



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 08:20 PM EST

PDB ID : 6QV2  
Title : Structure of ATPgS-bound outward-facing TM287/288 in complex with nanobody Nb\_TM#2  
Authors : Hutter, C.A.J.; Huerlimann, L.M.; Zimmermann, I.; Egloff, P.; Seeger, M.A.  
Deposited on : 2019-03-01  
Resolution : 4.23 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

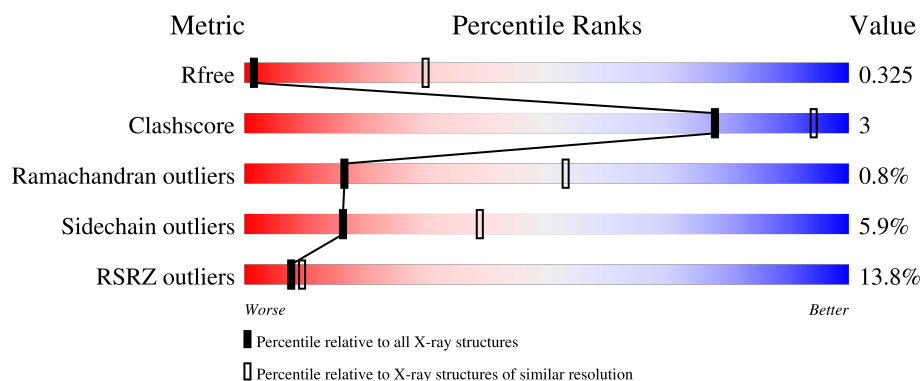
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.23 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))
$R_{free}$	164625	1004 (4.62-3.86)
Clashscore	180529	1022 (4.60-3.88)
Ramachandran outliers	177936	1021 (4.66-3.82)
Sidechain outliers	177891	1006 (4.66-3.82)
RSRZ outliers	164620	1002 (4.62-3.86)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	587	<div> <div>15%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>
1	C	587	<div> <div>17%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
2	B	599	<div> <div>9%</div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div>
2	D	599	<div> <div>10%</div> <div>83%</div> <div>12%</div> <div>• 5%</div> </div>
3	E	132	<div> <div>17%</div> <div>76%</div> <div>21%</div> <div>••</div> </div>
3	F	132	<div> <div>20%</div> <div>79%</div> <div>18%</div> <div>••</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20086 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 ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	19			
1	C	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9WYC3
A	-8	PRO	-	expression tag	UNP Q9WYC3
A	-7	SER	-	expression tag	UNP Q9WYC3
A	-6	GLY	-	expression tag	UNP Q9WYC3
A	-5	SER	-	expression tag	UNP Q9WYC3
A	-4	GLY	-	expression tag	UNP Q9WYC3
A	-3	GLY	-	expression tag	UNP Q9WYC3
A	-2	GLY	-	expression tag	UNP Q9WYC3
A	-1	GLY	-	expression tag	UNP Q9WYC3
A	0	GLY	-	expression tag	UNP Q9WYC3
A	1	SER	-	expression tag	UNP Q9WYC3
A	41	ALA	ASP	engineered mutation	UNP Q9WYC3
C	-9	GLY	-	expression tag	UNP Q9WYC3
C	-8	PRO	-	expression tag	UNP Q9WYC3
C	-7	SER	-	expression tag	UNP Q9WYC3
C	-6	GLY	-	expression tag	UNP Q9WYC3
C	-5	SER	-	expression tag	UNP Q9WYC3
C	-4	GLY	-	expression tag	UNP Q9WYC3
C	-3	GLY	-	expression tag	UNP Q9WYC3
C	-2	GLY	-	expression tag	UNP Q9WYC3
C	-1	GLY	-	expression tag	UNP Q9WYC3
C	0	GLY	-	expression tag	UNP Q9WYC3
C	1	SER	-	expression tag	UNP Q9WYC3
C	41	ALA	ASP	engineered mutation	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM\_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			
2	D	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			

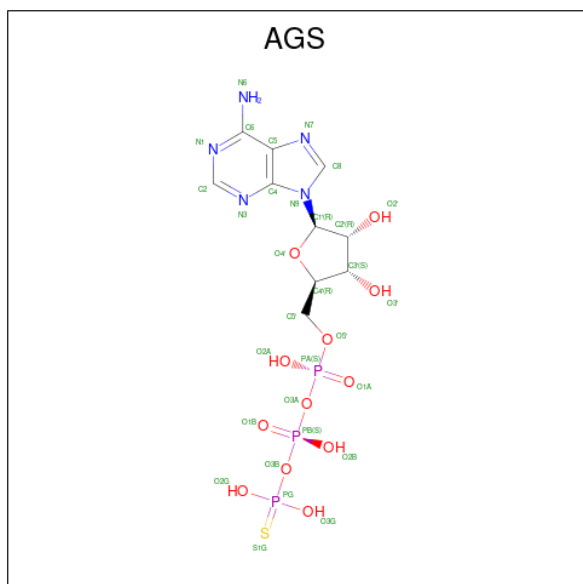
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	ALA	ASP	engineered mutation	UNP Q9WYC4
B	517	ALA	GLU	engineered mutation	UNP Q9WYC4
B	599	ALA	-	expression tag	UNP Q9WYC4
D	65	ALA	ASP	engineered mutation	UNP Q9WYC4
D	517	ALA	GLU	engineered mutation	UNP Q9WYC4
D	599	ALA	-	expression tag	UNP Q9WYC4

- Molecule 3 is a protein called Nb\_TM No.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	129	Total	C	N	O	S	0	0	0
			974	611	164	193	6			
3	F	129	Total	C	N	O	S	0	0	0
			974	611	164	193	6			

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



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

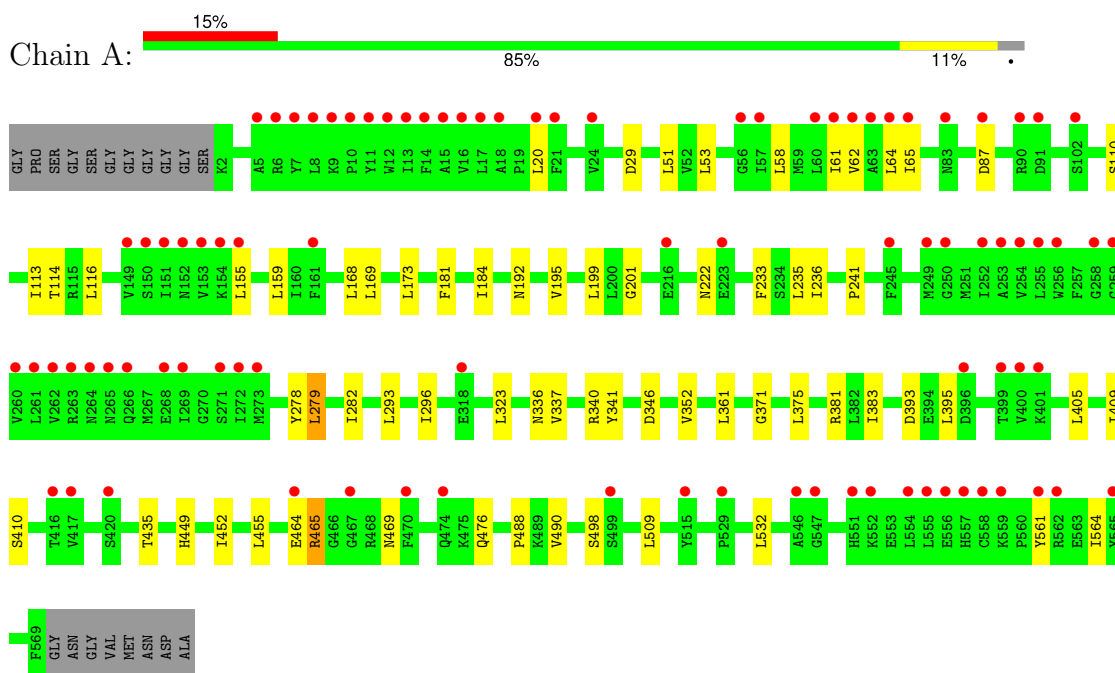
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

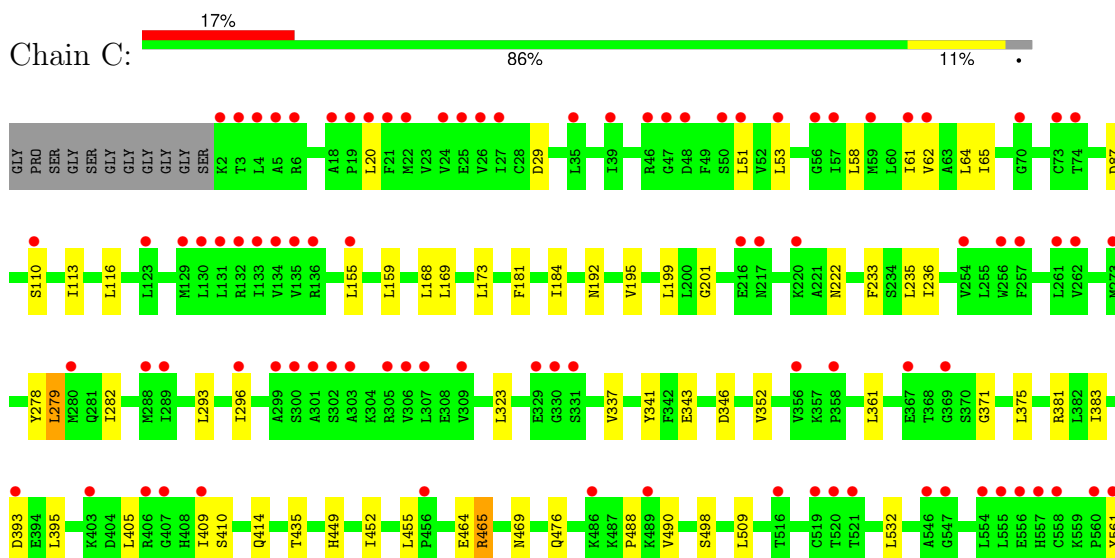
### 3 Residue-property plots [i](#)

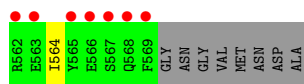
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: ABC transporter, ATP-binding protein

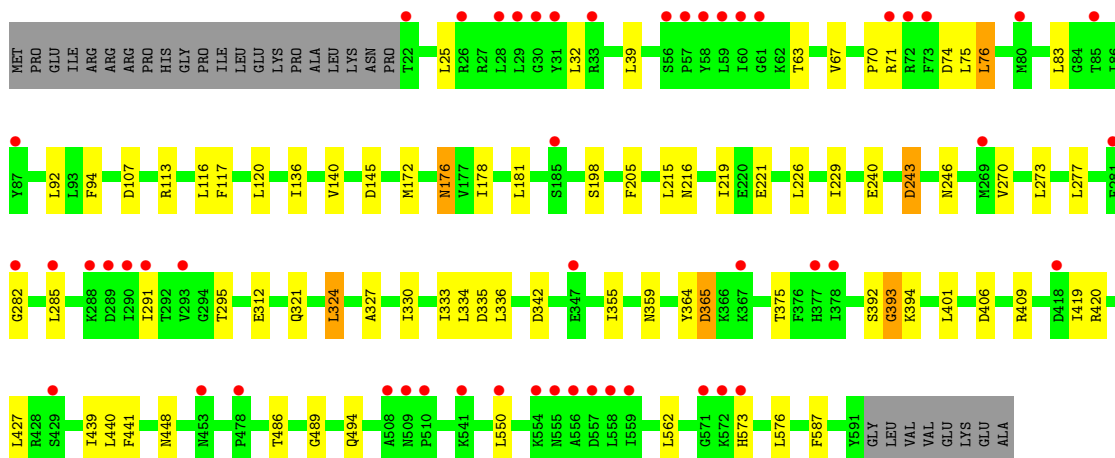
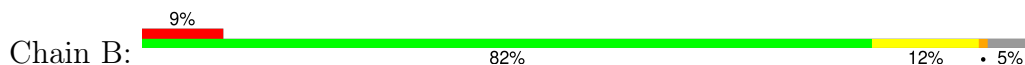


- Molecule 1: ABC transporter, ATP-binding protein

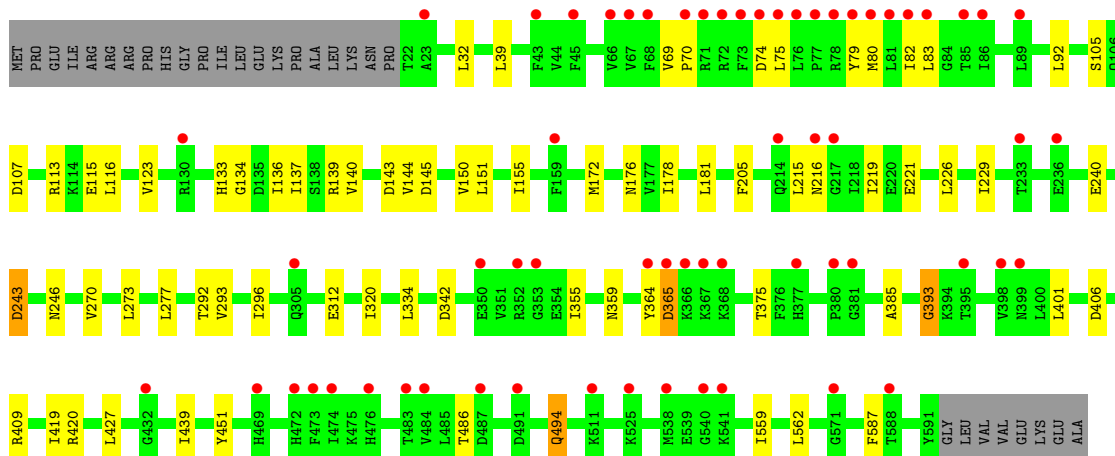
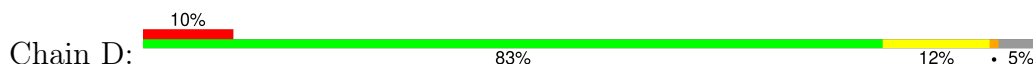




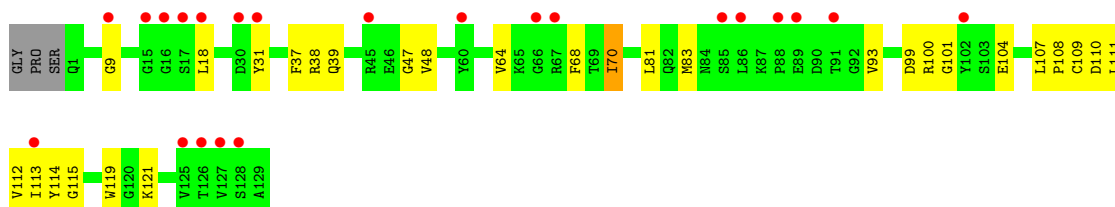
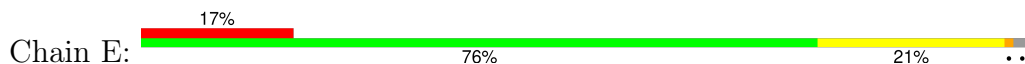
• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM\_0288



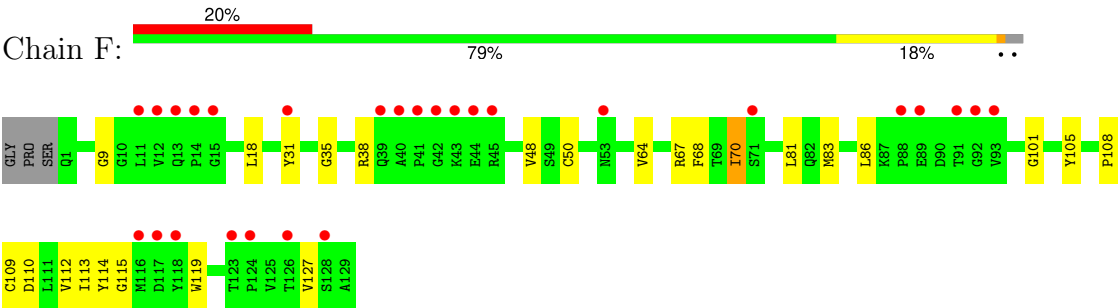
• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM\_0288



• Molecule 3: Nb\_TM No.2



● Molecule 3: Nb\_TM No.2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.60Å 113.07Å 126.89Å 83.18° 73.00° 67.37°	Depositor
Resolution (Å)	32.59 – 4.23 32.59 – 4.23	Depositor EDS
% Data completeness (in resolution range)	57.9 (32.59-4.23) 58.4 (32.59-4.23)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 4.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.306 , 0.330 0.343 , 0.325	Depositor DCC
$R_{free}$ test set	919 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	129.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.018 for -h,-h+k,-l	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	20086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.39	0/4539	0.53	0/6139
1	C	0.40	0/4539	0.53	0/6139
2	B	0.40	0/4619	0.55	0/6245
2	D	0.40	0/4619	0.55	0/6245
3	E	0.38	0/995	0.59	0/1345
3	F	0.40	0/995	0.59	0/1345
All	All	0.40	0/20306	0.55	0/27458

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	4464	0	4666	21	0
1	C	4464	0	4666	22	0
2	B	4541	0	4724	32	0
2	D	4541	0	4724	31	0
3	E	974	0	934	8	0
3	F	974	0	934	9	0
4	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	2	0
4	C	31	0	12	0	0
4	D	31	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	20086	0	20696	108	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 3.

All (108) 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)
3:F:38:ARG:HG2	3:F:48:VAL:HG22	1.79	0.64
2:D:216:ASN:HA	2:D:219:ILE:HD12	1.87	0.56
2:B:32:LEU:HB3	2:B:39:LEU:HD11	1.89	0.55
2:D:32:LEU:HB3	2:D:39:LEU:HD11	1.89	0.55
2:B:216:ASN:HA	2:B:219:ILE:HD12	1.89	0.55
3:E:9:GLY:HA2	3:E:18:LEU:HD22	1.89	0.55
2:B:198:SER:HB2	2:B:321:GLN:HG3	1.88	0.54
2:B:117:PHE:HA	2:B:120:LEU:HD12	1.89	0.54
1:C:465:ARG:HG3	2:D:221:GLU:HG3	1.89	0.54
2:B:176:ASN:HD21	2:B:291:ILE:HD13	1.73	0.54
1:C:199:LEU:HB3	2:D:133:HIS:HD2	1.73	0.53
3:F:9:GLY:HA2	3:F:18:LEU:HD22	1.91	0.53
1:A:465:ARG:HG3	2:B:221:GLU:HG3	1.91	0.52
2:B:333:ILE:HA	2:B:336:LEU:HD12	1.91	0.52
3:E:38:ARG:HG2	3:E:48:VAL:HG22	1.92	0.52
1:A:476:GLN:HE22	1:A:498:SER:H	1.58	0.52
2:B:226:LEU:HA	2:B:229:ILE:HD12	1.91	0.52
1:C:561:TYR:HA	1:C:564:ILE:HD12	1.92	0.52
3:E:37:PHE:HA	3:E:47:GLY:HA2	1.92	0.51
1:C:201:GLY:HA3	2:D:439:ILE:HG21	1.92	0.51
1:C:476:GLN:HE22	1:C:498:SER:H	1.58	0.51
1:A:561:TYR:HA	1:A:564:ILE:HD12	1.93	0.51
2:D:226:LEU:HA	2:D:229:ILE:HD12	1.91	0.51
2:D:150:VAL:HG23	2:D:320:ILE:HG22	1.93	0.51
1:A:201:GLY:HA3	2:B:439:ILE:HG21	1.92	0.50
2:D:113:ARG:HG3	2:D:144:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:35:GLY:HA3	3:F:50:CYS:HA	1.93	0.50
1:A:233:PHE:HA	1:A:236:ILE:HD12	1.94	0.50
2:D:365:ASP:HB3	4:D:600:AGS:H2	1.93	0.50
3:E:100:ARG:HB2	3:E:111:LEU:HD23	1.92	0.50
1:A:199:LEU:HD21	2:B:136:ILE:HD13	1.94	0.50
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.94	0.50
2:B:365:ASP:HB3	4:B:600:AGS:H2	1.93	0.50
3:F:70:ILE:HG23	3:F:81:LEU:HD23	1.95	0.49
1:C:181:PHE:HA	1:C:184:ILE:HD12	1.94	0.49
1:A:181:PHE:HA	1:A:184:ILE:HD12	1.94	0.49
3:F:64:VAL:HG13	3:F:67:ARG:HH11	1.78	0.48
3:E:70:ILE:HG23	3:E:81:LEU:HD23	1.96	0.48
1:A:222:ASN:HD21	2:B:113:ARG:HB3	1.77	0.48
1:A:464:GLU:HB2	1:A:469:ASN:HB3	1.95	0.48
1:A:279:LEU:HA	1:A:282:ILE:HD12	1.96	0.48
2:B:355:ILE:HD12	2:B:401:LEU:HD11	1.96	0.48
1:C:279:LEU:HA	1:C:282:ILE:HD12	1.95	0.48
2:D:79:TYR:HA	2:D:82:ILE:HD12	1.95	0.48
2:D:293:VAL:HA	2:D:296:ILE:HD12	1.96	0.48
1:C:464:GLU:HB2	1:C:469:ASN:HB3	1.95	0.47
2:D:355:ILE:HD12	2:D:401:LEU:HD11	1.96	0.47
1:C:337:VAL:HB	1:C:352:VAL:HB	1.96	0.47
1:A:337:VAL:HB	1:A:352:VAL:HB	1.96	0.47
1:C:199:LEU:HD21	2:D:136:ILE:HD13	1.98	0.46
2:D:409:ARG:HD2	3:F:105:TYR:HB2	1.98	0.46
2:D:105:SER:HA	2:D:151:LEU:HD22	1.99	0.45
2:B:67:VAL:HG13	2:B:70:PRO:HG2	1.98	0.45
2:B:441:PHE:H	2:B:448:ASN:HD21	1.64	0.45
1:C:410:SER:HB2	1:C:488:PRO:HG3	1.98	0.45
1:A:195:VAL:HG21	2:B:140:VAL:HG21	1.98	0.45
1:A:62:VAL:HA	1:A:65:ILE:HD12	1.98	0.45
2:D:80:MET:HA	2:D:83:LEU:HD12	1.98	0.45
2:B:327:ALA:HA	2:B:330:ILE:HD12	1.99	0.45
2:B:440:LEU:HD22	2:B:489:GLY:HA3	1.98	0.45
1:A:410:SER:HB2	1:A:488:PRO:HG3	1.98	0.45
3:E:39:GLN:HB2	3:E:93:VAL:O	2.17	0.45
1:A:409:ILE:HG12	1:A:490:VAL:HB	1.98	0.45
1:A:449:HIS:HA	1:A:452:ILE:HD12	1.99	0.45
1:C:293:LEU:HA	1:C:296:ILE:HD12	1.99	0.44
1:C:409:ILE:HG12	1:C:490:VAL:HB	1.98	0.44
1:C:449:HIS:HA	1:C:452:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:VAL:HA	2:D:273:LEU:HD12	1.98	0.44
2:B:419:ILE:HG23	2:B:420:ARG:HD3	2.00	0.44
1:C:62:VAL:HA	1:C:65:ILE:HD12	1.98	0.44
2:D:385:ALA:HB3	2:D:559:ILE:HG12	1.99	0.44
2:B:282:GLY:HA2	2:B:285:LEU:HD12	2.00	0.44
1:C:195:VAL:HG21	2:D:140:VAL:HG21	1.99	0.44
1:C:222:ASN:HD21	2:D:113:ARG:HB3	1.83	0.44
2:D:419:ILE:HG23	2:D:420:ARG:HD3	1.99	0.44
1:A:293:LEU:HA	1:A:296:ILE:HD12	1.99	0.44
2:B:270:VAL:HA	2:B:273:LEU:HD12	1.98	0.44
3:E:64:VAL:HB	3:E:68:PHE:CE2	2.53	0.44
2:B:67:VAL:HG11	2:B:76:LEU:HB2	2.00	0.43
2:B:25:LEU:HB2	2:B:324:LEU:HD21	1.99	0.42
2:B:409:ARG:HD3	3:E:107:LEU:HG	2.00	0.42
2:D:115:GLU:HB3	2:D:334:LEU:HD21	2.01	0.42
2:B:178:ILE:HA	2:B:181:LEU:HD12	2.01	0.42
1:A:452:ILE:HA	1:A:455:LEU:HD12	2.02	0.42
2:D:139:ARG:HA	2:D:143:ASP:HB2	2.00	0.42
2:B:63:THR:HG21	2:B:83:LEU:HD11	2.02	0.42
1:C:452:ILE:HA	1:C:455:LEU:HD12	2.02	0.42
1:C:110:SER:HA	1:C:113:ILE:HD12	2.02	0.42
2:D:178:ILE:HA	2:D:181:LEU:HD12	2.01	0.42
1:A:110:SER:HA	1:A:113:ILE:HD12	2.01	0.41
2:D:151:LEU:HA	2:D:155:ILE:HD12	2.03	0.41
2:D:134:GLY:HA2	2:D:137:ILE:HD12	2.03	0.41
2:B:392:SER:HB3	2:B:394:LYS:HZ3	1.86	0.41
1:C:58:LEU:HA	1:C:61:ILE:HD12	2.01	0.41
2:B:359:ASN:H	2:B:375:THR:HB	1.86	0.41
2:B:573:HIS:HA	2:B:576:LEU:HD12	2.03	0.41
1:A:58:LEU:HA	1:A:61:ILE:HD12	2.01	0.41
2:D:359:ASN:H	2:D:375:THR:HB	1.86	0.41
3:F:38:ARG:HH12	3:F:83:MET:HG2	1.85	0.41
3:F:86:LEU:HD13	3:F:127:VAL:HG11	2.02	0.41
1:C:414:GLN:HB3	2:D:494:GLN:HG3	2.03	0.41
1:A:241:PRO:HB3	2:B:94:PHE:HB3	2.02	0.40
2:D:393:GLY:HA2	4:D:600:AGS:H5'1	2.03	0.40
2:D:69:VAL:HB	2:D:70:PRO:HD3	2.03	0.40
2:D:240:GLU:HA	2:D:243:ASP:HB2	2.03	0.40
2:B:240:GLU:HA	2:B:243:ASP:HB2	2.03	0.40
2:B:393:GLY:HA2	4:B:600:AGS:H5'1	2.04	0.40
3:F:68:PHE:HB3	3:F:81:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/587 (96%)	544 (96%)	19 (3%)	3 (0%)	25	63
1	C	566/587 (96%)	542 (96%)	22 (4%)	2 (0%)	30	67
2	B	568/599 (95%)	541 (95%)	24 (4%)	3 (0%)	25	63
2	D	568/599 (95%)	540 (95%)	26 (5%)	2 (0%)	30	67
3	E	127/132 (96%)	93 (73%)	28 (22%)	6 (5%)	2	17
3	F	127/132 (96%)	94 (74%)	28 (22%)	5 (4%)	2	20
All	All	2522/2636 (96%)	2354 (93%)	147 (6%)	21 (1%)	16	53

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	108	PRO
3	F	108	PRO
3	E	101	GLY
2	B	71	ARG
3	F	113	ILE
2	B	74	ASP
2	D	74	ASP
3	E	113	ILE
3	E	121	LYS
3	F	101	GLY
3	F	112	VAL
1	A	336	ASN
1	C	371	GLY
1	A	371	GLY
1	A	381	ARG
1	C	381	ARG
3	E	112	VAL

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Mol	Chain	Res	Type
3	F	115	GLY
2	B	393	GLY
2	D	393	GLY
3	E	115	GLY

### 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	494/503 (98%)	463 (94%)	31 (6%)	15	37
1	C	494/503 (98%)	464 (94%)	30 (6%)	15	38
2	B	506/531 (95%)	478 (94%)	28 (6%)	18	41
2	D	506/531 (95%)	481 (95%)	25 (5%)	21	43
3	E	102/104 (98%)	93 (91%)	9 (9%)	8	26
3	F	102/104 (98%)	96 (94%)	6 (6%)	16	39
All	All	2204/2276 (97%)	2075 (94%)	129 (6%)	16	39

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	29	ASP
1	A	51	LEU
1	A	53	LEU
1	A	64	LEU
1	A	87	ASP
1	A	114	THR
1	A	116	LEU
1	A	155	LEU
1	A	159	LEU
1	A	168	LEU
1	A	169	LEU
1	A	173	LEU
1	A	192	ASN

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	278	TYR
1	A	279	LEU
1	A	323	LEU
1	A	340	ARG
1	A	341	TYR
1	A	346	ASP
1	A	361	LEU
1	A	375	LEU
1	A	383	ILE
1	A	393	ASP
1	A	395	LEU
1	A	405	LEU
1	A	435	THR
1	A	465	ARG
1	A	509	LEU
1	A	532	LEU
2	B	75	LEU
2	B	76	LEU
2	B	92	LEU
2	B	107	ASP
2	B	116	LEU
2	B	145	ASP
2	B	172	MET
2	B	176	ASN
2	B	205	PHE
2	B	215	LEU
2	B	243	ASP
2	B	246	ASN
2	B	277	LEU
2	B	295	THR
2	B	312	GLU
2	B	324	LEU
2	B	334	LEU
2	B	335	ASP
2	B	342	ASP
2	B	364	TYR
2	B	365	ASP
2	B	406	ASP
2	B	427	LEU
2	B	486	THR
2	B	494	GLN

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Mol	Chain	Res	Type
2	B	550	LEU
2	B	562	LEU
2	B	587	PHE
1	C	20	LEU
1	C	29	ASP
1	C	51	LEU
1	C	53	LEU
1	C	64	LEU
1	C	87	ASP
1	C	116	LEU
1	C	155	LEU
1	C	159	LEU
1	C	168	LEU
1	C	169	LEU
1	C	173	LEU
1	C	192	ASN
1	C	235	LEU
1	C	278	TYR
1	C	279	LEU
1	C	323	LEU
1	C	341	TYR
1	C	343	GLU
1	C	346	ASP
1	C	361	LEU
1	C	375	LEU
1	C	383	ILE
1	C	393	ASP
1	C	395	LEU
1	C	405	LEU
1	C	435	THR
1	C	465	ARG
1	C	509	LEU
1	C	532	LEU
2	D	75	LEU
2	D	92	LEU
2	D	107	ASP
2	D	116	LEU
2	D	123	VAL
2	D	145	ASP
2	D	172	MET
2	D	176	ASN
2	D	205	PHE

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Mol	Chain	Res	Type
2	D	215	LEU
2	D	243	ASP
2	D	246	ASN
2	D	277	LEU
2	D	292	THR
2	D	312	GLU
2	D	342	ASP
2	D	364	TYR
2	D	365	ASP
2	D	406	ASP
2	D	427	LEU
2	D	451	TYR
2	D	486	THR
2	D	494	GLN
2	D	562	LEU
2	D	587	PHE
3	E	31	TYR
3	E	70	ILE
3	E	83	MET
3	E	99	ASP
3	E	104	GLU
3	E	109	CYS
3	E	110	ASP
3	E	114	TYR
3	E	119	TRP
3	F	31	TYR
3	F	70	ILE
3	F	109	CYS
3	F	110	ASP
3	F	114	TYR
3	F	119	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	GLN
2	B	176	ASN
2	B	268	ASN
2	B	377	HIS
2	B	448	ASN
2	B	488	ASN
2	B	521	ASN

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Mol	Chain	Res	Type
2	B	551	ASN
2	B	590	GLN
1	C	222	ASN
1	C	474	GLN
1	C	476	GLN
2	D	133	HIS
2	D	176	ASN
2	D	268	ASN
2	D	377	HIS
2	D	448	ASN
2	D	521	ASN
3	F	84	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	AGS	B	600	5	28,33,33	0.63	0	31,52,52	0.71	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	AGS	D	600	5	28,33,33	0.62	0	31,52,52	0.71	1 (3%)
4	AGS	C	600	5	28,33,33	0.63	0	31,52,52	0.63	1 (3%)
4	AGS	A	600	5	28,33,33	0.63	0	31,52,52	0.65	1 (3%)

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	B	600	5	-	5/17/38/38	0/3/3/3
4	AGS	D	600	5	-	5/17/38/38	0/3/3/3
4	AGS	C	600	5	-	0/17/38/38	0/3/3/3
4	AGS	A	600	5	-	3/17/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	AGS	C5-C6-N6	2.29	123.80	120.31
4	D	600	AGS	C5-C6-N6	2.27	123.77	120.31
4	B	600	AGS	C5-C6-N6	2.27	123.76	120.31
4	C	600	AGS	C5-C6-N6	2.23	123.72	120.31

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	AGS	C5'-O5'-PA-O1A
4	B	600	AGS	C5'-O5'-PA-O3A
4	D	600	AGS	C5'-O5'-PA-O1A
4	D	600	AGS	C5'-O5'-PA-O3A
4	B	600	AGS	C5'-O5'-PA-O2A
4	D	600	AGS	C5'-O5'-PA-O2A
4	B	600	AGS	PA-O3A-PB-O1B
4	D	600	AGS	PA-O3A-PB-O1B
4	A	600	AGS	PB-O3B-PG-O3G
4	A	600	AGS	PG-O3B-PB-O1B
4	A	600	AGS	PG-O3B-PB-O2B
4	B	600	AGS	PA-O3A-PB-O2B

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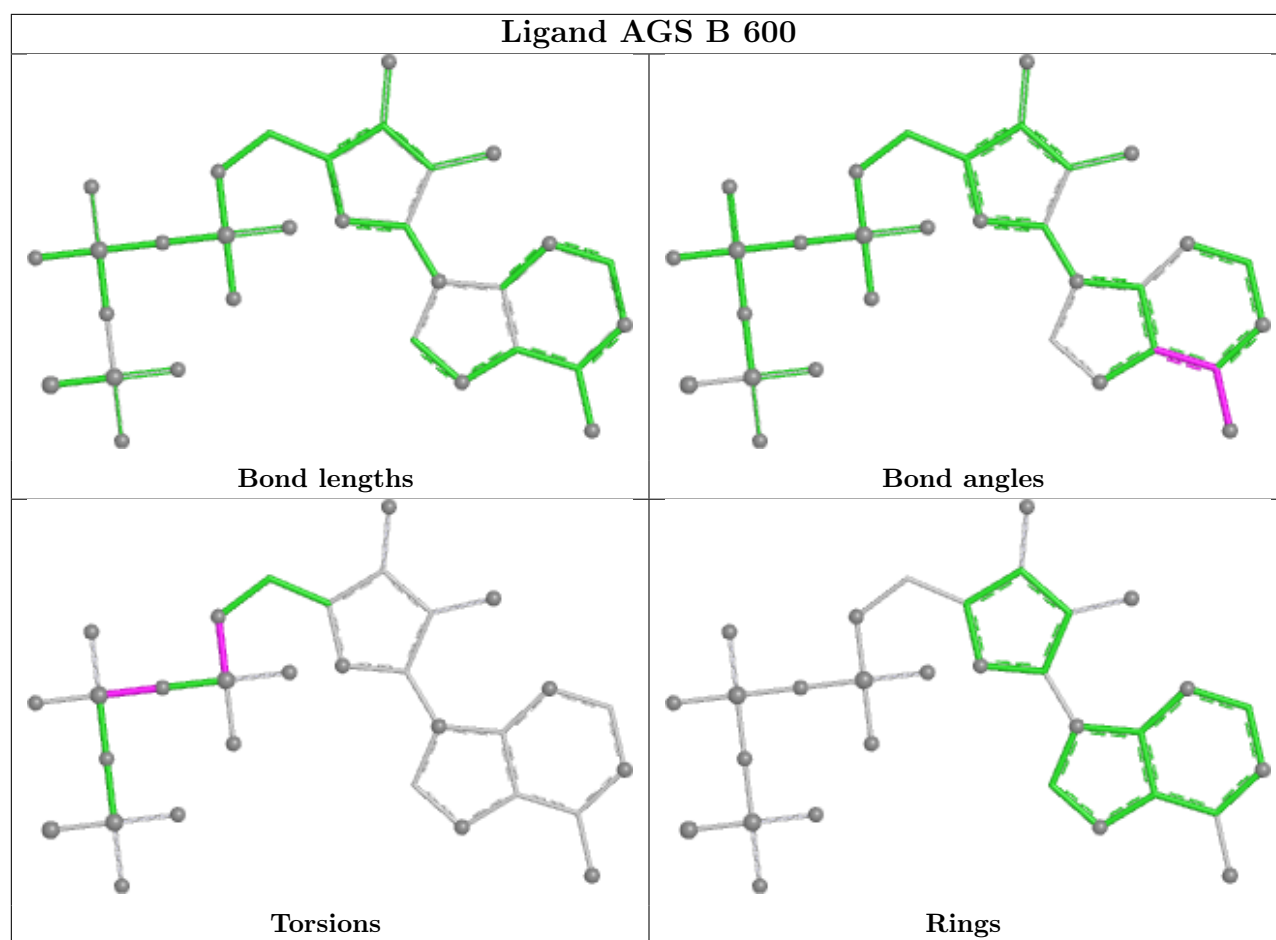
Mol	Chain	Res	Type	Atoms
4	D	600	AGS	PA-O3A-PB-O2B

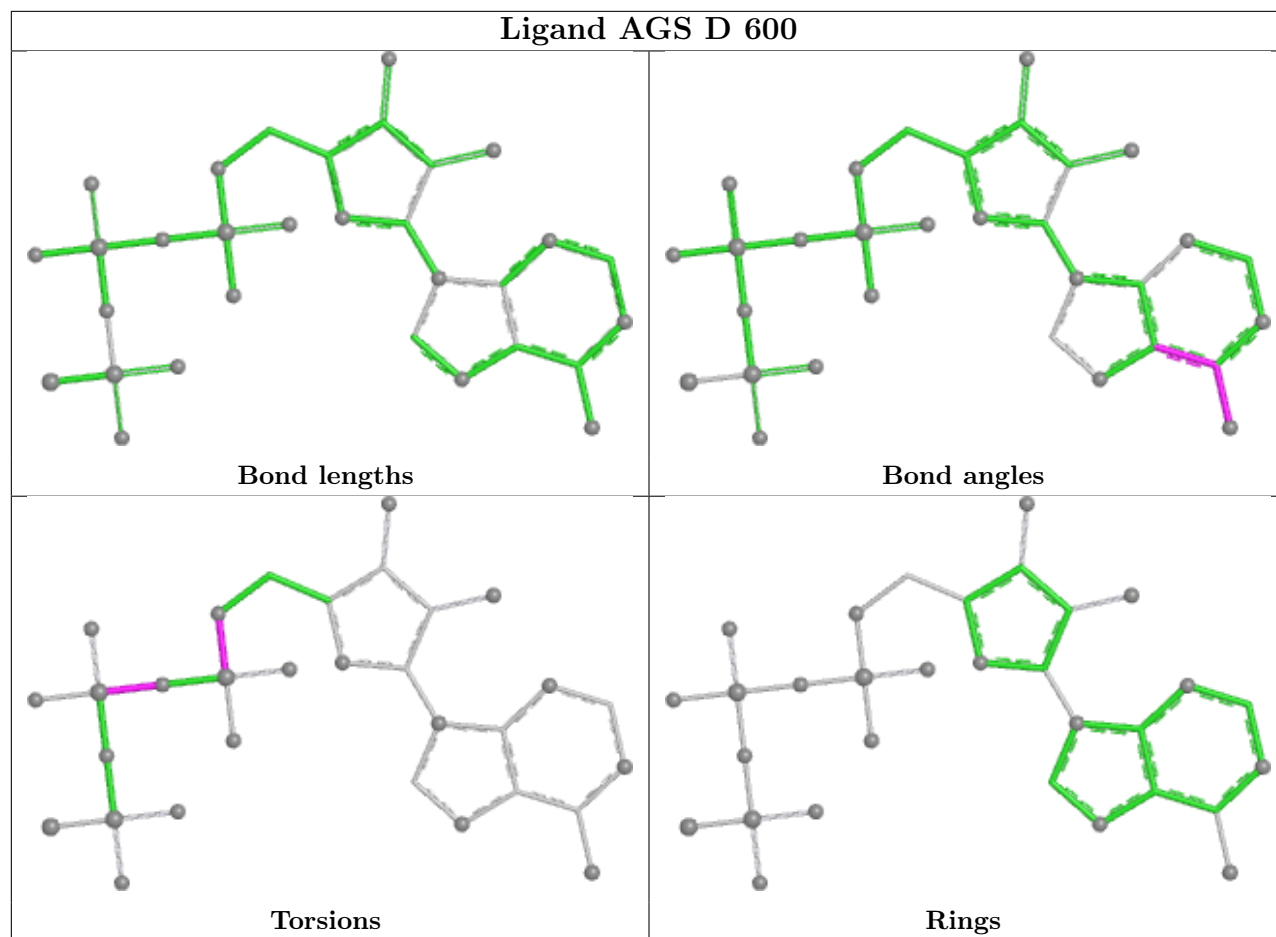
There are no ring outliers.

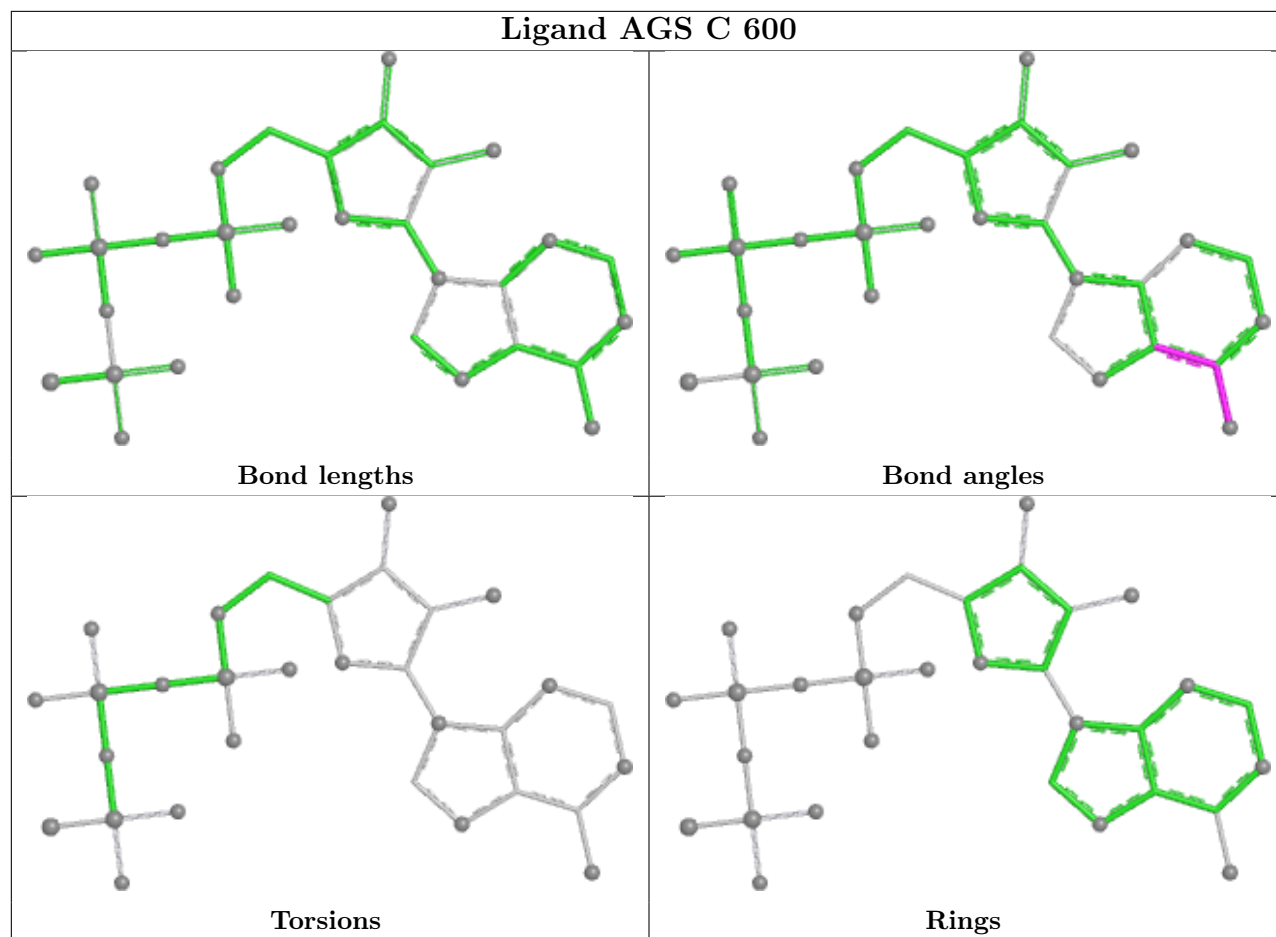
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	AGS	2	0
4	D	600	AGS	2	0

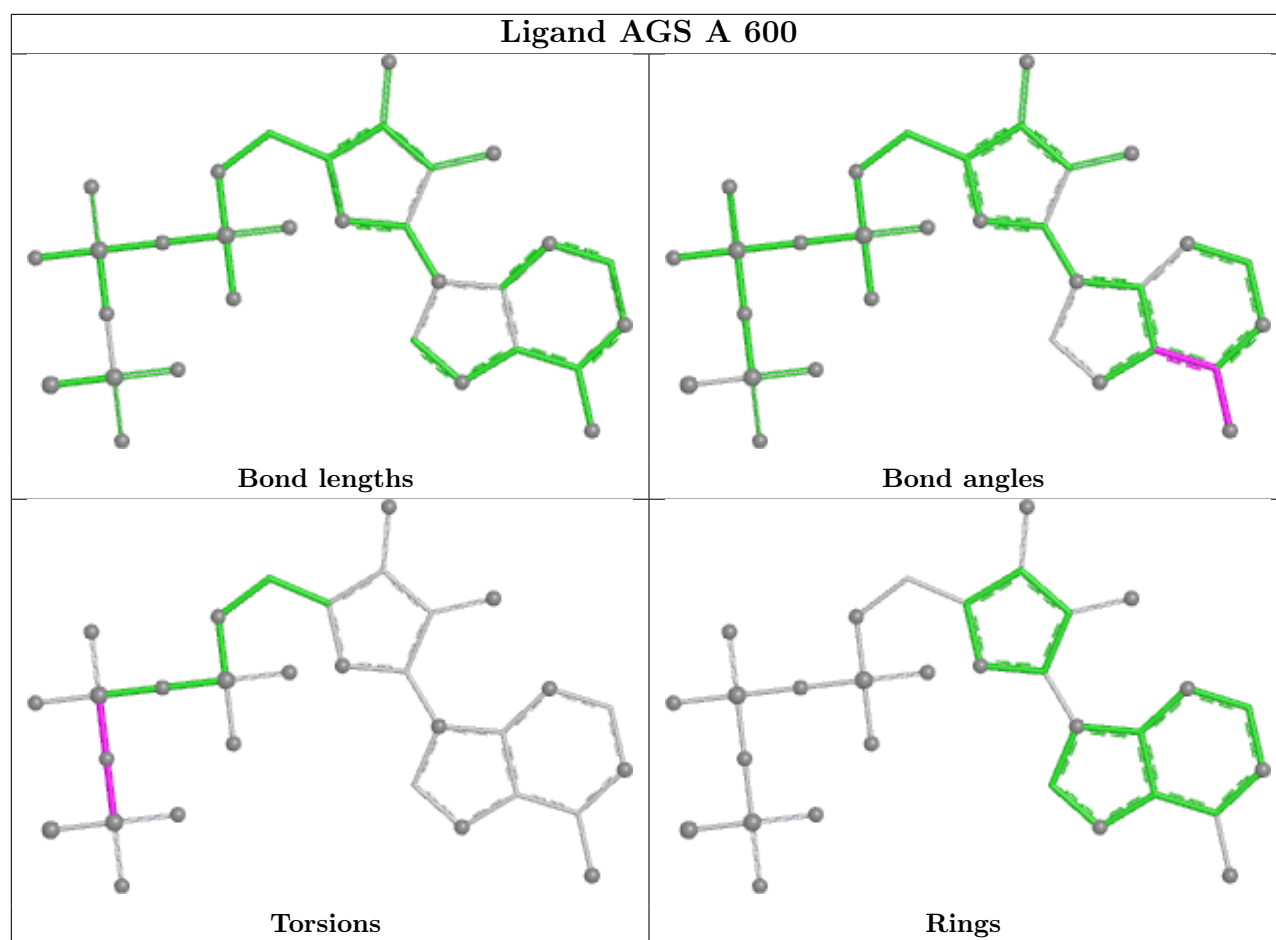
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

**Warning:** The R factor obtained from EDS is 0.4043, which does not match the depositor's R factor of 0.306. Please interpret the results in this section carefully.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	568/587 (96%)	0.88	90 (15%) 6 8	36, 173, 288, 300	0
1	C	568/587 (96%)	0.84	98 (17%) 5 6	23, 229, 269, 283	0
2	B	570/599 (95%)	0.30	51 (8%) 17 15	3, 94, 191, 232	0
2	D	570/599 (95%)	0.47	62 (10%) 12 12	19, 193, 267, 289	0
3	E	129/132 (97%)	1.08	22 (17%) 5 6	94, 178, 298, 300	0
3	F	129/132 (97%)	1.06	27 (20%) 3 5	80, 133, 277, 300	0
All	All	2534/2636 (96%)	0.67	350 (13%) 8 9	3, 180, 276, 300	0

All (350) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	57	PRO	13.2
3	F	42	GLY	12.9
1	A	15	ALA	12.3
1	C	2	LYS	12.2
1	A	558	CYS	11.9
1	A	153	VAL	11.6
2	B	288	LYS	11.4
2	B	555	ASN	11.1
1	A	264	ASN	11.1
1	C	519	CYS	10.8
2	D	540	GLY	10.8
1	A	87	ASP	10.6
2	B	291	ILE	10.5
1	A	10	PRO	10.4
1	A	265	ASN	10.3
1	A	57	ILE	9.4

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Mol	Chain	Res	Type	RSRZ
3	F	43	LYS	9.1
2	D	236	GLU	8.9
2	D	85	THR	8.8
1	A	253	ALA	8.5
2	B	56	SER	8.5
1	A	249	MET	8.3
3	F	39	GLN	8.3
3	E	128	SER	8.2
1	C	3	THR	8.2
2	D	365	ASP	7.9
1	A	11	TYR	7.8
1	C	130	LEU	7.7
1	C	557	HIS	7.4
1	A	268	GLU	7.4
1	C	134	VAL	7.4
1	A	266	GLN	7.4
1	C	135	VAL	7.4
1	C	393	ASP	7.3
1	A	149	VAL	7.0
1	C	50	SER	7.0
1	A	554	LEU	7.0
1	C	5	ALA	6.9
1	A	250	GLY	6.9
1	C	555	LEU	6.8
2	D	432	GLY	6.8
1	A	555	LEU	6.8
1	A	551	HIS	6.8
2	D	82	ILE	6.6
1	A	8	LEU	6.6
1	A	61	ILE	6.6
2	D	81	LEU	6.5
2	D	380	PRO	6.1
1	A	252	ILE	6.1
1	C	296	ILE	6.1
1	A	64	LEU	6.0
1	A	546	ALA	6.0
2	D	78	ARG	6.0
1	C	547	GLY	6.0
1	C	300	SER	6.0
1	A	562	ARG	5.9
3	E	88	PRO	5.9
2	B	508	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	20	LEU	5.9
3	E	85	SER	5.8
1	A	60	LEU	5.8
1	A	90	ARG	5.7
1	C	329	GLU	5.7
1	C	136	ARG	5.7
3	E	66	GLY	5.6
2	B	72	ARG	5.6
2	D	72	ARG	5.6
1	C	567	SER	5.6
1	A	259	GLY	5.5
1	C	46	ARG	5.5
2	B	71	ARG	5.5
1	A	152	ASN	5.5
1	C	302	SER	5.5
3	F	11	LEU	5.5
1	A	417	VAL	5.4
1	A	83	ASN	5.4
1	C	403	LYS	5.4
1	A	561	TYR	5.4
1	C	261	LEU	5.3
1	A	18	ALA	5.3
1	C	19	PRO	5.3
1	A	13	ILE	5.3
1	C	48	ASP	5.3
3	F	117	ASP	5.3
2	B	61	GLY	5.2
1	C	554	LEU	5.2
1	C	47	GLY	5.1
1	A	14	PHE	5.1
1	C	22	MET	5.0
2	D	381	GLY	4.9
1	C	566	GLU	4.9
2	D	77	PRO	4.9
1	C	407	GLY	4.8
2	B	572	LYS	4.8
1	C	521	THR	4.8
2	D	79	TYR	4.8
1	C	73	CYS	4.8
1	C	565	TYR	4.8
3	E	16	GLY	4.8
1	A	515	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	563	GLU	4.7
1	A	6	ARG	4.7
3	F	41	PRO	4.7
1	A	260	VAL	4.7
2	B	26	ARG	4.7
1	C	4	LEU	4.6
3	E	127	VAL	4.6
1	A	16	VAL	4.5
3	F	14	PRO	4.5
1	C	562	ARG	4.5
3	F	126	THR	4.5
3	F	13	GLN	4.5
3	F	88	PRO	4.5
1	A	318	GLU	4.5
2	D	216	ASN	4.5
3	F	40	ALA	4.5
1	A	91	ASP	4.5
1	C	305	ARG	4.4
3	F	15	GLY	4.4
1	C	301	ALA	4.4
3	F	123	THR	4.4
3	E	17	SER	4.4
1	C	155	LEU	4.4
2	B	378	ILE	4.4
1	C	486	LYS	4.3
2	B	347	GLU	4.3
1	C	59	MET	4.3
1	C	74	THR	4.3
2	D	473	PHE	4.3
1	C	132	ARG	4.2
1	A	272	ILE	4.2
2	B	541	LYS	4.2
2	D	233	THR	4.2
3	F	91	THR	4.2
2	B	22	THR	4.1
1	C	299	ALA	4.1
1	C	21	PHE	4.1
2	B	58	TYR	4.1
1	C	289	ILE	4.0
2	D	67	VAL	4.0
2	D	74	ASP	4.0
3	E	86	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	554	LYS	4.0
2	B	571	GLY	4.0
2	B	281	PHE	4.0
2	B	556	ALA	4.0
1	A	499	SER	3.9
1	C	35	LEU	3.9
2	D	511	LYS	3.9
1	A	396	ASP	3.8
1	C	556	GLU	3.8
1	C	558	CYS	3.8
1	C	57	ILE	3.8
1	C	307	LEU	3.8
1	C	131	LEU	3.8
2	B	59	LEU	3.8
2	B	290	ILE	3.8
1	C	546	ALA	3.8
1	A	62	VAL	3.8
3	F	44	GLU	3.8
1	A	399	THR	3.8
1	A	556	GLU	3.8
1	A	254	VAL	3.7
2	D	483	THR	3.7
1	C	24	VAL	3.7
2	D	484	VAL	3.7
1	C	123	LEU	3.7
1	A	258	GLY	3.7
1	C	256	TRP	3.7
1	A	17	LEU	3.7
2	B	29	LEU	3.7
2	D	469	HIS	3.7
1	A	154	LYS	3.7
1	C	358	PRO	3.7
1	A	269	ILE	3.7
2	B	185	SER	3.6
1	C	303	ALA	3.6
2	D	538	MET	3.6
1	A	271	SER	3.6
1	A	56	GLY	3.6
2	D	472	HIS	3.6
1	C	409	ILE	3.6
3	E	126	THR	3.6
3	E	31	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	217	GLY	3.5
3	F	89	GLU	3.5
2	D	86	ILE	3.5
1	C	53	LEU	3.4
1	A	547	GLY	3.4
2	D	367	LYS	3.4
1	A	150	SER	3.3
1	C	6	ARG	3.3
2	D	474	ILE	3.3
2	D	75	LEU	3.3
1	A	464	GLU	3.3
2	B	559	ILE	3.2
1	A	63	ALA	3.2
1	C	257	PHE	3.2
2	D	68	PHE	3.2
2	B	478	PRO	3.2
1	A	5	ALA	3.2
2	D	541	LYS	3.2
1	A	400	VAL	3.2
1	C	456	PRO	3.2
2	D	395	THR	3.2
2	D	89	LEU	3.2
2	B	453	ASN	3.2
1	C	20	LEU	3.2
2	B	377	HIS	3.1
2	D	43	PHE	3.1
3	F	92	GLY	3.1
2	D	73	PHE	3.1
3	E	125	VAL	3.1
1	A	552	LYS	3.1
3	E	15	GLY	3.0
1	C	25	GLU	3.0
1	A	467	GLY	3.0
2	D	588	THR	3.0
2	B	73	PHE	3.0
1	C	133	ILE	3.0
1	C	129	MET	3.0
2	D	80	MET	3.0
1	A	416	THR	3.0
2	D	350	GLU	3.0
3	E	89	GLU	2.9
1	A	273	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	21	PHE	2.9
2	D	398	VAL	2.9
3	F	116	MET	2.9
2	D	23	ALA	2.9
1	C	216	GLU	2.9
1	A	151	ILE	2.9
1	A	420	SER	2.9
1	C	306	VAL	2.9
1	A	12	TRP	2.8
3	E	18	LEU	2.8
1	A	155	LEU	2.8
3	F	12	VAL	2.8
1	C	51	LEU	2.8
2	B	28	LEU	2.8
2	B	30	GLY	2.8
2	D	571	GLY	2.8
3	E	113	ILE	2.8
2	B	510	PRO	2.8
1	C	288	MET	2.8
3	F	93	VAL	2.8
1	C	26	VAL	2.8
1	C	254	VAL	2.8
2	D	487	ASP	2.8
1	A	24	VAL	2.7
2	D	399	ASN	2.7
2	D	353	GLY	2.7
2	B	289	ASP	2.7
2	B	367	LYS	2.7
1	A	263	ARG	2.7
1	A	557	HIS	2.7
1	A	261	LEU	2.7
1	C	18	ALA	2.7
3	E	91	THR	2.7
2	D	159	PHE	2.7
2	D	377	HIS	2.7
1	A	65	ILE	2.7
2	D	364	TYR	2.6
1	C	70	GLY	2.6
2	B	558	LEU	2.6
3	E	60	TYR	2.6
1	C	217	ASN	2.6
1	A	401	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	573	HIS	2.6
3	F	128	SER	2.6
1	C	56	GLY	2.6
2	D	70	PRO	2.6
1	C	110	SER	2.6
1	C	27	ILE	2.6
1	C	220	LYS	2.6
2	B	60	ILE	2.6
1	C	61	ILE	2.6
1	C	356	VAL	2.6
1	A	256	TRP	2.5
1	A	565	TYR	2.5
1	C	406	ARG	2.5
3	E	102	TYR	2.5
1	A	245	PHE	2.5
1	A	7	TYR	2.5
1	A	9	LYS	2.5
2	D	476	HIS	2.5
3	E	67	ARG	2.5
2	B	509	ASN	2.5
2	D	130	ARG	2.5
1	C	39	ILE	2.5
1	A	529	PRO	2.4
2	B	31	TYR	2.4
3	F	31	TYR	2.4
3	F	53	ASN	2.4
3	E	45	ARG	2.4
1	C	561	TYR	2.4
2	D	83	LEU	2.4
2	B	293	VAL	2.4
2	B	550	LEU	2.4
2	B	418	ASP	2.4
3	F	71	SER	2.3
2	D	525	LYS	2.3
1	C	560	PRO	2.3
1	C	280	MET	2.3
1	C	516	THR	2.3
2	B	557	ASP	2.3
1	A	470	PHE	2.3
1	C	262	VAL	2.3
1	C	489	LYS	2.3
2	D	491	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	255	LEU	2.3
1	C	569	PHE	2.3
2	B	269	MET	2.3
2	D	45	PHE	2.3
2	D	71	ARG	2.3
3	F	118	TYR	2.3
1	A	102	SER	2.3
3	E	9	GLY	2.2
1	C	369	GLY	2.2
1	C	568	GLN	2.2
3	F	124	PRO	2.2
1	A	216	GLU	2.2
2	D	76	LEU	2.2
2	D	214	GLN	2.2
1	C	520	THR	2.2
3	F	45	ARG	2.2
1	A	559	LYS	2.2
1	A	223	GLU	2.2
1	C	62	VAL	2.2
2	D	352	ARG	2.2
2	D	366	LYS	2.2
1	C	273	MET	2.1
1	C	367	GLU	2.1
1	C	309	VAL	2.1
2	B	80	MET	2.1
1	A	262	VAL	2.1
2	D	66	VAL	2.1
3	E	30	ASP	2.1
2	D	305	GLN	2.1
2	B	33	ARG	2.1
2	B	429	SER	2.1
1	C	330	GLY	2.1
2	B	85	THR	2.1
2	B	87	TYR	2.1
2	D	368	LYS	2.1
1	A	474	GLN	2.1
1	C	331	SER	2.0
2	B	285	LEU	2.0
2	B	282	GLY	2.0
1	A	161	PHE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

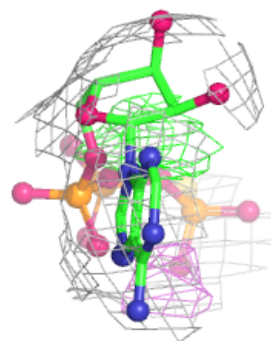
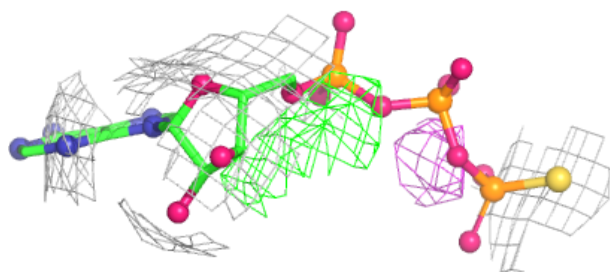
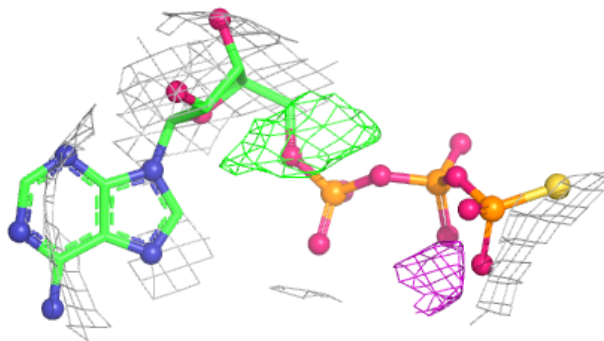
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	MG	D	601	1/1	0.84	0.12	176,176,176,176	0
4	AGS	A	600	31/31	0.91	0.12	99,135,179,183	0
5	MG	C	601	1/1	0.94	0.08	217,217,217,217	0
4	AGS	C	600	31/31	0.95	0.10	187,206,221,225	0
4	AGS	D	600	31/31	0.95	0.09	162,196,218,226	0
5	MG	A	601	1/1	0.96	0.15	116,116,116,116	0
4	AGS	B	600	31/31	0.97	0.08	4,26,78,82	0
5	MG	B	601	1/1	1.00	0.04	70,70,70,70	0

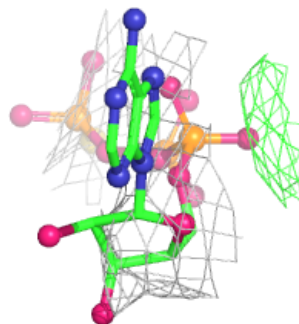
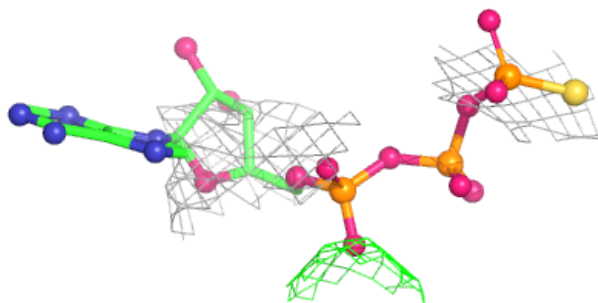
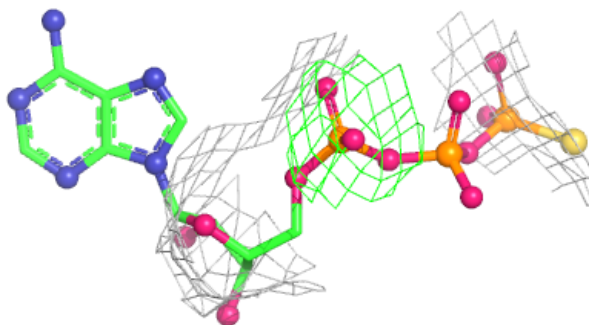
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AGS A 600:**

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

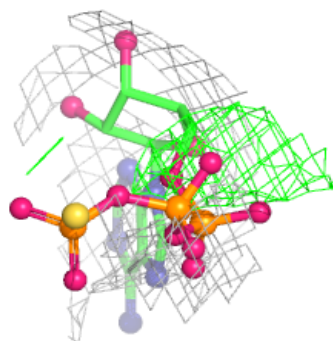
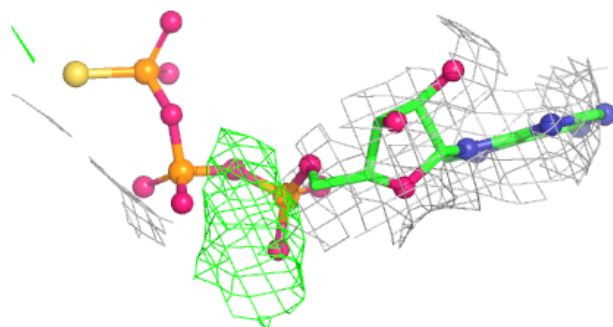
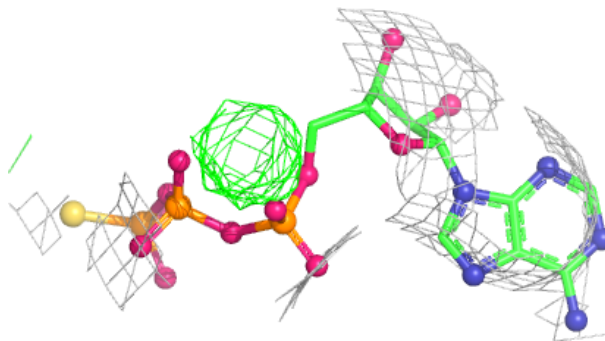
**Electron density around AGS C 600:**

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

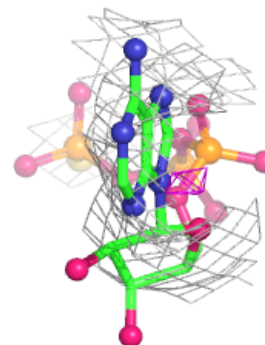
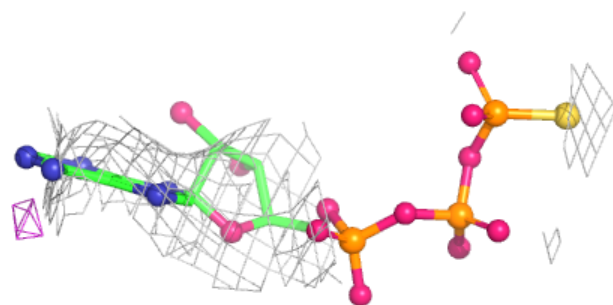
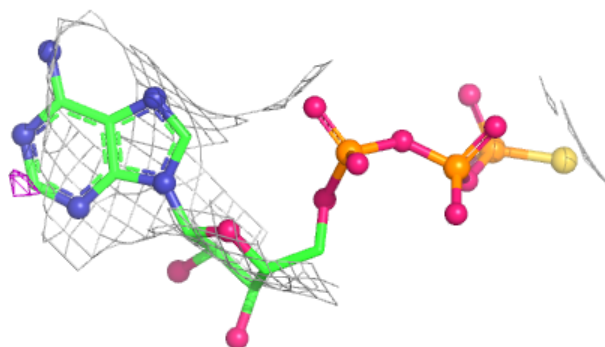


**Electron density around AGS D 600:**

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

**Electron density around AGS B 600:**

$2mF_o - DF_c$  (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.