Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2024 – 01:12 PM EST

PDB ID	:	3HU1
Title	:	Structure of p97 N-D1 R95G mutant in complex with ATPgS
Authors	:	Tang, W.-K.
Deposited on	:	2009-06-12
Resolution	:	2.81 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:

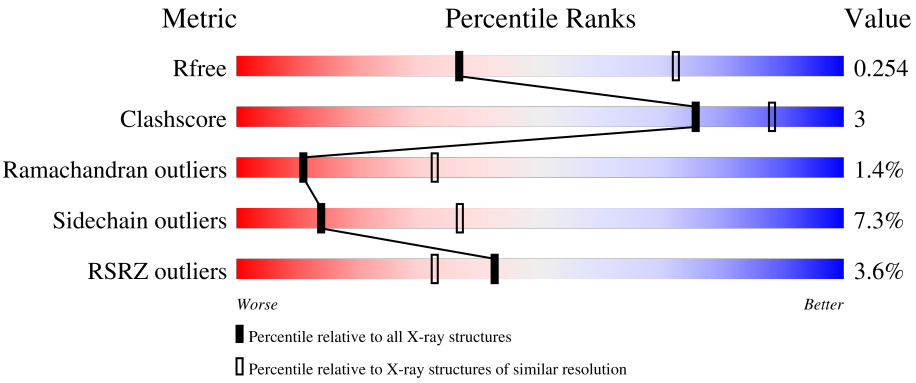
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 80% 11% • 8%
1	B	489	2% 78% 13% • 8%
1	C	489	2% 79% 12% • 8%
1	D	489	6% 80% 11% • 8%
1	E	489	5% 79% 11% • 8%

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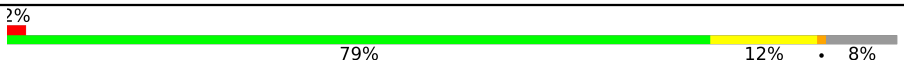
Mol	Chain	Length	Quality of chain
1	F	489	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21445 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	451	Total 3522	C 2211	N 623	O 670	S 18	0	0	0
1	B	451	Total 3522	C 2211	N 623	O 670	S 18	0	0	0
1	C	451	Total 3522	C 2211	N 623	O 670	S 18	0	0	0
1	D	451	Total 3522	C 2211	N 623	O 670	S 18	0	0	0
1	E	451	Total 3522	C 2211	N 623	O 670	S 18	0	0	0
1	F	451	Total 3522	C 2211	N 623	O 670	S 18	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	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	95	GLY	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

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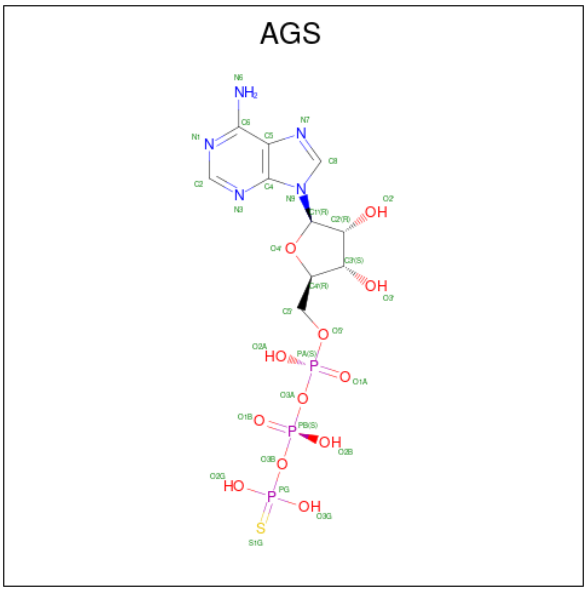
Chain	Residue	Modelled	Actual	Comment	Reference
B	489	HIS	-	expression tag	UNP P55072
C	95	GLY	ARG	engineered mutation	UNP P55072
C	482	ARG	-	expression tag	UNP P55072
C	483	SER	-	expression tag	UNP P55072
C	484	HIS	-	expression tag	UNP P55072
C	485	HIS	-	expression tag	UNP P55072
C	486	HIS	-	expression 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	95	GLY	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	95	GLY	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	95	GLY	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: $C_{10}H_{16}N_5O_{12}P_3S$).



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

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

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

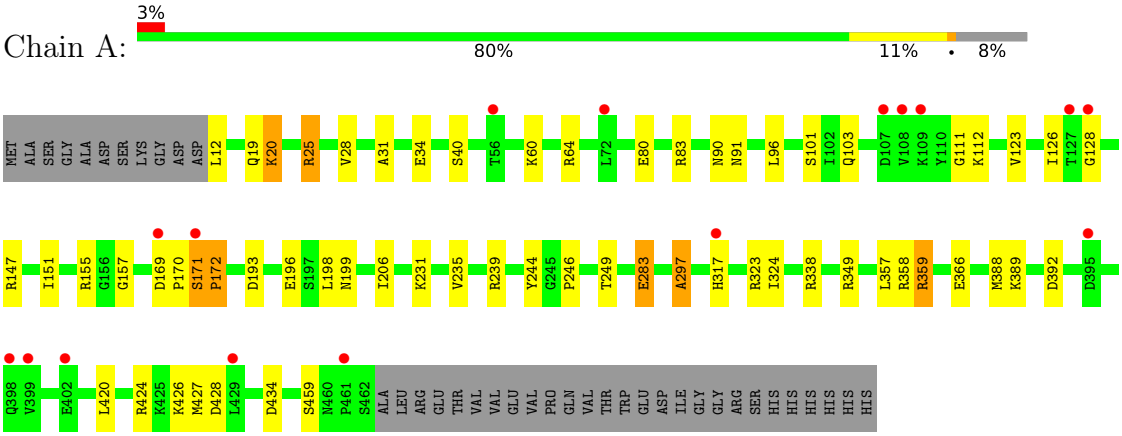
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O 27 27	0	0
4	B	22	Total O 22 22	0	0
4	C	22	Total O 22 22	0	0
4	D	16	Total O 16 16	0	0
4	E	19	Total O 19 19	0	0
4	F	15	Total O 15 15	0	0

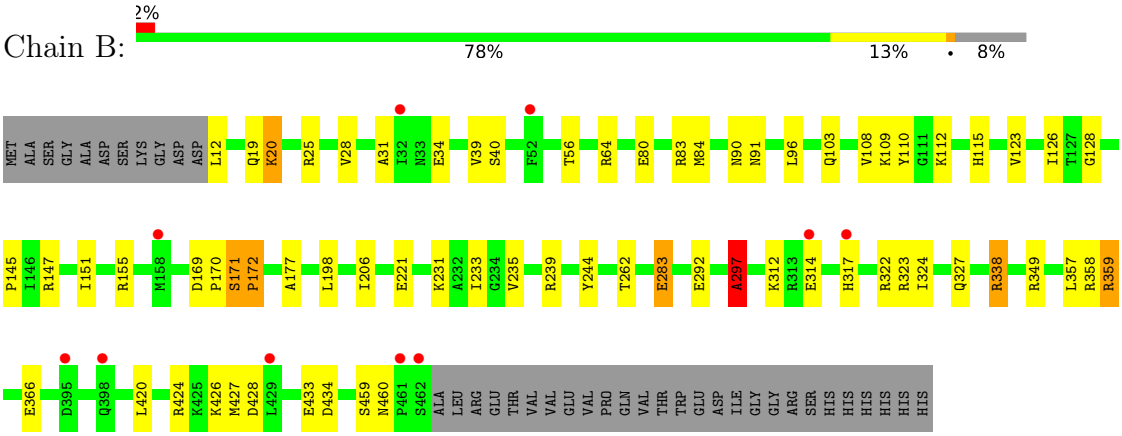
3 Residue-property plots (i)

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 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.

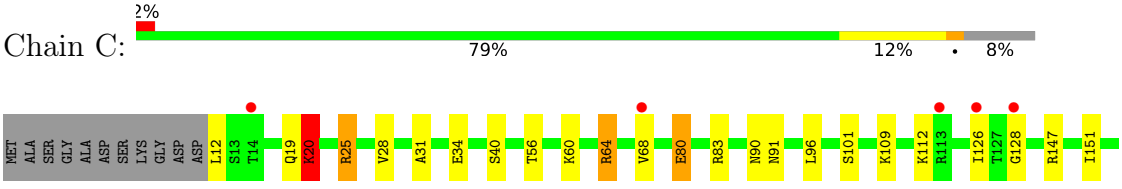
• Molecule 1: Transitional endoplasmic reticulum ATPase

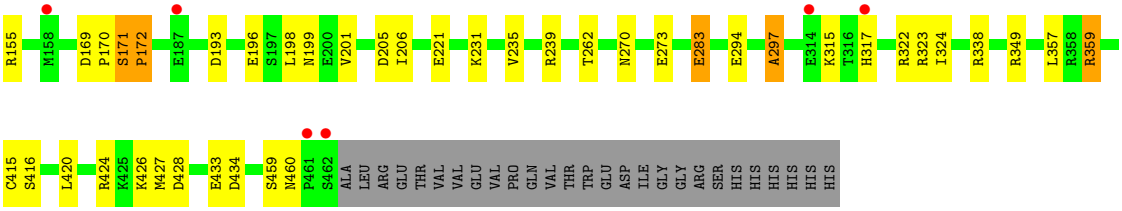


• Molecule 1: Transitional endoplasmic reticulum ATPase

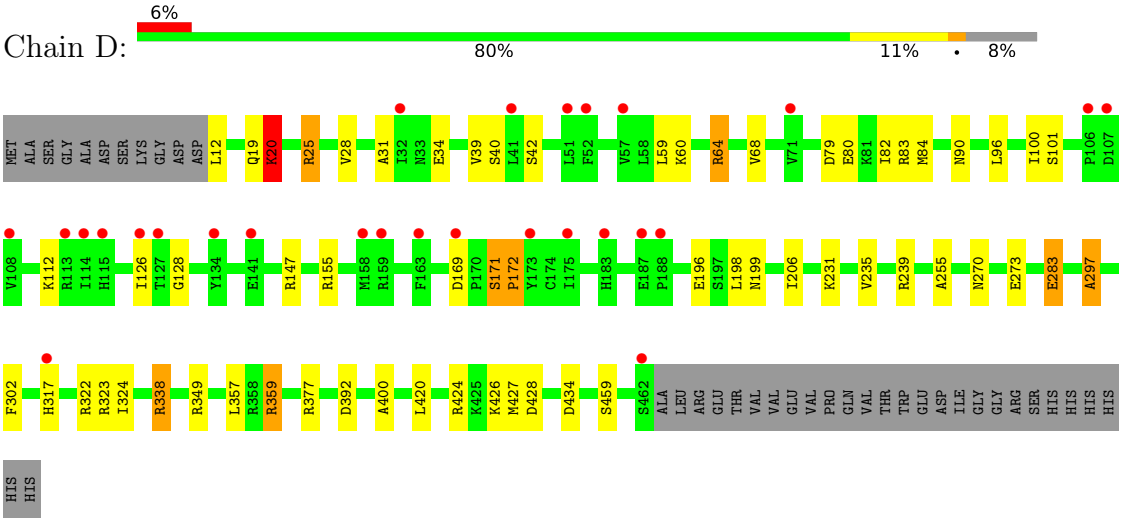


• Molecule 1: Transitional endoplasmic reticulum ATPase

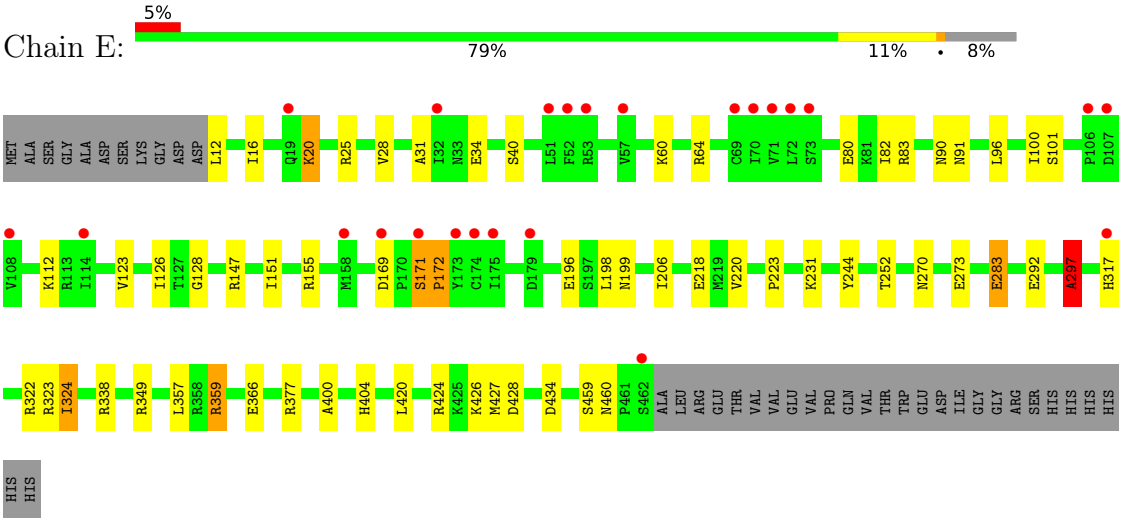




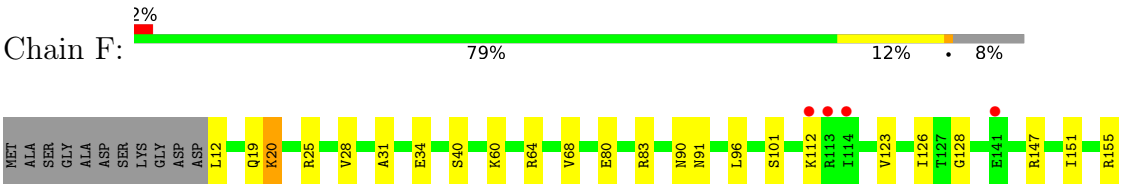
• Molecule 1: Transitional endoplasmic reticulum ATPase

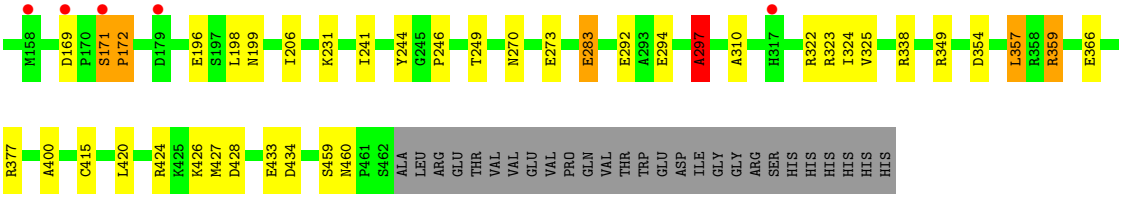


• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase




M158
D169
P170
S171
P172
D179
E196
S197
L198
N199
I206
K231
I241
Y244
G245
P246
T249
N270
E273
E283
E292
A293
E294
A297
A310
H317
R322
R323
I324
V325
R338
R349
D354
L357
R358
R359
E366
R377
A400
C415
L420
R424
K425
K426
M427
D428
E433
D434
S459
N460
P461
S462
ALA
LEU
ARG
GLU
THR
VAL
VAL
GLU
VAL
PRO
GLN
VAL
THR
TRP
GLU
ASP
ILE
GLY
GLY
ARG
SER
HIS
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HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.76Å 103.28Å 107.69Å 97.66° 91.88° 89.75°	Depositor
Resolution (Å)	25.00 – 2.81 43.92 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.2 (25.00-2.81) 90.1 (43.92-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.271 0.221 , 0.254	Depositor DCC
R_{free} test set	4328 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l 0.016 for -h,-l,-k 0.019 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21445	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 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	0.95	0/3576	0.73	0/4832
1	B	0.97	1/3576 (0.0%)	0.73	0/4832
1	C	0.97	1/3576 (0.0%)	0.73	0/4832
1	D	0.95	0/3576	0.73	0/4832
1	E	0.99	1/3576 (0.0%)	0.74	0/4832
1	F	0.98	2/3576 (0.1%)	0.73	1/4832 (0.0%)
All	All	0.97	5/21456 (0.0%)	0.73	1/28992 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	415	CYS	CB-SG	-7.06	1.70	1.82
1	F	415	CYS	CB-SG	-6.36	1.71	1.82
1	E	297	ALA	CA-CB	6.34	1.65	1.52
1	F	297	ALA	CA-CB	6.18	1.65	1.52
1	B	297	ALA	CA-CB	5.94	1.65	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	241	ILE	CG1-CB-CG2	-5.60	99.09	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ALA	Peptide
1	C	297	ALA	Peptide
1	D	297	ALA	Peptide
1	E	297	ALA	Peptide
1	F	297	ALA	Peptide

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	3522	0	3583	24	0
1	B	3522	0	3583	29	0
1	C	3522	0	3583	25	0
1	D	3522	0	3583	26	0
1	E	3522	0	3584	25	0
1	F	3522	0	3583	21	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	27	0	0	1	0
4	B	22	0	0	3	0
4	C	22	0	0	1	0
4	D	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	19	0	0	1	0
4	F	15	0	0	0	0
All	All	21445	0	21571	132	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 (132) 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:F:424:ARG:HA	1:F:427:MET:HG2	1.69	0.74
1:E:424:ARG:HA	1:E:427:MET:HG2	1.73	0.71
2:B:800:AGS:S1G	1:C:359:ARG:HG2	2.31	0.71
1:D:424:ARG:HA	1:D:427:MET:HG2	1.71	0.70
2:C:800:AGS:S1G	1:D:359:ARG:HG2	2.31	0.69
1:A:193:ASP:HA	1:B:338:ARG:HH12	1.57	0.68
1:C:424:ARG:HA	1:C:427:MET:HG2	1.75	0.68
2:E:800:AGS:S1G	1:F:359:ARG:HG2	2.33	0.68
1:B:424:ARG:HA	1:B:427:MET:HG2	1.76	0.67
1:A:193:ASP:HA	1:B:338:ARG:NH1	2.10	0.66
1:D:428:ASP:HA	1:E:20:LYS:HD3	1.78	0.66
1:E:428:ASP:HA	1:F:20:LYS:HD3	1.78	0.65
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.80	0.64
1:A:359:ARG:HG2	2:F:800:AGS:S1G	2.37	0.64
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.79	0.64
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.80	0.63
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.79	0.63
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.80	0.63
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.81	0.62
1:A:424:ARG:HA	1:A:427:MET:HG2	1.80	0.62
1:A:239:ARG:HD3	4:A:500:HOH:O	2.00	0.61
1:B:115:HIS:HB2	4:B:508:HOH:O	2.00	0.60
1:B:31:ALA:HA	1:B:83:ARG:HB3	1.84	0.59
1:C:317:HIS:HB2	1:D:322:ARG:HH12	1.68	0.59
1:F:377:ARG:NH1	1:F:400:ALA:O	2.36	0.59
1:E:252:THR:OG1	4:E:804:HOH:O	2.17	0.58
1:D:317:HIS:HB2	1:E:322:ARG:HH12	1.68	0.58
1:C:428:ASP:HA	1:D:20:LYS:HD2	1.86	0.57
1:A:317:HIS:HB2	1:B:322:ARG:HH12	1.71	0.56
1:B:317:HIS:HB2	1:C:322:ARG:HH12	1.72	0.55
1:E:60:LYS:HB2	1:E:101:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:HA	1:D:338:ARG:HH12	1.74	0.53
1:F:28:VAL:HG23	1:F:96:LEU:HA	1.91	0.53
1:B:110:TYR:HD2	1:B:177:ALA:HB2	1.75	0.52
2:D:800:AGS:S1G	1:E:359:ARG:HG2	2.48	0.52
1:E:91:ASN:HD21	1:E:151:ILE:H	1.57	0.52
1:B:283:GLU:HB3	1:B:327:GLN:HE21	1.75	0.52
1:A:428:ASP:HA	1:B:20:LYS:HD3	1.93	0.51
1:C:112:LYS:HB3	1:C:169:ASP:HB3	1.92	0.51
1:A:31:ALA:HA	1:A:83:ARG:HB3	1.91	0.51
1:E:28:VAL:HG23	1:E:96:LEU:HA	1.93	0.51
1:C:109:LYS:HD2	1:C:170:PRO:HB3	1.92	0.50
1:B:171:SER:CB	1:B:172:PRO:HD3	2.41	0.50
1:F:60:LYS:HB2	1:F:101:SER:HB2	1.94	0.50
1:C:221:GLU:OE2	1:C:262:THR:HG22	2.12	0.50
1:D:283:GLU:OE2	1:D:323:ARG:HD2	2.11	0.50
1:E:270:ASN:HB2	1:E:273:GLU:HB2	1.94	0.50
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.93	0.49
1:A:283:GLU:OE2	1:A:323:ARG:HD2	2.12	0.49
1:B:428:ASP:HA	1:C:20:LYS:HD2	1.94	0.49
1:D:31:ALA:HA	1:D:83:ARG:HB3	1.94	0.48
1:F:91:ASN:HD21	1:F:151:ILE:H	1.62	0.48
1:C:201:VAL:HG13	1:C:205:ASP:HB2	1.95	0.48
1:C:91:ASN:HD21	1:C:151:ILE:H	1.61	0.48
1:F:270:ASN:HB2	1:F:273:GLU:HB2	1.96	0.48
1:A:91:ASN:HD21	1:A:151:ILE:H	1.62	0.47
1:B:109:LYS:HD2	1:B:170:PRO:HB3	1.95	0.47
1:E:31:ALA:HA	1:E:83:ARG:HB3	1.97	0.47
1:C:433:GLU:HG3	1:D:25:ARG:HH21	1.80	0.47
1:F:31:ALA:HA	1:F:83:ARG:HB3	1.97	0.47
1:F:244:TYR:HE2	1:F:366:GLU:HB3	1.81	0.46
1:D:60:LYS:HB2	1:D:101:SER:HB2	1.97	0.46
2:A:800:AGS:S1G	1:B:359:ARG:HG2	2.55	0.46
1:E:283:GLU:OE2	1:E:323:ARG:HD2	2.16	0.46
1:C:28:VAL:HG23	1:C:96:LEU:HA	1.97	0.46
1:D:171:SER:HB2	1:D:172:PRO:HD3	1.98	0.46
1:C:31:ALA:HA	1:C:83:ARG:HB3	1.97	0.45
1:E:196:GLU:HA	1:E:199:ASN:HB2	1.98	0.45
1:D:28:VAL:HG23	1:D:96:LEU:HA	1.97	0.45
1:A:112:LYS:HB3	1:A:169:ASP:HB3	1.99	0.45
1:D:82:ILE:HG21	1:D:100:ILE:HD11	1.98	0.45
1:F:91:ASN:ND2	1:F:151:ILE:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLU:OE2	1:B:323:ARG:HD2	2.17	0.44
1:C:283:GLU:OE2	1:C:323:ARG:HD2	2.17	0.44
1:A:171:SER:CB	1:A:172:PRO:HD3	2.46	0.44
1:C:60:LYS:HB2	1:C:101:SER:HB2	1.99	0.44
1:E:244:TYR:HE2	1:E:366:GLU:HB3	1.83	0.44
1:A:389:LYS:HE3	4:B:496:HOH:O	2.16	0.44
1:A:60:LYS:HB2	1:A:101:SER:HB2	1.99	0.44
1:A:244:TYR:HE2	1:A:366:GLU:HB3	1.83	0.44
1:E:16:ILE:HG21	1:E:218:GLU:HG3	1.99	0.44
1:A:25:ARG:HH21	1:F:433:GLU:HG3	1.82	0.44
1:B:56:THR:HG22	1:B:145:PRO:HG3	2.00	0.43
1:B:91:ASN:HD21	1:B:151:ILE:H	1.65	0.43
1:B:221:GLU:OE2	1:B:262:THR:HG22	2.18	0.43
1:D:42:SER:OG	1:D:79:ASP:HA	2.18	0.43
1:D:196:GLU:HA	1:D:199:ASN:HB2	2.00	0.43
1:B:39:VAL:HG12	1:B:84:MET:HB3	2.01	0.43
1:E:283:GLU:HG3	1:E:324:ILE:HG13	2.00	0.43
1:C:171:SER:HB2	1:C:172:PRO:HD3	2.01	0.43
1:C:171:SER:CB	1:C:172:PRO:HD3	2.48	0.43
1:D:255:ALA:HB2	1:D:302:PHE:CZ	2.54	0.43
1:A:246:PRO:HD2	1:A:249:THR:HG21	2.00	0.43
1:D:270:ASN:HB2	1:D:273:GLU:HB2	2.01	0.43
1:E:220:VAL:O	1:E:223:PRO:HD2	2.18	0.42
1:F:354:ASP:HB3	1:F:357:LEU:HD12	2.01	0.42
1:A:91:ASN:ND2	1:A:151:ILE:H	2.17	0.42
1:B:171:SER:HB2	1:B:172:PRO:HD3	2.00	0.42
1:F:283:GLU:OE2	1:F:323:ARG:HD2	2.19	0.42
1:F:310:ALA:HA	1:F:325:VAL:HG22	2.01	0.42
1:A:196:GLU:HA	1:A:199:ASN:HB2	2.00	0.42
1:C:80:GLU:HB3	4:C:498:HOH:O	2.19	0.42
1:E:171:SER:CB	1:E:172:PRO:HD3	2.50	0.42
1:A:28:VAL:HG23	1:A:96:LEU:HA	2.02	0.42
1:B:110:TYR:CD2	1:B:177:ALA:HB2	2.54	0.42
1:B:433:GLU:HG3	1:C:25:ARG:HH21	1.84	0.42
1:D:171:SER:CB	1:D:172:PRO:HD3	2.50	0.42
1:F:112:LYS:HB3	1:F:169:ASP:HB3	2.02	0.42
1:A:388:MET:HA	1:B:233:ILE:O	2.20	0.41
1:D:64:ARG:O	1:D:64:ARG:HG3	2.20	0.41
1:E:317:HIS:HB2	1:F:322:ARG:HH12	1.85	0.41
1:F:196:GLU:HA	1:F:199:ASN:HB2	2.01	0.41
1:B:312:LYS:HB3	1:B:314:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:ARG:NH1	1:E:400:ALA:O	2.48	0.41
1:D:317:HIS:HB2	1:E:322:ARG:NH1	2.34	0.41
1:A:171:SER:HB2	1:A:172:PRO:HD3	2.02	0.41
1:B:297:ALA:O	4:B:500:HOH:O	2.22	0.41
1:D:112:LYS:HB3	1:D:169:ASP:HB3	2.01	0.41
1:E:82:ILE:HG21	1:E:100:ILE:HD11	2.02	0.41
1:D:39:VAL:HG11	1:D:59:LEU:HD11	2.02	0.41
1:A:111:GLY:HA2	1:A:170:PRO:HG2	2.03	0.41
1:B:112:LYS:HB3	1:B:169:ASP:HB3	2.02	0.41
1:B:244:TYR:HE2	1:B:366:GLU:HB3	1.84	0.41
1:C:64:ARG:O	1:C:64:ARG:HG3	2.21	0.41
1:E:112:LYS:HB3	1:E:169:ASP:HB3	2.02	0.41
1:F:246:PRO:HD2	1:F:249:THR:HG21	2.02	0.41
1:D:377:ARG:NH1	1:D:400:ALA:O	2.47	0.40
1:D:39:VAL:HG12	1:D:84:MET:HB3	2.02	0.40
1:E:91:ASN:ND2	1:E:151:ILE:H	2.18	0.40
1:F:171:SER:HB2	1:F:172:PRO:HD3	2.04	0.40
1:C:196:GLU:HA	1:C:199:ASN:HB2	2.03	0.40
1:C:270:ASN:HB2	1:C:273:GLU:HB2	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	449/489 (92%)	419 (93%)	23 (5%)	7 (2%)	9 29
1	B	449/489 (92%)	422 (94%)	21 (5%)	6 (1%)	12 34
1	C	449/489 (92%)	421 (94%)	22 (5%)	6 (1%)	12 34
1	D	449/489 (92%)	420 (94%)	23 (5%)	6 (1%)	12 34
1	E	449/489 (92%)	420 (94%)	23 (5%)	6 (1%)	12 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	449/489 (92%)	419 (93%)	24 (5%)	6 (1%)	12	34
All	All	2694/2934 (92%)	2521 (94%)	136 (5%)	37 (1%)	11	32

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	B	171	SER
1	C	171	SER
1	D	171	SER
1	E	171	SER
1	F	171	SER
1	A	126	ILE
1	A	128	GLY
1	A	297	ALA
1	B	20	LYS
1	B	126	ILE
1	B	128	GLY
1	C	126	ILE
1	D	126	ILE
1	E	20	LYS
1	E	126	ILE
1	E	128	GLY
1	F	20	LYS
1	F	126	ILE
1	F	128	GLY
1	A	20	LYS
1	A	172	PRO
1	B	172	PRO
1	B	297	ALA
1	C	20	LYS
1	C	172	PRO
1	C	297	ALA
1	D	20	LYS
1	D	128	GLY
1	D	172	PRO
1	D	297	ALA
1	E	172	PRO
1	E	297	ALA
1	F	172	PRO
1	F	297	ALA
1	C	128	GLY

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Mol	Chain	Res	Type
1	A	157	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/417 (93%)	358 (93%)	28 (7%)	14	37
1	B	386/417 (93%)	356 (92%)	30 (8%)	12	33
1	C	386/417 (93%)	355 (92%)	31 (8%)	12	32
1	D	386/417 (93%)	359 (93%)	27 (7%)	15	39
1	E	386/417 (93%)	361 (94%)	25 (6%)	17	43
1	F	386/417 (93%)	358 (93%)	28 (7%)	14	37
All	All	2316/2502 (93%)	2147 (93%)	169 (7%)	14	37

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	19	GLN
1	A	20	LYS
1	A	25	ARG
1	A	34	GLU
1	A	64	ARG
1	A	80	GLU
1	A	90	ASN
1	A	103	GLN
1	A	123	VAL
1	A	147	ARG
1	A	155	ARG
1	A	198	LEU
1	A	206	ILE
1	A	231	LYS
1	A	235	VAL
1	A	283	GLU

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Mol	Chain	Res	Type
1	A	324	ILE
1	A	338	ARG
1	A	349	ARG
1	A	357	LEU
1	A	358	ARG
1	A	359	ARG
1	A	392	ASP
1	A	420	LEU
1	A	426	LYS
1	A	434	ASP
1	A	459	SER
1	B	12	LEU
1	B	19	GLN
1	B	25	ARG
1	B	34	GLU
1	B	64	ARG
1	B	80	GLU
1	B	90	ASN
1	B	103	GLN
1	B	108	VAL
1	B	123	VAL
1	B	147	ARG
1	B	155	ARG
1	B	198	LEU
1	B	206	ILE
1	B	231	LYS
1	B	235	VAL
1	B	239	ARG
1	B	283	GLU
1	B	292	GLU
1	B	324	ILE
1	B	338	ARG
1	B	349	ARG
1	B	357	LEU
1	B	358	ARG
1	B	359	ARG
1	B	420	LEU
1	B	426	LYS
1	B	434	ASP
1	B	459	SER
1	B	460	ASN
1	C	12	LEU

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Mol	Chain	Res	Type
1	C	19	GLN
1	C	20	LYS
1	C	25	ARG
1	C	34	GLU
1	C	56	THR
1	C	64	ARG
1	C	68	VAL
1	C	80	GLU
1	C	90	ASN
1	C	147	ARG
1	C	155	ARG
1	C	198	LEU
1	C	206	ILE
1	C	231	LYS
1	C	235	VAL
1	C	239	ARG
1	C	283	GLU
1	C	294	GLU
1	C	315	LYS
1	C	324	ILE
1	C	338	ARG
1	C	349	ARG
1	C	357	LEU
1	C	359	ARG
1	C	416	SER
1	C	420	LEU
1	C	426	LYS
1	C	434	ASP
1	C	459	SER
1	C	460	ASN
1	D	12	LEU
1	D	19	GLN
1	D	20	LYS
1	D	25	ARG
1	D	34	GLU
1	D	64	ARG
1	D	68	VAL
1	D	80	GLU
1	D	90	ASN
1	D	147	ARG
1	D	155	ARG
1	D	198	LEU

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Mol	Chain	Res	Type
1	D	206	ILE
1	D	231	LYS
1	D	235	VAL
1	D	239	ARG
1	D	283	GLU
1	D	324	ILE
1	D	338	ARG
1	D	349	ARG
1	D	357	LEU
1	D	359	ARG
1	D	392	ASP
1	D	420	LEU
1	D	426	LYS
1	D	434	ASP
1	D	459	SER
1	E	12	LEU
1	E	25	ARG
1	E	34	GLU
1	E	64	ARG
1	E	80	GLU
1	E	90	ASN
1	E	123	VAL
1	E	147	ARG
1	E	155	ARG
1	E	198	LEU
1	E	206	ILE
1	E	231	LYS
1	E	283	GLU
1	E	292	GLU
1	E	324	ILE
1	E	338	ARG
1	E	349	ARG
1	E	357	LEU
1	E	359	ARG
1	E	404	HIS
1	E	420	LEU
1	E	426	LYS
1	E	434	ASP
1	E	459	SER
1	E	460	ASN
1	F	12	LEU
1	F	19	GLN

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Mol	Chain	Res	Type
1	F	25	ARG
1	F	34	GLU
1	F	64	ARG
1	F	68	VAL
1	F	80	GLU
1	F	90	ASN
1	F	123	VAL
1	F	147	ARG
1	F	155	ARG
1	F	198	LEU
1	F	206	ILE
1	F	231	LYS
1	F	283	GLU
1	F	292	GLU
1	F	294	GLU
1	F	324	ILE
1	F	338	ARG
1	F	349	ARG
1	F	357	LEU
1	F	359	ARG
1	F	420	LEU
1	F	426	LYS
1	F	428	ASP
1	F	434	ASP
1	F	459	SER
1	F	460	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	260	ASN
1	A	285	ASN
1	A	327	GLN
1	B	91	ASN
1	B	260	ASN
1	B	285	ASN
1	B	327	GLN
1	C	91	ASN
1	C	260	ASN
1	C	327	GLN
1	D	91	ASN

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Mol	Chain	Res	Type
1	D	260	ASN
1	D	285	ASN
1	D	327	GLN
1	E	91	ASN
1	E	260	ASN
1	E	285	ASN
1	E	327	GLN
1	F	91	ASN
1	F	260	ASN
1	F	285	ASN
1	F	327	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1.49	3 (11%)	26,52,52	1.43	5 (19%)
2	AGS	E	800	3	26,33,33	1.30	3 (11%)	26,52,52	1.32	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	AGS	D	800	3	26,33,33	1.42	2 (7%)	26,52,52	1.44	6 (23%)
2	AGS	C	800	3	26,33,33	1.51	3 (11%)	26,52,52	1.41	5 (19%)
2	AGS	F	800	3	26,33,33	1.48	3 (11%)	26,52,52	1.29	3 (11%)
2	AGS	A	800	3	26,33,33	1.39	3 (11%)	26,52,52	1.45	5 (19%)

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	-	5/17/38/38	0/3/3/3
2	AGS	E	800	3	-	3/17/38/38	0/3/3/3
2	AGS	D	800	3	-	3/17/38/38	0/3/3/3
2	AGS	C	800	3	-	3/17/38/38	0/3/3/3
2	AGS	F	800	3	-	3/17/38/38	0/3/3/3
2	AGS	A	800	3	-	5/17/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	AGS	PG-S1G	5.12	2.01	1.90
2	F	800	AGS	PG-S1G	5.10	2.01	1.90
2	B	800	AGS	PG-S1G	5.10	2.01	1.90
2	A	800	AGS	PG-S1G	4.71	2.00	1.90
2	D	800	AGS	PG-S1G	4.64	2.00	1.90
2	E	800	AGS	PG-S1G	4.07	1.99	1.90
2	C	800	AGS	C2-N3	2.91	1.36	1.32
2	F	800	AGS	C2-N3	2.24	1.35	1.32
2	B	800	AGS	C2-N3	2.22	1.35	1.32
2	D	800	AGS	C5-C4	2.20	1.46	1.40
2	E	800	AGS	C5-N7	-2.18	1.31	1.39
2	B	800	AGS	C5-N7	-2.10	1.32	1.39
2	F	800	AGS	C5-C4	2.07	1.46	1.40
2	A	800	AGS	C5-C4	2.03	1.46	1.40
2	C	800	AGS	C5-N7	-2.03	1.32	1.39
2	A	800	AGS	C2-N3	2.02	1.35	1.32
2	E	800	AGS	C2-N3	2.01	1.35	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	AGS	N3-C2-N1	-4.06	122.33	128.68
2	D	800	AGS	N3-C2-N1	-3.93	122.54	128.68
2	B	800	AGS	N3-C2-N1	-3.89	122.60	128.68
2	F	800	AGS	N3-C2-N1	-3.73	122.84	128.68
2	E	800	AGS	N3-C2-N1	-3.61	123.03	128.68
2	C	800	AGS	N3-C2-N1	-3.58	123.08	128.68
2	C	800	AGS	C4-C5-N7	-2.76	106.53	109.40
2	E	800	AGS	C3'-C2'-C1'	2.55	104.82	100.98
2	B	800	AGS	PA-O3A-PB	-2.52	124.19	132.83
2	B	800	AGS	C3'-C2'-C1'	2.46	104.69	100.98
2	A	800	AGS	PA-O3A-PB	-2.45	124.42	132.83
2	C	800	AGS	C3'-C2'-C1'	2.39	104.58	100.98
2	A	800	AGS	C4-C5-N7	-2.38	106.92	109.40
2	A	800	AGS	C3'-C2'-C1'	2.36	104.53	100.98
2	C	800	AGS	PA-O3A-PB	-2.29	124.95	132.83
2	D	800	AGS	C3'-C2'-C1'	2.29	104.43	100.98
2	B	800	AGS	C4-C5-N7	-2.25	107.06	109.40
2	F	800	AGS	C4-C5-N7	-2.19	107.11	109.40
2	D	800	AGS	C2-N1-C6	2.18	122.48	118.75
2	A	800	AGS	O3G-PG-O3B	2.14	111.80	104.64
2	D	800	AGS	O3G-PG-O3B	2.13	111.75	104.64
2	F	800	AGS	C3'-C2'-C1'	2.12	104.17	100.98
2	E	800	AGS	PA-O3A-PB	-2.12	125.56	132.83
2	B	800	AGS	O3G-PG-O3B	2.10	111.66	104.64
2	D	800	AGS	PA-O3A-PB	-2.10	125.62	132.83
2	C	800	AGS	O2B-PB-O1B	2.05	122.38	112.24
2	D	800	AGS	O2B-PB-O1B	2.02	122.24	112.24

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	A	800	AGS	PA-O3A-PB-O1B
2	B	800	AGS	PA-O3A-PB-O1B
2	E	800	AGS	C5'-O5'-PA-O2A
2	A	800	AGS	C5'-O5'-PA-O3A
2	B	800	AGS	C5'-O5'-PA-O3A
2	C	800	AGS	C5'-O5'-PA-O3A
2	D	800	AGS	C5'-O5'-PA-O3A
2	E	800	AGS	C5'-O5'-PA-O3A
2	F	800	AGS	C5'-O5'-PA-O3A
2	A	800	AGS	PA-O3A-PB-O2B
2	B	800	AGS	PA-O3A-PB-O2B

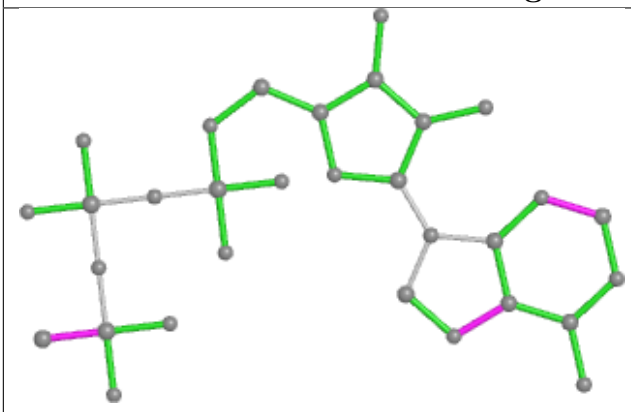
There are no ring outliers.

6 monomers are involved in 6 short contacts:

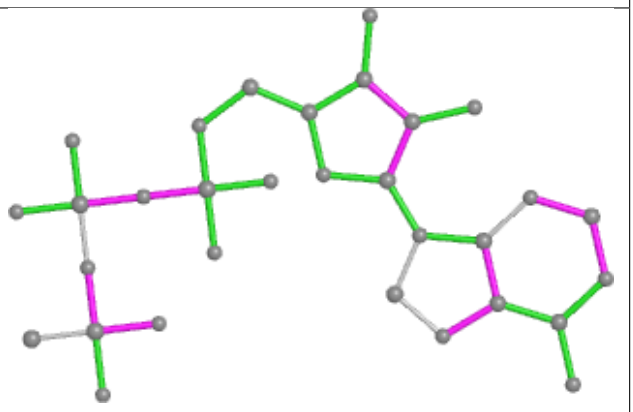
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	AGS	1	0
2	E	800	AGS	1	0
2	D	800	AGS	1	0
2	C	800	AGS	1	0
2	F	800	AGS	1	0
2	A	800	AGS	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

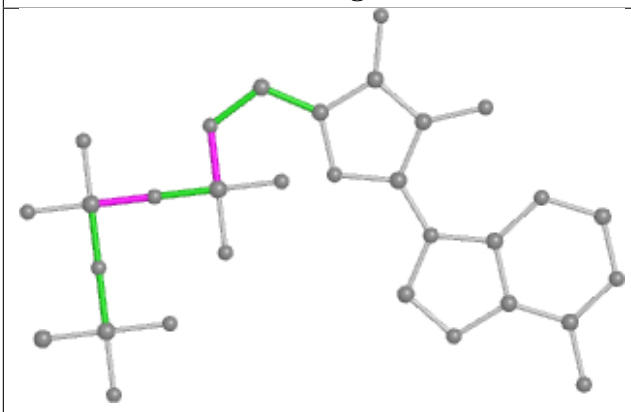
Ligand AGS B 800



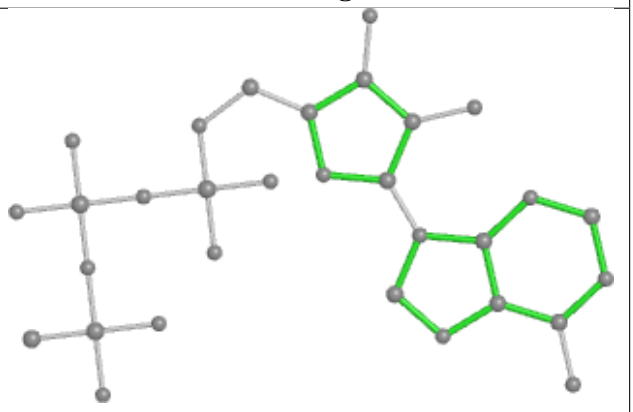
Bond lengths



Bond angles

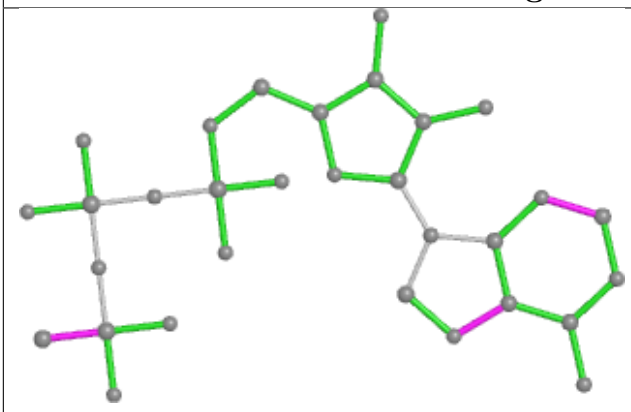


Torsions

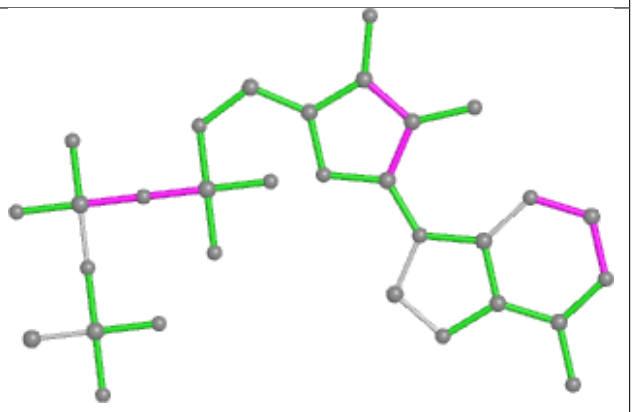


Rings

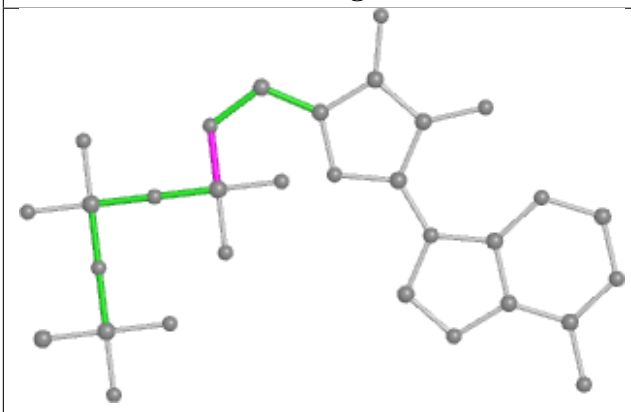
Ligand AGS E 800



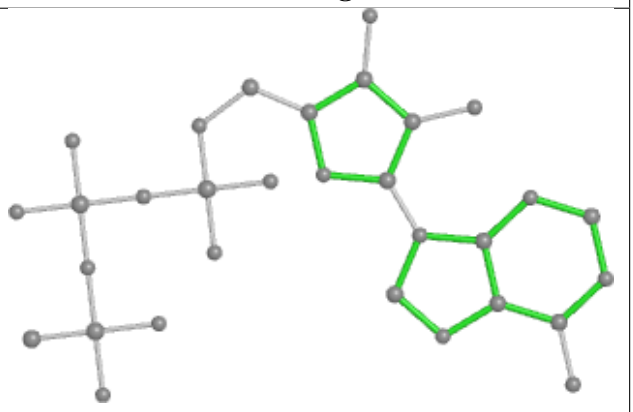
Bond lengths



Bond angles

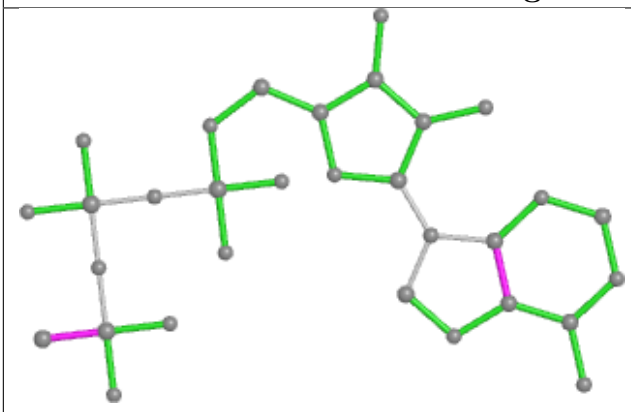


Torsions

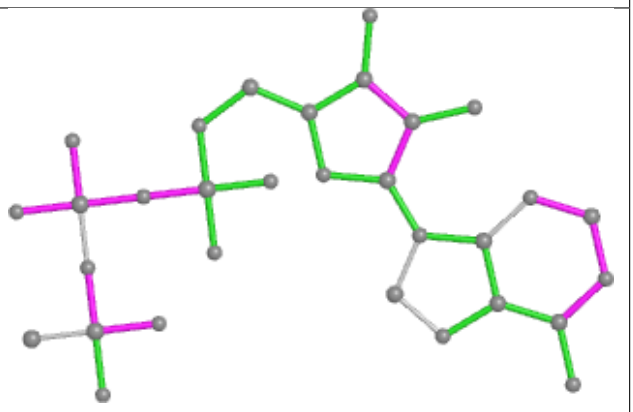


Rings

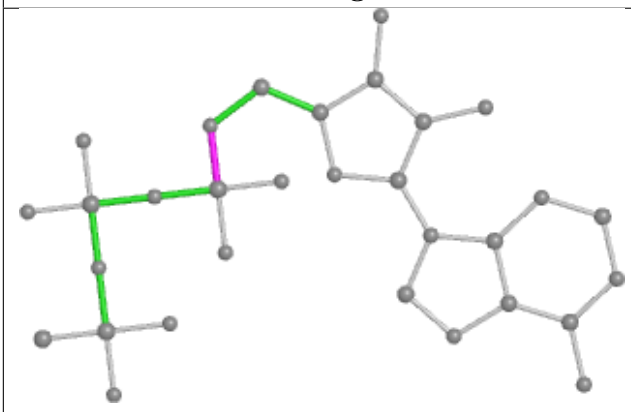
Ligand AGS D 800



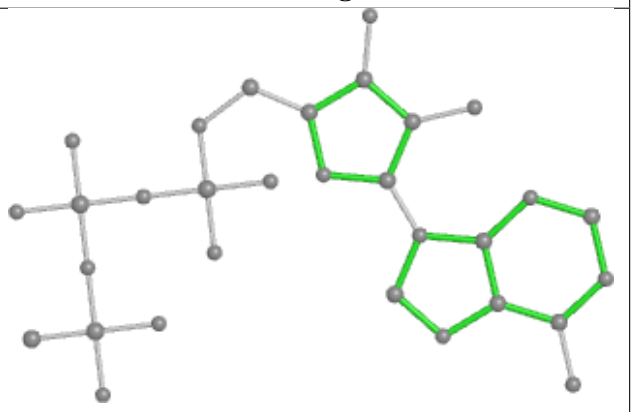
Bond lengths



Bond angles

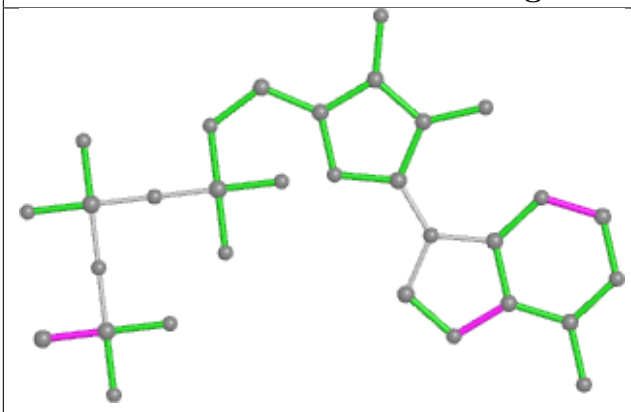


Torsions

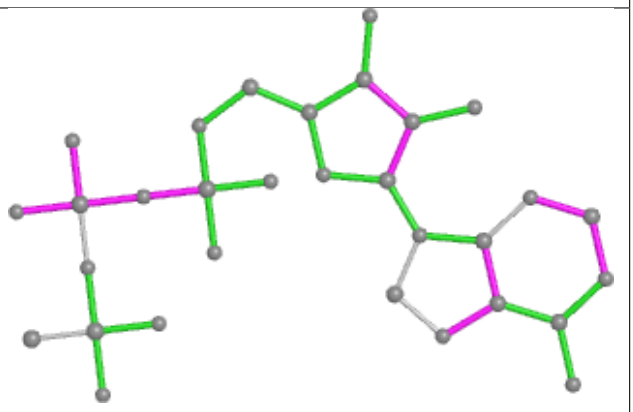


Rings

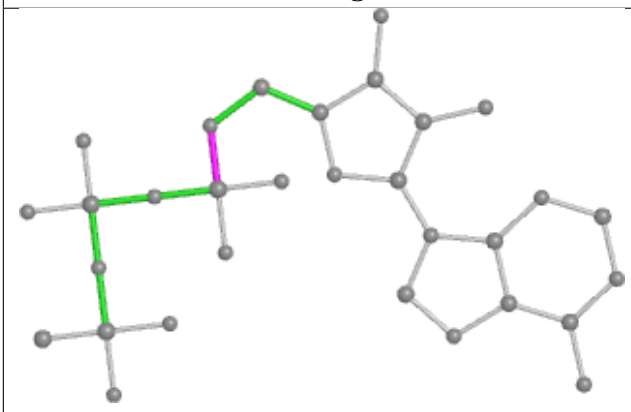
Ligand AGS C 800



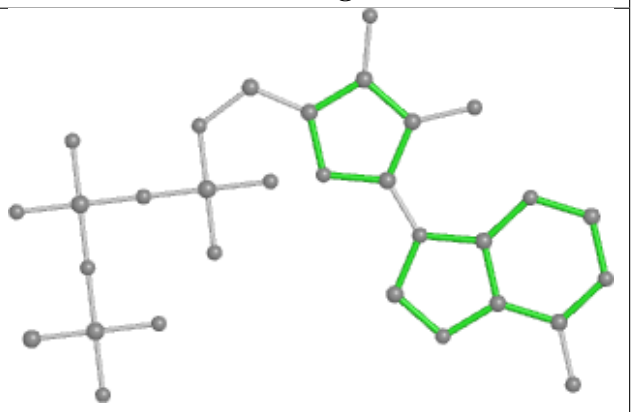
Bond lengths



Bond angles

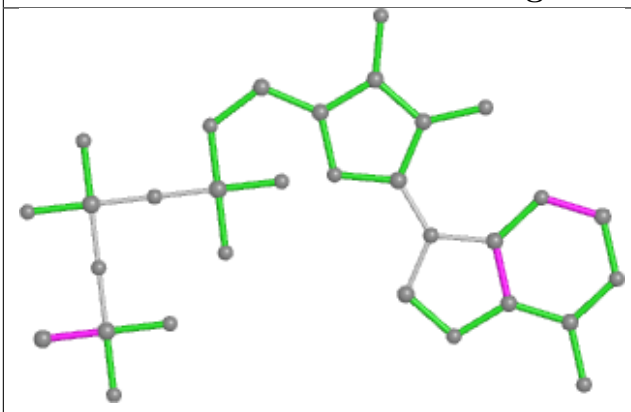


Torsions

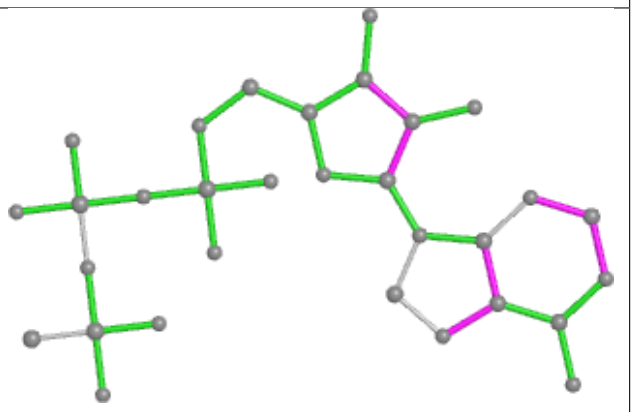


Rings

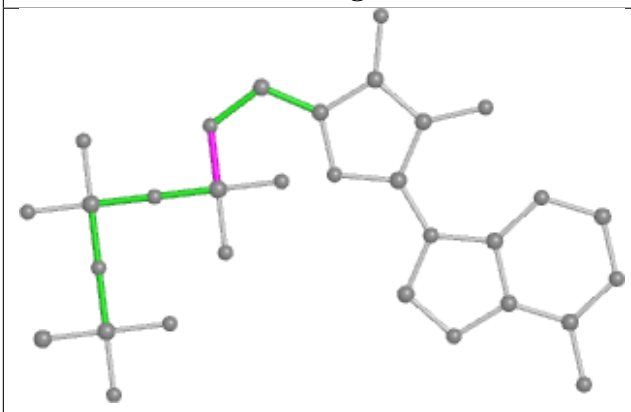
Ligand AGS F 800



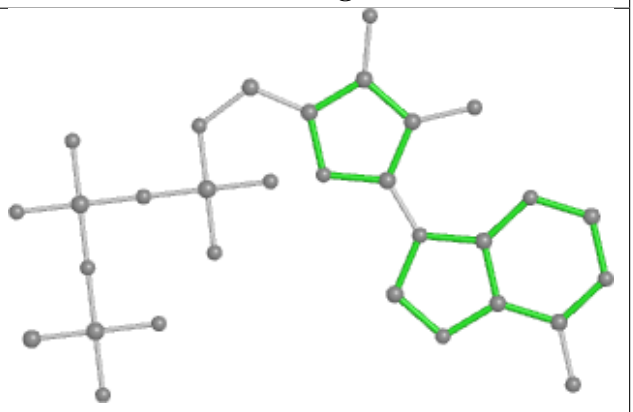
Bond lengths



Bond angles

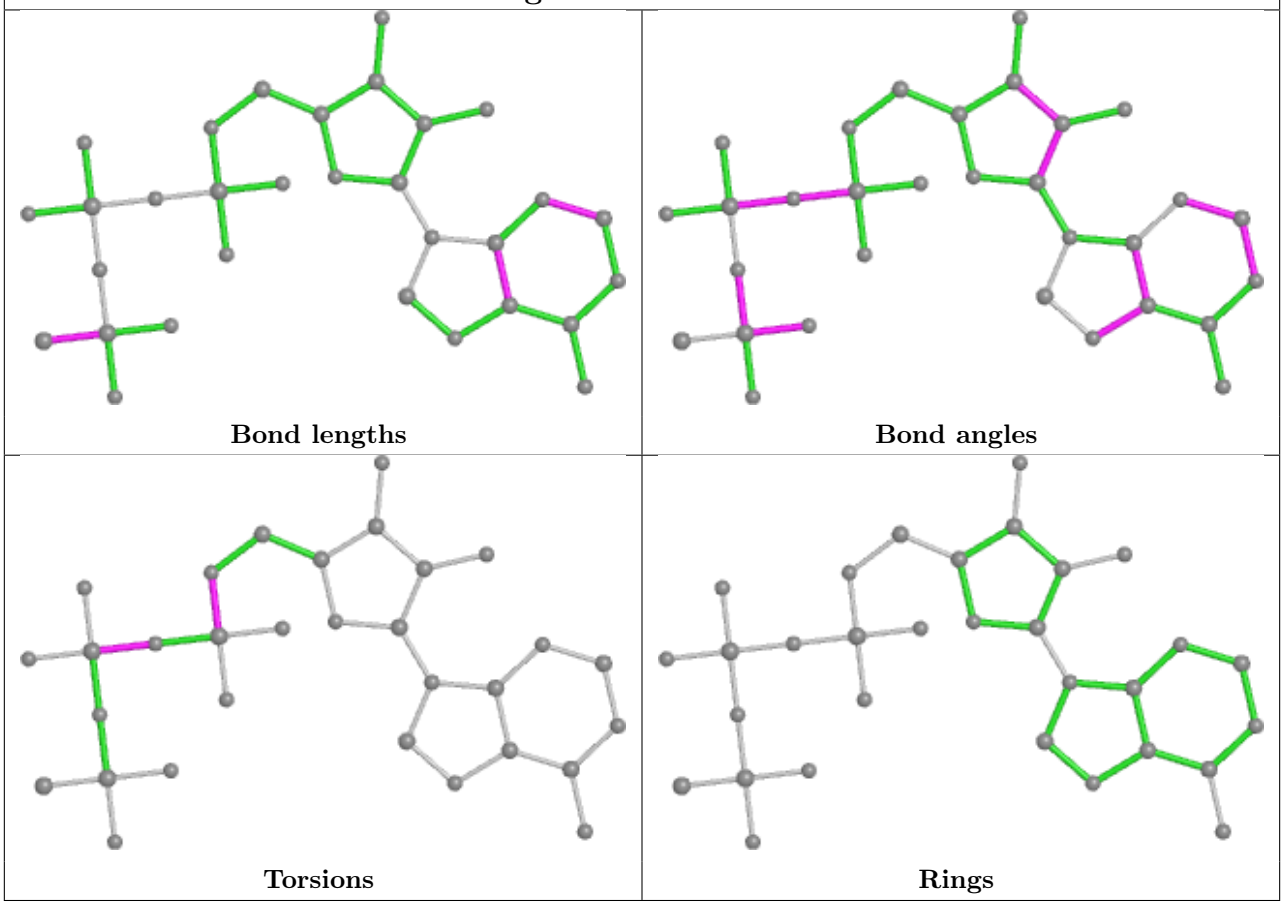


Torsions



Rings

Ligand AGS A 800



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, 95^{th} 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	451/489 (92%)	0.26	16 (3%)	44	34	62, 65, 67, 72	0
1	B	451/489 (92%)	0.18	10 (2%)	62	52	62, 65, 67, 71	0
1	C	451/489 (92%)	0.20	11 (2%)	59	49	62, 65, 67, 70	0
1	D	451/489 (92%)	0.36	27 (5%)	21	14	62, 65, 67, 71	0
1	E	451/489 (92%)	0.29	24 (5%)	26	18	62, 65, 67, 77	0
1	F	451/489 (92%)	0.22	9 (1%)	65	56	62, 65, 67, 70	0
All	All	2706/2934 (92%)	0.25	97 (3%)	42	32	62, 65, 67, 77	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	MET	4.4
1	E	106	PRO	4.1
1	D	169	ASP	4.0
1	D	114	ILE	3.8
1	E	158	MET	3.7
1	C	462	SER	3.6
1	E	173	TYR	3.6
1	F	114	ILE	3.5
1	A	128	GLY	3.5
1	E	52	PHE	3.5
1	E	169	ASP	3.4
1	E	114	ILE	3.4
1	E	462	SER	3.3
1	D	32	ILE	3.3
1	F	113	ARG	3.3
1	E	171	SER	3.2
1	A	109	LYS	3.2
1	D	57	VAL	3.1
1	D	187	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	171	SER	3.1
1	B	462	SER	3.1
1	D	183	HIS	3.1
1	D	106	PRO	3.1
1	A	72	LEU	3.0
1	A	317	HIS	3.0
1	D	52	PHE	3.0
1	D	173	TYR	3.0
1	A	169	ASP	3.0
1	C	461	PRO	2.9
1	C	317	HIS	2.9
1	D	113	ARG	2.9
1	A	395	ASP	2.9
1	D	159	ARG	2.8
1	F	158	MET	2.8
1	D	141	GLU	2.7
1	E	175	ILE	2.7
1	E	107	ASP	2.7
1	E	179	ASP	2.7
1	C	158	MET	2.7
1	E	19	GLN	2.7
1	E	317	HIS	2.7
1	A	402	GLU	2.7
1	E	57	VAL	2.6
1	E	72	LEU	2.6
1	C	126	ILE	2.5
1	A	107	ASP	2.5
1	D	41	LEU	2.5
1	A	127	THR	2.5
1	B	395	ASP	2.5
1	D	107	ASP	2.5
1	E	69	CYS	2.5
1	F	112	LYS	2.5
1	C	128	GLY	2.5
1	D	175	ILE	2.4
1	C	187	GLU	2.4
1	E	51	LEU	2.4
1	E	108	VAL	2.4
1	B	158	MET	2.4
1	D	51	LEU	2.4
1	A	461	PRO	2.4
1	F	169	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	462	SER	2.4
1	F	171	SER	2.4
1	D	126	ILE	2.4
1	F	141	GLU	2.3
1	D	108	VAL	2.3
1	D	188	PRO	2.3
1	B	461	PRO	2.3
1	E	32	ILE	2.3
1	B	317	HIS	2.3
1	E	70	ILE	2.3
1	F	179	ASP	2.3
1	C	14	THR	2.3
1	B	429	LEU	2.2
1	A	108	VAL	2.2
1	D	317	HIS	2.2
1	D	163	PHE	2.2
1	A	399	VAL	2.2
1	C	113	ARG	2.2
1	A	398	GLN	2.2
1	F	317	HIS	2.2
1	C	68	VAL	2.2
1	D	134	TYR	2.2
1	E	53	ARG	2.2
1	D	71	VAL	2.2
1	B	32	ILE	2.1
1	E	71	VAL	2.1
1	C	314	GLU	2.1
1	E	174	CYS	2.1
1	E	73	SER	2.0
1	A	429	LEU	2.0
1	B	398	GLN	2.0
1	A	56	THR	2.0
1	B	314	GLU	2.0
1	D	115	HIS	2.0
1	D	127	THR	2.0
1	B	52	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)

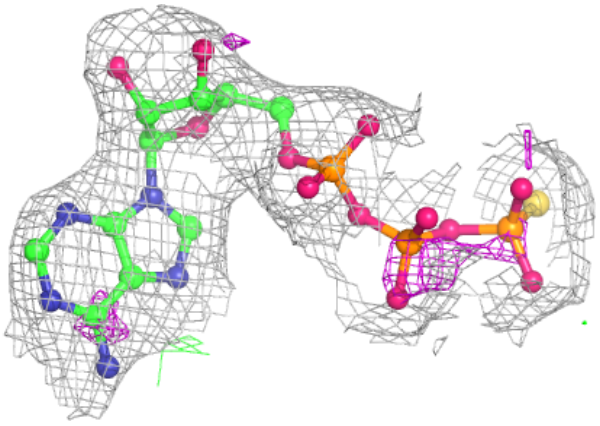
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

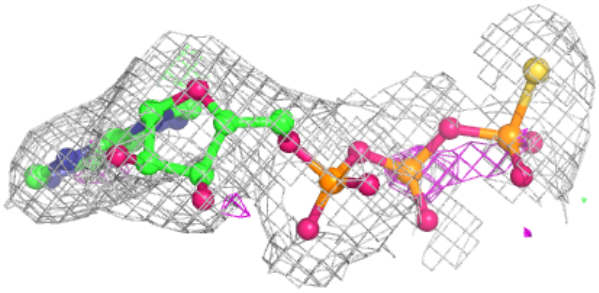
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	801	1/1	0.96	0.18	55,55,55,55	0
3	MG	D	801	1/1	0.96	0.12	55,55,55,55	0
3	MG	B	801	1/1	0.97	0.10	55,55,55,55	0
2	AGS	A	800	31/31	0.97	0.17	53,60,62,64	0
3	MG	F	801	1/1	0.97	0.09	55,55,55,55	0
2	AGS	F	800	31/31	0.98	0.13	51,60,62,64	0
2	AGS	B	800	31/31	0.98	0.14	51,60,63,65	0
2	AGS	C	800	31/31	0.98	0.14	53,61,62,65	0
3	MG	C	801	1/1	0.98	0.12	54,54,54,54	0
2	AGS	D	800	31/31	0.98	0.12	53,60,62,65	0
2	AGS	E	800	31/31	0.98	0.15	51,60,62,64	0
3	MG	E	801	1/1	0.99	0.14	54,54,54,54	0

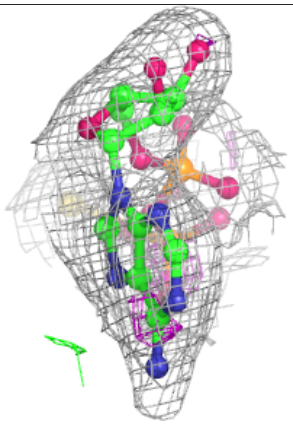
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

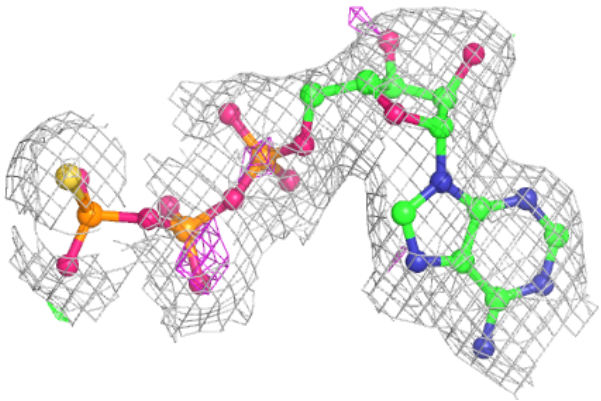


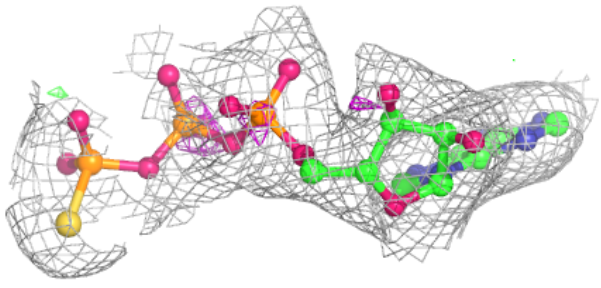


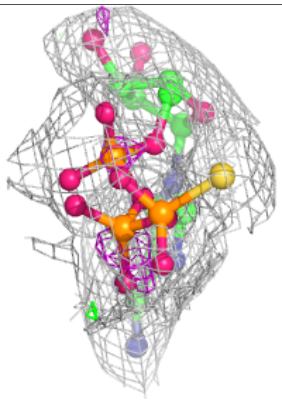


Electron density around AGS F 800:

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

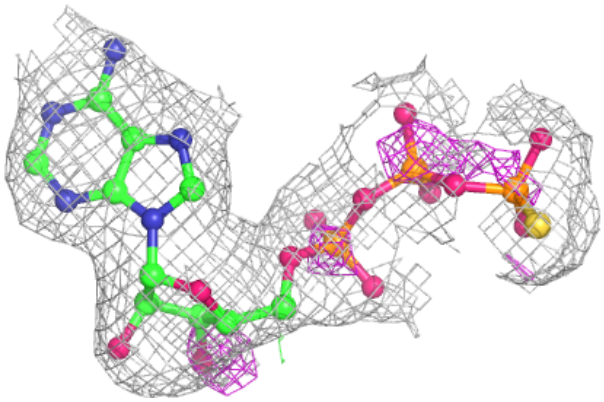


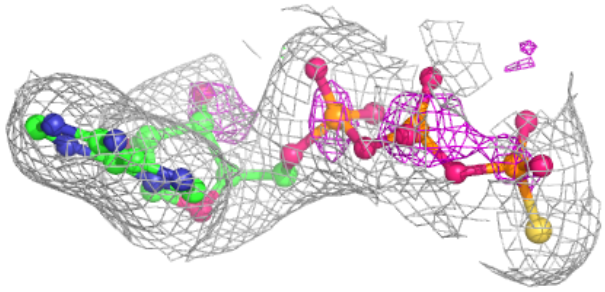


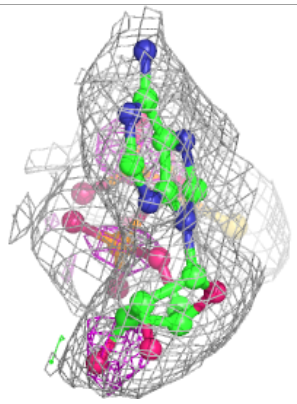


Electron density around AGS B 800:

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

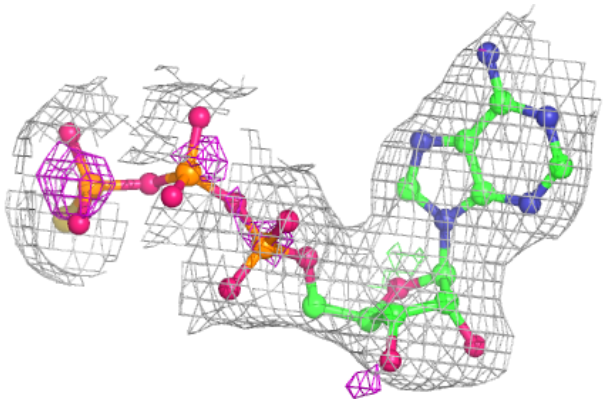


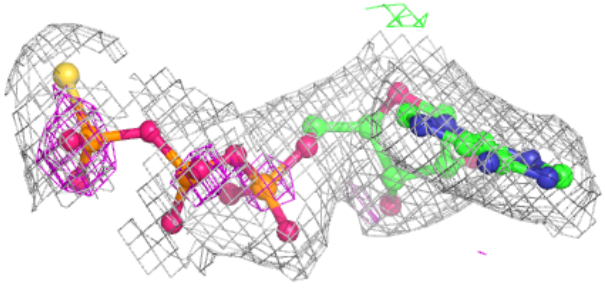


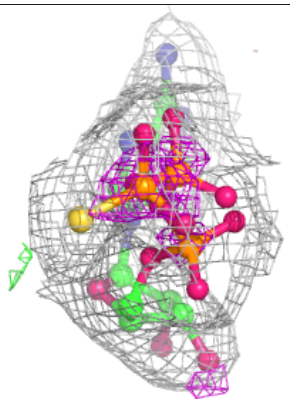


Electron density around AGS C 800:

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

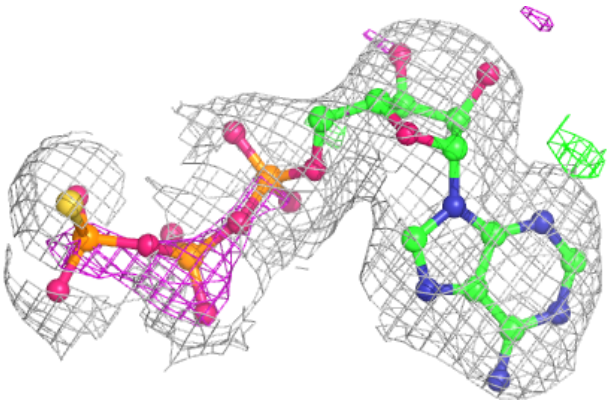


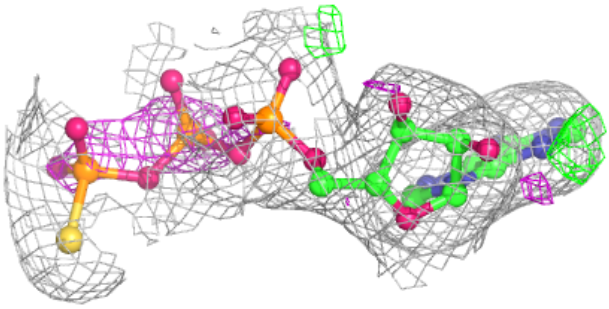


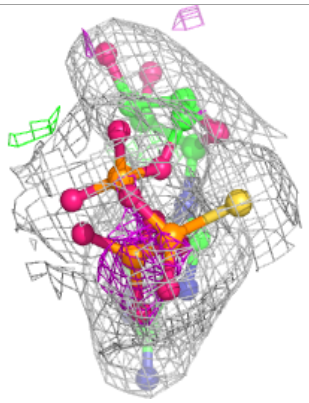


Electron density around AGS D 800:

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

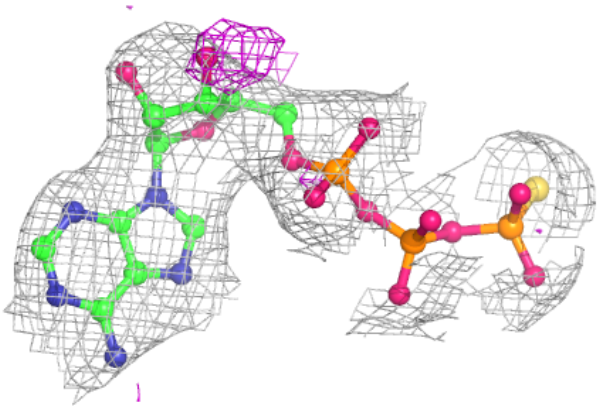


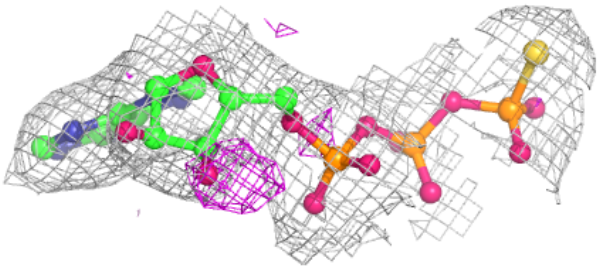


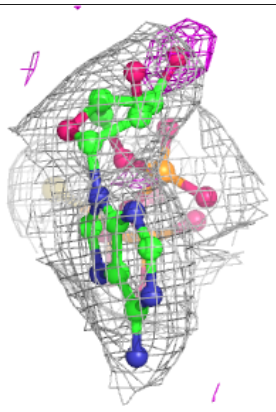


Electron density around AGS E 800:

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







6.5 Other polymers (i)

There are no such residues in this entry.