	AGS	A	800	3	-	4/17/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	F	800	3	-	4/17/38/38	0/3/3/3
2	AGS	E	800	3	-	4/17/38/38	0/3/3/3
2	AGS	D	800	3	-	4/17/38/38	0/3/3/3
2	AGS	C	800	3	-	4/17/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	AGS	PG-S1G	5.29	2.02	1.90
2	F	800	AGS	PG-S1G	5.13	2.01	1.90
2	A	800	AGS	PG-S1G	4.94	2.01	1.90
2	D	800	AGS	PG-S1G	4.64	2.00	1.90
2	B	800	AGS	PG-S1G	4.62	2.00	1.90
2	E	800	AGS	PG-S1G	3.86	1.99	1.90
2	E	800	AGS	C2-N3	2.96	1.36	1.32
2	F	800	AGS	C2-N3	2.96	1.36	1.32
2	B	800	AGS	C2-N3	2.69	1.36	1.32
2	C	800	AGS	C2-N3	2.56	1.36	1.32
2	D	800	AGS	C2-N3	2.39	1.35	1.32
2	C	800	AGS	C2'-C1'	-2.28	1.50	1.53
2	A	800	AGS	C2-N3	2.27	1.35	1.32
2	D	800	AGS	C5-C4	2.18	1.46	1.40
2	B	800	AGS	PG-O2G	-2.03	1.48	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	AGS	N3-C2-N1	-3.83	122.69	128.68
2	D	800	AGS	N3-C2-N1	-3.82	122.70	128.68
2	A	800	AGS	N3-C2-N1	-3.71	122.88	128.68
2	B	800	AGS	N3-C2-N1	-3.63	123.01	128.68
2	E	800	AGS	N3-C2-N1	-3.58	123.09	128.68
2	F	800	AGS	N3-C2-N1	-3.30	123.52	128.68
2	F	800	AGS	PA-O3A-PB	-3.24	121.72	132.83
2	C	800	AGS	C4-C5-N7	-3.16	106.11	109.40
2	F	800	AGS	C3'-C2'-C1'	3.09	105.63	100.98
2	C	800	AGS	C3'-C2'-C1'	2.99	105.47	100.98
2	E	800	AGS	C3'-C2'-C1'	2.86	105.28	100.98
2	D	800	AGS	PA-O3A-PB	-2.81	123.17	132.83
2	D	800	AGS	C3'-C2'-C1'	2.63	104.94	100.98
2	C	800	AGS	PA-O3A-PB	-2.56	124.04	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	AGS	C4-C5-N7	-2.56	106.73	109.40
2	B	800	AGS	C3'-C2'-C1'	2.54	104.80	100.98
2	A	800	AGS	PA-O3A-PB	-2.49	124.28	132.83
2	B	800	AGS	C4-C5-N7	-2.41	106.89	109.40
2	F	800	AGS	C4-C5-N7	-2.28	107.03	109.40
2	D	800	AGS	C4-C5-N7	-2.27	107.03	109.40
2	E	800	AGS	C4-C5-N7	-2.12	107.19	109.40
2	A	800	AGS	C3'-C2'-C1'	2.09	104.13	100.98
2	B	800	AGS	PA-O3A-PB	-2.08	125.67	132.83
2	A	800	AGS	O2G-PG-O3B	2.06	111.52	104.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

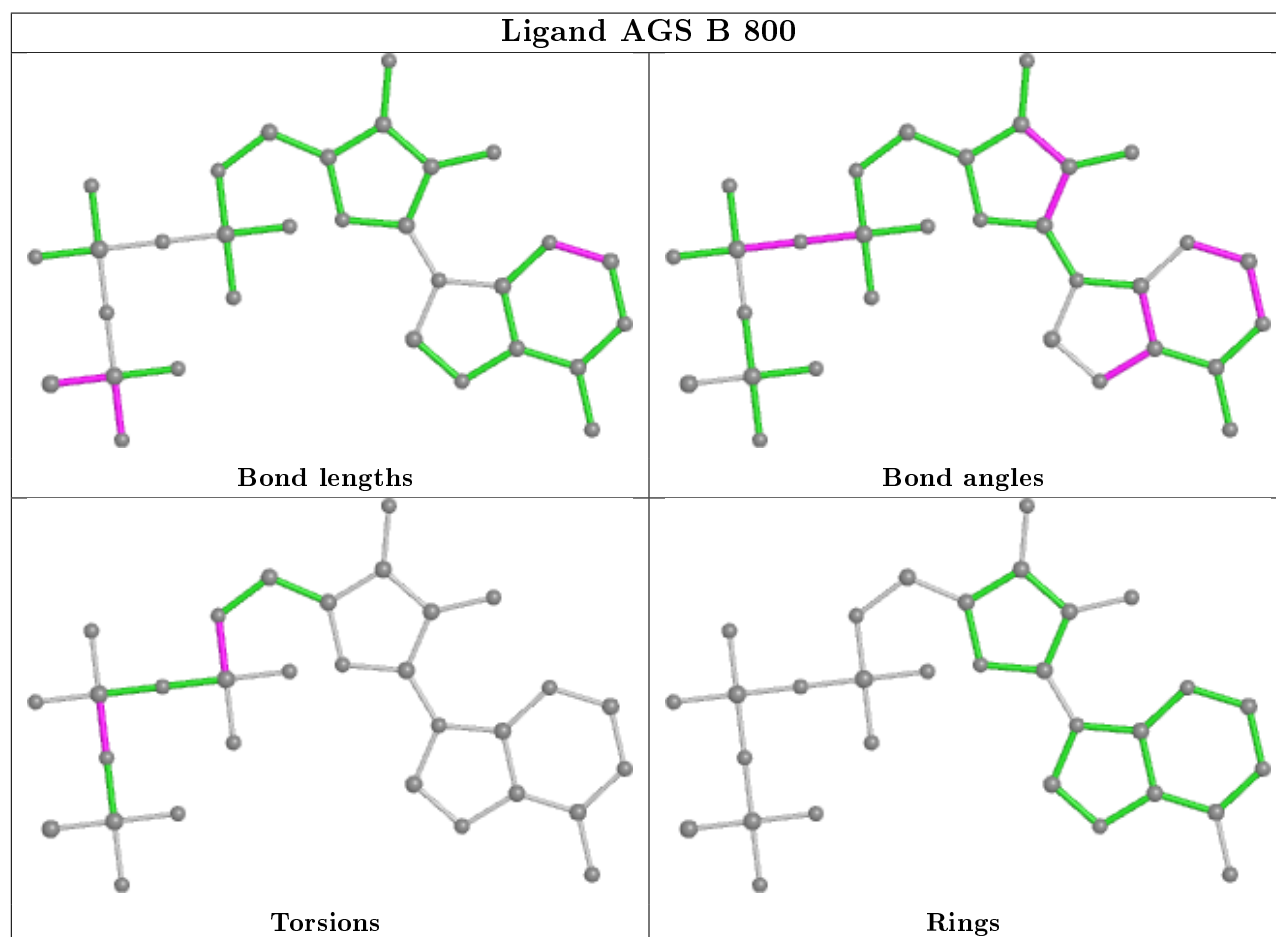
Mol	Chain	Res	Type	Atoms
2	B	800	AGS	C5'-O5'-PA-O1A
2	A	800	AGS	C5'-O5'-PA-O1A
2	F	800	AGS	C5'-O5'-PA-O1A
2	E	800	AGS	C5'-O5'-PA-O1A
2	D	800	AGS	C5'-O5'-PA-O2A
2	C	800	AGS	C5'-O5'-PA-O2A
2	B	800	AGS	C5'-O5'-PA-O3A
2	A	800	AGS	C5'-O5'-PA-O3A
2	F	800	AGS	C5'-O5'-PA-O3A
2	E	800	AGS	C5'-O5'-PA-O3A
2	D	800	AGS	C5'-O5'-PA-O3A
2	C	800	AGS	C5'-O5'-PA-O3A
2	B	800	AGS	C5'-O5'-PA-O2A
2	A	800	AGS	C5'-O5'-PA-O2A
2	F	800	AGS	C5'-O5'-PA-O2A
2	E	800	AGS	C5'-O5'-PA-O2A
2	D	800	AGS	C5'-O5'-PA-O1A
2	C	800	AGS	C5'-O5'-PA-O1A
2	F	800	AGS	PG-O3B-PB-O2B
2	B	800	AGS	PG-O3B-PB-O2B
2	A	800	AGS	PG-O3B-PB-O2B
2	E	800	AGS	PG-O3B-PB-O2B
2	D	800	AGS	PG-O3B-PB-O2B
2	C	800	AGS	PG-O3B-PB-O2B

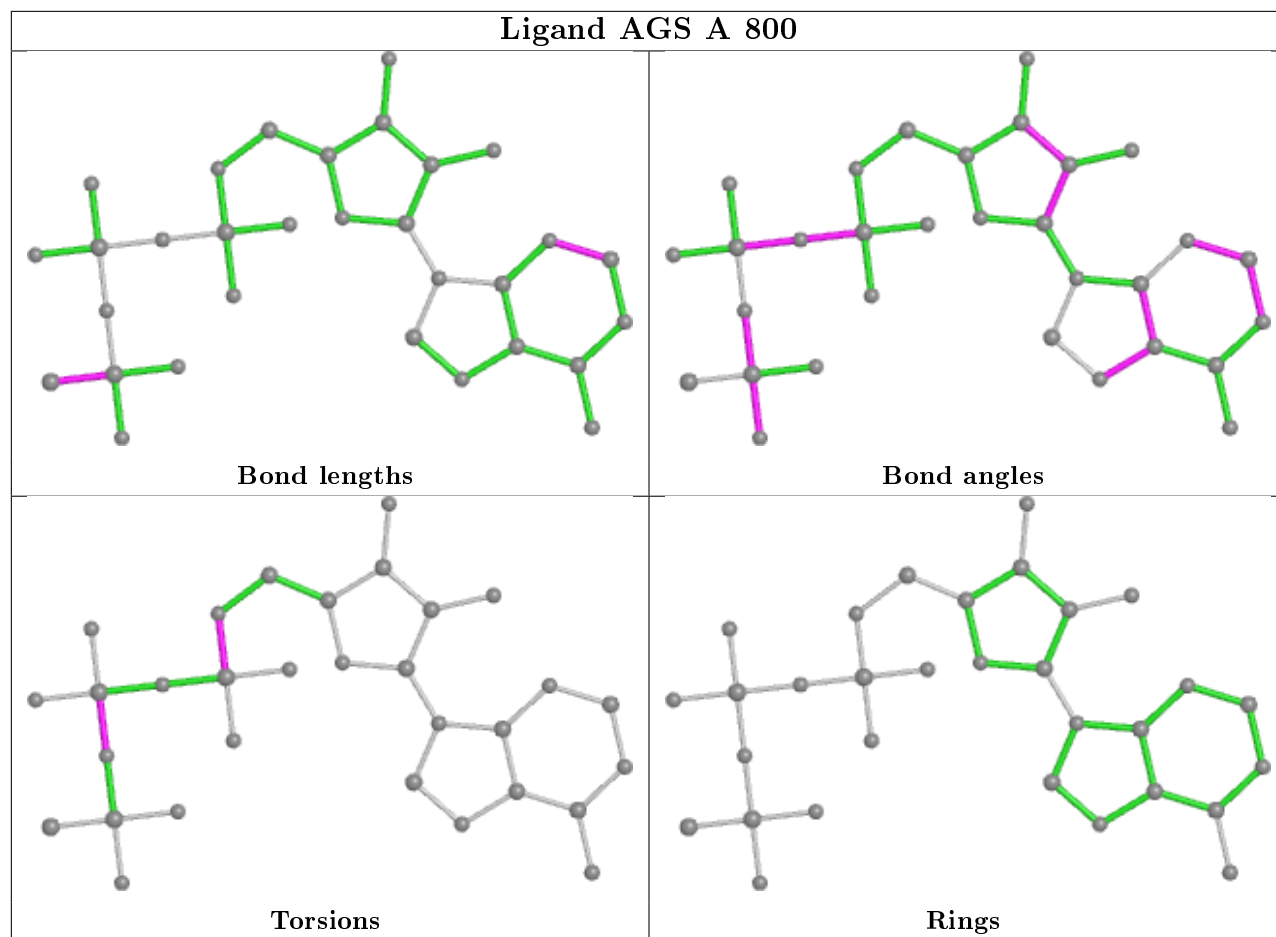
There are no ring outliers.

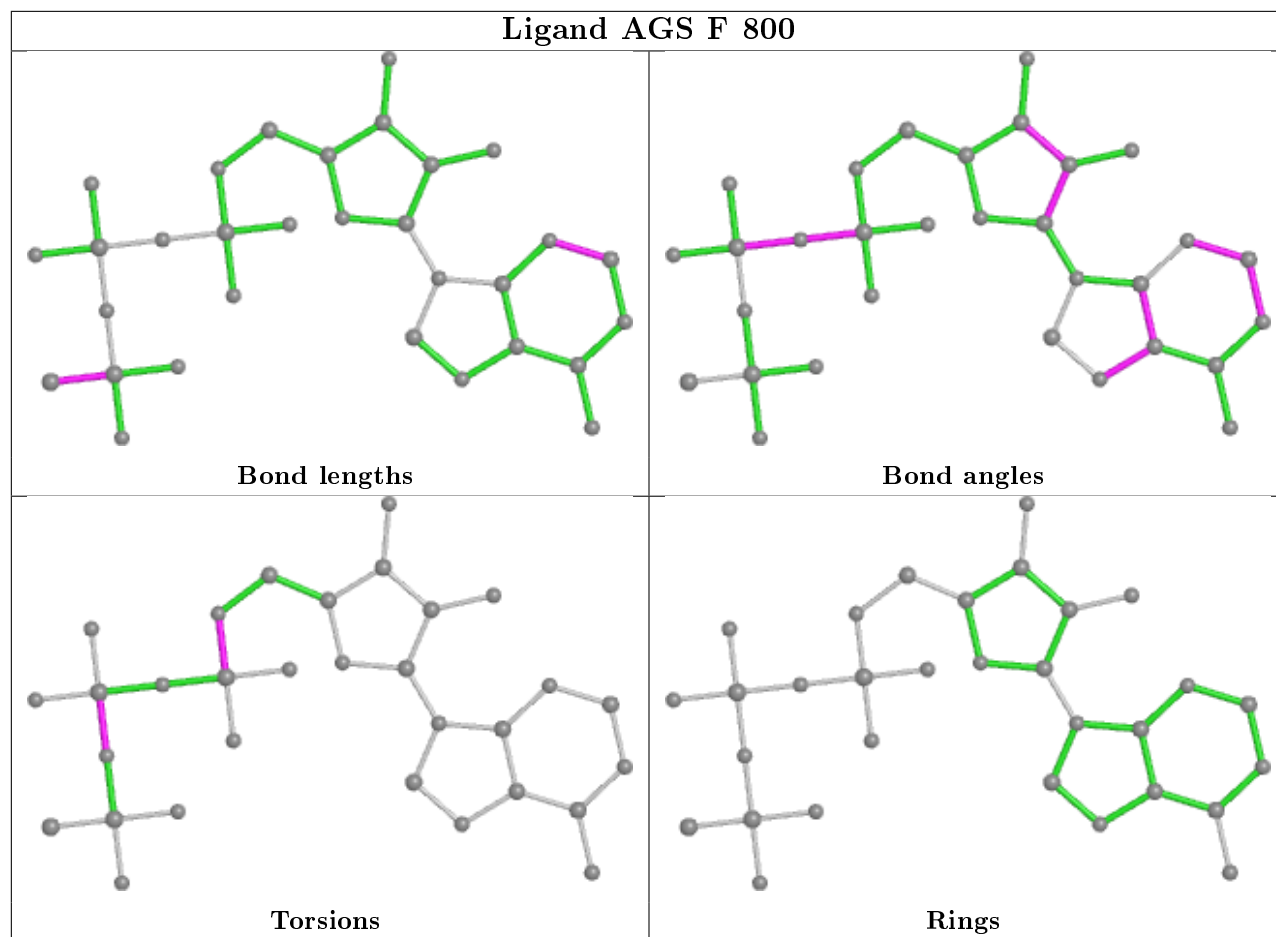
6 monomers are involved in 6 short contacts:

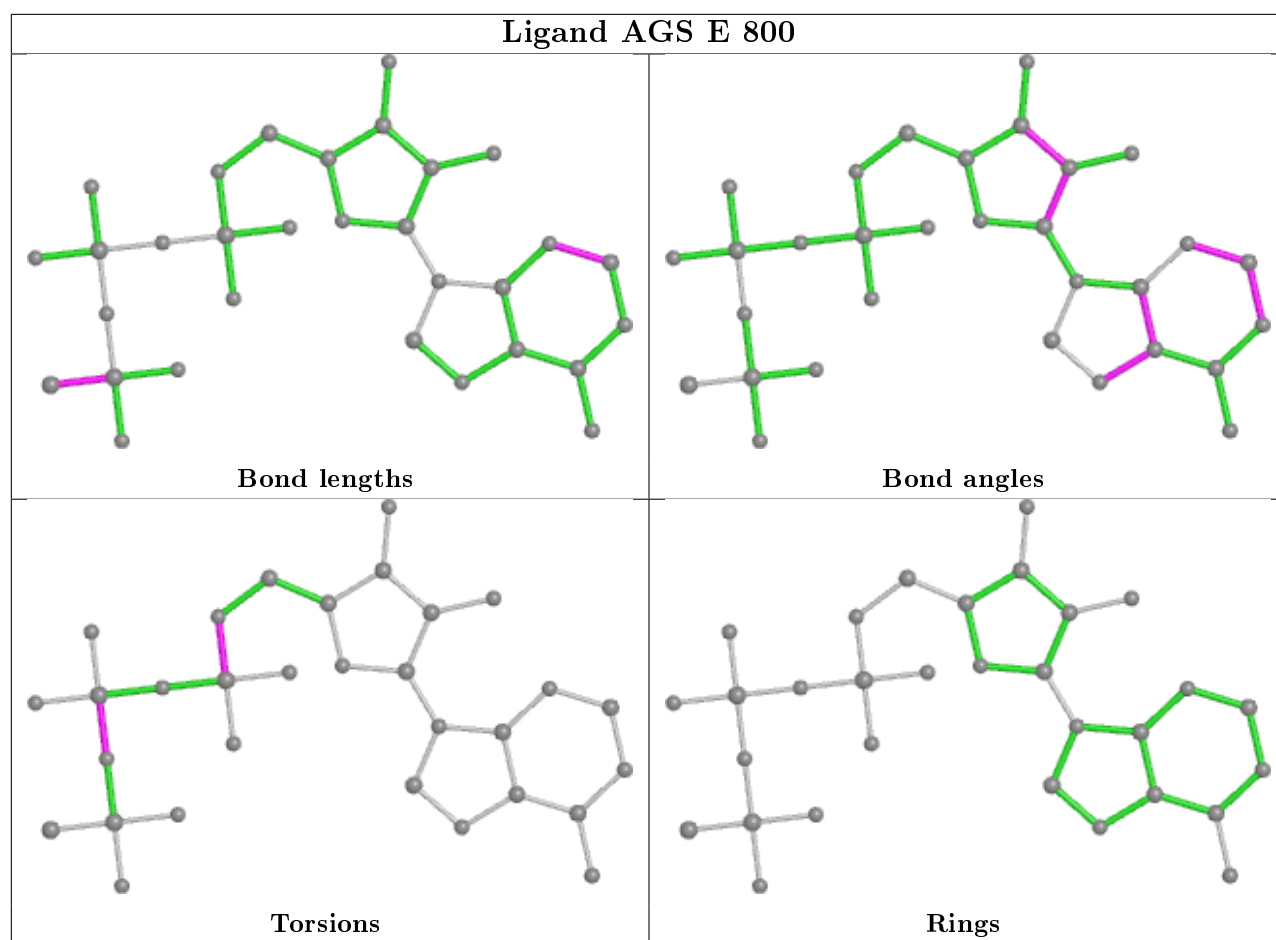
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	AGS	1	0
2	A	800	AGS	1	0
2	F	800	AGS	1	0
2	E	800	AGS	1	0
2	D	800	AGS	1	0
2	C	800	AGS	1	0

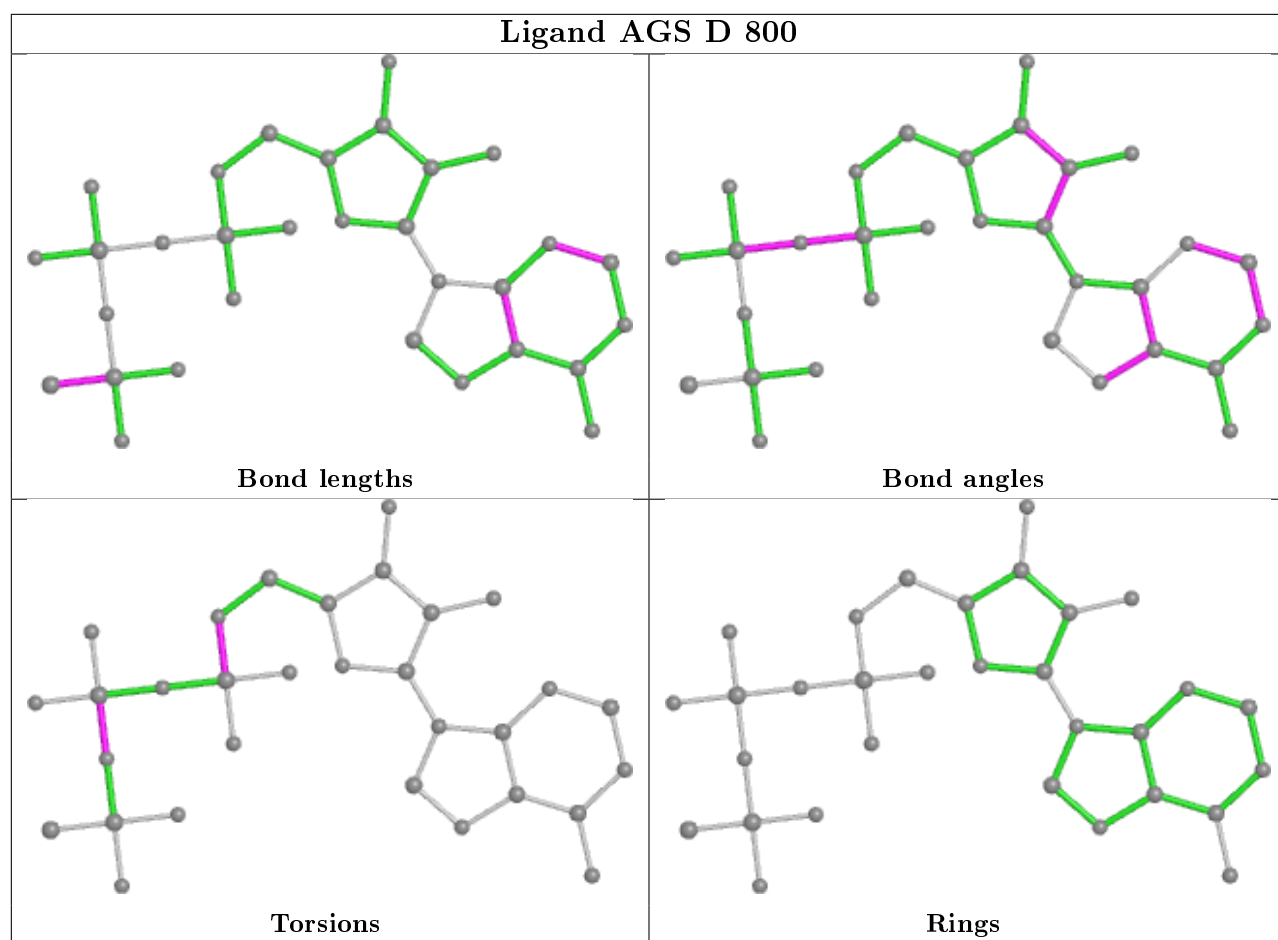
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

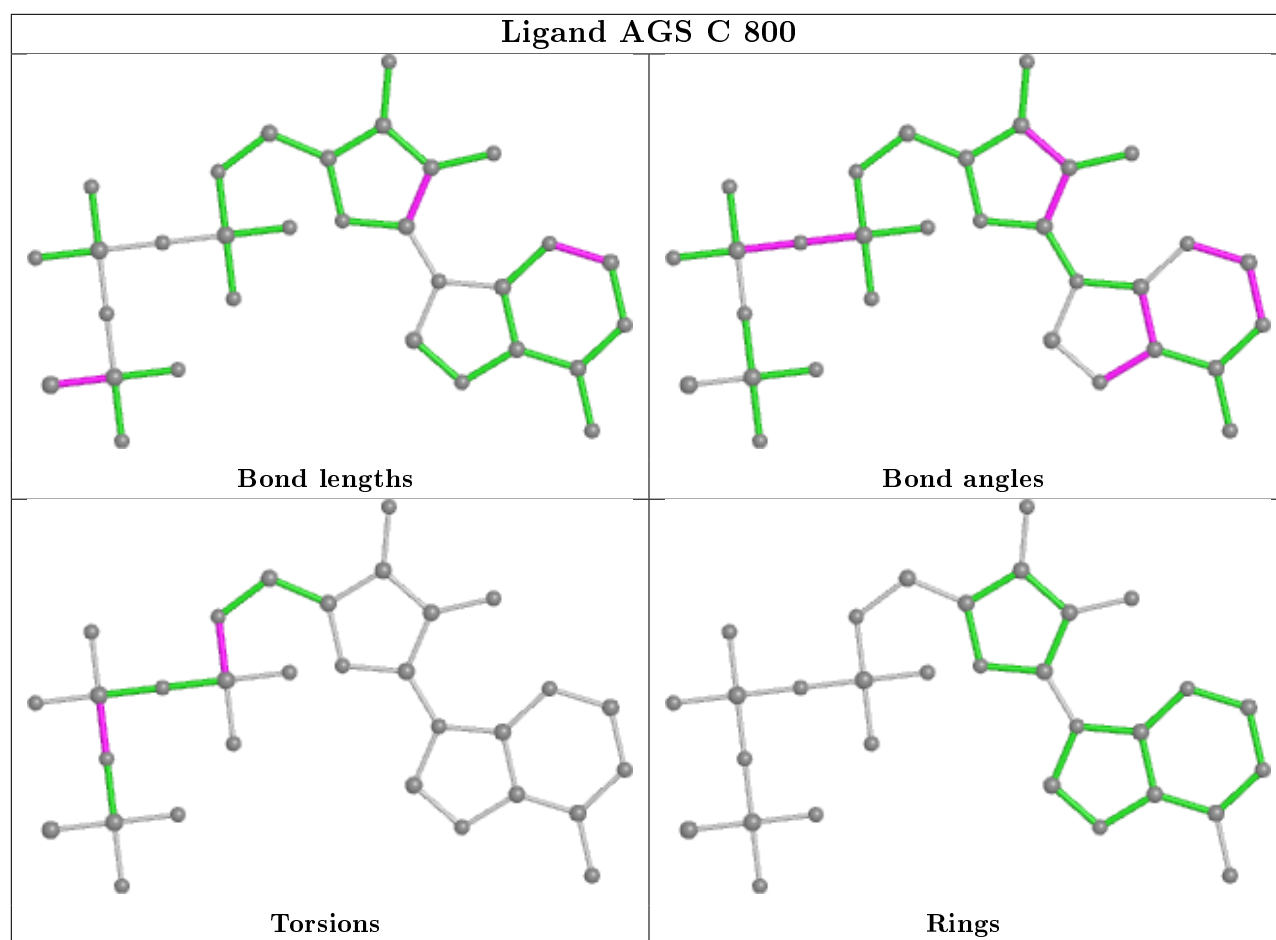












5.7 Other polymers [i](#)

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	452/489 (92%)	0.24	16 (3%)	44	38	68, 71, 73, 84	0
1	B	452/489 (92%)	0.31	22 (4%)	29	25	68, 71, 73, 81	0
1	C	452/489 (92%)	0.25	18 (3%)	38	32	68, 71, 73, 81	0
1	D	452/489 (92%)	0.40	33 (7%)	15	11	68, 71, 73, 80	0
1	E	452/489 (92%)	0.42	30 (6%)	18	14	68, 71, 73, 83	0
1	F	452/489 (92%)	0.23	14 (3%)	49	44	68, 71, 73, 80	0
All	All	2712/2934 (92%)	0.31	133 (4%)	29	25	68, 71, 73, 84	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	MET	6.1
1	D	32	ILE	6.0
1	C	158	MET	5.5
1	D	188	PRO	5.2
1	E	52	PHE	5.1
1	F	158	MET	4.9
1	C	126	ILE	4.8
1	D	126	ILE	4.7
1	D	187	GLU	4.6
1	F	32	ILE	4.5
1	A	463	ALA	4.3
1	B	32	ILE	4.2
1	E	463	ALA	4.1
1	E	158	MET	4.0
1	B	463	ALA	3.9
1	B	126	ILE	3.8
1	D	52	PHE	3.7
1	C	32	ILE	3.7
1	E	315	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	19	GLN	3.6
1	A	127	THR	3.6
1	C	187	GLU	3.6
1	E	53	ARG	3.5
1	A	72	LEU	3.5
1	D	27	ILE	3.4
1	A	315	LYS	3.4
1	A	128	GLY	3.4
1	E	112	LYS	3.3
1	D	113	ARG	3.3
1	E	462	SER	3.3
1	C	14	THR	3.1
1	E	80	GLU	3.1
1	D	463	ALA	3.1
1	C	52	PHE	3.1
1	E	114	ILE	3.1
1	C	315	LYS	3.0
1	E	128	GLY	3.0
1	E	21	ASN	3.0
1	D	127	THR	2.9
1	F	141	GLU	2.9
1	D	338	ARG	2.9
1	D	117	LEU	2.9
1	E	120	ASP	2.9
1	E	179	ASP	2.9
1	B	80	GLU	2.9
1	B	315	LYS	2.9
1	B	158	MET	2.9
1	D	128	GLY	2.9
1	C	463	ALA	2.9
1	E	32	ILE	2.8
1	A	32	ILE	2.8
1	D	129	ASN	2.7
1	E	27	ILE	2.7
1	D	106	PRO	2.7
1	F	171	SER	2.7
1	E	51	LEU	2.6
1	A	41	LEU	2.6
1	E	72	LEU	2.6
1	E	157	GLY	2.6
1	A	78	SER	2.6
1	C	15	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	104	PRO	2.6
1	D	78	SER	2.5
1	C	125	GLY	2.5
1	E	127	THR	2.5
1	B	314	GLU	2.5
1	D	186	GLY	2.5
1	D	104	PRO	2.5
1	B	26	LEU	2.5
1	B	51	LEU	2.5
1	D	99	VAL	2.5
1	C	12	LEU	2.5
1	E	23	PRO	2.5
1	D	71	VAL	2.5
1	B	52	PHE	2.5
1	A	52	PHE	2.5
1	D	132	GLU	2.4
1	E	173	TYR	2.4
1	A	171	SER	2.4
1	B	19	GLN	2.4
1	D	19	GLN	2.4
1	E	141	GLU	2.3
1	B	75	ASP	2.3
1	B	462	SER	2.3
1	B	49	LEU	2.3
1	B	195	GLU	2.3
1	D	80	GLU	2.3
1	C	461	PRO	2.3
1	E	110	TYR	2.3
1	F	112	LYS	2.3
1	B	27	ILE	2.3
1	C	188	PRO	2.3
1	C	171	SER	2.2
1	F	47	ASP	2.2
1	E	106	PRO	2.2
1	A	27	ILE	2.2
1	F	109	LYS	2.2
1	F	126	ILE	2.2
1	A	50	GLN	2.2
1	E	187	GLU	2.2
1	F	72	LEU	2.2
1	A	51	LEU	2.2
1	E	171	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	115	HIS	2.2
1	B	53	ARG	2.2
1	D	190	LYS	2.1
1	E	178	PRO	2.1
1	E	174	CYS	2.1
1	D	163	PHE	2.1
1	D	199	ASN	2.1
1	C	106	PRO	2.1
1	B	338	ARG	2.1
1	D	51	LEU	2.1
1	A	80	GLU	2.1
1	B	82	ILE	2.1
1	E	126	ILE	2.1
1	C	112	LYS	2.1
1	D	118	PRO	2.1
1	F	104	PRO	2.1
1	F	163	PHE	2.1
1	F	159	ARG	2.1
1	B	78	SER	2.0
1	B	395	ASP	2.0
1	A	109	LYS	2.0
1	D	159	ARG	2.0
1	D	102	ILE	2.0
1	C	53	ARG	2.0
1	F	152	PHE	2.0
1	F	338	ARG	2.0
1	D	157	GLY	2.0
1	C	462	SER	2.0
1	D	173	TYR	2.0
1	B	106	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

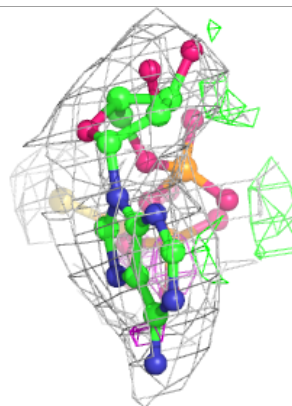
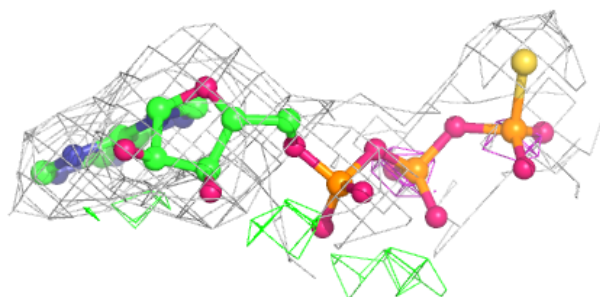
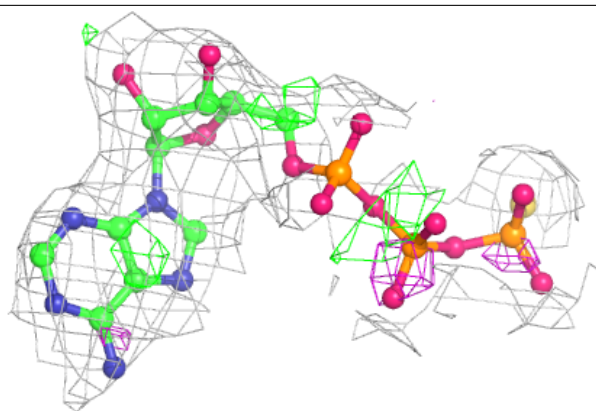
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	801	1/1	0.94	0.12	61,61,61,61	0
3	MG	A	801	1/1	0.95	0.13	61,61,61,61	0
3	MG	D	801	1/1	0.96	0.15	61,61,61,61	0
2	AGS	A	800	31/31	0.97	0.14	60,66,68,72	0
3	MG	F	801	1/1	0.97	0.08	61,61,61,61	0
2	AGS	F	800	31/31	0.97	0.12	60,66,68,71	0
2	AGS	E	800	31/31	0.97	0.12	60,66,68,71	0
2	AGS	D	800	31/31	0.97	0.13	61,66,68,71	0
2	AGS	C	800	31/31	0.97	0.11	60,66,68,71	0
3	MG	C	801	1/1	0.98	0.03	61,61,61,61	0
3	MG	E	801	1/1	0.98	0.08	60,60,60,60	0
2	AGS	B	800	31/31	0.98	0.12	60,66,68,71	0

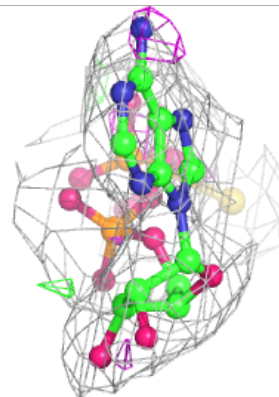
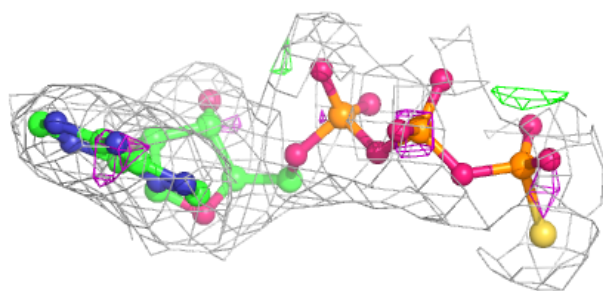
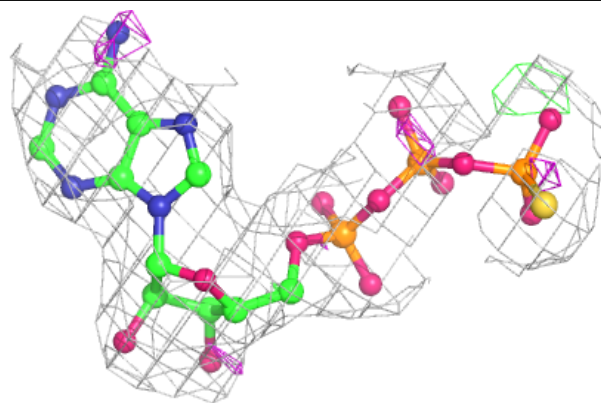
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS A 800:

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

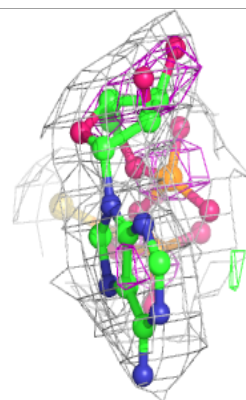
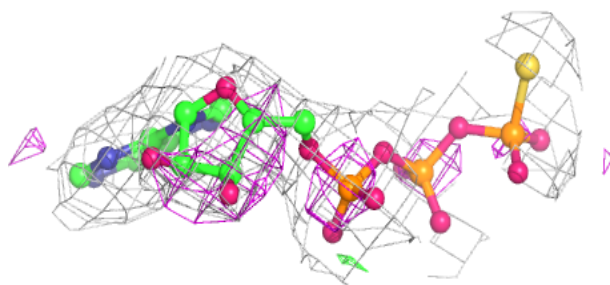
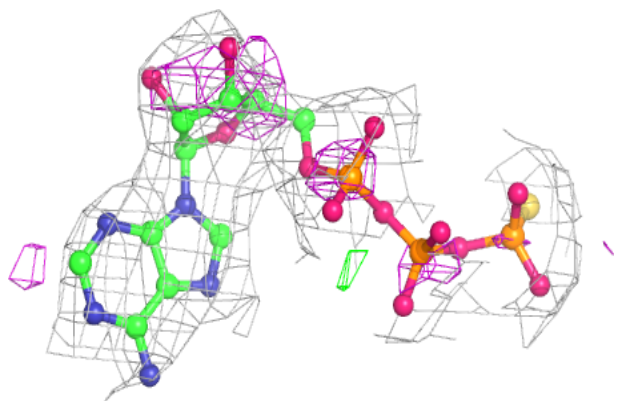
**Electron density around AGS F 800:**

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

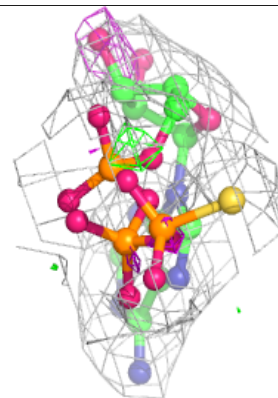
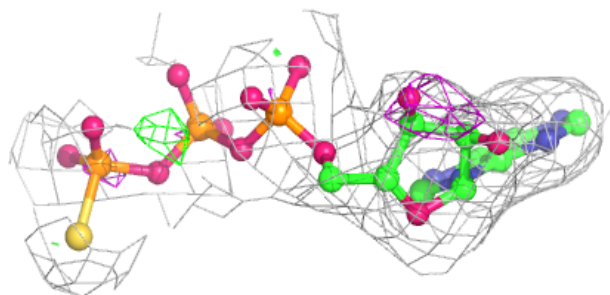
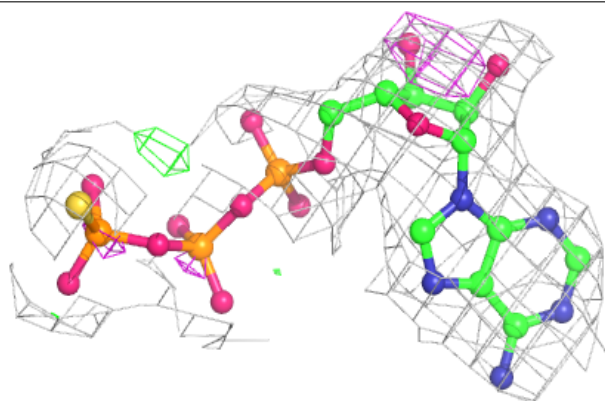


Electron density around AGS E 800:

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

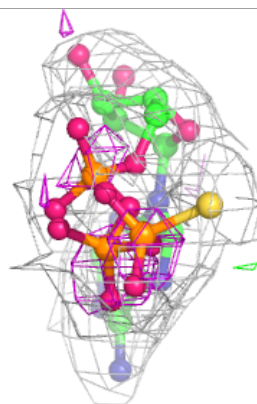
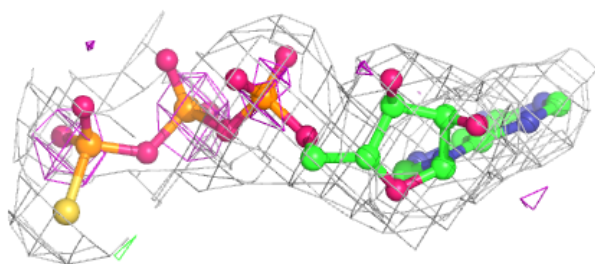
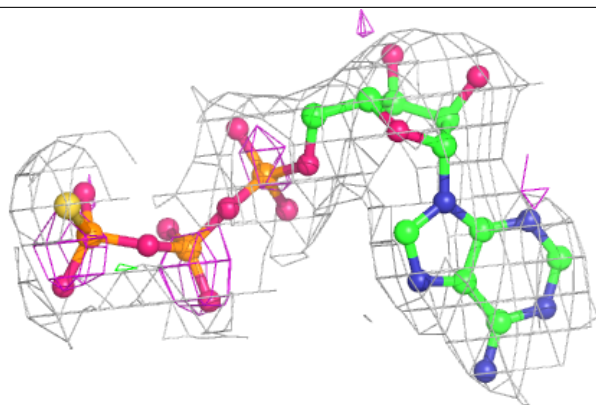
**Electron density around AGS D 800:**

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

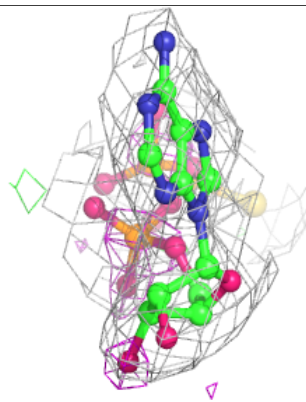
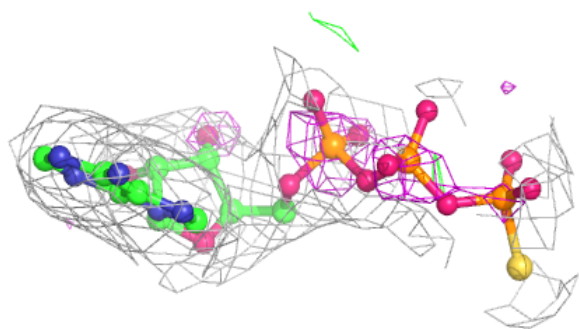
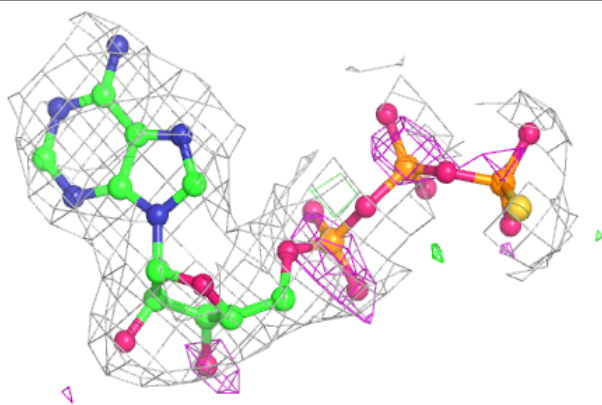


Electron density around AGS C 800:

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

**Electron density around AGS B 800:**

$2mF_o-DF_c$ (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.