



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:41 PM UTC

PDB ID : 4KLN / pdb_00004klh
Title : Structure of p97 N-D1 A232E mutant in complex with ATPgS
Authors : Xia, D.; Tang, W.K.
Deposited on : 2013-05-07
Resolution : 2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

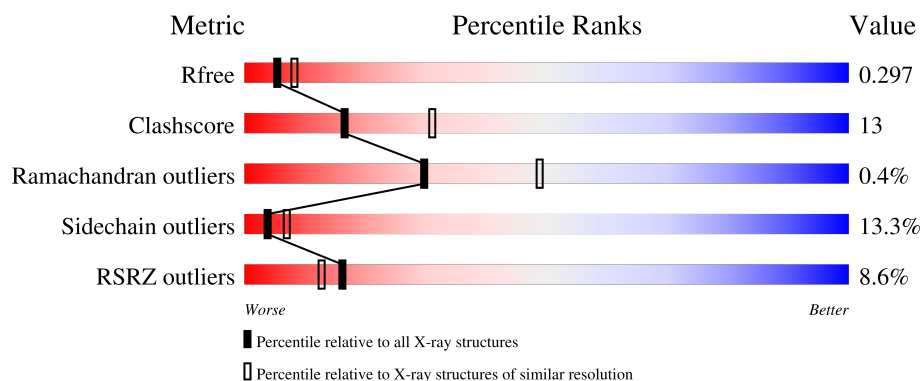
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	489	7% 60% 29% 8%
1	B	489	6% 63% 26% 8%
1	C	489	10% 61% 28% 8%
1	D	489	7% 61% 28% 8%
1	E	489	11% 60% 29% 8%

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Mol	Chain	Length	Quality of chain
1	F	489	6% 62% 26% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21556 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	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	B	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	C	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	D	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	E	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	F	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			

There are 54 discrepancies between the modelled and reference sequences:

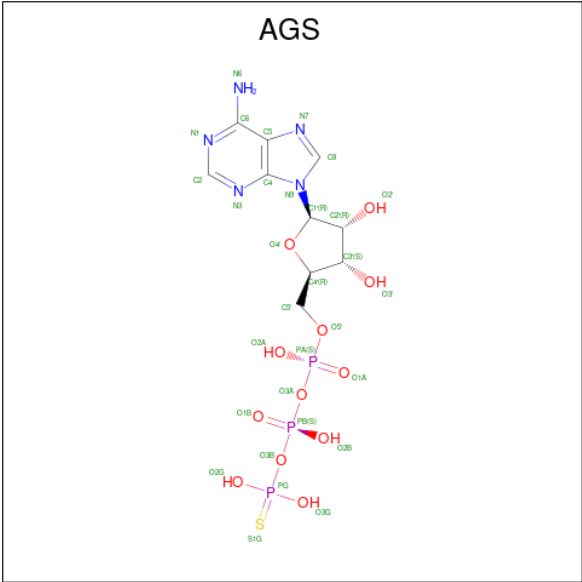
Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLU	ALA	engineered mutation	UNP P55072
A	482	ARG	-	expression tag	UNP P55072
A	483	SER	-	expression tag	UNP P55072
A	484	HIS	-	expression tag	UNP P55072
A	485	HIS	-	expression tag	UNP P55072
A	486	HIS	-	expression tag	UNP P55072
A	487	HIS	-	expression tag	UNP P55072
A	488	HIS	-	expression tag	UNP P55072
A	489	HIS	-	expression tag	UNP P55072
B	232	GLU	ALA	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	232	GLU	ALA	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	232	GLU	ALA	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	232	GLU	ALA	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	232	GLU	ALA	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 (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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 (CCD ID: 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		

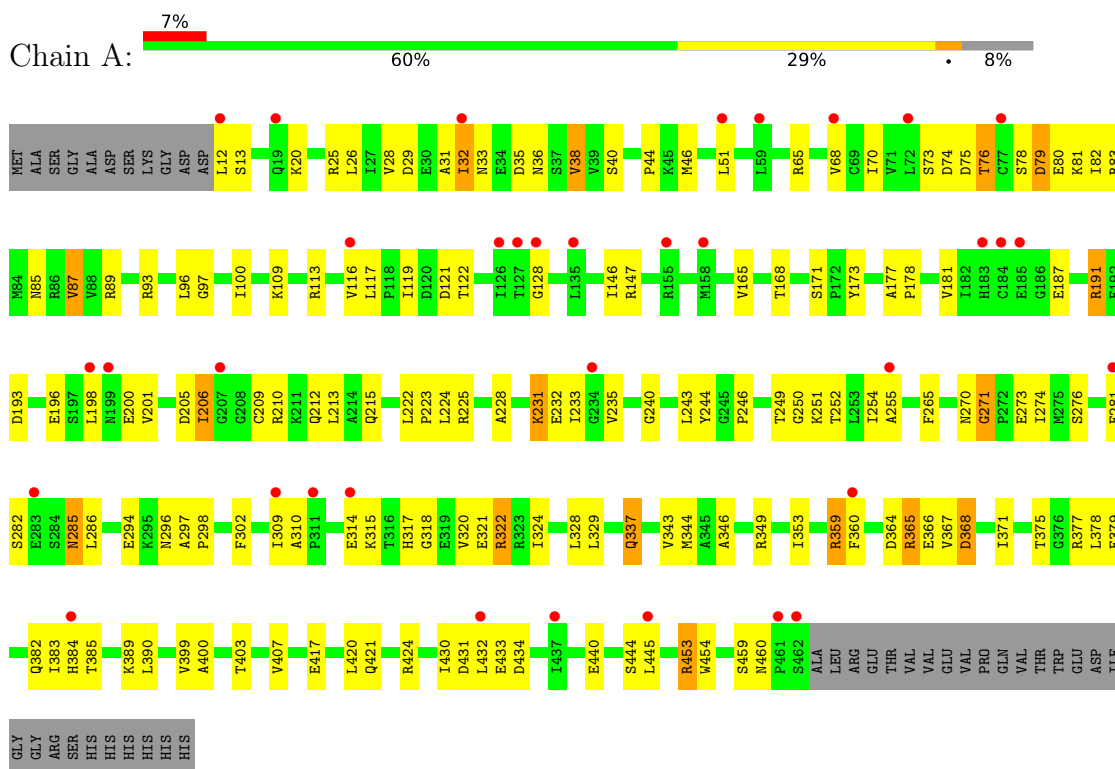
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	28	Total 28	O 28	0	0
4	C	30	Total 30	O 30	0	0
4	D	26	Total 26	O 26	0	0
4	E	25	Total 25	O 25	0	0
4	F	24	Total 24	O 24	0	0

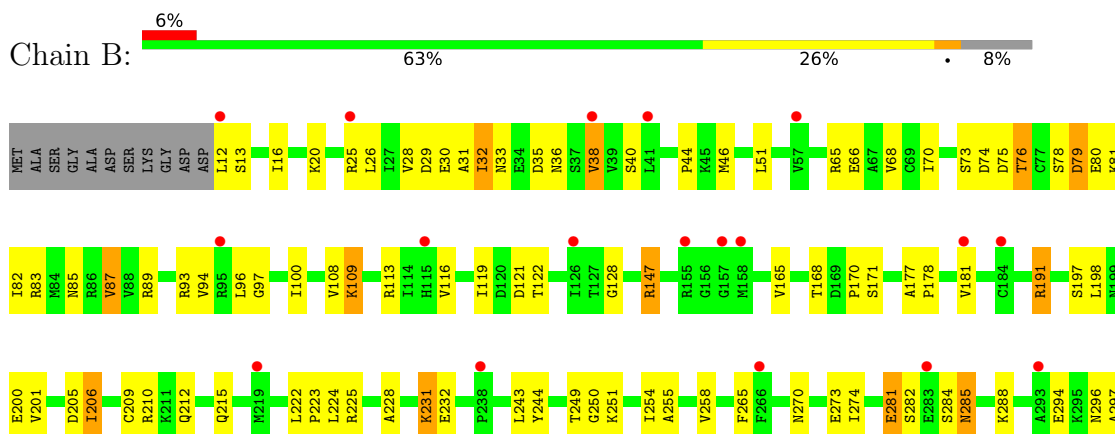
3 Residue-property plots

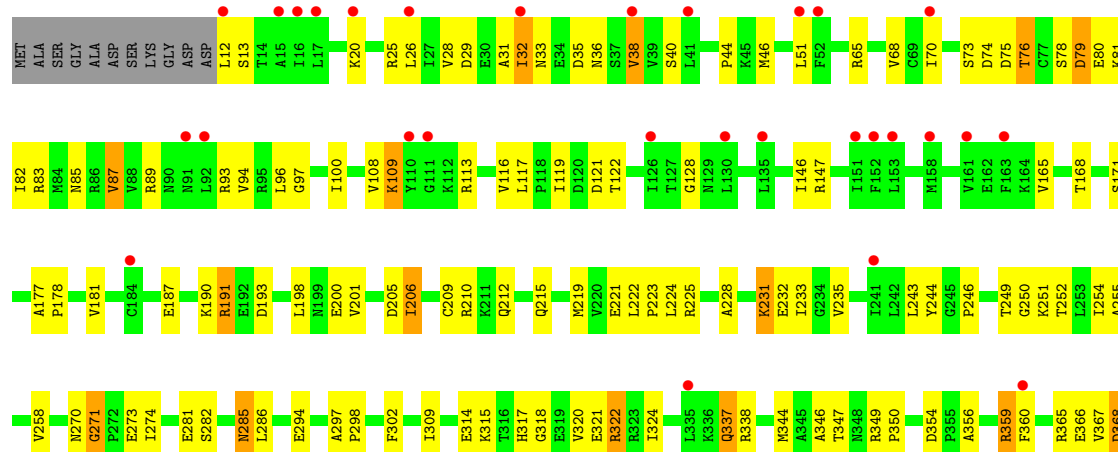
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transitional endoplasmic reticulum ATPase



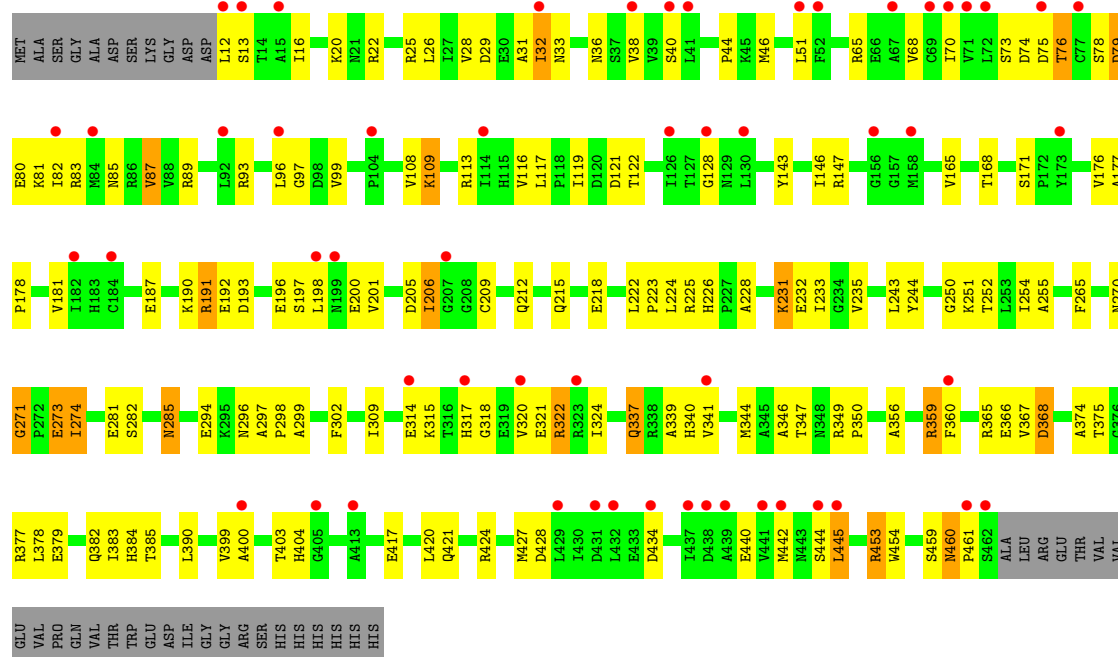
- Molecule 1: Transitional endoplasmic reticulum ATPase



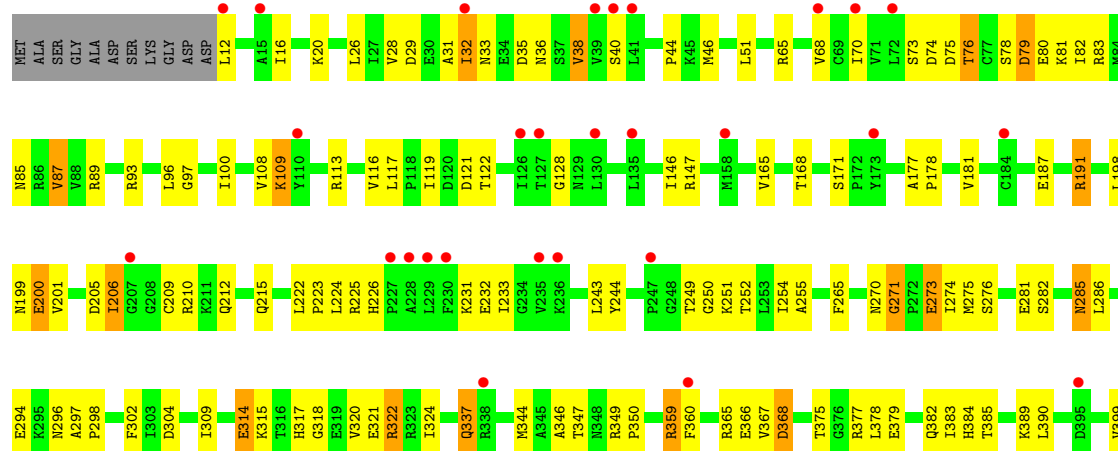


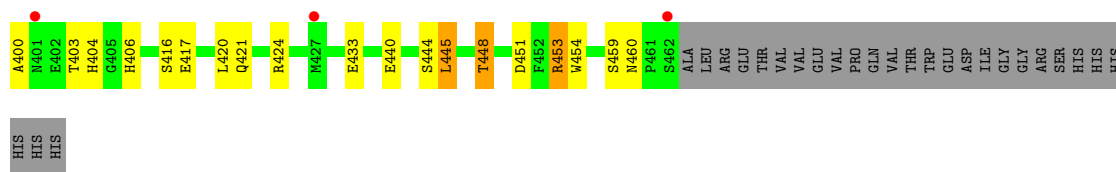


• Molecule 1: Transitional endoplasmic reticulum ATPase



• 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	91.15Å 104.51Å 109.53Å 98.11° 90.55° 92.72°	Depositor
Resolution (Å)	46.29 – 2.62 46.29 – 2.62	Depositor EDS
% Data completeness (in resolution range)	83.1 (46.29-2.62) 83.1 (46.29-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.274 , 0.289 0.284 , 0.297	Depositor DCC
R_{free} test set	6020 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21556	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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	0.40	0/3587	0.86	1/4846 (0.0%)
1	B	0.43	1/3587 (0.0%)	0.87	1/4846 (0.0%)
1	C	0.42	1/3587 (0.0%)	0.86	3/4846 (0.1%)
1	D	0.40	0/3587	0.86	3/4846 (0.1%)
1	E	0.40	0/3587	0.85	1/4846 (0.0%)
1	F	0.44	0/3587	0.87	0/4846
All	All	0.42	2/21522 (0.0%)	0.86	9/29076 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	THR	C-O	-6.78	1.15	1.23
1	B	285	ASN	CG-OD1	-6.45	1.11	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	SER	N-CA-C	-5.66	104.95	113.89
1	C	262	THR	CB-CA-C	-5.64	99.16	109.54
1	E	13	SER	N-CA-C	-5.57	105.09	113.89
1	B	13	SER	N-CA-C	-5.43	105.31	113.89
1	D	13	SER	N-CA-C	-5.35	105.43	113.89
1	C	13	SER	N-CA-C	-5.30	105.51	113.89
1	D	354	ASP	CA-C-N	5.09	124.75	119.56
1	D	354	ASP	C-N-CA	5.09	124.75	119.56
1	C	262	THR	CA-C-O	-5.03	116.08	121.56

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	3533	0	3594	102	0
1	B	3533	0	3594	94	0
1	C	3533	0	3594	105	0
1	D	3533	0	3594	106	0
1	E	3533	0	3594	102	0
1	F	3533	0	3594	95	0
2	A	31	0	12	6	0
2	B	31	0	12	5	0
2	C	31	0	12	4	0
2	D	31	0	12	4	0
2	E	31	0	12	5	0
2	F	31	0	12	6	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	33	0	0	0	0
4	B	28	0	0	0	0
4	C	30	0	0	0	0
4	D	26	0	0	6	0
4	E	25	0	0	0	0
4	F	24	0	0	0	0
All	All	21556	0	21636	554	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 13.

All (554) 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:C:399:VAL:O	1:C:403:THR:HG23	1.42	1.14
1:D:399:VAL:O	1:D:403:THR:HG23	1.47	1.11
2:E:800:AGS:S1G	1:F:359:ARG:HG2	2.04	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:AGS:S1G	1:C:359:ARG:CG	2.55	0.95
2:B:800:AGS:S1G	1:C:359:ARG:HG2	2.05	0.95
1:F:399:VAL:O	1:F:403:THR:HG23	1.69	0.93
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.50	0.93
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.50	0.93
1:C:428:ASP:HA	1:D:20:LYS:HE2	1.50	0.92
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.52	0.92
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.52	0.91
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.52	0.91
2:E:800:AGS:S1G	1:F:359:ARG:CG	2.59	0.90
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.51	0.90
1:D:433:GLU:HG3	1:E:25:ARG:HH21	1.36	0.89
1:A:359:ARG:CG	2:F:800:AGS:S1G	2.63	0.87
1:B:399:VAL:O	1:B:403:THR:HG23	1.73	0.87
1:C:251:LYS:HE3	2:C:800:AGS:O2B	1.75	0.87
1:A:359:ARG:HG2	2:F:800:AGS:S1G	2.16	0.86
1:D:251:LYS:HE3	2:D:800:AGS:O2B	1.77	0.85
1:B:32:ILE:HG23	1:B:83:ARG:HH11	1.42	0.82
1:C:31:ALA:HA	1:C:83:ARG:HB3	1.62	0.82
2:C:800:AGS:S1G	1:D:359:ARG:HG2	2.21	0.81
1:C:250:GLY:O	1:C:254:ILE:HG13	1.81	0.80
1:D:206:ILE:HD11	1:D:209:CYS:HB2	1.63	0.80
1:F:31:ALA:HA	1:F:83:ARG:HB3	1.64	0.80
1:E:206:ILE:HD11	1:E:209:CYS:HB2	1.64	0.80
1:C:206:ILE:HD11	1:C:209:CYS:HB2	1.65	0.79
1:E:399:VAL:O	1:E:403:THR:HG23	1.81	0.79
1:B:32:ILE:HG23	1:B:83:ARG:NH1	1.96	0.79
1:A:31:ALA:HA	1:A:83:ARG:HB3	1.63	0.79
1:B:206:ILE:HD11	1:B:209:CYS:HB2	1.62	0.79
1:E:31:ALA:HA	1:E:83:ARG:HB3	1.63	0.79
1:A:206:ILE:HD11	1:A:209:CYS:HB2	1.66	0.79
1:B:31:ALA:HA	1:B:83:ARG:HB3	1.65	0.78
1:C:249:THR:OG1	1:C:251:LYS:HE2	1.83	0.78
2:A:800:AGS:S1G	1:B:359:ARG:HG2	2.24	0.78
1:D:31:ALA:HA	1:D:83:ARG:HB3	1.64	0.77
1:F:206:ILE:HD11	1:F:209:CYS:HB2	1.64	0.77
2:C:800:AGS:S1G	1:D:359:ARG:CG	2.73	0.77
1:E:302:PHE:CE2	1:E:344:MET:HE2	2.20	0.76
2:A:800:AGS:S1G	1:B:359:ARG:CG	2.72	0.76
1:C:399:VAL:O	1:C:403:THR:CG2	2.30	0.76
1:B:251:LYS:HE3	2:B:800:AGS:O2B	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:HD2	1:C:403:THR:OG1	1.87	0.74
2:D:800:AGS:S1G	1:E:359:ARG:HG2	2.29	0.73
1:D:244:TYR:CZ	1:D:368:ASP:HB2	2.23	0.73
1:D:433:GLU:HG3	1:E:25:ARG:NH2	2.02	0.73
1:A:244:TYR:CZ	1:A:368:ASP:HB2	2.23	0.73
1:E:317:HIS:HB2	1:F:322:ARG:HH22	1.54	0.73
1:E:243:LEU:HD22	1:E:367:VAL:HB	1.71	0.73
1:F:244:TYR:CZ	1:F:368:ASP:HB2	2.24	0.72
1:A:251:LYS:HE3	2:A:800:AGS:O2B	1.90	0.71
1:D:89:ARG:HD3	4:D:917:HOH:O	1.89	0.71
1:A:25:ARG:HH21	1:F:433:GLU:HG3	1.54	0.71
2:B:800:AGS:S1G	1:C:359:ARG:HG3	2.30	0.71
1:C:377:ARG:CD	1:C:403:THR:OG1	2.38	0.70
2:D:800:AGS:S1G	1:E:359:ARG:CG	2.79	0.70
1:D:109:LYS:H	1:D:109:LYS:HD2	1.57	0.70
1:F:302:PHE:CE2	1:F:344:MET:HE2	2.28	0.68
1:B:244:TYR:CZ	1:B:368:ASP:HB2	2.29	0.68
1:E:109:LYS:H	1:E:109:LYS:HD2	1.59	0.68
1:F:109:LYS:H	1:F:109:LYS:HD2	1.59	0.68
1:A:399:VAL:O	1:A:403:THR:HG23	1.94	0.68
1:B:416:SER:HA	1:C:235:VAL:HG21	1.76	0.68
1:E:337:GLN:HA	1:E:337:GLN:HE21	1.59	0.68
1:C:109:LYS:H	1:C:109:LYS:HD2	1.58	0.67
1:F:252:THR:O	1:F:255:ALA:HB3	1.95	0.67
1:C:277:LYS:HB3	1:C:281:GLU:HB3	1.76	0.67
1:B:109:LYS:H	1:B:109:LYS:HD2	1.60	0.67
1:A:196:GLU:OE2	1:B:337:GLN:HB2	1.94	0.66
1:E:243:LEU:CD2	1:E:367:VAL:HB	2.25	0.66
1:F:377:ARG:NH1	1:F:400:ALA:O	2.28	0.66
1:E:244:TYR:CZ	1:E:368:ASP:HB2	2.30	0.66
1:B:243:LEU:HD22	1:B:367:VAL:HB	1.78	0.66
1:D:377:ARG:HD2	1:D:403:THR:OG1	1.95	0.66
1:E:377:ARG:NH2	1:E:404:HIS:HA	2.10	0.65
1:F:243:LEU:HD22	1:F:367:VAL:HB	1.79	0.65
1:A:337:GLN:HE21	1:A:337:GLN:HA	1.61	0.65
1:C:249:THR:HG1	1:C:251:LYS:HE2	1.62	0.65
1:F:337:GLN:HA	1:F:337:GLN:HE21	1.62	0.65
1:C:377:ARG:HD2	1:C:403:THR:HG1	1.62	0.65
1:C:302:PHE:CE2	1:C:344:MET:HE2	2.32	0.65
1:A:433:GLU:HG3	1:B:25:ARG:HH21	1.62	0.65
1:C:278:LEU:O	1:C:281:GLU:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:GLN:HE21	1:D:337:GLN:HA	1.62	0.64
1:B:317:HIS:HB2	1:C:322:ARG:HH22	1.60	0.64
1:C:337:GLN:HE21	1:C:337:GLN:HA	1.60	0.64
1:B:433:GLU:HG3	1:C:25:ARG:NH2	2.12	0.64
1:E:385:THR:HB	1:E:390:LEU:HD11	1.80	0.64
1:B:377:ARG:HD2	1:B:403:THR:OG1	1.97	0.64
1:D:317:HIS:HB2	1:E:322:ARG:HH22	1.63	0.64
1:E:222:LEU:HB3	1:E:223:PRO:HD3	1.80	0.63
1:B:206:ILE:CD1	1:B:209:CYS:HB2	2.28	0.63
1:C:378:LEU:HG	1:C:382:GLN:NE2	2.14	0.63
1:E:377:ARG:HD2	1:E:403:THR:OG1	1.98	0.63
1:C:243:LEU:HD22	1:C:367:VAL:HB	1.80	0.63
1:C:385:THR:HB	1:C:390:LEU:HD11	1.81	0.63
1:D:378:LEU:HG	1:D:382:GLN:NE2	2.14	0.63
1:F:378:LEU:HG	1:F:382:GLN:NE2	2.13	0.63
1:B:222:LEU:HB3	1:B:223:PRO:HD3	1.81	0.63
1:B:385:THR:HB	1:B:390:LEU:HD11	1.80	0.62
1:D:302:PHE:CE2	1:D:344:MET:HE2	2.34	0.62
1:B:337:GLN:HE21	1:B:337:GLN:HA	1.64	0.62
1:C:416:SER:HA	1:D:235:VAL:HG21	1.81	0.62
1:D:206:ILE:CD1	1:D:209:CYS:HB2	2.29	0.62
1:E:378:LEU:HG	1:E:382:GLN:NE2	2.13	0.62
1:A:206:ILE:CD1	1:A:209:CYS:HB2	2.29	0.62
1:D:377:ARG:CD	1:D:403:THR:OG1	2.47	0.62
1:A:359:ARG:HG3	2:F:800:AGS:S1G	2.39	0.62
1:A:385:THR:HB	1:A:390:LEU:HD11	1.82	0.62
1:B:74:ASP:OD1	1:B:76:THR:HG23	1.99	0.62
1:B:378:LEU:HG	1:B:382:GLN:NE2	2.14	0.62
1:E:318:GLY:HA3	1:E:321:GLU:HG3	1.81	0.62
1:F:251:LYS:HE3	2:F:800:AGS:O2B	2.00	0.62
1:C:206:ILE:CD1	1:C:209:CYS:HB2	2.29	0.61
1:E:206:ILE:CD1	1:E:209:CYS:HB2	2.30	0.61
1:D:28:VAL:HG21	4:D:917:HOH:O	2.00	0.61
1:F:249:THR:OG1	1:F:251:LYS:HE2	2.00	0.61
1:D:219:MET:O	1:D:223:PRO:HG2	1.99	0.61
1:B:36:ASN:HA	1:B:85:ASN:HD21	1.65	0.61
1:E:285:ASN:N	1:E:285:ASN:HD22	1.99	0.61
1:D:243:LEU:HD22	1:D:367:VAL:HB	1.82	0.61
1:D:250:GLY:O	1:D:254:ILE:HG13	2.01	0.61
1:F:385:THR:HB	1:F:390:LEU:HD11	1.82	0.61
1:F:403:THR:O	1:F:406:HIS:ND1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HB3	1:A:223:PRO:HD3	1.81	0.60
1:C:428:ASP:HA	1:D:20:LYS:CE	2.27	0.60
1:C:201:VAL:HG13	1:C:205:ASP:HB2	1.82	0.60
1:D:320:VAL:O	1:D:324:ILE:HD12	2.02	0.60
1:A:378:LEU:HG	1:A:382:GLN:NE2	2.16	0.60
1:B:29:ASP:O	1:B:83:ARG:HA	2.01	0.59
1:C:222:LEU:HB3	1:C:223:PRO:HD3	1.82	0.59
1:A:431:ASP:HB2	1:B:20:LYS:HD3	1.84	0.59
1:B:201:VAL:HG13	1:B:205:ASP:HB2	1.84	0.59
1:E:20:LYS:HD2	1:E:20:LYS:N	2.17	0.59
1:B:302:PHE:CE2	1:B:344:MET:HE2	2.38	0.59
1:F:222:LEU:HB3	1:F:223:PRO:HD3	1.83	0.59
1:A:25:ARG:NH2	1:F:433:GLU:HG3	2.18	0.59
1:A:285:ASN:HD22	1:A:285:ASN:N	2.00	0.59
1:C:320:VAL:O	1:C:324:ILE:HD12	2.03	0.59
1:F:201:VAL:HG13	1:F:205:ASP:HB2	1.84	0.59
1:B:20:LYS:HD2	1:B:20:LYS:N	2.18	0.58
1:F:206:ILE:CD1	1:F:209:CYS:HB2	2.31	0.58
1:D:243:LEU:CD2	1:D:367:VAL:HB	2.34	0.58
1:D:385:THR:HB	1:D:390:LEU:HD11	1.85	0.58
1:F:243:LEU:CD2	1:F:367:VAL:HB	2.33	0.58
1:F:377:ARG:HD2	1:F:403:THR:OG1	2.03	0.58
2:E:800:AGS:S1G	1:F:359:ARG:HG3	2.44	0.58
1:A:201:VAL:HG13	1:A:205:ASP:HB2	1.85	0.58
2:A:800:AGS:S1G	1:B:359:ARG:HG3	2.43	0.57
1:E:192:GLU:O	1:E:196:GLU:HG3	2.04	0.57
1:C:244:TYR:CZ	1:C:368:ASP:HB2	2.38	0.57
1:A:32:ILE:HG23	1:A:83:ARG:NH1	2.19	0.57
1:C:32:ILE:HG23	1:C:83:ARG:NH1	2.20	0.57
1:A:431:ASP:CB	1:B:20:LYS:HD3	2.35	0.57
1:D:399:VAL:O	1:D:403:THR:CG2	2.38	0.57
1:F:250:GLY:HA2	2:F:800:AGS:O1A	2.05	0.57
1:F:318:GLY:HA3	1:F:321:GLU:HG3	1.86	0.57
1:E:29:ASP:O	1:E:83:ARG:HA	2.04	0.57
1:B:320:VAL:O	1:B:324:ILE:HD12	2.05	0.57
1:C:417:GLU:OE2	1:C:454:TRP:HZ3	1.87	0.57
1:F:74:ASP:OD1	1:F:76:THR:HG23	2.05	0.57
1:F:285:ASN:N	1:F:285:ASN:HD22	2.02	0.57
1:A:250:GLY:O	1:A:254:ILE:HG13	2.05	0.57
1:A:417:GLU:OE2	1:A:454:TRP:HZ3	1.87	0.57
1:C:285:ASN:N	1:C:285:ASN:HD22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ILE:HG23	1:D:83:ARG:NH1	2.20	0.57
1:C:428:ASP:CA	1:D:20:LYS:HE2	2.30	0.56
1:D:285:ASN:N	1:D:285:ASN:HD22	2.02	0.56
1:E:377:ARG:CZ	1:E:404:HIS:HA	2.34	0.56
1:E:428:ASP:HA	1:F:20:LYS:HE2	1.86	0.56
1:B:255:ALA:HB2	1:B:302:PHE:CZ	2.41	0.56
1:A:320:VAL:O	1:A:324:ILE:HD12	2.05	0.56
1:E:32:ILE:HG23	1:E:83:ARG:NH1	2.20	0.56
1:B:243:LEU:CD2	1:B:367:VAL:HB	2.35	0.56
2:C:800:AGS:S1G	1:D:359:ARG:HG3	2.45	0.56
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.88	0.56
1:E:442:MET:HG3	1:F:232:GLU:HG2	1.87	0.56
1:A:74:ASP:OD1	1:A:76:THR:HG23	2.06	0.56
1:D:417:GLU:OE2	1:D:454:TRP:HZ3	1.88	0.56
1:E:320:VAL:O	1:E:324:ILE:HD12	2.06	0.56
1:F:32:ILE:HG23	1:F:83:ARG:NH1	2.21	0.56
1:A:377:ARG:NH1	1:A:400:ALA:O	2.38	0.56
1:B:212:GLN:HA	1:B:215:GLN:HG3	1.88	0.56
1:B:318:GLY:HA3	1:B:321:GLU:HG3	1.88	0.56
1:A:20:LYS:N	1:A:20:LYS:HD2	2.21	0.55
1:E:36:ASN:HA	1:E:85:ASN:HD21	1.71	0.55
1:A:29:ASP:O	1:A:83:ARG:HA	2.06	0.55
1:C:29:ASP:O	1:C:83:ARG:HA	2.06	0.55
1:F:417:GLU:OE2	1:F:454:TRP:HZ3	1.89	0.55
1:E:298:PRO:HA	1:E:340:HIS:O	2.06	0.55
1:F:252:THR:OG1	1:F:304:ASP:OD2	2.25	0.55
1:B:250:GLY:O	1:B:254:ILE:HG13	2.06	0.55
1:F:320:VAL:O	1:F:324:ILE:HD12	2.07	0.55
1:A:36:ASN:HA	1:A:85:ASN:HD21	1.71	0.55
1:A:235:VAL:HG21	1:F:416:SER:HA	1.89	0.55
1:B:65:ARG:HG3	1:B:93:ARG:CG	2.37	0.55
1:D:29:ASP:O	1:D:83:ARG:HA	2.06	0.55
1:A:273:GLU:HG3	1:B:330:THR:HG23	1.89	0.55
1:E:299:ALA:HB3	1:E:341:VAL:HG22	1.89	0.55
1:A:212:GLN:HA	1:A:215:GLN:HG3	1.89	0.55
1:D:212:GLN:HA	1:D:215:GLN:HG3	1.89	0.54
1:B:65:ARG:HG3	1:B:93:ARG:HG2	1.89	0.54
1:A:243:LEU:HD22	1:A:367:VAL:HB	1.89	0.54
1:A:317:HIS:HB2	1:B:322:ARG:HH22	1.71	0.54
1:D:20:LYS:N	1:D:20:LYS:HD2	2.22	0.54
1:D:74:ASP:OD1	1:D:76:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:LYS:HE3	2:E:800:AGS:O2B	2.06	0.54
1:F:36:ASN:HA	1:F:85:ASN:HD21	1.73	0.54
1:D:201:VAL:HG13	1:D:205:ASP:HB2	1.89	0.54
1:A:65:ARG:HG3	1:A:93:ARG:CG	2.38	0.54
1:E:250:GLY:O	1:E:254:ILE:HG13	2.08	0.54
1:E:252:THR:O	1:E:255:ALA:HB3	2.08	0.54
1:B:35:ASP:O	1:B:38:VAL:HG12	2.07	0.54
1:C:212:GLN:HA	1:C:215:GLN:HG3	1.89	0.54
1:A:377:ARG:HD2	1:A:403:THR:OG1	2.07	0.54
1:C:74:ASP:OD1	1:C:76:THR:HG23	2.07	0.54
1:F:20:LYS:N	1:F:20:LYS:HD2	2.23	0.53
1:E:417:GLU:OE2	1:E:454:TRP:HZ3	1.90	0.53
1:B:377:ARG:NH2	1:B:404:HIS:HA	2.24	0.53
1:E:116:VAL:HG12	1:E:165:VAL:HA	1.90	0.53
1:F:65:ARG:HG3	1:F:93:ARG:CG	2.38	0.53
1:B:89:ARG:HD3	1:B:96:LEU:HG	1.90	0.53
1:C:20:LYS:HD2	1:C:20:LYS:N	2.23	0.53
1:C:377:ARG:HD3	1:C:403:THR:OG1	2.09	0.53
1:D:35:ASP:O	1:D:38:VAL:HG12	2.09	0.53
1:D:36:ASN:HA	1:D:85:ASN:HD21	1.74	0.53
1:F:212:GLN:HA	1:F:215:GLN:HG3	1.90	0.53
1:C:318:GLY:HA3	1:C:321:GLU:HG3	1.90	0.53
1:E:297:ALA:CB	1:E:339:ALA:O	2.57	0.53
1:F:65:ARG:HG3	1:F:93:ARG:HG2	1.91	0.53
1:F:250:GLY:O	1:F:254:ILE:HG13	2.09	0.53
1:A:35:ASP:O	1:A:38:VAL:HG12	2.09	0.52
1:B:116:VAL:HG12	1:B:165:VAL:HA	1.92	0.52
1:B:377:ARG:NH1	1:B:400:ALA:O	2.43	0.52
1:C:35:ASP:O	1:C:38:VAL:HG12	2.09	0.52
1:E:74:ASP:OD1	1:E:76:THR:HG23	2.10	0.52
1:F:29:ASP:O	1:F:83:ARG:HA	2.08	0.52
1:E:212:GLN:HA	1:E:215:GLN:HG3	1.90	0.52
1:C:243:LEU:CD2	1:C:367:VAL:HB	2.38	0.52
1:A:433:GLU:HB2	1:B:25:ARG:NH2	2.24	0.52
1:B:417:GLU:OE2	1:B:454:TRP:HZ3	1.93	0.52
1:C:116:VAL:HG12	1:C:165:VAL:HA	1.91	0.52
1:C:262:THR:HG23	1:C:262:THR:O	2.09	0.52
1:D:65:ARG:HG3	1:D:93:ARG:CG	2.40	0.51
1:C:36:ASN:HA	1:C:85:ASN:HD21	1.74	0.51
1:F:116:VAL:HG12	1:F:165:VAL:HA	1.91	0.51
1:B:224:LEU:HD22	1:B:298:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:VAL:HG13	1:E:205:ASP:HB2	1.92	0.51
1:C:377:ARG:NH1	1:C:400:ALA:O	2.44	0.51
1:C:65:ARG:HG3	1:C:93:ARG:CG	2.41	0.51
1:A:121:ASP:OD2	1:A:191:ARG:HD2	2.11	0.51
1:D:89:ARG:HG2	4:D:917:HOH:O	2.10	0.51
1:D:116:VAL:HG12	1:D:165:VAL:HA	1.91	0.51
1:D:252:THR:O	1:D:255:ALA:HB3	2.11	0.51
1:E:224:LEU:HD22	1:E:298:PRO:HB3	1.93	0.50
1:A:65:ARG:HG3	1:A:93:ARG:HG2	1.94	0.50
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.93	0.50
1:A:116:VAL:HG12	1:A:165:VAL:HA	1.91	0.50
1:C:121:ASP:OD2	1:C:191:ARG:HD2	2.11	0.50
1:A:297:ALA:HA	1:A:298:PRO:C	2.37	0.50
1:A:379:GLU:O	1:A:383:ILE:HG13	2.11	0.50
1:B:121:ASP:OD2	1:B:191:ARG:HD2	2.11	0.50
1:B:281:GLU:O	1:B:285:ASN:ND2	2.36	0.50
1:D:377:ARG:NH1	1:D:400:ALA:O	2.43	0.50
1:E:445:LEU:HD22	1:F:233:ILE:HD12	1.94	0.50
1:E:32:ILE:HG13	1:E:33:ASN:H	1.76	0.50
1:F:32:ILE:HG13	1:F:33:ASN:H	1.77	0.50
1:B:433:GLU:HG3	1:C:25:ARG:HH21	1.75	0.50
1:E:297:ALA:HA	1:E:298:PRO:C	2.36	0.50
1:A:196:GLU:CD	1:B:337:GLN:HB2	2.36	0.50
1:F:113:ARG:HG2	1:F:181:VAL:HB	1.94	0.50
1:C:32:ILE:HG23	1:C:83:ARG:HH11	1.77	0.49
1:A:113:ARG:HG2	1:A:181:VAL:HB	1.94	0.49
1:B:30:GLU:O	1:B:83:ARG:HG2	2.12	0.49
1:F:35:ASP:O	1:F:38:VAL:HG12	2.12	0.49
1:D:224:LEU:HD22	1:D:298:PRO:HB3	1.94	0.49
1:A:233:ILE:HD12	1:F:445:LEU:HD22	1.93	0.49
1:A:360:PHE:CD1	1:A:360:PHE:C	2.90	0.49
1:C:364:ASP:O	1:C:365:ARG:HD3	2.12	0.49
1:D:421:GLN:HA	1:D:424:ARG:HE	1.78	0.49
1:D:434:ASP:CG	1:E:22:ARG:HH12	2.20	0.49
1:E:379:GLU:O	1:E:383:ILE:HG13	2.12	0.49
1:A:32:ILE:HG23	1:A:83:ARG:HH11	1.76	0.49
1:D:32:ILE:HG13	1:D:33:ASN:H	1.78	0.49
1:D:46:MET:HE2	1:D:51:LEU:O	2.13	0.49
1:D:243:LEU:O	1:D:346:ALA:HA	2.13	0.49
1:E:113:ARG:HG2	1:E:181:VAL:HB	1.94	0.49
1:A:46:MET:HE2	1:A:51:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:HB2	1:A:302:PHE:CZ	2.48	0.49
1:A:270:ASN:O	1:A:273:GLU:N	2.43	0.49
1:A:224:LEU:HD22	1:A:298:PRO:HB3	1.95	0.49
1:B:297:ALA:HA	1:B:298:PRO:C	2.38	0.48
1:A:32:ILE:HG13	1:A:33:ASN:H	1.77	0.48
1:F:379:GLU:O	1:F:383:ILE:HG13	2.13	0.48
1:C:32:ILE:HG13	1:C:33:ASN:H	1.77	0.48
1:C:243:LEU:O	1:C:346:ALA:HA	2.13	0.48
1:D:113:ARG:HG2	1:D:181:VAL:HB	1.95	0.48
1:D:318:GLY:HA3	1:D:321:GLU:HG3	1.95	0.48
1:C:224:LEU:HD22	1:C:298:PRO:HB3	1.95	0.48
1:E:378:LEU:HG	1:E:382:GLN:HE21	1.78	0.48
1:F:121:ASP:OD2	1:F:191:ARG:HD2	2.13	0.48
1:C:389:LYS:HE2	1:D:232:GLU:O	2.14	0.48
1:D:297:ALA:HA	1:D:298:PRO:C	2.39	0.48
1:F:297:ALA:HA	1:F:298:PRO:C	2.39	0.48
1:A:433:GLU:HB2	1:B:25:ARG:HH22	1.79	0.47
1:D:121:ASP:OD2	1:D:191:ARG:HD2	2.14	0.47
1:F:224:LEU:HD22	1:F:298:PRO:HB3	1.95	0.47
1:B:378:LEU:HG	1:B:382:GLN:HE21	1.79	0.47
1:C:252:THR:O	1:C:255:ALA:HB3	2.15	0.47
1:D:32:ILE:HG23	1:D:83:ARG:HH11	1.77	0.47
1:E:349:ARG:HH12	1:F:314:GLU:HG2	1.78	0.47
1:F:378:LEU:HG	1:F:382:GLN:HE21	1.78	0.47
1:B:44:PRO:HB2	1:B:79:ASP:OD2	2.14	0.47
1:E:32:ILE:HG23	1:E:83:ARG:HH11	1.78	0.47
1:E:65:ARG:HG3	1:E:93:ARG:CG	2.45	0.47
1:B:46:MET:HE2	1:B:51:LEU:O	2.15	0.47
1:B:377:ARG:CD	1:B:403:THR:OG1	2.63	0.47
1:A:360:PHE:CE1	2:F:800:AGS:H4'	2.50	0.47
1:B:317:HIS:HB2	1:C:322:ARG:NH2	2.29	0.47
1:C:378:LEU:HG	1:C:382:GLN:HE21	1.80	0.47
1:B:379:GLU:O	1:B:383:ILE:HG13	2.15	0.47
1:F:421:GLN:HA	1:F:424:ARG:HE	1.79	0.47
1:C:421:GLN:HA	1:C:424:ARG:HE	1.80	0.47
1:D:379:GLU:O	1:D:383:ILE:HG13	2.14	0.47
2:D:800:AGS:S1G	1:E:359:ARG:HG3	2.55	0.47
1:F:377:ARG:NH2	1:F:404:HIS:HA	2.29	0.47
1:A:244:TYR:OH	1:A:368:ASP:HB2	2.15	0.47
1:C:113:ARG:HG2	1:C:181:VAL:HB	1.97	0.47
1:A:243:LEU:CD2	1:A:367:VAL:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:SER:O	1:B:82:ILE:HG13	2.15	0.47
1:D:65:ARG:HG3	1:D:93:ARG:HG2	1.96	0.47
1:D:378:LEU:HG	1:D:382:GLN:HE21	1.79	0.47
1:D:249:THR:OG1	1:D:251:LYS:HE2	2.15	0.47
1:E:377:ARG:CD	1:E:403:THR:OG1	2.63	0.47
1:C:379:GLU:O	1:C:383:ILE:HG13	2.14	0.46
1:F:32:ILE:HG23	1:F:83:ARG:HH11	1.79	0.46
1:F:270:ASN:O	1:F:273:GLU:N	2.43	0.46
1:A:302:PHE:CE2	1:A:344:MET:HE2	2.51	0.46
1:C:46:MET:HE2	1:C:51:LEU:O	2.15	0.46
1:F:28:VAL:HG23	1:F:96:LEU:HA	1.96	0.46
1:B:113:ARG:HG2	1:B:181:VAL:HB	1.95	0.46
1:E:421:GLN:HA	1:E:424:ARG:HE	1.79	0.46
1:C:206:ILE:C	1:C:206:ILE:HD12	2.41	0.46
1:D:28:VAL:HG23	1:D:97:GLY:H	1.81	0.46
1:A:318:GLY:HA3	1:A:321:GLU:HG3	1.98	0.46
1:C:337:GLN:HE21	1:C:337:GLN:CA	2.27	0.46
1:A:270:ASN:O	1:A:271:GLY:C	2.59	0.46
1:E:46:MET:HE2	1:E:51:LEU:O	2.15	0.46
1:B:270:ASN:O	1:B:273:GLU:N	2.47	0.46
1:A:421:GLN:HA	1:A:424:ARG:HE	1.81	0.46
1:C:28:VAL:HG23	1:C:96:LEU:HA	1.97	0.46
1:E:121:ASP:OD2	1:E:191:ARG:HD2	2.16	0.46
1:E:377:ARG:NH1	1:E:400:ALA:O	2.50	0.45
1:C:270:ASN:O	1:C:273:GLU:N	2.47	0.45
1:D:377:ARG:HD3	1:D:403:THR:OG1	2.16	0.45
1:E:65:ARG:HG3	1:E:93:ARG:HG2	1.98	0.45
1:A:273:GLU:HG3	1:B:330:THR:CG2	2.46	0.45
1:B:89:ARG:CD	1:B:96:LEU:HG	2.45	0.45
1:F:360:PHE:CD1	1:F:360:PHE:C	2.94	0.45
1:A:378:LEU:HG	1:A:382:GLN:HE21	1.80	0.45
1:E:28:VAL:HG23	1:E:96:LEU:HA	1.99	0.45
1:F:206:ILE:C	1:F:206:ILE:HD12	2.41	0.45
1:B:177:ALA:HB1	1:B:178:PRO:CD	2.46	0.45
1:B:421:GLN:HA	1:B:424:ARG:HE	1.82	0.45
1:C:65:ARG:HG3	1:C:93:ARG:HG2	1.99	0.45
1:C:317:HIS:HB2	1:D:322:ARG:HH22	1.82	0.45
1:D:445:LEU:HD22	1:E:233:ILE:HD12	1.99	0.45
1:F:46:MET:HE2	1:F:51:LEU:O	2.15	0.45
1:C:297:ALA:HA	1:C:298:PRO:C	2.42	0.45
1:D:434:ASP:OD1	1:D:434:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:LEU:O	1:E:346:ALA:HA	2.17	0.45
1:B:284:SER:O	1:B:288:LYS:HB2	2.16	0.45
1:D:206:ILE:HD12	1:D:206:ILE:C	2.42	0.45
1:E:28:VAL:HG23	1:E:97:GLY:H	1.81	0.45
1:A:28:VAL:HG23	1:A:96:LEU:HA	1.98	0.45
1:A:44:PRO:HB2	1:A:79:ASP:OD2	2.17	0.45
1:E:434:ASP:O	1:F:226:HIS:HE1	1.99	0.45
1:A:209:CYS:O	1:A:210:ARG:C	2.60	0.44
1:C:44:PRO:HB2	1:C:79:ASP:OD2	2.17	0.44
1:C:192:GLU:OE1	1:D:338:ARG:HB2	2.17	0.44
1:F:243:LEU:O	1:F:346:ALA:HA	2.17	0.44
1:A:273:GLU:O	1:A:276:SER:OG	2.35	0.44
1:C:431:ASP:OD2	1:D:25:ARG:NH2	2.49	0.44
1:C:428:ASP:O	1:D:20:LYS:HG2	2.18	0.44
1:E:44:PRO:HB2	1:E:79:ASP:OD2	2.18	0.44
1:B:377:ARG:CZ	1:B:404:HIS:HA	2.47	0.44
1:F:249:THR:OG1	1:F:251:LYS:CE	2.64	0.44
1:A:265:PHE:CD2	1:A:296:ASN:HB2	2.52	0.44
1:D:44:PRO:HB2	1:D:79:ASP:OD2	2.18	0.44
1:B:78:SER:HB2	1:B:81:LYS:HB2	2.00	0.44
1:E:16:ILE:HG21	1:E:218:GLU:HG3	1.98	0.44
1:E:302:PHE:HE2	1:E:344:MET:HE2	1.77	0.44
1:E:274:ILE:HD13	1:E:274:ILE:HA	1.90	0.44
1:A:328:LEU:O	1:A:329:LEU:C	2.61	0.43
1:D:94:VAL:HG23	4:D:917:HOH:O	2.17	0.43
1:E:360:PHE:CD1	1:E:360:PHE:C	2.96	0.43
1:B:250:GLY:HA2	2:B:800:AGS:O1A	2.18	0.43
1:D:377:ARG:NH2	1:D:404:HIS:HA	2.32	0.43
2:A:800:AGS:H4'	1:B:360:PHE:CE1	2.54	0.43
1:E:337:GLN:HA	1:E:337:GLN:NE2	2.31	0.43
1:A:28:VAL:HG23	1:A:97:GLY:H	1.83	0.43
1:A:364:ASP:O	1:A:365:ARG:CD	2.65	0.43
1:A:430:ILE:O	1:B:20:LYS:NZ	2.49	0.43
1:E:177:ALA:HB1	1:E:178:PRO:CD	2.48	0.43
1:A:177:ALA:HB1	1:A:178:PRO:CD	2.48	0.43
1:E:299:ALA:O	1:E:341:VAL:HA	2.19	0.43
1:F:265:PHE:CD2	1:F:296:ASN:HB2	2.53	0.43
1:B:249:THR:OG1	1:B:251:LYS:HE2	2.18	0.43
1:B:360:PHE:CD1	1:B:360:PHE:C	2.96	0.43
1:C:274:ILE:HD13	1:C:274:ILE:HA	1.89	0.43
1:D:117:LEU:HD13	1:D:187:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:SER:HA	1:E:235:VAL:HG21	2.00	0.43
1:C:424:ARG:O	1:C:427:MET:HB2	2.19	0.43
1:F:271:GLY:O	1:F:275:MET:HG2	2.18	0.43
1:A:85:ASN:OD1	1:A:87:VAL:HB	2.19	0.43
1:B:32:ILE:HG13	1:B:33:ASN:H	1.84	0.43
1:D:78:SER:HB2	1:D:81:LYS:HB2	2.01	0.43
1:C:377:ARG:NH2	1:C:404:HIS:HA	2.33	0.43
1:D:177:ALA:HB1	1:D:178:PRO:CD	2.48	0.43
1:D:40:SER:O	1:D:82:ILE:HG13	2.19	0.42
1:F:177:ALA:HB1	1:F:178:PRO:CD	2.49	0.42
1:F:205:ASP:HA	1:F:383:ILE:HG21	2.01	0.42
1:F:377:ARG:CZ	1:F:404:HIS:HA	2.49	0.42
1:A:78:SER:HB2	1:A:81:LYS:HB2	2.01	0.42
1:A:389:LYS:HE2	1:B:232:GLU:O	2.19	0.42
1:C:249:THR:OG1	1:C:251:LYS:CE	2.62	0.42
1:E:117:LEU:HD13	1:E:187:GLU:O	2.19	0.42
1:F:270:ASN:O	1:F:271:GLY:C	2.62	0.42
1:A:344:MET:HE2	1:A:344:MET:HB3	1.90	0.42
1:B:100:ILE:C	1:B:100:ILE:HD12	2.44	0.42
1:C:177:ALA:HB1	1:C:178:PRO:CD	2.48	0.42
1:C:270:ASN:O	1:C:271:GLY:C	2.62	0.42
1:D:246:PRO:HG3	1:D:371:ILE:HD12	2.02	0.42
1:E:40:SER:O	1:E:82:ILE:HG13	2.19	0.42
1:C:62:LYS:O	1:C:63:LYS:C	2.62	0.42
1:D:254:ILE:O	1:D:258:VAL:HG23	2.19	0.42
1:F:117:LEU:HD13	1:F:187:GLU:O	2.19	0.42
1:F:347:THR:HG21	1:F:350:PRO:HA	1.99	0.42
1:C:205:ASP:N	1:C:205:ASP:OD1	2.52	0.42
1:C:445:LEU:HD22	1:D:233:ILE:HD12	2.01	0.42
1:D:28:VAL:CG2	4:D:917:HOH:O	2.63	0.42
1:E:78:SER:HB2	1:E:81:LYS:HB2	2.01	0.42
1:F:302:PHE:CD2	1:F:344:MET:HE2	2.54	0.42
1:B:66:GLU:OE1	1:B:147:ARG:NH1	2.52	0.42
1:B:254:ILE:O	1:B:258:VAL:HG23	2.20	0.42
1:C:284:SER:O	1:C:288:LYS:HB2	2.19	0.42
1:E:205:ASP:OD1	1:E:205:ASP:N	2.53	0.42
1:E:460:ASN:CG	1:E:461:PRO:HD2	2.44	0.42
1:A:240:GLY:HA2	1:A:343:VAL:O	2.19	0.42
1:A:246:PRO:HG3	1:A:371:ILE:HD12	2.02	0.42
1:C:228:ALA:HA	1:C:231:LYS:HB2	2.02	0.42
1:D:209:CYS:O	1:D:210:ARG:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:O	1:D:273:GLU:N	2.47	0.42
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.88	0.42
1:A:100:ILE:HD12	1:A:100:ILE:C	2.44	0.42
1:A:205:ASP:HA	1:A:383:ILE:HG21	2.01	0.42
1:C:78:SER:HB2	1:C:81:LYS:HB2	2.02	0.42
1:D:434:ASP:O	1:E:226:HIS:HE1	2.02	0.42
1:F:44:PRO:HB2	1:F:79:ASP:OD2	2.18	0.42
1:F:209:CYS:O	1:F:210:ARG:C	2.63	0.42
1:F:453:ARG:HE	1:F:453:ARG:HB2	1.71	0.42
1:A:250:GLY:HA2	2:A:800:AGS:O1A	2.20	0.42
1:D:244:TYR:OH	1:D:368:ASP:HB2	2.20	0.42
1:E:190:LYS:HB2	1:E:193:ASP:OD2	2.20	0.42
1:E:356:ALA:HA	1:E:359:ARG:HD2	2.02	0.42
1:E:374:ALA:HA	1:E:377:ARG:NH1	2.35	0.42
1:E:434:ASP:O	1:F:226:HIS:CE1	2.73	0.42
1:A:310:ALA:O	1:A:353:ILE:HA	2.20	0.42
1:C:28:VAL:HG23	1:C:97:GLY:H	1.85	0.42
1:C:273:GLU:O	1:C:276:SER:OG	2.37	0.42
1:C:337:GLN:HA	1:C:337:GLN:NE2	2.32	0.42
1:D:344:MET:HE2	1:D:344:MET:HB3	1.88	0.42
1:D:347:THR:HG21	1:D:350:PRO:HA	2.02	0.42
1:E:270:ASN:O	1:E:273:GLU:N	2.49	0.42
1:F:40:SER:O	1:F:82:ILE:HG13	2.20	0.41
1:F:100:ILE:HD12	1:F:100:ILE:C	2.45	0.41
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.88	0.41
1:A:377:ARG:NE	1:A:403:THR:O	2.53	0.41
1:B:28:VAL:HG23	1:B:97:GLY:H	1.84	0.41
1:D:360:PHE:CD1	1:D:360:PHE:C	2.98	0.41
1:E:302:PHE:CD2	1:E:344:MET:HE2	2.54	0.41
1:F:448:THR:O	1:F:451:ASP:HB2	2.20	0.41
1:A:228:ALA:HA	1:A:231:LYS:HB2	2.02	0.41
1:A:249:THR:OG1	1:A:251:LYS:HE2	2.19	0.41
1:A:252:THR:O	1:A:255:ALA:HB3	2.19	0.41
1:C:209:CYS:O	1:C:210:ARG:C	2.64	0.41
1:D:89:ARG:HD3	1:D:96:LEU:HG	2.02	0.41
1:D:100:ILE:C	1:D:100:ILE:HD12	2.46	0.41
1:A:96:LEU:HD12	1:A:96:LEU:H	1.85	0.41
1:B:109:LYS:HD3	1:B:170:PRO:CG	2.51	0.41
1:D:424:ARG:O	1:D:427:MET:HB2	2.20	0.41
1:E:89:ARG:HD3	1:E:96:LEU:HG	2.02	0.41
1:E:347:THR:HG21	1:E:350:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ASN:OD1	1:F:87:VAL:HB	2.20	0.41
1:F:89:ARG:HD3	1:F:96:LEU:HG	2.02	0.41
1:A:205:ASP:OD1	1:A:205:ASP:N	2.52	0.41
1:B:265:PHE:CD2	1:B:296:ASN:HB2	2.54	0.41
1:C:206:ILE:HD11	1:C:213:LEU:HD11	2.02	0.41
1:C:369:ILE:O	1:C:369:ILE:HG22	2.20	0.41
1:D:85:ASN:OD1	1:D:87:VAL:HB	2.20	0.41
1:E:85:ASN:OD1	1:E:87:VAL:HB	2.20	0.41
1:E:228:ALA:HA	1:E:231:LYS:HB2	2.02	0.41
1:F:28:VAL:HG23	1:F:97:GLY:H	1.84	0.41
1:A:89:ARG:HD3	1:A:96:LEU:HG	2.02	0.41
1:A:322:ARG:HH22	1:F:317:HIS:HB2	1.85	0.41
1:C:226:HIS:HB2	1:C:229:LEU:HD12	2.02	0.41
1:A:206:ILE:HD11	1:A:213:LEU:HD11	2.03	0.41
1:A:432:LEU:HD13	1:B:16:ILE:HD11	2.01	0.41
1:C:354:ASP:HA	1:C:355:PRO:HD2	1.93	0.41
1:D:337:GLN:HA	1:D:337:GLN:NE2	2.34	0.41
1:F:199:ASN:O	1:F:200:GLU:C	2.63	0.41
1:F:337:GLN:HA	1:F:337:GLN:NE2	2.34	0.41
1:C:89:ARG:HD3	1:C:96:LEU:HG	2.02	0.41
1:D:96:LEU:H	1:D:96:LEU:HD12	1.86	0.41
1:D:190:LYS:HB2	1:D:193:ASP:OD2	2.21	0.41
1:D:205:ASP:OD1	1:D:205:ASP:N	2.53	0.41
1:F:286:LEU:HD23	1:F:286:LEU:HA	1.86	0.41
1:A:117:LEU:HD13	1:A:187:GLU:O	2.21	0.41
1:B:209:CYS:O	1:B:210:ARG:C	2.63	0.41
1:B:424:ARG:O	1:B:427:MET:HB2	2.21	0.41
1:C:117:LEU:HD13	1:C:187:GLU:O	2.21	0.41
1:D:442:MET:HG3	1:E:232:GLU:HG2	2.02	0.41
1:E:206:ILE:HD12	1:E:206:ILE:C	2.46	0.41
1:E:265:PHE:CD2	1:E:296:ASN:HB2	2.56	0.41
1:F:273:GLU:O	1:F:276:SER:OG	2.36	0.41
1:C:96:LEU:H	1:C:96:LEU:HD12	1.85	0.41
1:D:89:ARG:CG	4:D:917:HOH:O	2.69	0.41
1:E:40:SER:CB	1:E:83:ARG:HB2	2.37	0.41
1:E:250:GLY:HA2	2:E:800:AGS:O1A	2.21	0.41
1:B:96:LEU:H	1:B:96:LEU:HD12	1.86	0.40
1:C:254:ILE:O	1:C:258:VAL:HG23	2.21	0.40
1:D:228:ALA:HA	1:D:231:LYS:HB2	2.02	0.40
1:E:143:TYR:HA	1:E:176:VAL:O	2.20	0.40
1:A:243:LEU:O	1:A:346:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:OD1	1:C:87:VAL:HB	2.20	0.40
1:C:255:ALA:HB2	1:C:302:PHE:CZ	2.56	0.40
1:D:270:ASN:O	1:D:271:GLY:C	2.64	0.40
1:E:424:ARG:O	1:E:427:MET:HB2	2.20	0.40
1:E:427:MET:HE2	1:F:16:ILE:HG13	2.03	0.40
1:A:40:SER:O	1:A:82:ILE:HG13	2.21	0.40
1:A:232:GLU:O	1:F:389:LYS:HE2	2.22	0.40
1:A:249:THR:HG22	1:A:407:VAL:HB	2.03	0.40
1:B:85:ASN:OD1	1:B:87:VAL:HB	2.21	0.40
1:C:440:GLU:CD	1:C:440:GLU:C	2.89	0.40
1:A:453:ARG:HE	1:A:453:ARG:HB2	1.71	0.40
1:B:32:ILE:CG2	1:B:83:ARG:NH1	2.76	0.40
1:C:244:TYR:OH	1:C:368:ASP:HB2	2.21	0.40
1:E:453:ARG:HE	1:E:453:ARG:HB2	1.72	0.40
1:B:228:ALA:HA	1:B:231:LYS:HB2	2.02	0.40
1:D:356:ALA:HA	1:D:359:ARG:HD2	2.04	0.40
1:E:270:ASN:O	1:E:271:GLY:C	2.63	0.40
1:F:78:SER:HB2	1:F:81:LYS:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/489 (92%)	426 (95%)	21 (5%)	2 (0%)	30	49
1	B	449/489 (92%)	427 (95%)	21 (5%)	1 (0%)	43	64
1	C	449/489 (92%)	425 (95%)	22 (5%)	2 (0%)	30	49
1	D	449/489 (92%)	428 (95%)	19 (4%)	2 (0%)	30	49
1	E	449/489 (92%)	427 (95%)	20 (4%)	2 (0%)	30	49
1	F	449/489 (92%)	429 (96%)	18 (4%)	2 (0%)	30	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2694/2934 (92%)	2562 (95%)	121 (4%)	11 (0%)	30	49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	B	128	GLY
1	E	128	GLY
1	C	128	GLY
1	D	128	GLY
1	F	128	GLY
1	A	271	GLY
1	F	271	GLY
1	C	271	GLY
1	D	271	GLY
1	E	271	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	388/419 (93%)	336 (87%)	52 (13%)	4	7
1	B	388/419 (93%)	337 (87%)	51 (13%)	4	7
1	C	388/419 (93%)	337 (87%)	51 (13%)	4	7
1	D	388/419 (93%)	336 (87%)	52 (13%)	4	7
1	E	388/419 (93%)	336 (87%)	52 (13%)	4	7
1	F	388/419 (93%)	336 (87%)	52 (13%)	4	7
All	All	2328/2514 (93%)	2018 (87%)	310 (13%)	4	7

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	ILE
1	A	38	VAL
1	A	68	VAL
1	A	70	ILE
1	A	73	SER
1	A	75	ASP
1	A	76	THR
1	A	79	ASP
1	A	80	GLU
1	A	87	VAL
1	A	109	LYS
1	A	119	ILE
1	A	122	THR
1	A	146	ILE
1	A	147	ARG
1	A	168	THR
1	A	171	SER
1	A	173	TYR
1	A	191	ARG
1	A	193	ASP
1	A	198	LEU
1	A	200	GLU
1	A	206	ILE
1	A	225	ARG
1	A	231	LYS
1	A	274	ILE
1	A	281	GLU
1	A	282	SER
1	A	285	ASN
1	A	294	GLU
1	A	309	ILE
1	A	314	GLU
1	A	315	LYS
1	A	322	ARG
1	A	337	GLN
1	A	349	ARG
1	A	359	ARG
1	A	365	ARG
1	A	366	GLU
1	A	368	ASP
1	A	375	THR

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Mol	Chain	Res	Type
1	A	384	HIS
1	A	420	LEU
1	A	434	ASP
1	A	440	GLU
1	A	444	SER
1	A	445	LEU
1	A	453	ARG
1	A	459	SER
1	A	460	ASN
1	B	12	LEU
1	B	26	LEU
1	B	32	ILE
1	B	38	VAL
1	B	68	VAL
1	B	70	ILE
1	B	73	SER
1	B	75	ASP
1	B	76	THR
1	B	79	ASP
1	B	80	GLU
1	B	87	VAL
1	B	94	VAL
1	B	108	VAL
1	B	109	LYS
1	B	119	ILE
1	B	122	THR
1	B	147	ARG
1	B	168	THR
1	B	171	SER
1	B	191	ARG
1	B	197	SER
1	B	198	LEU
1	B	200	GLU
1	B	206	ILE
1	B	225	ARG
1	B	231	LYS
1	B	274	ILE
1	B	281	GLU
1	B	282	SER
1	B	294	GLU
1	B	309	ILE
1	B	314	GLU

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Mol	Chain	Res	Type
1	B	315	LYS
1	B	322	ARG
1	B	337	GLN
1	B	349	ARG
1	B	359	ARG
1	B	365	ARG
1	B	366	GLU
1	B	368	ASP
1	B	375	THR
1	B	384	HIS
1	B	420	LEU
1	B	434	ASP
1	B	440	GLU
1	B	444	SER
1	B	445	LEU
1	B	453	ARG
1	B	459	SER
1	B	460	ASN
1	C	12	LEU
1	C	26	LEU
1	C	32	ILE
1	C	38	VAL
1	C	68	VAL
1	C	70	ILE
1	C	73	SER
1	C	75	ASP
1	C	76	THR
1	C	79	ASP
1	C	80	GLU
1	C	87	VAL
1	C	108	VAL
1	C	109	LYS
1	C	119	ILE
1	C	122	THR
1	C	146	ILE
1	C	147	ARG
1	C	168	THR
1	C	171	SER
1	C	191	ARG
1	C	197	SER
1	C	198	LEU
1	C	200	GLU

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Mol	Chain	Res	Type
1	C	206	ILE
1	C	225	ARG
1	C	231	LYS
1	C	274	ILE
1	C	281	GLU
1	C	282	SER
1	C	285	ASN
1	C	294	GLU
1	C	309	ILE
1	C	314	GLU
1	C	315	LYS
1	C	322	ARG
1	C	337	GLN
1	C	349	ARG
1	C	359	ARG
1	C	366	GLU
1	C	368	ASP
1	C	375	THR
1	C	384	HIS
1	C	420	LEU
1	C	434	ASP
1	C	440	GLU
1	C	444	SER
1	C	445	LEU
1	C	453	ARG
1	C	459	SER
1	C	460	ASN
1	D	12	LEU
1	D	26	LEU
1	D	32	ILE
1	D	38	VAL
1	D	68	VAL
1	D	70	ILE
1	D	73	SER
1	D	75	ASP
1	D	76	THR
1	D	79	ASP
1	D	80	GLU
1	D	87	VAL
1	D	108	VAL
1	D	109	LYS
1	D	119	ILE

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Mol	Chain	Res	Type
1	D	122	THR
1	D	146	ILE
1	D	147	ARG
1	D	168	THR
1	D	171	SER
1	D	191	ARG
1	D	198	LEU
1	D	200	GLU
1	D	206	ILE
1	D	221	GLU
1	D	225	ARG
1	D	231	LYS
1	D	274	ILE
1	D	281	GLU
1	D	282	SER
1	D	285	ASN
1	D	294	GLU
1	D	309	ILE
1	D	314	GLU
1	D	315	LYS
1	D	322	ARG
1	D	337	GLN
1	D	349	ARG
1	D	359	ARG
1	D	365	ARG
1	D	366	GLU
1	D	368	ASP
1	D	375	THR
1	D	384	HIS
1	D	420	LEU
1	D	434	ASP
1	D	440	GLU
1	D	444	SER
1	D	445	LEU
1	D	453	ARG
1	D	459	SER
1	D	460	ASN
1	E	12	LEU
1	E	26	LEU
1	E	32	ILE
1	E	38	VAL
1	E	68	VAL

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Mol	Chain	Res	Type
1	E	70	ILE
1	E	73	SER
1	E	75	ASP
1	E	76	THR
1	E	79	ASP
1	E	80	GLU
1	E	87	VAL
1	E	99	VAL
1	E	108	VAL
1	E	109	LYS
1	E	119	ILE
1	E	122	THR
1	E	146	ILE
1	E	147	ARG
1	E	168	THR
1	E	171	SER
1	E	191	ARG
1	E	197	SER
1	E	198	LEU
1	E	200	GLU
1	E	206	ILE
1	E	225	ARG
1	E	231	LYS
1	E	273	GLU
1	E	274	ILE
1	E	281	GLU
1	E	282	SER
1	E	285	ASN
1	E	294	GLU
1	E	309	ILE
1	E	314	GLU
1	E	315	LYS
1	E	322	ARG
1	E	337	GLN
1	E	359	ARG
1	E	365	ARG
1	E	366	GLU
1	E	368	ASP
1	E	375	THR
1	E	384	HIS
1	E	420	LEU
1	E	440	GLU

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Mol	Chain	Res	Type
1	E	444	SER
1	E	445	LEU
1	E	453	ARG
1	E	459	SER
1	E	460	ASN
1	F	12	LEU
1	F	26	LEU
1	F	32	ILE
1	F	38	VAL
1	F	68	VAL
1	F	70	ILE
1	F	73	SER
1	F	75	ASP
1	F	76	THR
1	F	79	ASP
1	F	80	GLU
1	F	87	VAL
1	F	108	VAL
1	F	109	LYS
1	F	119	ILE
1	F	122	THR
1	F	146	ILE
1	F	147	ARG
1	F	168	THR
1	F	171	SER
1	F	191	ARG
1	F	198	LEU
1	F	200	GLU
1	F	206	ILE
1	F	225	ARG
1	F	231	LYS
1	F	273	GLU
1	F	274	ILE
1	F	281	GLU
1	F	282	SER
1	F	285	ASN
1	F	294	GLU
1	F	309	ILE
1	F	314	GLU
1	F	315	LYS
1	F	322	ARG
1	F	337	GLN

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Mol	Chain	Res	Type
1	F	349	ARG
1	F	359	ARG
1	F	365	ARG
1	F	366	GLU
1	F	368	ASP
1	F	375	THR
1	F	384	HIS
1	F	420	LEU
1	F	440	GLU
1	F	444	SER
1	F	445	LEU
1	F	448	THR
1	F	453	ARG
1	F	459	SER
1	F	460	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	43	GLN
1	A	90	ASN
1	A	91	ASN
1	A	226	HIS
1	A	285	ASN
1	A	337	GLN
1	A	382	GLN
1	A	460	ASN
1	B	24	ASN
1	B	90	ASN
1	B	91	ASN
1	B	226	HIS
1	B	337	GLN
1	B	382	GLN
1	B	387	ASN
1	B	460	ASN
1	C	24	ASN
1	C	43	GLN
1	C	90	ASN
1	C	91	ASN
1	C	285	ASN
1	C	337	GLN

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Mol	Chain	Res	Type
1	C	382	GLN
1	C	387	ASN
1	C	460	ASN
1	D	24	ASN
1	D	43	GLN
1	D	90	ASN
1	D	91	ASN
1	D	226	HIS
1	D	285	ASN
1	D	337	GLN
1	D	382	GLN
1	D	460	ASN
1	E	43	GLN
1	E	90	ASN
1	E	91	ASN
1	E	226	HIS
1	E	285	ASN
1	E	337	GLN
1	E	387	ASN
1	E	398	GLN
1	E	460	ASN
1	F	43	GLN
1	F	90	ASN
1	F	91	ASN
1	F	226	HIS
1	F	285	ASN
1	F	337	GLN
1	F	382	GLN
1	F	398	GLN
1	F	404	HIS
1	F	460	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 [i](#)

There are no oligosaccharides 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	E	800	3	32,33,33	1.87	6 (18%)	45,52,52	1.85	10 (22%)
2	AGS	C	800	3	32,33,33	1.91	7 (21%)	45,52,52	1.76	10 (22%)
2	AGS	D	800	3	32,33,33	1.91	6 (18%)	45,52,52	1.85	11 (24%)
2	AGS	F	800	3	32,33,33	2.06	7 (21%)	45,52,52	1.91	8 (17%)
2	AGS	A	800	3	32,33,33	1.88	6 (18%)	45,52,52	1.88	10 (22%)
2	AGS	B	800	3	32,33,33	1.89	7 (21%)	45,52,52	1.83	9 (20%)

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	E	800	3	-	4/21/38/38	0/3/3/3
2	AGS	C	800	3	-	4/21/38/38	0/3/3/3
2	AGS	D	800	3	-	4/21/38/38	0/3/3/3
2	AGS	F	800	3	-	3/21/38/38	0/3/3/3
2	AGS	A	800	3	-	3/21/38/38	0/3/3/3
2	AGS	B	800	3	-	4/21/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	800	AGS	PG-S1G	8.31	2.08	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	AGS	PG-S1G	7.11	2.06	1.90
2	A	800	AGS	PG-S1G	7.10	2.06	1.90
2	C	800	AGS	PG-S1G	6.85	2.05	1.90
2	B	800	AGS	PG-S1G	6.84	2.05	1.90
2	E	800	AGS	PG-S1G	6.79	2.05	1.90
2	C	800	AGS	C5-C4	5.27	1.48	1.39
2	E	800	AGS	C5-C4	4.84	1.47	1.39
2	B	800	AGS	C5-C4	4.83	1.47	1.39
2	A	800	AGS	C5-C4	4.76	1.47	1.39
2	D	800	AGS	C5-C4	4.76	1.47	1.39
2	F	800	AGS	C5-C4	4.61	1.47	1.39
2	A	800	AGS	C5-C6	2.68	1.48	1.41
2	E	800	AGS	C5-C6	2.67	1.48	1.41
2	F	800	AGS	C5-C6	2.66	1.48	1.41
2	B	800	AGS	C5-C6	2.63	1.48	1.41
2	D	800	AGS	C5-C6	2.62	1.48	1.41
2	B	800	AGS	C5-N7	-2.62	1.34	1.39
2	C	800	AGS	C5-C6	2.62	1.48	1.41
2	D	800	AGS	C5-N7	-2.59	1.34	1.39
2	C	800	AGS	C5-N7	-2.58	1.34	1.39
2	F	800	AGS	C5-N7	-2.56	1.34	1.39
2	C	800	AGS	C8-N7	2.54	1.36	1.31
2	E	800	AGS	C5-N7	-2.51	1.34	1.39
2	A	800	AGS	C5-N7	-2.45	1.34	1.39
2	F	800	AGS	C8-N7	2.45	1.36	1.31
2	A	800	AGS	C8-N7	2.41	1.36	1.31
2	B	800	AGS	C8-N7	2.32	1.36	1.31
2	B	800	AGS	PG-O3G	-2.25	1.47	1.54
2	C	800	AGS	PG-O3G	-2.25	1.47	1.54
2	E	800	AGS	C8-N7	2.24	1.36	1.31
2	D	800	AGS	C8-N7	2.24	1.36	1.31
2	E	800	AGS	PG-O3G	-2.19	1.47	1.54
2	A	800	AGS	PG-O3G	-2.19	1.47	1.54
2	F	800	AGS	PA-O3A	2.17	1.61	1.59
2	D	800	AGS	PG-O3G	-2.17	1.47	1.54
2	F	800	AGS	PG-O3G	-2.10	1.47	1.54
2	B	800	AGS	PG-O2G	2.06	1.61	1.54
2	C	800	AGS	PG-O2G	2.05	1.61	1.54

All (58) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	800	AGS	C5-C4-N3	-6.28	118.07	126.72
2	A	800	AGS	C5-C4-N3	-6.19	118.20	126.72
2	E	800	AGS	C5-C4-N3	-6.06	118.37	126.72
2	B	800	AGS	C5-C4-N3	-6.04	118.40	126.72
2	D	800	AGS	C5-C4-N3	-6.00	118.45	126.72
2	C	800	AGS	C5-C4-N3	-5.55	119.07	126.72
2	F	800	AGS	N3-C4-N9	4.77	135.28	127.17
2	D	800	AGS	N3-C4-N9	4.70	135.16	127.17
2	A	800	AGS	N3-C4-N9	4.69	135.15	127.17
2	E	800	AGS	N3-C4-N9	4.68	135.12	127.17
2	B	800	AGS	N3-C4-N9	4.65	135.08	127.17
2	C	800	AGS	N3-C4-N9	4.42	134.68	127.17
2	F	800	AGS	C2-N3-C4	4.04	121.69	111.83
2	A	800	AGS	C2-N3-C4	3.97	121.53	111.83
2	D	800	AGS	C2-N3-C4	3.92	121.39	111.83
2	E	800	AGS	C2-N3-C4	3.88	121.30	111.83
2	B	800	AGS	C2-N3-C4	3.84	121.21	111.83
2	F	800	AGS	N3-C2-N1	-3.72	122.94	128.58
2	C	800	AGS	C2-N3-C4	3.72	120.91	111.83
2	D	800	AGS	N3-C2-N1	-3.68	123.01	128.58
2	A	800	AGS	N3-C2-N1	-3.67	123.03	128.58
2	C	800	AGS	N3-C2-N1	-3.60	123.13	128.58
2	E	800	AGS	N3-C2-N1	-3.54	123.22	128.58
2	B	800	AGS	N3-C2-N1	-3.54	123.23	128.58
2	A	800	AGS	C4-C5-N7	-3.39	106.71	110.58
2	E	800	AGS	C4-C5-N7	-3.36	106.74	110.58
2	F	800	AGS	C4-C5-N7	-3.36	106.74	110.58
2	B	800	AGS	C4-C5-N7	-3.29	106.82	110.58
2	D	800	AGS	C4-C5-N7	-3.26	106.86	110.58
2	F	800	AGS	O2G-PG-O3B	2.85	114.16	104.64
2	C	800	AGS	C4-C5-N7	-2.78	107.41	110.58
2	C	800	AGS	O2G-PG-O3B	2.49	112.95	104.64
2	A	800	AGS	O2G-PG-O3B	2.47	112.89	104.64
2	A	800	AGS	C5-N7-C8	2.47	107.33	103.45
2	D	800	AGS	C5-N7-C8	2.46	107.31	103.45
2	E	800	AGS	C5-N7-C8	2.46	107.31	103.45
2	D	800	AGS	O2G-PG-O3B	2.45	112.82	104.64
2	E	800	AGS	O2G-PG-O3B	2.44	112.79	104.64
2	F	800	AGS	C5-N7-C8	2.44	107.28	103.45
2	C	800	AGS	PB-O3B-PG	-2.41	124.36	133.17
2	B	800	AGS	O2G-PG-O3B	2.39	112.63	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	AGS	O3G-PG-O3B	2.38	112.57	104.64
2	B	800	AGS	C5-N7-C8	2.37	107.17	103.45
2	E	800	AGS	PB-O3B-PG	-2.36	124.53	133.17
2	A	800	AGS	O3G-PG-O3B	2.30	112.33	104.64
2	D	800	AGS	O3G-PG-O3B	2.26	112.19	104.64
2	E	800	AGS	O3G-PG-O3B	2.24	112.11	104.64
2	B	800	AGS	PB-O3B-PG	-2.23	125.00	133.17
2	B	800	AGS	O3G-PG-O3B	2.23	112.07	104.64
2	F	800	AGS	O3G-PG-O3B	2.21	112.02	104.64
2	A	800	AGS	PB-O3B-PG	-2.19	125.16	133.17
2	D	800	AGS	PB-O3B-PG	-2.17	125.23	133.17
2	C	800	AGS	C2-N1-C6	2.08	122.14	118.73
2	A	800	AGS	C6-C5-N7	2.04	136.02	132.09
2	D	800	AGS	C6-C5-N7	2.03	136.01	132.09
2	C	800	AGS	C6-C5-N7	2.02	135.99	132.09
2	E	800	AGS	C6-C5-N7	2.01	135.96	132.09
2	D	800	AGS	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	D	800	AGS	PA-O3A-PB-O2B
2	F	800	AGS	PA-O3A-PB-O2B

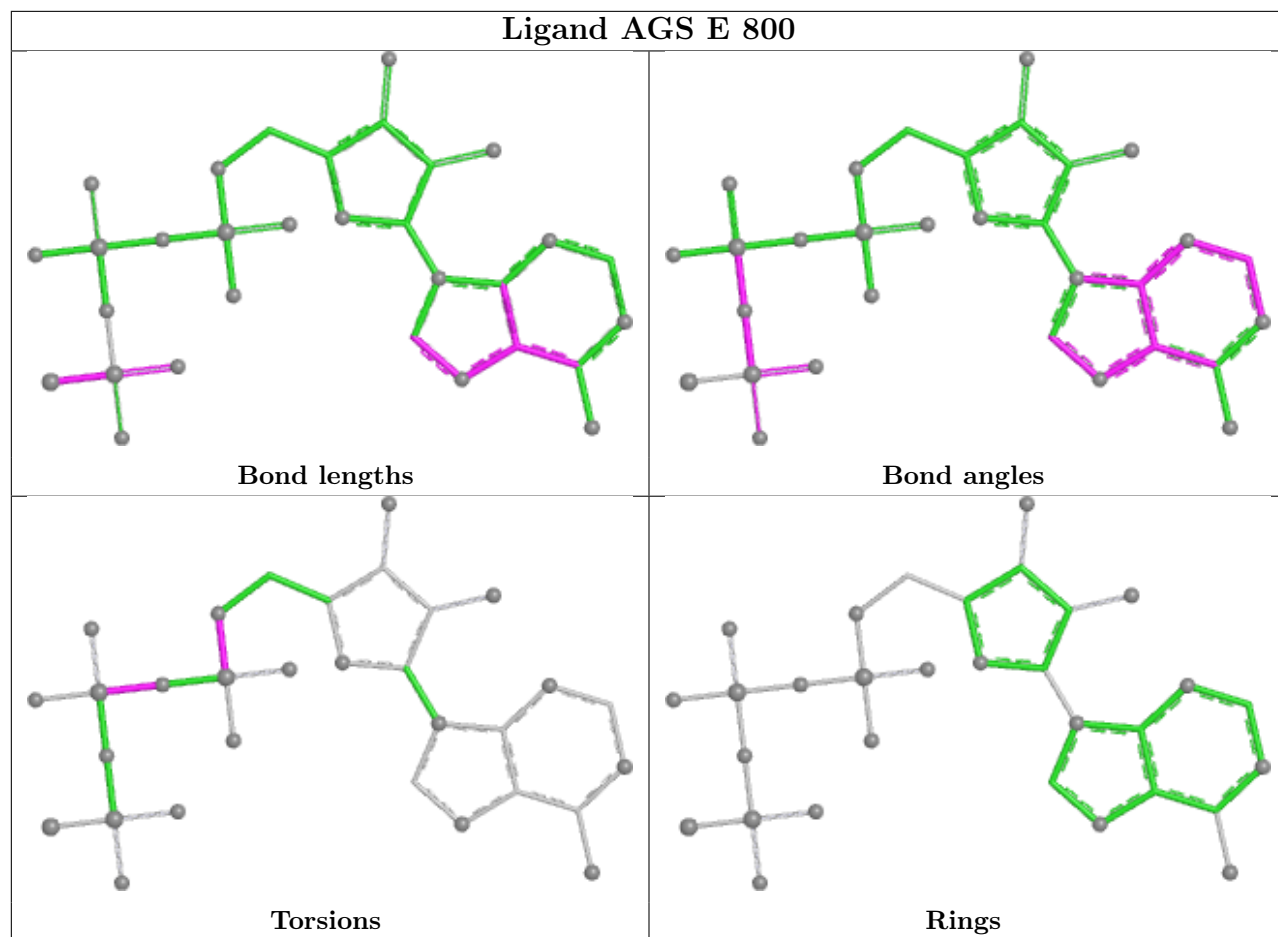
There are no ring outliers.

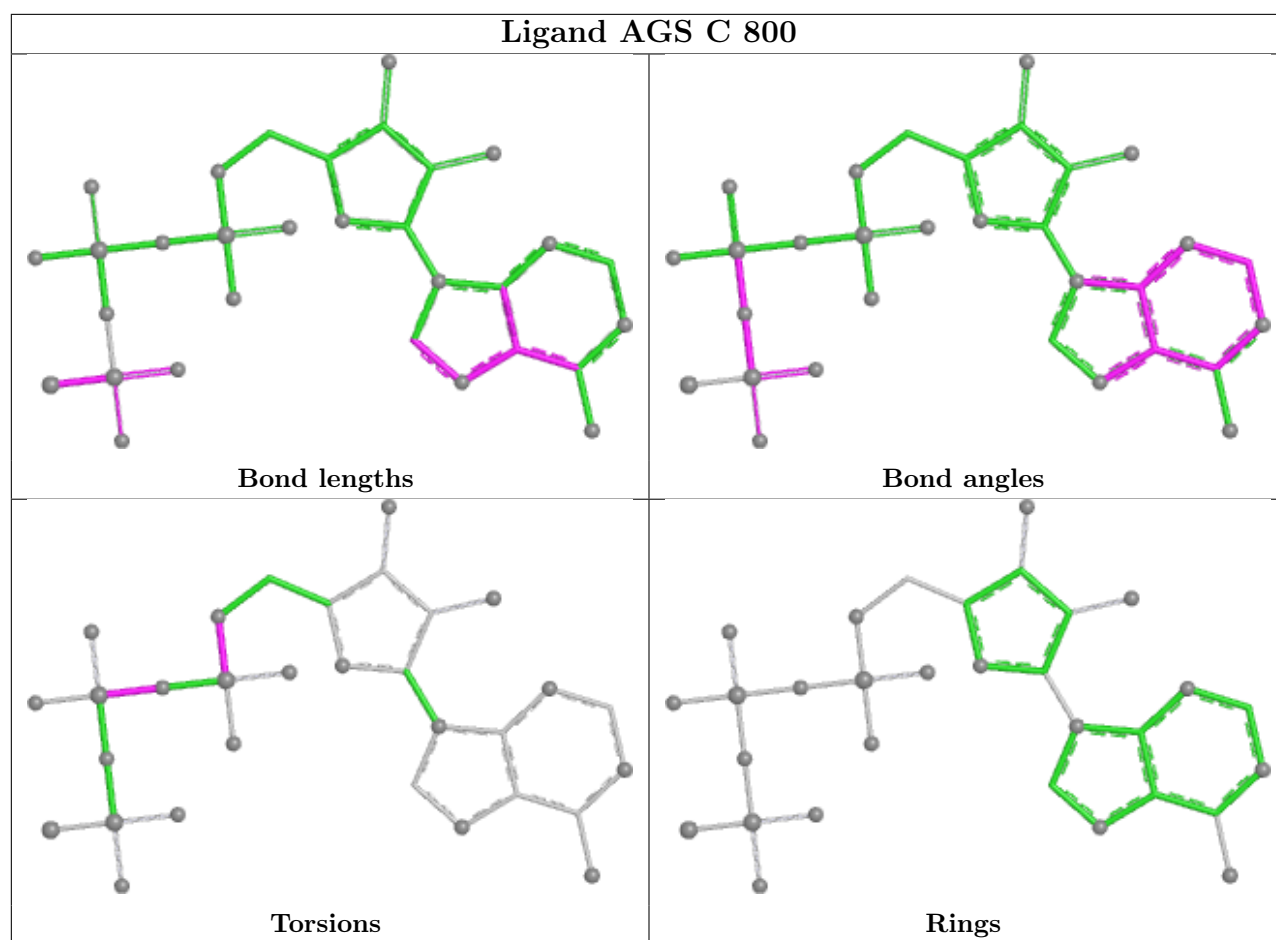
6 monomers are involved in 30 short contacts:

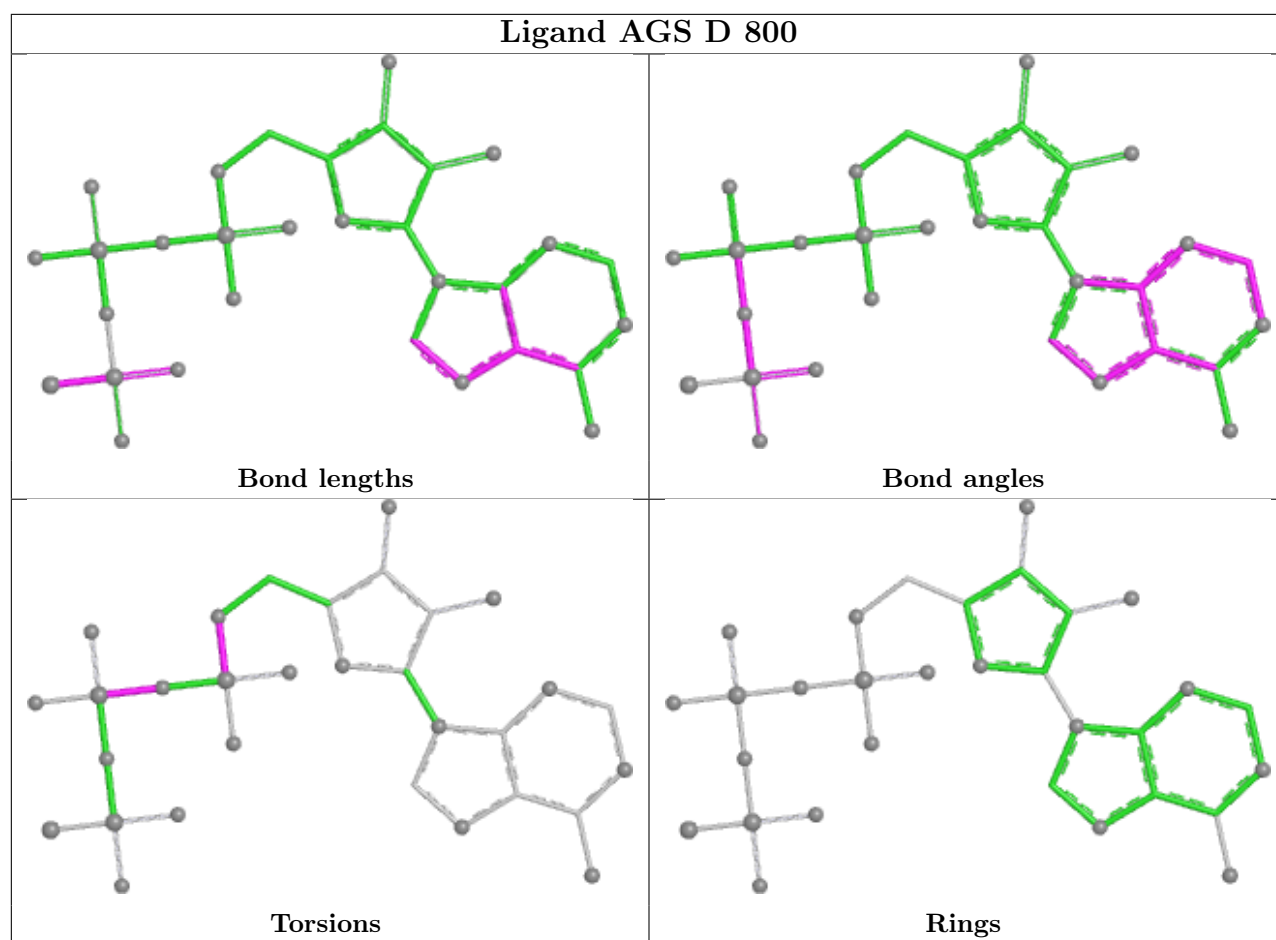
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	800	AGS	5	0
2	C	800	AGS	4	0
2	D	800	AGS	4	0
2	F	800	AGS	6	0
2	A	800	AGS	6	0
2	B	800	AGS	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

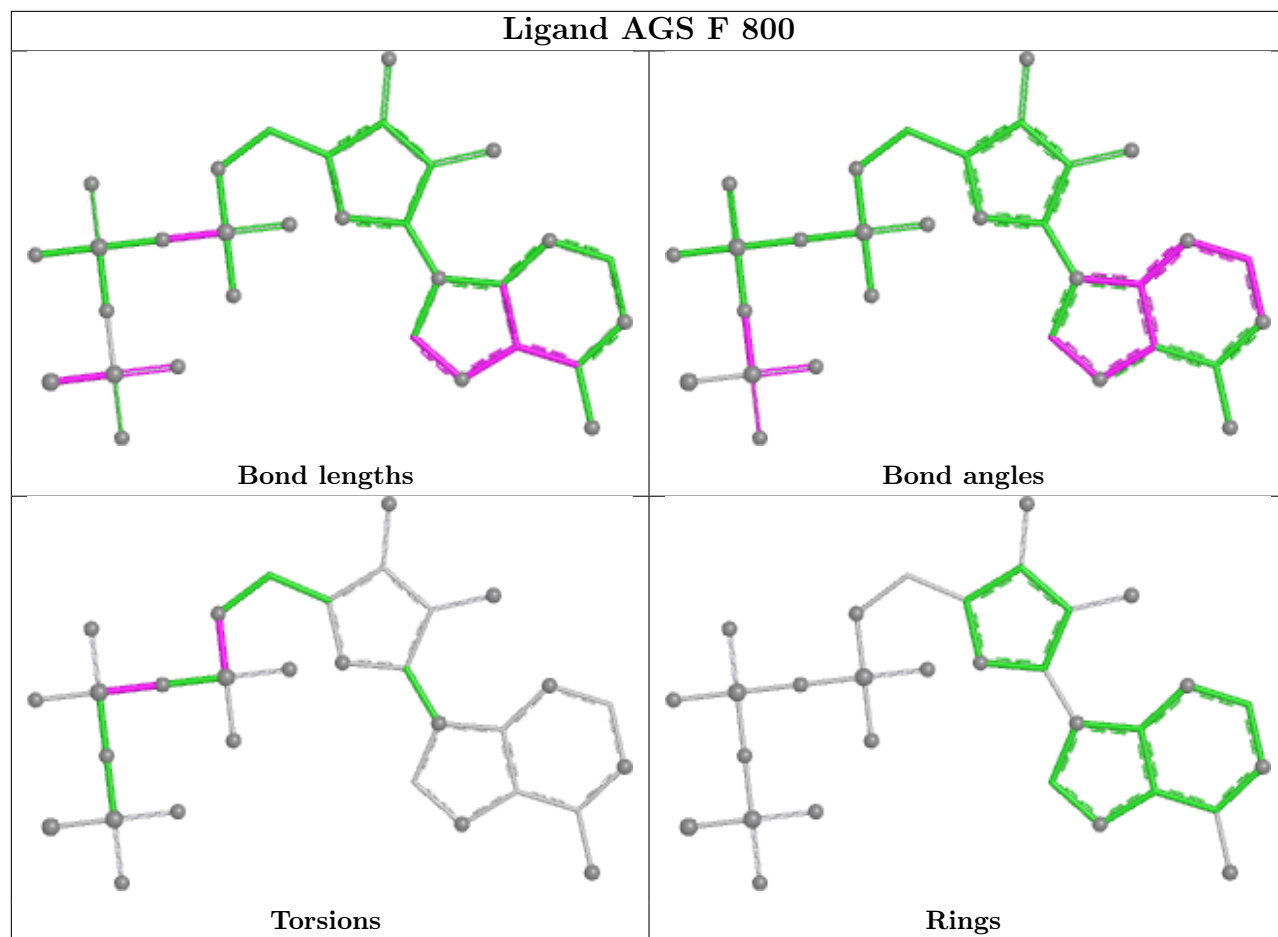
Ligand AGS E 800

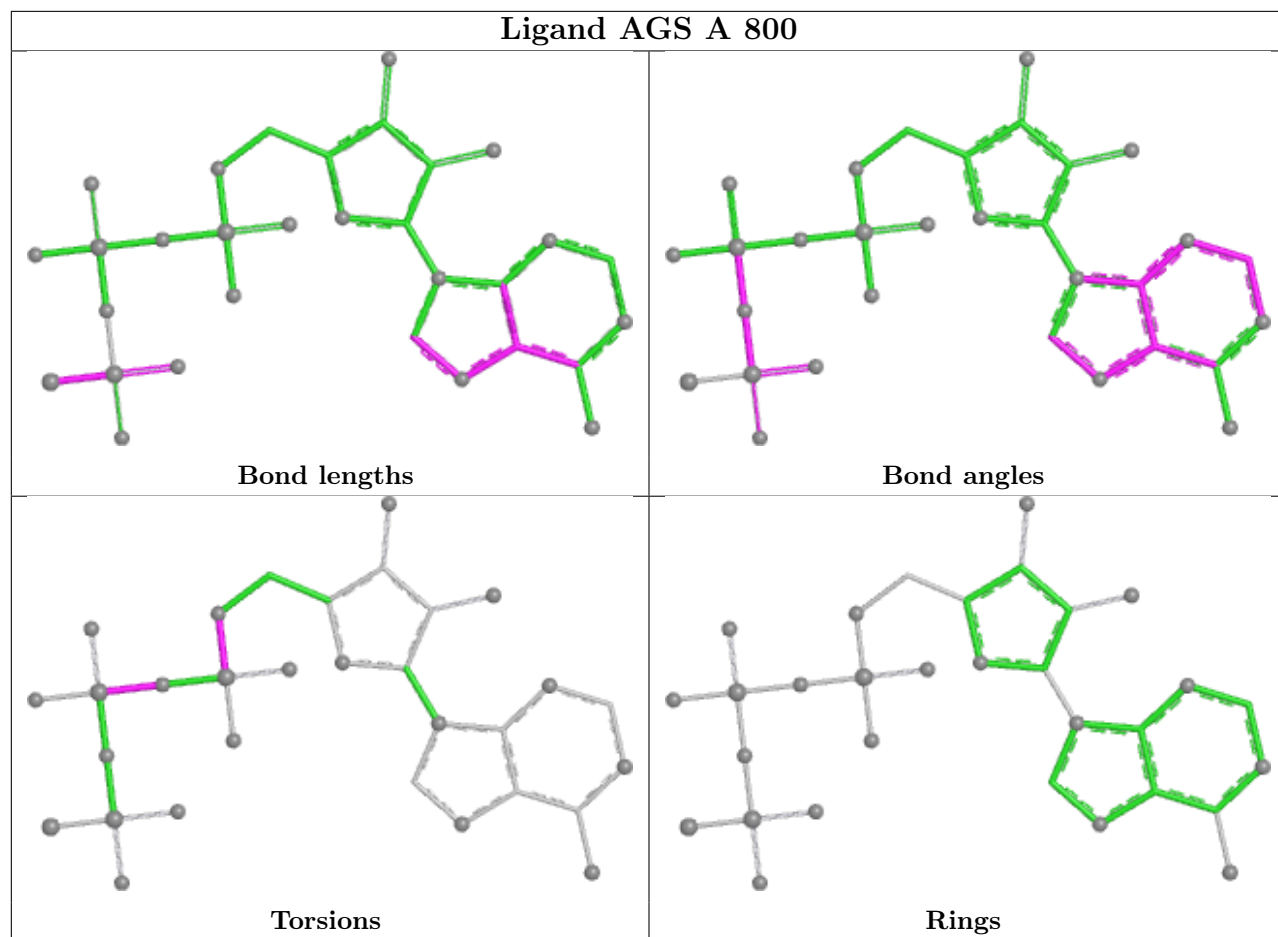


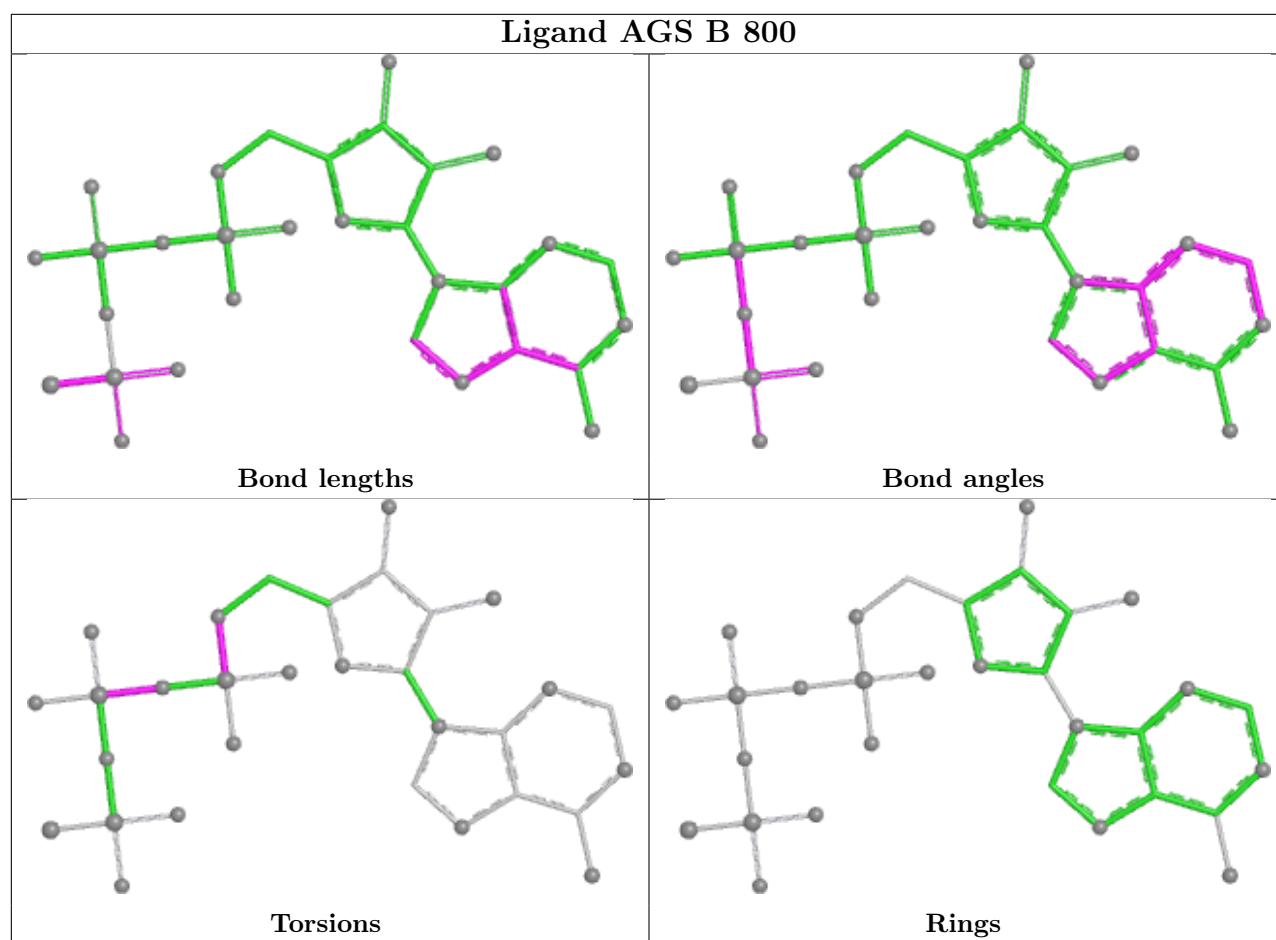




Ligand AGS F 800







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, 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	451/489 (92%)	0.77	35 (7%) 19 15	47, 81, 123, 137	0
1	B	451/489 (92%)	0.81	29 (6%) 25 21	47, 77, 110, 129	0
1	C	451/489 (92%)	0.90	47 (10%) 11 9	43, 89, 130, 150	0
1	D	451/489 (92%)	0.86	36 (7%) 18 14	45, 95, 144, 163	0
1	E	451/489 (92%)	1.02	55 (12%) 8 6	52, 93, 156, 173	0
1	F	451/489 (92%)	0.85	31 (6%) 23 19	37, 89, 132, 152	0
All	All	2706/2934 (92%)	0.87	233 (8%) 16 13	37, 86, 136, 173	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	LEU	6.1
1	D	12	LEU	6.1
1	F	12	LEU	5.5
1	C	15	ALA	5.2
1	A	12	LEU	5.2
1	A	72	LEU	5.2
1	C	12	LEU	4.8
1	C	16	ILE	4.7
1	E	12	LEU	4.6
1	E	72	LEU	4.6
1	C	13	SER	4.6
1	B	184	CYS	4.6
1	E	69	CYS	4.6
1	E	156	GLY	4.5
1	B	314	GLU	4.3
1	D	462	SER	4.1
1	C	72	LEU	3.9
1	F	427	MET	3.8
1	E	198	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	429	LEU	3.7
1	C	462	SER	3.7
1	C	201	VAL	3.7
1	F	126	ILE	3.6
1	F	32	ILE	3.6
1	E	462	SER	3.5
1	C	133	VAL	3.5
1	B	445	LEU	3.4
1	F	462	SER	3.4
1	C	14	THR	3.3
1	E	432	LEU	3.3
1	F	401	ASN	3.2
1	F	235	VAL	3.2
1	E	128	GLY	3.2
1	E	439	ALA	3.2
1	E	173	TYR	3.2
1	E	51	LEU	3.1
1	E	442	MET	3.1
1	F	229	LEU	3.1
1	F	72	LEU	3.0
1	A	183	HIS	3.0
1	A	360	PHE	3.0
1	D	360	PHE	3.0
1	E	40	SER	3.0
1	E	437	ILE	3.0
1	D	126	ILE	2.9
1	C	452	PHE	2.9
1	E	360	PHE	2.9
1	A	283	GLU	2.9
1	D	92	LEU	2.9
1	D	70	ILE	2.8
1	E	431	ASP	2.8
1	F	228	ALA	2.8
1	D	158	MET	2.8
1	B	432	LEU	2.8
1	D	41	LEU	2.8
1	E	441	VAL	2.8
1	D	184	CYS	2.8
1	A	461	PRO	2.8
1	F	70	ILE	2.8
1	E	92	LEU	2.8
1	D	15	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	320	VAL	2.8
1	F	338	ARG	2.8
1	F	184	CYS	2.7
1	A	445	LEU	2.7
1	B	157	GLY	2.7
1	C	157	GLY	2.7
1	A	158	MET	2.7
1	C	70	ILE	2.7
1	D	17	LEU	2.7
1	E	41	LEU	2.7
1	E	413	ALA	2.7
1	F	360	PHE	2.7
1	C	398	GLN	2.7
1	E	84	MET	2.7
1	A	281	GLU	2.7
1	C	314	GLU	2.7
1	D	163	PHE	2.7
1	B	238	PRO	2.7
1	D	110	TYR	2.6
1	E	182	ILE	2.6
1	F	227	PRO	2.6
1	E	207	GLY	2.6
1	A	32	ILE	2.6
1	E	314	GLU	2.6
1	E	405	GLY	2.6
1	B	181	VAL	2.6
1	C	68	VAL	2.6
1	C	346	ALA	2.6
1	A	126	ILE	2.6
1	E	32	ILE	2.6
1	A	462	SER	2.5
1	B	462	SER	2.5
1	B	158	MET	2.5
1	E	434	ASP	2.5
1	F	395	ASP	2.5
1	D	20	LYS	2.5
1	E	130	LEU	2.5
1	C	402	GLU	2.5
1	C	127	THR	2.5
1	C	184	CYS	2.5
1	E	126	ILE	2.5
1	C	92	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	317	HIS	2.5
1	C	110	TYR	2.5
1	D	26	LEU	2.5
1	D	32	ILE	2.5
1	F	39	VAL	2.5
1	F	68	VAL	2.5
1	A	384	HIS	2.4
1	B	283	GLU	2.4
1	A	234	GLY	2.4
1	D	461	PRO	2.4
1	E	71	VAL	2.4
1	D	153	LEU	2.4
1	E	96	LEU	2.4
1	D	405	GLY	2.4
1	B	398	GLN	2.4
1	E	52	PHE	2.4
1	A	432	LEU	2.4
1	F	130	LEU	2.4
1	F	40	SER	2.4
1	C	461	PRO	2.4
1	D	130	LEU	2.4
1	D	91	ASN	2.4
1	C	69	CYS	2.4
1	F	247	PRO	2.4
1	A	19	GLN	2.4
1	B	441	VAL	2.4
1	D	161	VAL	2.4
1	E	38	VAL	2.4
1	E	323	ARG	2.4
1	D	241	ILE	2.3
1	A	127	THR	2.3
1	C	247	PRO	2.3
1	E	184	CYS	2.3
1	D	370	GLY	2.3
1	C	181	VAL	2.3
1	C	163	PHE	2.3
1	D	52	PHE	2.3
1	C	126	ILE	2.3
1	C	317	HIS	2.3
1	E	158	MET	2.3
1	F	158	MET	2.3
1	E	13	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	155	ARG	2.3
1	A	77	CYS	2.3
1	A	184	CYS	2.3
1	B	41	LEU	2.3
1	C	339	ALA	2.3
1	E	67	ALA	2.3
1	E	114	ILE	2.3
1	F	127	THR	2.3
1	B	427	MET	2.3
1	B	355	PRO	2.3
1	E	461	PRO	2.3
1	C	17	LEU	2.3
1	F	41	LEU	2.3
1	F	135	LEU	2.3
1	E	70	ILE	2.3
1	E	400	ALA	2.3
1	B	95	ARG	2.3
1	C	179	ASP	2.3
1	A	128	GLY	2.3
1	D	111	GLY	2.3
1	B	57	VAL	2.3
1	D	335	LEU	2.3
1	E	15	ALA	2.2
1	E	77	CYS	2.2
1	F	15	ALA	2.2
1	E	199	ASN	2.2
1	C	128	GLY	2.2
1	A	255	ALA	2.2
1	A	437	ILE	2.2
1	B	266	PHE	2.2
1	A	311	PRO	2.2
1	E	75	ASP	2.2
1	C	439	ALA	2.2
1	A	199	ASN	2.2
1	F	173	TYR	2.2
1	A	68	VAL	2.2
1	A	314	GLU	2.2
1	B	415	CYS	2.2
1	B	461	PRO	2.2
1	F	110	TYR	2.2
1	A	198	LEU	2.2
1	A	207	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	198	LEU	2.2
1	C	405	GLY	2.2
1	D	51	LEU	2.2
1	D	432	LEU	2.2
1	D	445	LEU	2.2
1	C	189	ILE	2.2
1	D	447	VAL	2.2
1	E	82	ILE	2.2
1	D	152	PHE	2.2
1	C	225	ARG	2.1
1	F	236	LYS	2.1
1	A	59	LEU	2.1
1	A	135	LEU	2.1
1	B	293	ALA	2.1
1	C	26	LEU	2.1
1	C	158	MET	2.1
1	F	207	GLY	2.1
1	B	115	HIS	2.1
1	D	151	ILE	2.1
1	B	155	ARG	2.1
1	C	338	ARG	2.1
1	E	104	PRO	2.1
1	C	51	LEU	2.1
1	C	429	LEU	2.1
1	B	348	ASN	2.1
1	D	16	ILE	2.1
1	A	185	GLU	2.1
1	B	25	ARG	2.1
1	C	278	LEU	2.1
1	C	445	LEU	2.1
1	E	445	LEU	2.1
1	B	126	ILE	2.1
1	E	341	VAL	2.1
1	F	230	PHE	2.1
1	C	112	LYS	2.0
1	C	432	LEU	2.0
1	A	309	ILE	2.0
1	C	146	ILE	2.0
1	A	116	VAL	2.0
1	D	38	VAL	2.0
1	E	438	ASP	2.0
1	E	444	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	219	MET	2.0
1	A	51	LEU	2.0
1	D	135	LEU	2.0
1	B	38	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

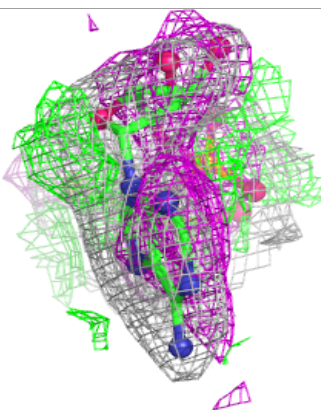
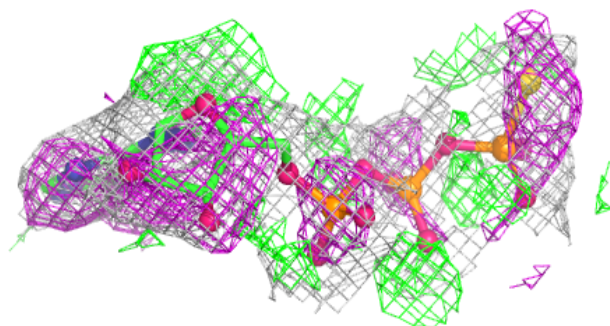
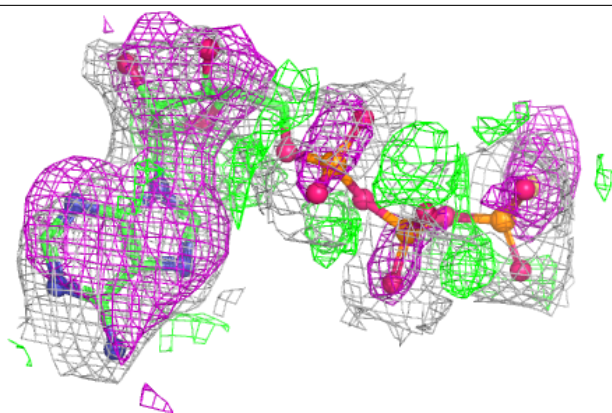
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AGS	A	800	31/31	0.90	0.11	24,27,29,29	0
2	AGS	B	800	31/31	0.92	0.09	28,29,30,30	0
2	AGS	F	800	31/31	0.92	0.10	12,12,13,14	0
2	AGS	E	800	31/31	0.94	0.09	39,40,42,43	0
2	AGS	D	800	31/31	0.94	0.08	34,43,45,46	0
2	AGS	C	800	31/31	0.95	0.08	25,31,36,37	0
3	MG	F	801	1/1	0.97	0.05	4,4,4,4	0
3	MG	E	801	1/1	0.98	0.05	19,19,19,19	0
3	MG	A	801	1/1	0.98	0.04	12,12,12,12	0
3	MG	D	801	1/1	0.99	0.03	24,24,24,24	0
3	MG	B	801	1/1	0.99	0.03	14,14,14,14	0
3	MG	C	801	1/1	0.99	0.05	13,13,13,13	0

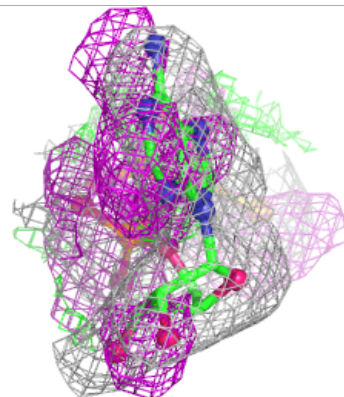
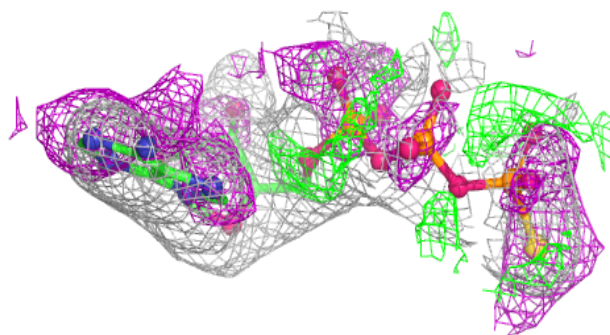
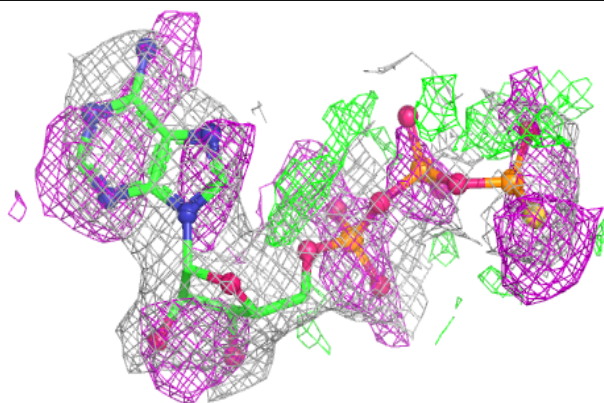
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

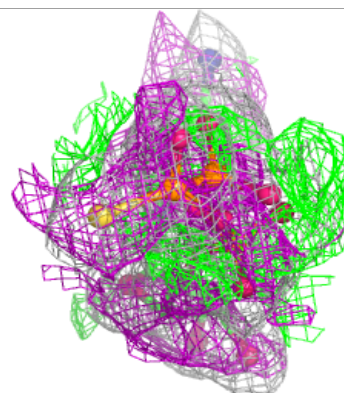
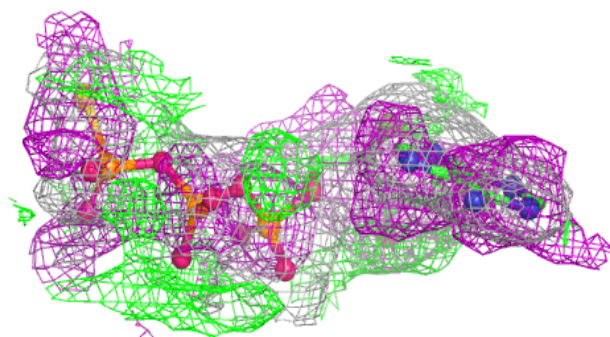
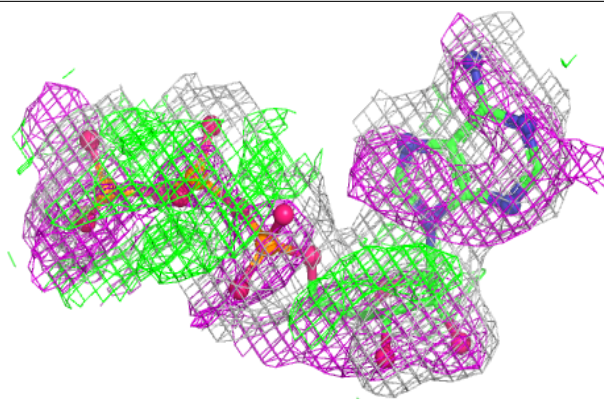
**Electron density around AGS B 800:**

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

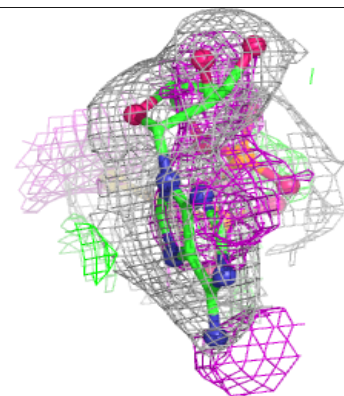
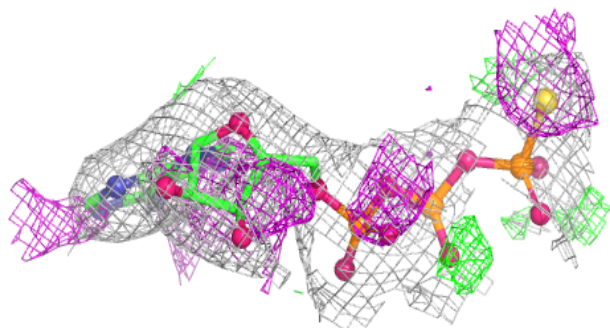
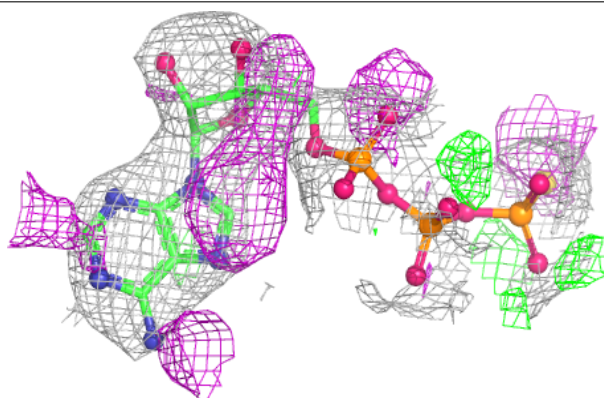


Electron density around AGS F 800:

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

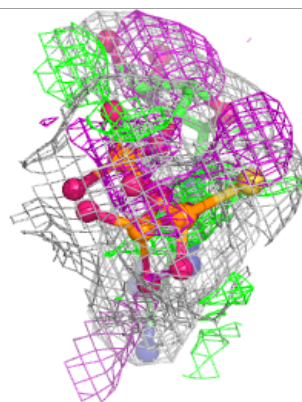
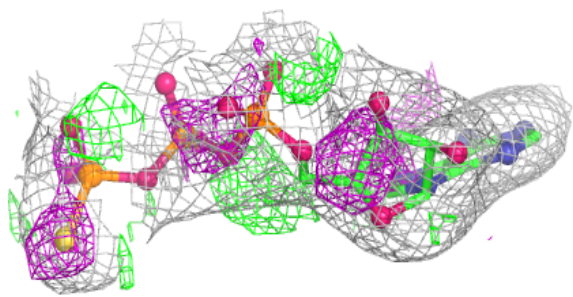
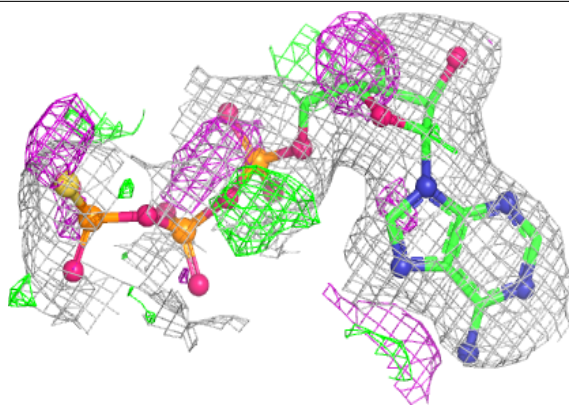
**Electron density around AGS E 800:**

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

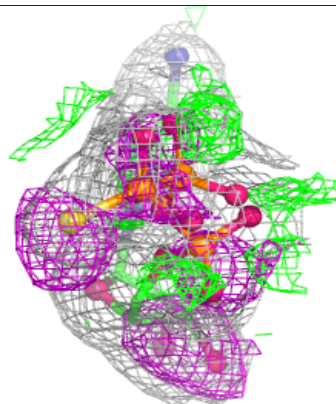
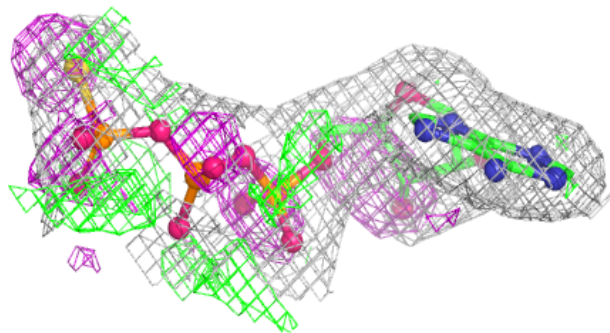
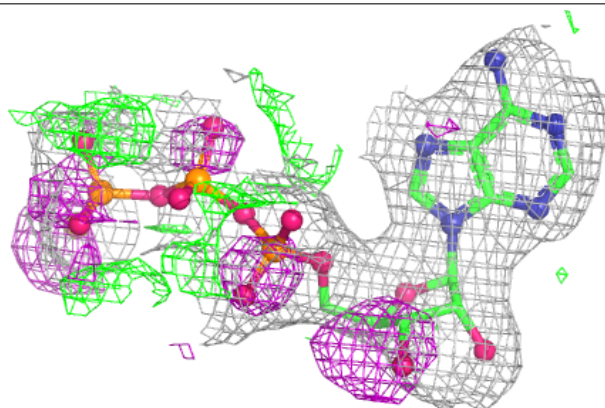


Electron density around AGS D 800:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.