



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:14 PM UTC

PDB ID : 5NXA / pdb_00005nxa
Title : Crystal structure of Neanderthal Adenylosuccinate Lyase (ADSL)in complex with its products AICAR and fumarate
Authors : Van Laer, B.; Kapp, U.; Soler-Lopez, M.; Leonard, G.; Mueller-Dieckmann, C.
Deposited on : 2017-05-09
Resolution : 2.40 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

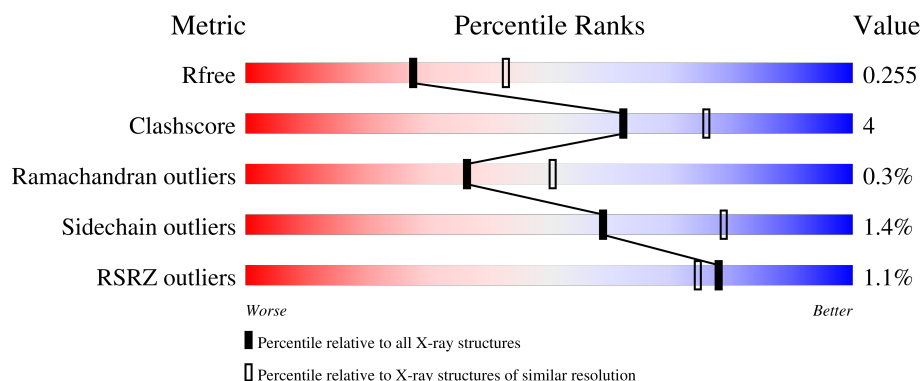
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	487	89% 7% 5%
1	B	487	78% 6% 15%
1	C	487	77% 8% 14%
1	D	487	82% 7% 10%

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Mol	Chain	Length	Quality of chain
1	E	487	 89% 2% 6% ..
1	F	487	 87% % 7% ..
1	G	487	 89% 5% 5% 5%
1	H	487	 92% 6% 6% .

2 Entry composition

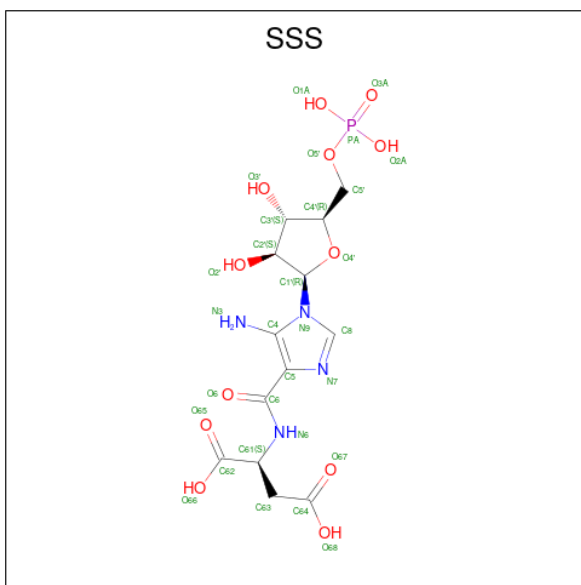
There are 6 unique types of molecules in this entry. The entry contains 29423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3696	2328	657	684	27			
1	B	415	Total	C	N	O	S	0	0	0
			3312	2092	586	611	23			
1	C	418	Total	C	N	O	S	0	0	0
			3355	2123	592	615	25			
1	D	440	Total	C	N	O	S	0	0	0
			3521	2218	625	653	25			
1	E	466	Total	C	N	O	S	0	0	0
			3723	2350	657	689	27			
1	F	466	Total	C	N	O	S	0	0	0
			3716	2342	659	688	27			
1	G	463	Total	C	N	O	S	0	0	0
			3692	2326	656	683	27			
1	H	477	Total	C	N	O	S	0	0	0
			3799	2394	673	704	28			

- Molecule 2 is N-{[5-AMINO-1-(5-O-PHOSPHONO-BETA-D-ARABINOFURANOSYL)-1H-IMIDAZOL-4-YL]CARBONYL}-L-ASPARTIC ACID (CCD ID: SSS) (formula: C₁₃H₁₉N₄O₁₂P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	13	4	12	1		
2	B	1	Total	C	N	O	P	0	0
			30	13	4	12	1		
2	D	1	Total	C	N	O	P	0	0
			30	13	4	12	1		
2	F	1	Total	C	N	O	P	0	0
			30	13	4	12	1		
2	G	1	Total	C	N	O	P	0	0
			30	13	4	12	1		
2	H	1	Total	C	N	O	P	0	0
			30	13	4	12	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

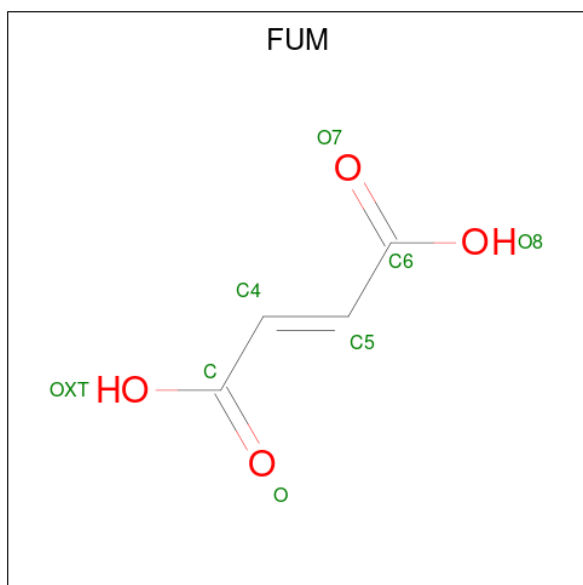
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

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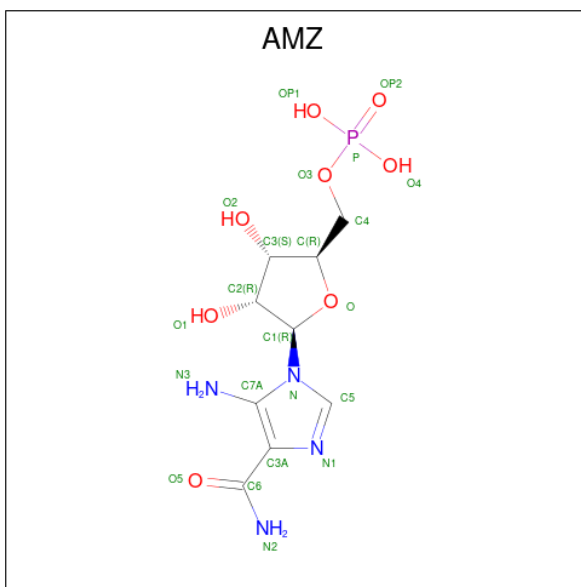
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	4	4		
4	E	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (CCD ID: AMZ) (formula: $C_9H_{15}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			22	9	4	8	1		
5	H	1	Total	C	N	O	P	0	0
			22	9	4	8	1		

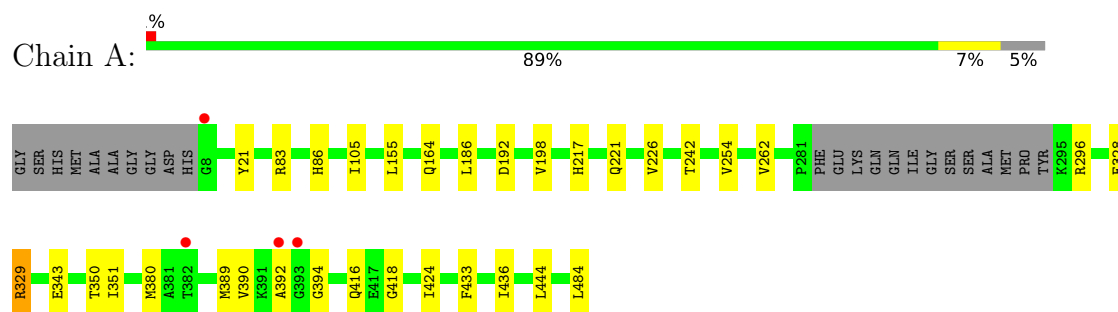
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total	O	0	0
			35	35		
6	B	39	Total	O	0	0
			39	39		
6	C	27	Total	O	0	0
			27	27		
6	D	33	Total	O	0	0
			33	33		
6	E	62	Total	O	0	0
			62	62		
6	F	41	Total	O	0	0
			41	41		
6	G	53	Total	O	0	0
			53	53		
6	H	71	Total	O	0	0
			71	71		

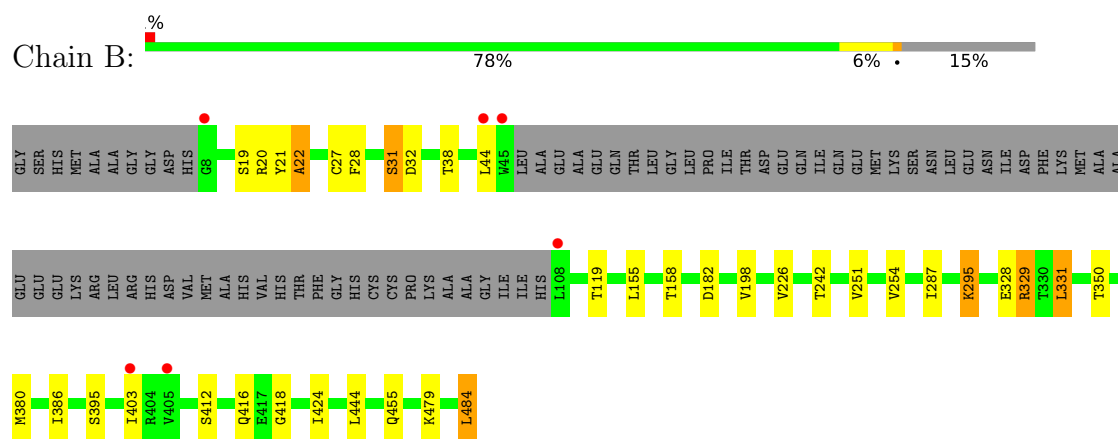
3 Residue-property plots [i](#)

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.

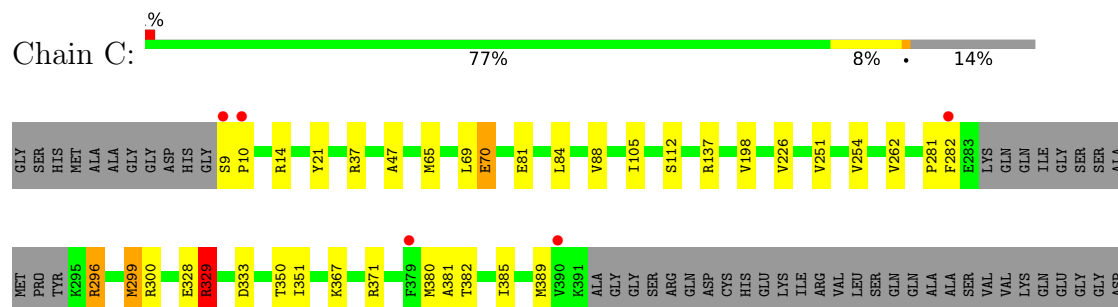
- Molecule 1: Adenylosuccinate lyase

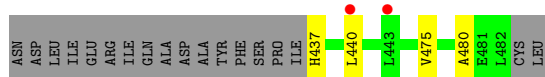


- Molecule 1: Adenylosuccinate lyase

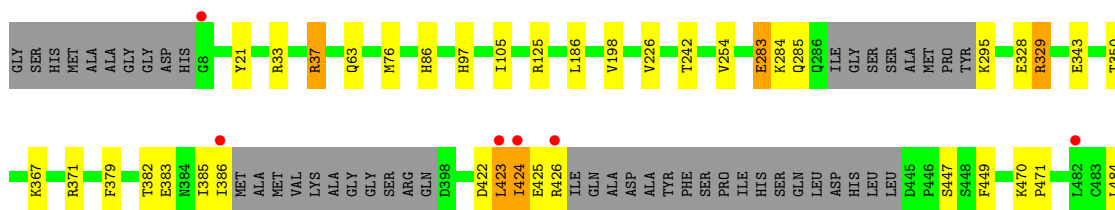
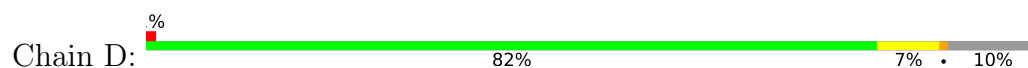


- Molecule 1: Adenylosuccinate lyase

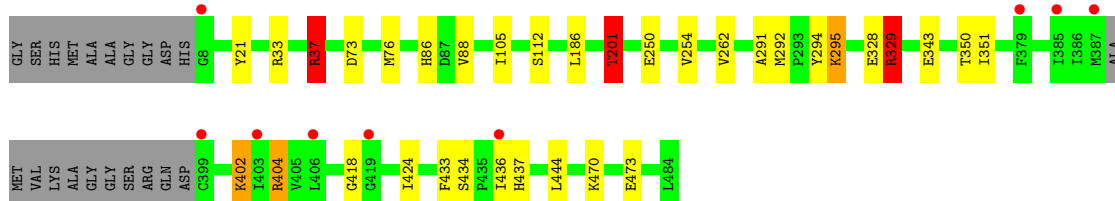
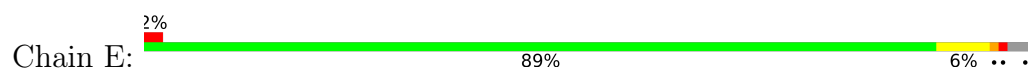




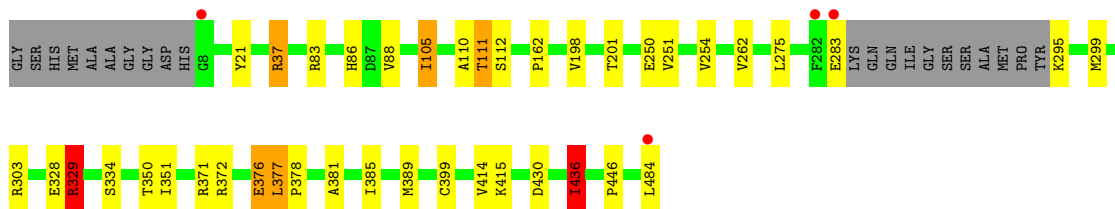
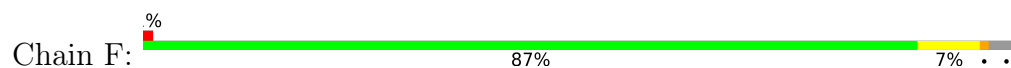
- Molecule 1: Adenylosuccinate lyase



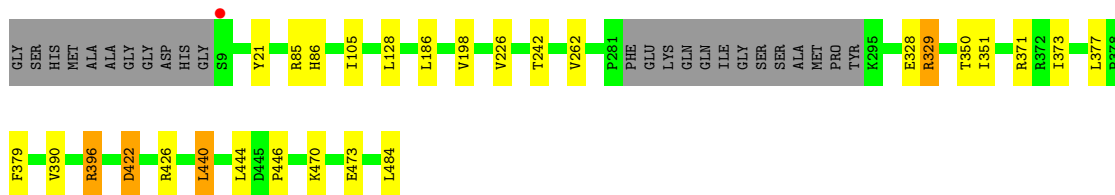
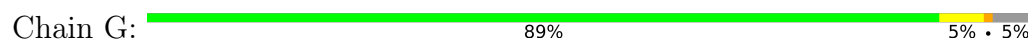
- Molecule 1: Adenylosuccinate lyase



- Molecule 1: Adenylosuccinate lyase



- Molecule 1: Adenylosuccinate lyase



- Molecule 1: Adenylosuccinate lyase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	356.53Å 74.21Å 160.31Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	47.85 – 2.40 47.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.85-2.40) 98.9 (47.85-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.220 , 0.254 0.224 , 0.255	Depositor DCC
R_{free} test set	7694 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29423	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUM, AMZ, SSS, CL

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	0.73	0/3761	0.77	0/5076
1	B	0.85	2/3371 (0.1%)	0.86	2/4550 (0.0%)
1	C	0.74	0/3416	0.83	3/4610 (0.1%)
1	D	0.76	0/3580	0.90	7/4827 (0.1%)
1	E	0.74	1/3791 (0.0%)	0.81	4/5118 (0.1%)
1	F	0.81	3/3782 (0.1%)	0.82	3/5104 (0.1%)
1	G	0.77	2/3757 (0.1%)	0.81	1/5071 (0.0%)
1	H	0.77	1/3868 (0.0%)	0.80	1/5221 (0.0%)
All	All	0.77	9/29326 (0.0%)	0.82	21/39577 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	422	ASP	C-O	-6.33	1.15	1.24
1	F	446	PRO	C-O	-6.22	1.16	1.24
1	G	422	ASP	C-O	5.97	1.31	1.23
1	E	201	THR	C-O	-5.63	1.17	1.24
1	B	22	ALA	N-CA	5.61	1.53	1.46
1	G	446	PRO	C-O	-5.59	1.17	1.24
1	B	19	SER	N-CA	5.55	1.53	1.46
1	F	250	GLU	C-O	-5.45	1.17	1.24
1	F	381	ALA	C-O	-5.17	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	424	ILE	N-CA-C	-25.53	87.42	111.67
1	C	480	ALA	N-CA-C	9.36	122.40	110.33
1	D	283	GLU	N-CA-C	8.09	120.84	110.65
1	B	295	LYS	N-CA-C	7.87	122.52	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	295	LYS	N-CA-C	7.48	121.18	109.96
1	E	37	ARG	CB-CG-CD	7.41	128.33	111.30
1	D	447	SER	N-CA-C	6.69	119.43	111.33
1	E	37	ARG	CA-CB-CG	6.53	127.15	114.10
1	D	449	PHE	N-CA-C	6.27	120.67	112.89
1	C	299	MET	N-CA-C	5.83	117.64	111.28
1	B	44	LEU	N-CA-C	-5.83	105.06	111.82
1	G	440	LEU	N-CA-C	5.75	117.55	111.28
1	H	329	ARG	CG-CD-NE	5.52	124.14	112.00
1	F	329	ARG	CG-CD-NE	5.38	123.83	112.00
1	F	110	ALA	N-CA-C	5.37	118.74	110.42
1	D	423	LEU	CA-C-N	5.37	129.02	122.63
1	D	423	LEU	C-N-CA	5.37	129.02	122.63
1	C	440	LEU	N-CA-C	5.32	117.08	111.28
1	E	329	ARG	CG-CD-NE	5.20	123.44	112.00
1	D	422	ASP	N-CA-C	5.10	117.67	107.62
1	F	436	ILE	N-CA-C	5.02	117.72	112.90

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	3696	0	3730	33	0
1	B	3312	0	3352	24	0
1	C	3355	0	3393	40	0
1	D	3521	0	3552	43	0
1	E	3723	0	3751	29	0
1	F	3716	0	3745	46	0
1	G	3692	0	3727	26	0
1	H	3799	0	3829	22	0
2	A	30	0	15	1	0
2	B	30	0	15	0	0
2	D	30	0	15	2	0
2	F	30	0	15	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	30	0	15	2	0
2	H	30	0	15	2	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
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	8	0	1	0	0
4	E	8	0	1	0	0
5	C	22	0	13	1	0
5	H	22	0	13	0	0
6	A	35	0	0	1	0
6	B	39	0	0	2	0
6	C	27	0	0	0	0
6	D	33	0	0	0	0
6	E	62	0	0	0	0
6	F	41	0	0	2	0
6	G	53	0	0	0	0
6	H	71	0	0	0	0
All	All	29423	0	29197	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (238) 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:283:GLU:OE1	1:G:85:ARG:NH1	1.80	1.15
1:C:10:PRO:HA	1:C:14:ARG:HH21	1.12	1.09
1:C:10:PRO:CA	1:C:14:ARG:HH21	1.72	1.02
1:D:385:ILE:HD12	1:D:426:ARG:NH1	1.76	1.01
1:C:10:PRO:CA	1:C:14:ARG:NH2	2.25	0.99
1:C:10:PRO:HA	1:C:14:ARG:NH2	1.80	0.97
1:A:217:HIS:NE2	1:A:221:GLN:NE2	2.22	0.88
1:E:402:LYS:N	1:E:402:LYS:HD2	1.89	0.87
1:D:37:ARG:HG3	1:D:37:ARG:HH11	1.38	0.87
1:E:402:LYS:HD2	1:E:402:LYS:H	1.41	0.85
1:F:111:THR:HG21	1:F:201:THR:HA	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:ILE:HD12	1:D:426:ARG:HH12	1.46	0.81
1:H:328:GLU:O	1:H:329:ARG:HB3	1.82	0.79
1:F:303:ARG:HH12	1:F:484:LEU:CD2	1.96	0.79
1:C:475:VAL:HG12	1:C:475:VAL:O	1.82	0.79
1:F:328:GLU:O	1:F:329:ARG:HB3	1.82	0.79
1:B:418:GLY:O	1:D:371:ARG:HD2	1.83	0.78
1:F:303:ARG:HH12	1:F:484:LEU:HD23	1.47	0.78
1:E:328:GLU:O	1:E:329:ARG:HB3	1.83	0.78
1:D:385:ILE:CD1	1:D:426:ARG:NH1	2.46	0.77
1:C:328:GLU:O	1:C:329:ARG:HB3	1.84	0.77
1:D:423:LEU:HB3	1:D:426:ARG:HG2	1.65	0.77
1:H:37:ARG:HD3	1:H:37:ARG:C	2.09	0.77
1:A:217:HIS:CD2	1:A:221:GLN:NE2	2.53	0.77
1:A:389:MET:N	1:A:436:ILE:HD11	2.01	0.76
1:D:283:GLU:O	1:D:285:GLN:N	2.19	0.75
1:A:389:MET:HG2	1:A:436:ILE:HD12	1.70	0.73
1:F:83:ARG:HG2	1:F:83:ARG:HH21	1.53	0.72
1:G:328:GLU:O	1:G:329:ARG:HB2	1.89	0.72
1:C:137:ARG:NH2	1:C:475:VAL:HG12	2.04	0.72
1:A:389:MET:CE	1:A:433:PHE:HA	2.20	0.71
1:D:328:GLU:O	1:D:329:ARG:HB2	1.90	0.71
1:A:328:GLU:O	1:A:329:ARG:HB2	1.90	0.71
1:E:86:HIS:HA	2:H:501:SSS:H2'	1.72	0.71
1:A:192:ASP:OD2	6:A:601:HOH:O	2.09	0.70
1:B:328:GLU:O	1:B:329:ARG:HB2	1.89	0.70
1:C:381:ALA:O	1:C:382:THR:OG1	2.06	0.70
1:C:10:PRO:CB	1:C:14:ARG:NH2	2.56	0.69
1:F:86:HIS:HA	2:F:502:SSS:H2'	1.74	0.68
1:F:299:MET:CE	1:F:484:LEU:HD13	2.23	0.67
1:B:455:GLN:HG3	6:B:631:HOH:O	1.94	0.67
1:A:186:LEU:HD12	1:A:254:VAL:CG1	2.25	0.67
1:A:390:VAL:HA	1:A:394:GLY:HA2	1.75	0.67
1:C:10:PRO:CB	1:C:14:ARG:HH22	2.08	0.67
1:E:186:LEU:HD12	1:E:254:VAL:CG1	2.26	0.65
1:F:299:MET:HE1	1:F:484:LEU:HD13	1.78	0.65
1:D:186:LEU:HD12	1:D:254:VAL:CG1	2.25	0.65
1:C:37:ARG:HG3	1:C:70:GLU:HG3	1.78	0.64
1:C:10:PRO:HB3	1:C:14:ARG:HH22	1.61	0.64
1:F:303:ARG:NH1	1:F:484:LEU:HD23	2.13	0.64
1:G:422:ASP:OD2	1:G:426:ARG:NH1	2.31	0.64
1:F:484:LEU:HB2	1:G:85:ARG:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ILE:O	1:C:389:MET:HG2	1.98	0.64
1:D:423:LEU:HD13	1:D:426:ARG:NH2	2.13	0.63
1:D:423:LEU:HD13	1:D:426:ARG:HH21	1.62	0.63
1:A:389:MET:CA	1:A:436:ILE:HD11	2.28	0.63
1:F:275:LEU:O	1:F:372:ARG:NH2	2.31	0.63
1:C:47:ALA:CB	1:C:65:MET:HE1	2.29	0.62
1:G:262:VAL:HG11	1:G:351:ILE:HG23	1.81	0.62
1:A:86:HIS:HA	2:A:501:SSS:H2'	1.80	0.62
1:F:262:VAL:HG11	1:F:351:ILE:HG23	1.82	0.62
1:A:262:VAL:HG11	1:A:351:ILE:HG23	1.82	0.61
1:F:484:LEU:HD12	1:G:85:ARG:CG	2.31	0.61
1:G:86:HIS:HA	2:G:502:SSS:H2'	1.83	0.61
1:C:475:VAL:O	1:C:475:VAL:CG1	2.49	0.61
1:E:262:VAL:HG11	1:E:351:ILE:HG23	1.83	0.60
1:D:423:LEU:HB3	1:D:426:ARG:CG	2.30	0.60
1:D:425:GLU:O	1:D:426:ARG:C	2.43	0.60
1:B:182:ASP:OD1	6:B:601:HOH:O	2.16	0.60
1:C:10:PRO:N	1:C:14:ARG:NH2	2.49	0.60
1:F:303:ARG:NH1	1:F:484:LEU:CD2	2.64	0.60
1:C:10:PRO:HB3	1:C:14:ARG:NH2	2.15	0.60
1:D:423:LEU:HD22	1:D:426:ARG:HE	1.67	0.60
1:B:416:GLN:O	1:D:367:LYS:HG3	2.00	0.59
1:D:37:ARG:HG3	1:D:37:ARG:NH1	2.09	0.59
1:E:404:ARG:CG	1:E:404:ARG:HH11	2.15	0.59
1:E:418:GLY:O	1:G:371:ARG:HD2	2.03	0.58
1:C:262:VAL:HG11	1:C:351:ILE:HG23	1.84	0.58
1:A:262:VAL:HG11	1:A:351:ILE:CG2	2.33	0.58
1:G:262:VAL:HG11	1:G:351:ILE:CG2	2.34	0.58
1:H:21:TYR:CE1	1:H:303:ARG:HD2	2.39	0.58
1:C:9:SER:O	1:C:14:ARG:HD2	2.03	0.58
1:F:262:VAL:HG11	1:F:351:ILE:CG2	2.34	0.57
1:A:389:MET:HE1	1:A:433:PHE:HA	1.85	0.57
1:B:21:TYR:HB3	1:B:350:THR:HG21	1.86	0.57
1:B:424:ILE:HD12	1:B:444:LEU:HD11	1.86	0.57
1:C:65:MET:O	1:C:69:LEU:CD1	2.52	0.57
1:E:434:SER:HA	1:E:437:HIS:ND1	2.20	0.57
1:A:217:HIS:CE1	1:A:221:GLN:HE21	2.21	0.56
1:D:86:HIS:HA	2:D:502:SSS:H2'	1.86	0.56
1:C:137:ARG:HH21	1:C:475:VAL:HG12	1.70	0.56
1:E:262:VAL:HG11	1:E:351:ILE:CG2	2.35	0.56
1:F:83:ARG:HG2	1:F:83:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:VAL:HG11	1:C:351:ILE:CG2	2.35	0.56
1:B:386:ILE:CG1	1:B:403:ILE:HD12	2.36	0.56
1:A:389:MET:HE3	1:A:433:PHE:HA	1.86	0.56
1:C:10:PRO:N	1:C:14:ARG:HH21	2.03	0.56
1:E:424:ILE:HD12	1:E:444:LEU:HD11	1.88	0.56
1:D:382:THR:HG23	1:D:426:ARG:NH2	2.21	0.56
1:F:37:ARG:HG3	1:F:37:ARG:HH11	1.72	0.55
1:F:389:MET:HB3	1:F:399:CYS:SG	2.46	0.55
1:C:282:PHE:HB3	1:C:296:ARG:NH1	2.21	0.55
1:D:383:GLU:O	1:D:386:ILE:HG13	2.07	0.54
1:D:423:LEU:HD22	1:D:426:ARG:NE	2.22	0.54
1:E:201:THR:HG21	1:H:292:MET:HE2	1.90	0.54
1:A:424:ILE:HD12	1:A:444:LEU:HD11	1.88	0.54
1:H:289:SER:OG	2:H:501:SSS:H631	2.07	0.54
1:H:424:ILE:HD12	1:H:444:LEU:HD11	1.89	0.54
1:B:20:ARG:NH2	1:C:81:GLU:OE2	2.40	0.54
1:E:470:LYS:NZ	1:E:473:GLU:OE1	2.38	0.54
1:E:33:ARG:O	1:E:37:ARG:HB3	2.07	0.54
1:F:111:THR:CG2	1:F:201:THR:HA	2.34	0.53
1:D:33:ARG:O	1:D:37:ARG:HB3	2.08	0.53
1:E:436:ILE:O	1:E:436:ILE:HG22	2.08	0.53
1:F:414:VAL:HG11	1:H:276:LYS:HE3	1.90	0.52
1:D:383:GLU:HA	1:D:386:ILE:HG12	1.92	0.52
1:D:382:THR:CG2	1:D:426:ARG:NH2	2.73	0.52
1:A:389:MET:HA	1:A:436:ILE:HD11	1.89	0.52
1:A:436:ILE:HG22	1:A:436:ILE:O	2.10	0.52
1:E:294:TYR:HB2	1:G:379:PHE:CD1	2.45	0.52
1:F:484:LEU:CD1	1:G:85:ARG:HB3	2.40	0.51
1:G:242:THR:HG23	1:G:329:ARG:HG3	1.92	0.51
1:D:242:THR:HG23	1:D:329:ARG:HG3	1.92	0.51
1:E:433:PHE:O	1:E:437:HIS:ND1	2.44	0.51
1:A:242:THR:HG23	1:A:329:ARG:HG3	1.92	0.51
1:D:379:PHE:O	1:D:382:THR:OG1	2.24	0.51
1:F:371:ARG:NH2	1:H:420:ASP:OD1	2.42	0.51
1:F:37:ARG:HH11	1:F:37:ARG:CG	2.24	0.51
1:F:385:ILE:HG23	1:F:436:ILE:HD13	1.91	0.51
1:H:198:VAL:HG23	1:H:226:VAL:HG21	1.93	0.51
1:B:329:ARG:CZ	1:B:331:LEU:HD23	2.40	0.50
2:F:502:SSS:O2'	2:F:502:SSS:H8	2.11	0.50
1:H:80:GLU:OE1	1:H:83:ARG:NH1	2.44	0.50
1:A:418:GLY:O	1:C:371:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:ARG:HH11	1:E:404:ARG:HG3	1.76	0.50
1:B:386:ILE:HG13	1:B:403:ILE:HD12	1.92	0.50
1:E:292:MET:HE2	1:H:201:THR:HG21	1.94	0.50
1:B:28:PHE:HA	1:B:31:SER:HB3	1.93	0.49
2:D:502:SSS:H8	2:D:502:SSS:O2'	2.12	0.49
1:D:76:MET:HE1	1:D:97:HIS:ND1	2.27	0.49
1:F:484:LEU:HD12	1:G:85:ARG:HB3	1.94	0.49
1:A:389:MET:HE2	1:A:436:ILE:HD12	1.94	0.49
1:D:424:ILE:O	1:D:425:GLU:C	2.52	0.49
1:B:242:THR:HG23	1:B:329:ARG:HG3	1.93	0.48
1:B:386:ILE:HG13	1:B:403:ILE:CD1	2.43	0.48
1:D:37:ARG:NH1	1:D:37:ARG:CG	2.73	0.48
1:C:65:MET:O	1:C:69:LEU:HD13	2.13	0.48
1:F:484:LEU:HD12	1:G:85:ARG:CD	2.44	0.48
1:A:198:VAL:HG23	1:A:226:VAL:HG21	1.96	0.47
1:G:390:VAL:CG2	1:G:396:ARG:HB3	2.44	0.47
1:C:198:VAL:HG23	1:C:226:VAL:HG21	1.96	0.47
1:C:251:VAL:O	1:C:254:VAL:HG22	2.15	0.47
1:B:21:TYR:HB3	1:B:350:THR:CG2	2.45	0.47
1:F:251:VAL:O	1:F:254:VAL:HG22	2.15	0.47
1:G:470:LYS:NZ	1:G:473:GLU:OE1	2.40	0.47
1:A:186:LEU:HD12	1:A:254:VAL:HG11	1.96	0.46
1:B:20:ARG:NH1	5:C:502:AMZ:O4	2.47	0.46
1:F:83:ARG:HB2	1:F:83:ARG:CZ	2.45	0.46
1:G:390:VAL:HG21	1:G:396:ARG:HB3	1.97	0.46
1:A:21:TYR:HB3	1:A:350:THR:HG21	1.97	0.46
1:D:385:ILE:CD1	1:D:426:ARG:HH11	2.25	0.46
1:F:334:SER:OG	2:F:502:SSS:O2A	2.23	0.46
1:F:415:LYS:HB3	1:H:365:TYR:CG	2.51	0.46
1:B:251:VAL:O	1:B:254:VAL:HG22	2.16	0.46
1:E:294:TYR:CB	1:G:379:PHE:CD1	2.99	0.46
1:D:21:TYR:HB3	1:D:350:THR:HG21	1.98	0.46
1:F:430:ASP:OD2	6:F:601:HOH:O	2.21	0.46
1:D:76:MET:HE1	1:D:97:HIS:CE1	2.51	0.45
1:F:303:ARG:HH12	1:F:484:LEU:HD22	1.79	0.45
1:B:287:ILE:CD1	1:C:84:LEU:HD22	2.47	0.45
1:H:251:VAL:O	1:H:254:VAL:HG22	2.15	0.45
1:A:389:MET:HG2	1:A:436:ILE:CD1	2.44	0.45
1:G:198:VAL:HG23	1:G:226:VAL:HG21	1.97	0.45
1:C:21:TYR:HB3	1:C:350:THR:HG21	1.99	0.45
1:D:198:VAL:HG23	1:D:226:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:C	1:A:105:ILE:HD12	2.42	0.45
1:D:385:ILE:CD1	1:D:426:ARG:HH12	2.20	0.45
1:E:21:TYR:HB3	1:E:350:THR:HG21	1.97	0.45
1:E:105:ILE:HD12	1:E:105:ILE:C	2.42	0.45
1:G:21:TYR:HB3	1:G:350:THR:HG21	1.99	0.45
1:F:295:LYS:NZ	1:H:158:THR:OG1	2.48	0.44
1:F:83:ARG:NH2	1:F:83:ARG:CG	2.73	0.44
1:F:303:ARG:NH1	1:F:484:LEU:HD22	2.32	0.44
1:F:37:ARG:CG	1:F:37:ARG:NH1	2.79	0.44
1:H:21:TYR:HB3	1:H:350:THR:HG21	1.98	0.44
1:A:155:LEU:CD1	1:A:380:MET:HE1	2.48	0.44
1:A:436:ILE:O	1:A:436:ILE:CG2	2.66	0.44
1:C:105:ILE:C	1:C:105:ILE:HD12	2.43	0.44
1:D:105:ILE:C	1:D:105:ILE:HD12	2.43	0.44
1:F:21:TYR:HB3	1:F:350:THR:HG21	1.99	0.44
1:G:128:LEU:CD2	1:G:186:LEU:HD22	2.48	0.44
1:B:484:LEU:C	1:B:484:LEU:HD23	2.42	0.43
1:F:377:LEU:HB3	1:F:378:PRO:HD3	2.00	0.43
1:D:186:LEU:HD12	1:D:254:VAL:HG11	1.97	0.43
1:E:73:ASP:CG	1:E:76:MET:HG2	2.44	0.43
1:G:373:ILE:HG22	1:G:377:LEU:HD13	1.99	0.43
1:G:105:ILE:HD12	1:G:105:ILE:C	2.43	0.43
1:H:21:TYR:HE1	1:H:303:ARG:HD2	1.82	0.43
1:C:281:PRO:O	1:C:300:ARG:NH2	2.51	0.43
1:D:382:THR:HG23	1:D:426:ARG:HH22	1.83	0.43
1:E:291:ALA:HB3	1:H:201:THR:HG23	1.99	0.43
1:G:422:ASP:CG	1:G:426:ARG:HH11	2.27	0.43
1:C:282:PHE:CB	1:C:296:ARG:NH1	2.81	0.43
1:B:22:ALA:HB3	1:B:27:CYS:SG	2.59	0.42
1:F:162:PRO:HG2	6:F:636:HOH:O	2.19	0.42
1:D:423:LEU:HD13	1:D:426:ARG:CZ	2.49	0.42
1:H:105:ILE:C	1:H:105:ILE:HD12	2.44	0.42
1:F:88:VAL:HG21	1:F:112:SER:HB3	2.01	0.42
1:H:88:VAL:HG21	1:H:112:SER:HB3	2.02	0.42
1:B:38:THR:HG21	1:B:119:THR:HG23	2.01	0.42
1:A:83:ARG:HH11	1:D:285:GLN:CD	2.28	0.42
1:C:329:ARG:NH2	1:C:333:ASP:OD1	2.52	0.42
1:D:423:LEU:HD23	1:D:423:LEU:HA	1.85	0.42
1:F:385:ILE:HG23	1:F:436:ILE:CD1	2.49	0.42
1:A:416:GLN:O	1:C:367:LYS:HG3	2.20	0.42
1:B:158:THR:OG1	1:D:295:LYS:NZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:ARG:CG	1:E:404:ARG:NH1	2.78	0.42
1:C:65:MET:O	1:C:69:LEU:HD12	2.20	0.42
1:A:343:GLU:OE2	1:D:343:GLU:OE1	2.38	0.41
1:B:155:LEU:CD1	1:B:380:MET:HE1	2.50	0.41
1:E:186:LEU:HD12	1:E:254:VAL:HG11	2.01	0.41
1:F:105:ILE:HA	1:F:105:ILE:HD12	1.59	0.41
1:E:343:GLU:OE2	1:H:343:GLU:OE1	2.39	0.41
1:E:73:ASP:OD2	1:E:76:MET:HG2	2.21	0.41
1:B:198:VAL:HG23	1:B:226:VAL:HG21	2.02	0.41
1:G:440:LEU:O	1:G:444:LEU:HG	2.20	0.41
1:D:423:LEU:HD13	1:D:426:ARG:NE	2.35	0.41
1:C:88:VAL:HG21	1:C:112:SER:HB3	2.03	0.41
1:E:88:VAL:HG21	1:E:112:SER:HB3	2.03	0.41
1:F:376:GLU:OE2	1:H:276:LYS:NZ	2.50	0.41
1:F:389:MET:CB	1:F:399:CYS:SG	3.09	0.41
2:G:502:SSS:O2'	2:G:502:SSS:H8	2.20	0.41
1:A:217:HIS:O	1:A:221:GLN:HG3	2.21	0.41
1:C:47:ALA:HB2	1:C:65:MET:HE1	2.03	0.41
1:C:137:ARG:NH2	1:C:475:VAL:CG1	2.78	0.40
1:H:84:LEU:HD11	1:H:93:HIS:HD2	1.86	0.40
1:F:484:LEU:HD12	1:G:85:ARG:CB	2.51	0.40
1:D:470:LYS:HB3	1:D:471:PRO:HD3	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	460/487 (94%)	449 (98%)	9 (2%)	2 (0%)	30	43
1	B	411/487 (84%)	403 (98%)	7 (2%)	1 (0%)	43	58
1	C	412/487 (85%)	401 (97%)	10 (2%)	1 (0%)	43	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	432/487 (89%)	420 (97%)	10 (2%)	2 (0%)	24	37
1	E	462/487 (95%)	454 (98%)	7 (2%)	1 (0%)	43	58
1	F	462/487 (95%)	453 (98%)	8 (2%)	1 (0%)	43	58
1	G	459/487 (94%)	451 (98%)	7 (2%)	1 (0%)	43	58
1	H	475/487 (98%)	467 (98%)	7 (2%)	1 (0%)	43	58
All	All	3573/3896 (92%)	3498 (98%)	65 (2%)	10 (0%)	36	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ARG
1	B	329	ARG
1	C	329	ARG
1	D	284	LYS
1	D	329	ARG
1	E	329	ARG
1	F	329	ARG
1	G	329	ARG
1	H	329	ARG
1	A	392	ALA

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	406/422 (96%)	403 (99%)	3 (1%)	76	88
1	B	365/422 (86%)	357 (98%)	8 (2%)	45	67
1	C	370/422 (88%)	364 (98%)	6 (2%)	55	76
1	D	388/422 (92%)	384 (99%)	4 (1%)	68	84
1	E	410/422 (97%)	403 (98%)	7 (2%)	53	74
1	F	408/422 (97%)	400 (98%)	8 (2%)	48	70
1	G	406/422 (96%)	404 (100%)	2 (0%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	417/422 (99%)	411 (99%)	6 (1%)	59 79
All	All	3170/3376 (94%)	3126 (99%)	44 (1%)	59 79

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	296	ARG
1	A	484	LEU
1	B	31	SER
1	B	32	ASP
1	B	295	LYS
1	B	331	LEU
1	B	395	SER
1	B	412	SER
1	B	479	LYS
1	B	484	LEU
1	C	70	GLU
1	C	296	ARG
1	C	299	MET
1	C	329	ARG
1	C	380	MET
1	C	437	HIS
1	D	37	ARG
1	D	63	GLN
1	D	125	ARG
1	D	484	LEU
1	E	37	ARG
1	E	201	THR
1	E	250	GLU
1	E	295	LYS
1	E	329	ARG
1	E	402	LYS
1	E	404	ARG
1	F	37	ARG
1	F	105	ILE
1	F	111	THR
1	F	198	VAL
1	F	329	ARG
1	F	376	GLU
1	F	377	LEU
1	F	436	ILE

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Mol	Chain	Res	Type
1	G	396	ARG
1	G	484	LEU
1	H	37	ARG
1	H	66	LYS
1	H	201	THR
1	H	295	LYS
1	H	329	ARG
1	H	484	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	217	HIS
1	B	221	GLN
1	B	397	GLN
1	B	458	GLN
1	C	177	GLN
1	C	353	ASN
1	D	71	ASN
1	D	177	GLN
1	D	217	HIS
1	D	297	ASN
1	D	384	ASN
1	D	455	GLN
1	E	97	HIS
1	E	221	GLN
1	F	41	GLN
1	F	164	GLN
1	F	177	GLN
1	F	217	HIS
1	F	221	GLN
1	F	297	ASN
1	G	71	ASN
1	G	93	HIS
1	G	164	GLN
1	G	177	GLN
1	G	353	ASN
1	G	437	HIS
1	H	71	ASN
1	H	93	HIS
1	H	217	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	SSS	F	502	-	30,31,31	1.26	2 (6%)	43,46,46	3.92	12 (27%)
2	SSS	H	501	-	30,31,31	1.23	2 (6%)	43,46,46	3.80	18 (41%)
4	FUM	E	502	-	7,7,7	1.29	0	8,8,8	1.15	0
2	SSS	D	502	-	30,31,31	1.29	3 (10%)	43,46,46	3.42	14 (32%)
5	AMZ	C	502	-	22,23,23	1.20	2 (9%)	32,35,35	3.69	7 (21%)
2	SSS	B	502	-	30,31,31	1.45	4 (13%)	43,46,46	4.98	14 (32%)
2	SSS	A	501	-	30,31,31	1.31	3 (10%)	43,46,46	3.13	13 (30%)
4	FUM	B	503	-	7,7,7	1.23	1 (14%)	8,8,8	1.29	1 (12%)
5	AMZ	H	503	-	22,23,23	1.06	1 (4%)	32,35,35	3.65	9 (28%)
2	SSS	G	502	-	30,31,31	1.03	2 (6%)	43,46,46	3.41	10 (23%)

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	SSS	F	502	-	-	9/26/42/42	0/2/2/2
2	SSS	H	501	-	-	4/26/42/42	0/2/2/2
4	FUM	E	502	-	-	1/5/5/5	-
2	SSS	D	502	-	-	4/26/42/42	0/2/2/2
5	AMZ	C	502	-	-	3/14/30/30	0/2/2/2
2	SSS	B	502	-	-	8/26/42/42	0/2/2/2
2	SSS	A	501	-	-	11/26/42/42	0/2/2/2
4	FUM	B	503	-	-	0/5/5/5	-
5	AMZ	H	503	-	-	2/14/30/30	0/2/2/2
2	SSS	G	502	-	-	7/26/42/42	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	SSS	C5-C4	4.64	1.47	1.39
2	F	502	SSS	C5-C4	4.22	1.46	1.39
2	H	501	SSS	C5-C4	3.97	1.46	1.39
5	C	502	AMZ	C3A-C7A	3.86	1.46	1.39
2	A	501	SSS	C5-C4	3.76	1.45	1.39
5	H	503	AMZ	C3A-C7A	3.64	1.45	1.39
2	D	502	SSS	C5-C4	3.58	1.45	1.39
2	B	502	SSS	C8-N7	2.99	1.40	1.32
2	D	502	SSS	C5-N7	-2.80	1.33	1.39
2	H	501	SSS	C5-N7	-2.68	1.33	1.39
2	A	501	SSS	C5-N7	-2.62	1.33	1.39
2	B	502	SSS	C5-C6	2.43	1.53	1.48
2	F	502	SSS	C5-N7	-2.33	1.34	1.39
2	D	502	SSS	O4'-C4'	-2.29	1.39	1.45
2	G	502	SSS	C5-C4	2.29	1.43	1.39
4	B	503	FUM	OXT-C	-2.26	1.24	1.30
2	A	501	SSS	O68-C64	-2.25	1.23	1.30
2	B	502	SSS	C1'-N9	2.12	1.53	1.47
2	G	502	SSS	C5-N7	-2.10	1.34	1.39
5	C	502	AMZ	C3A-N1	-2.02	1.35	1.39

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	SSS	C4-C5-N7	-20.19	102.28	109.91
2	F	502	SSS	C4-C5-N7	-17.88	103.15	109.91
2	B	502	SSS	C5-C4-N9	17.63	112.97	105.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	AMZ	C7A-C3A-N1	-15.74	103.96	109.91
2	D	502	SSS	C4-C5-N7	-14.95	104.26	109.91
5	H	503	AMZ	C7A-C3A-N1	-14.90	104.28	109.91
2	H	501	SSS	C4-C5-N7	-14.89	104.28	109.91
2	F	502	SSS	C5-C4-N9	13.80	111.40	105.75
2	G	502	SSS	C4-C5-N7	-13.46	104.82	109.91
2	H	501	SSS	C5-C4-N9	12.08	110.69	105.75
2	G	502	SSS	C5-C4-N9	11.75	110.56	105.75
2	B	502	SSS	C6-C5-N7	11.02	137.00	120.34
2	D	502	SSS	C5-C4-N9	10.90	110.21	105.75
2	A	501	SSS	C5-C4-N9	10.89	110.21	105.75
2	A	501	SSS	C4-C5-N7	-10.79	105.83	109.91
5	C	502	AMZ	C3A-C7A-N	10.09	109.88	105.75
5	H	503	AMZ	C3A-C7A-N	9.06	109.46	105.75
2	H	501	SSS	C6-C5-N7	7.98	132.39	120.34
2	G	502	SSS	C6-C5-N7	7.52	131.70	120.34
2	B	502	SSS	C5-C6-N6	7.01	125.33	114.27
2	F	502	SSS	C6-C5-N7	6.55	130.24	120.34
2	B	502	SSS	C5-C4-N3	-6.51	121.65	130.63
2	A	501	SSS	C6-C5-N7	6.45	130.09	120.34
2	H	501	SSS	C5-C6-N6	6.25	124.12	114.27
2	B	502	SSS	C6-C5-C4	-6.09	120.72	125.92
5	H	503	AMZ	C3A-C6-N2	5.55	126.52	116.73
2	G	502	SSS	C5-C4-N3	-5.45	123.12	130.63
5	H	503	AMZ	C6-C3A-C7A	5.25	130.20	125.92
2	D	502	SSS	C6-C5-N7	4.96	127.83	120.34
2	H	501	SSS	C61-N6-C6	4.88	130.21	122.00
2	A	501	SSS	C5-C4-N3	-4.75	124.07	130.63
5	C	502	AMZ	C3A-C6-N2	4.65	124.94	116.73
5	H	503	AMZ	O5-C6-C3A	-4.60	111.40	120.11
2	F	502	SSS	C5-C4-N3	-4.56	124.33	130.63
2	D	502	SSS	C5-C6-N6	-4.53	107.12	114.27
5	C	502	AMZ	C6-C3A-C7A	4.35	129.47	125.92
2	D	502	SSS	C5-C4-N3	-4.30	124.70	130.63
2	B	502	SSS	O6-C6-N6	-4.21	115.67	123.09
2	A	501	SSS	C5-C6-N6	-4.11	107.78	114.27
2	D	502	SSS	C61-N6-C6	4.04	128.79	122.00
2	A	501	SSS	O6-C6-N6	3.81	129.81	123.09
2	D	502	SSS	O6-C6-N6	3.75	129.70	123.09
2	G	502	SSS	C6-C5-C4	-3.63	122.82	125.92
2	A	501	SSS	C6-C5-C4	-3.58	122.87	125.92
2	B	502	SSS	O5'-PA-O3A	-3.51	96.95	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	SSS	C5-C4-N3	-3.43	125.90	130.63
2	H	501	SSS	O6-C6-C5	-3.40	116.13	121.60
2	G	502	SSS	O2'-C2'-C1'	3.35	121.65	110.10
2	H	501	SSS	O3'-C3'-C2'	-3.34	101.09	111.82
2	B	502	SSS	C61-N6-C6	3.32	127.58	122.00
2	A	501	SSS	C61-N6-C6	3.22	127.42	122.00
2	H	501	SSS	C6-C5-C4	-3.16	123.23	125.92
2	D	502	SSS	O1A-PA-O5'	-3.14	98.49	106.67
2	F	502	SSS	C5-C6-N6	-3.03	109.49	114.27
2	H	501	SSS	C2'-C3'-C4'	3.03	108.46	102.61
2	G	502	SSS	O1A-PA-O5'	-3.02	98.78	106.67
2	H	501	SSS	C63-C61-C62	-2.97	104.86	110.79
2	B	502	SSS	C8-N7-C5	2.92	109.46	104.26
2	B	502	SSS	C8-N9-C4	-2.81	104.46	106.62
2	B	502	SSS	C2'-C1'-N9	2.81	121.07	113.25
2	H	501	SSS	O2'-C2'-C1'	2.79	119.73	110.10
5	C	502	AMZ	O5-C6-C3A	-2.76	114.87	120.11
5	H	503	AMZ	O3-P-OP2	-2.76	98.99	106.44
2	H	501	SSS	C63-C61-N6	-2.75	105.39	110.64
2	A	501	SSS	O2'-C2'-C1'	2.74	119.55	110.10
2	G	502	SSS	O3'-C3'-C2'	-2.74	103.02	111.82
5	H	503	AMZ	C3A-C7A-N3	-2.73	126.86	130.63
5	C	502	AMZ	C5-N1-C3A	2.67	109.02	104.26
2	D	502	SSS	C8-N7-C5	2.59	108.88	104.26
2	A	501	SSS	O1A-PA-O5'	-2.52	100.09	106.67
2	F	502	SSS	O2A-PA-O5'	-2.51	100.12	106.67
5	H	503	AMZ	C5-N1-C3A	2.47	108.66	104.26
2	F	502	SSS	C8-N7-C5	2.47	108.66	104.26
5	C	502	AMZ	C3A-C7A-N3	-2.38	127.35	130.63
2	H	501	SSS	O2A-PA-O1A	2.36	116.64	107.80
2	F	502	SSS	O4'-C4'-C3'	2.35	109.83	105.15
2	A	501	SSS	O4'-C1'-N9	2.34	113.67	108.36
2	B	502	SSS	O4'-C1'-N9	2.32	113.61	108.36
4	B	503	FUM	OXT-C-O	-2.31	118.00	122.70
2	A	501	SSS	O4'-C4'-C3'	2.28	109.67	105.15
2	F	502	SSS	O1A-PA-O5'	-2.26	100.78	106.67
2	A	501	SSS	C8-N9-C4	-2.24	104.89	106.62
2	D	502	SSS	O2A-PA-O1A	2.24	116.21	107.80
2	H	501	SSS	C8-N7-C5	2.21	108.19	104.26
5	H	503	AMZ	O4-P-OP1	2.17	115.93	107.80
2	D	502	SSS	O4'-C4'-C5'	-2.14	102.47	109.33
2	F	502	SSS	O2A-PA-O1A	2.13	115.81	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	502	SSS	O2'-C2'-C1'	2.13	117.42	110.10
2	G	502	SSS	O6-C6-N6	2.12	126.83	123.09
2	H	501	SSS	C1'-N9-C8	2.08	132.65	126.73
2	D	502	SSS	C3'-C2'-C1'	2.08	105.40	101.46
2	G	502	SSS	C8-N7-C5	2.07	107.95	104.26
2	H	501	SSS	C62-C61-N6	2.05	115.33	110.57
2	F	502	SSS	C8-N9-C4	-2.05	105.05	106.62
2	D	502	SSS	C8-N9-C4	-2.04	105.05	106.62
2	H	501	SSS	O6-C6-N6	-2.04	119.50	123.09
2	B	502	SSS	C1'-N9-C8	2.04	132.52	126.73
2	D	502	SSS	O66-C62-C61	2.00	120.29	113.51

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	SSS	C5'-O5'-PA-O1A
2	A	501	SSS	C5'-O5'-PA-O2A
2	A	501	SSS	C4-C5-C6-O6
2	A	501	SSS	C4-C5-C6-N6
2	A	501	SSS	N7-C5-C6-N6
2	B	502	SSS	C5'-O5'-PA-O1A
2	B	502	SSS	C5'-O5'-PA-O2A
2	B	502	SSS	C5'-O5'-PA-O3A
2	B	502	SSS	O6-C6-N6-C61
2	B	502	SSS	C5-C6-N6-C61
2	D	502	SSS	C4-C5-C6-O6
2	D	502	SSS	C4-C5-C6-N6
2	F	502	SSS	C4-C5-C6-O6
2	F	502	SSS	C4-C5-C6-N6
2	F	502	SSS	N7-C5-C6-N6
2	G	502	SSS	C5-C6-N6-C61
2	H	501	SSS	O6-C6-N6-C61
2	H	501	SSS	C5-C6-N6-C61
2	B	502	SSS	O4'-C4'-C5'-O5'
2	B	502	SSS	C3'-C4'-C5'-O5'
2	F	502	SSS	C5-C6-N6-C61
2	A	501	SSS	N6-C61-C63-C64
2	F	502	SSS	N6-C61-C63-C64
2	G	502	SSS	N6-C61-C63-C64
2	F	502	SSS	O4'-C4'-C5'-O5'
2	F	502	SSS	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	501	SSS	N7-C5-C6-O6
2	D	502	SSS	N7-C5-C6-N6
2	A	501	SSS	O4'-C4'-C5'-O5'
2	A	501	SSS	C3'-C4'-C5'-O5'
2	H	501	SSS	O4'-C4'-C5'-O5'
2	G	502	SSS	C4-C5-C6-N6
5	H	503	AMZ	O-C-C4-O3
2	F	502	SSS	C61-C63-C64-O68
2	H	501	SSS	C3'-C4'-C5'-O5'
2	A	501	SSS	N6-C61-C62-O66
2	G	502	SSS	C61-C63-C64-O67
5	C	502	AMZ	O-C1-N-C7A
2	F	502	SSS	C61-C63-C64-O67
2	G	502	SSS	C61-C63-C64-O68
2	A	501	SSS	N6-C61-C62-O65
5	C	502	AMZ	O-C1-N-C5
5	H	503	AMZ	C3-C-C4-O3
2	D	502	SSS	C5-C6-N6-C61
5	C	502	AMZ	O-C-C4-O3
2	G	502	SSS	O6-C6-N6-C61
4	E	502	FUM	C4-C5-C6-O7
2	B	502	SSS	N6-C61-C63-C64
2	G	502	SSS	O4'-C4'-C5'-O5'

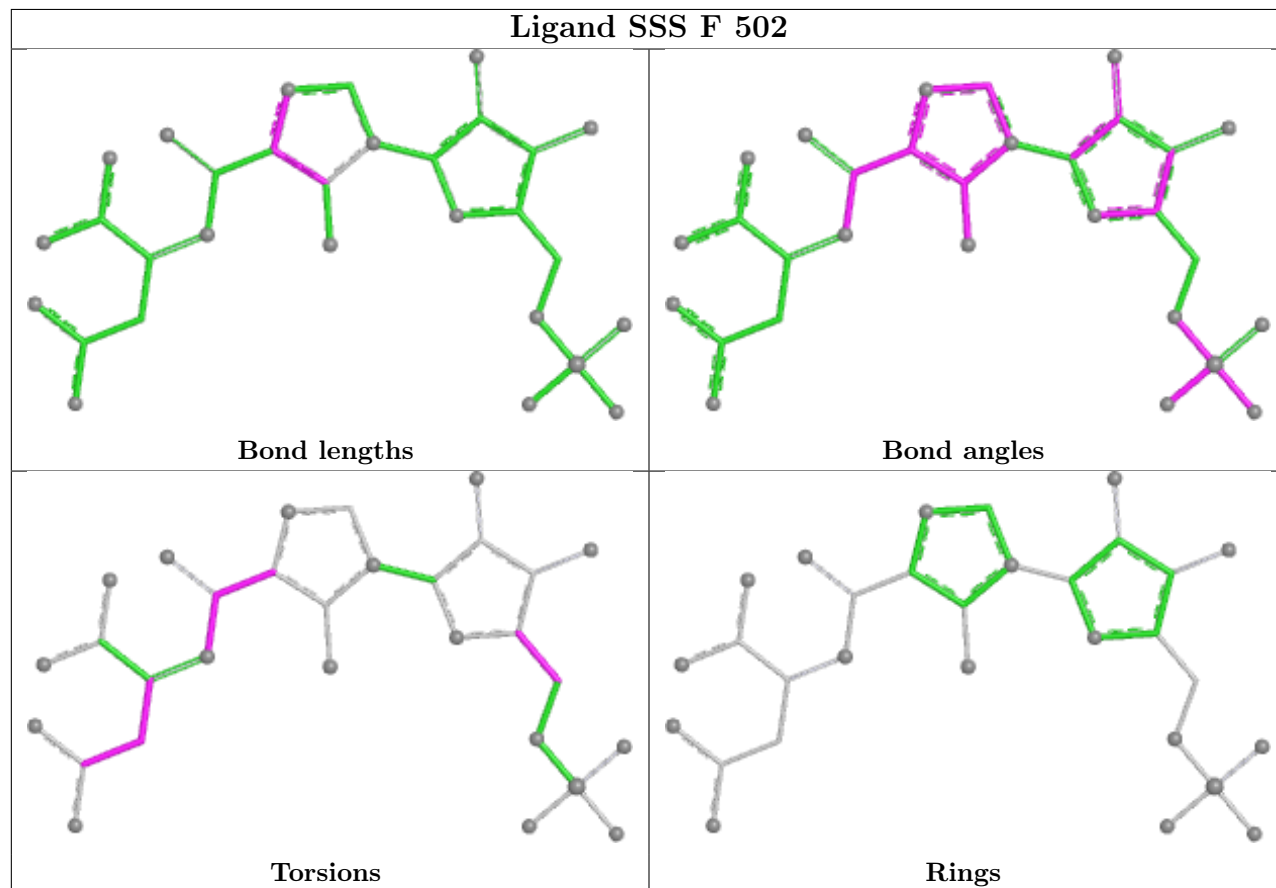
There are no ring outliers.

6 monomers are involved in 11 short contacts:

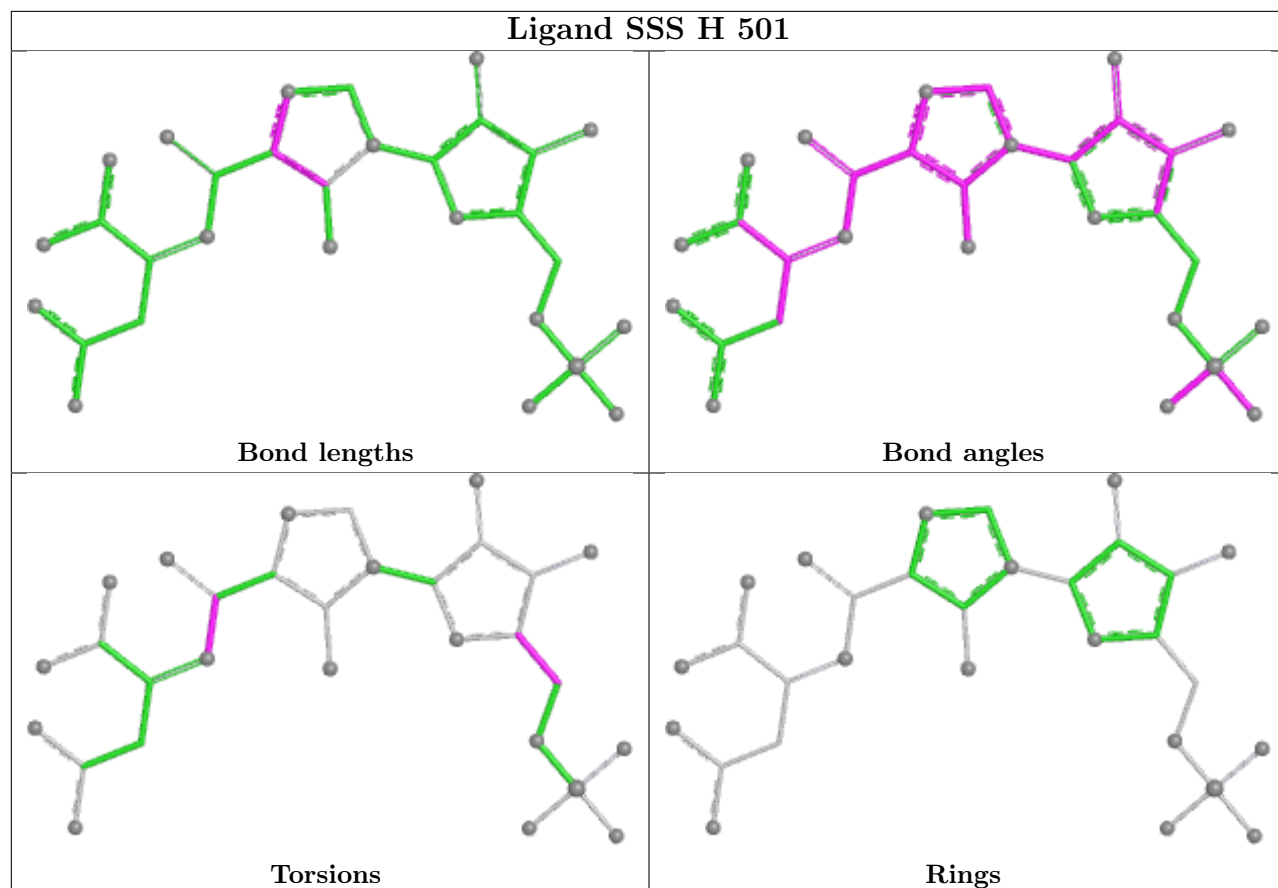
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	502	SSS	3	0
2	H	501	SSS	2	0
2	D	502	SSS	2	0
5	C	502	AMZ	1	0
2	A	501	SSS	1	0
2	G	502	SSS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

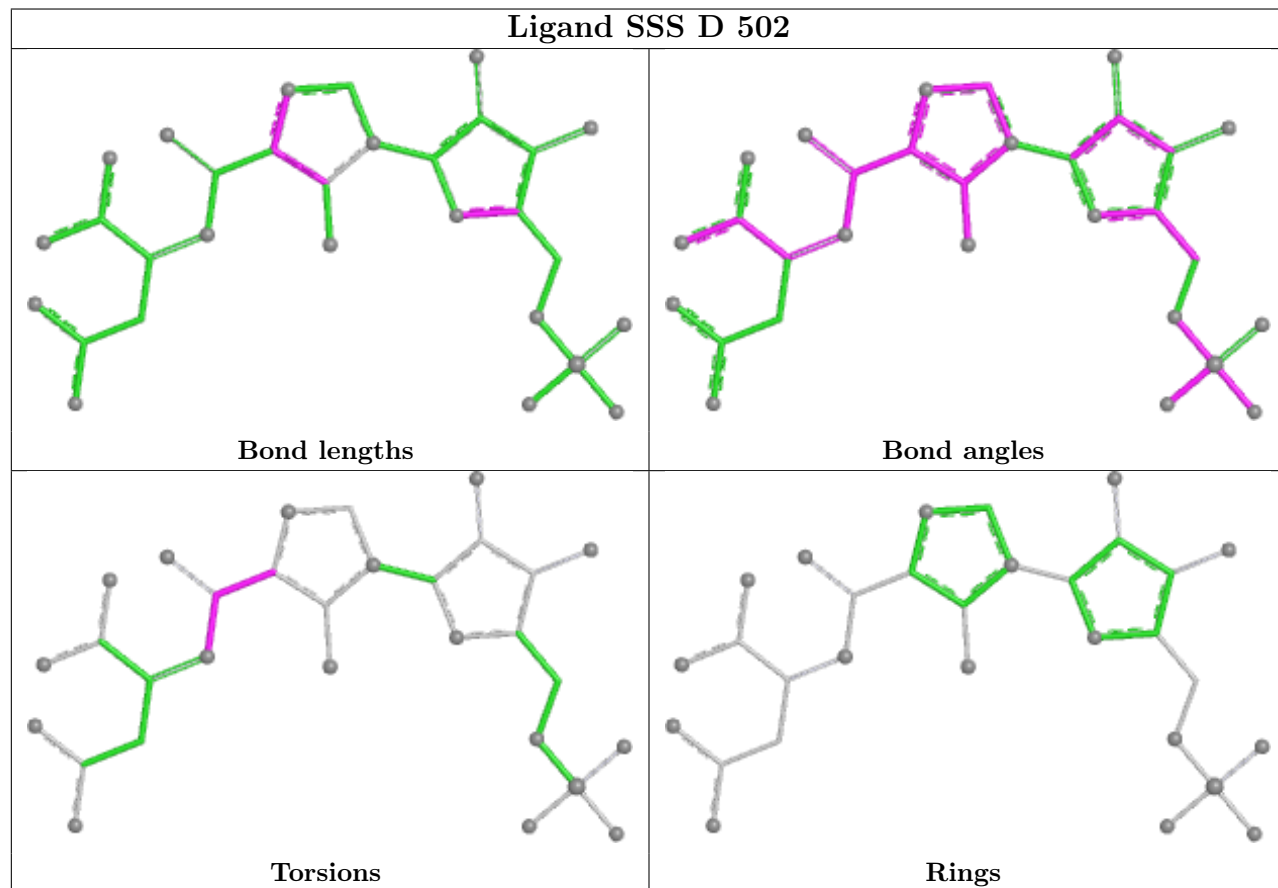
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

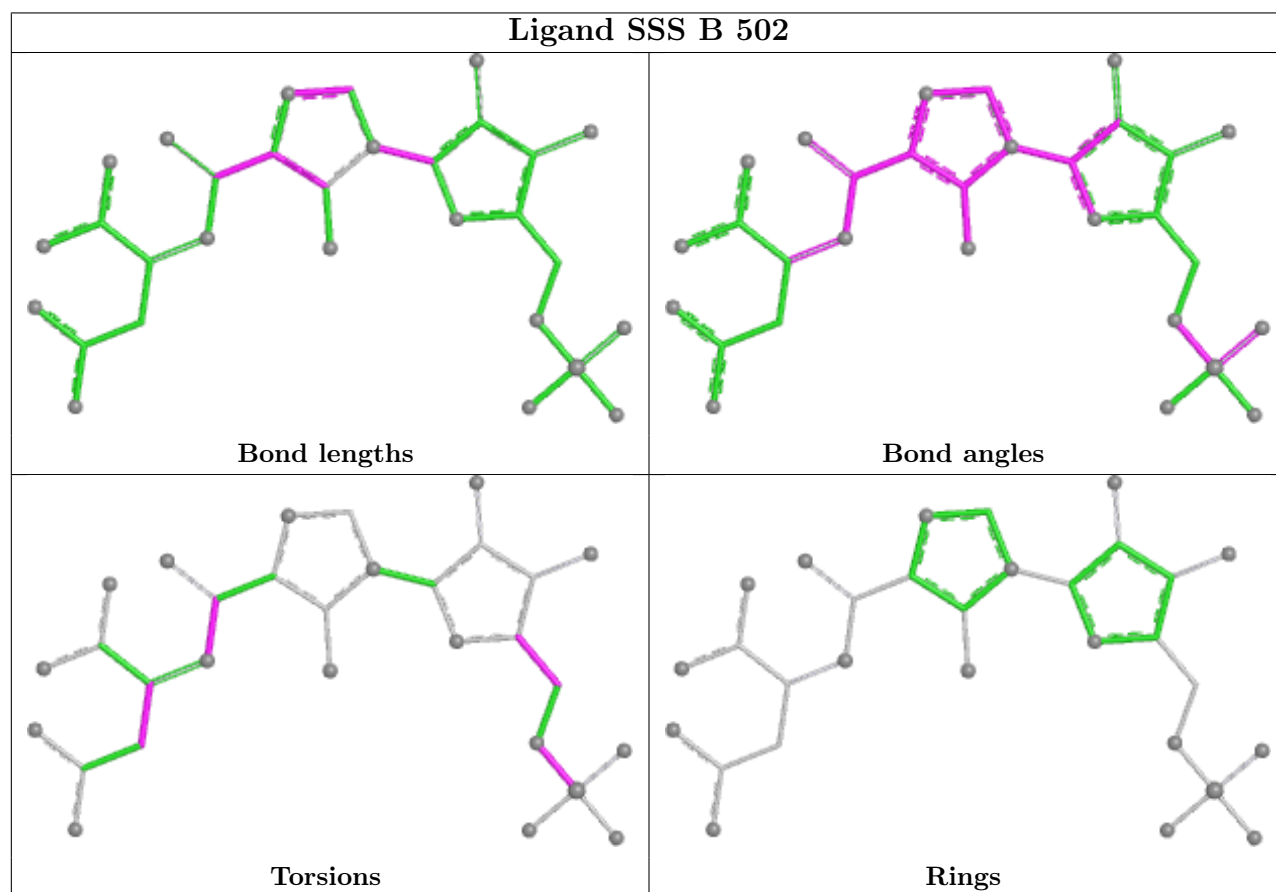
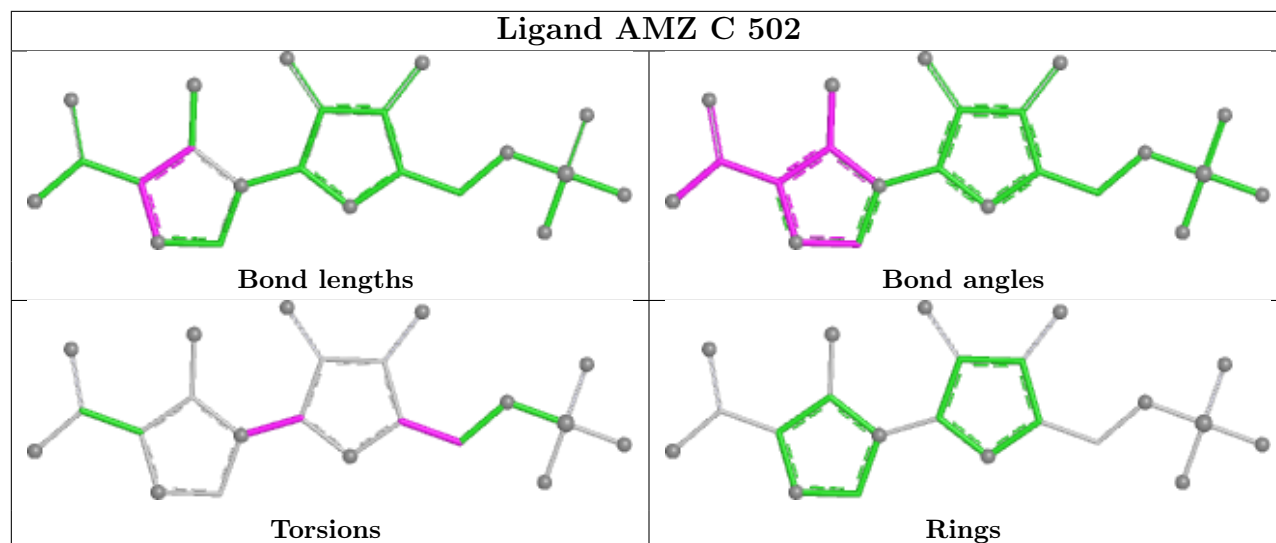


Ligand SSS H 501

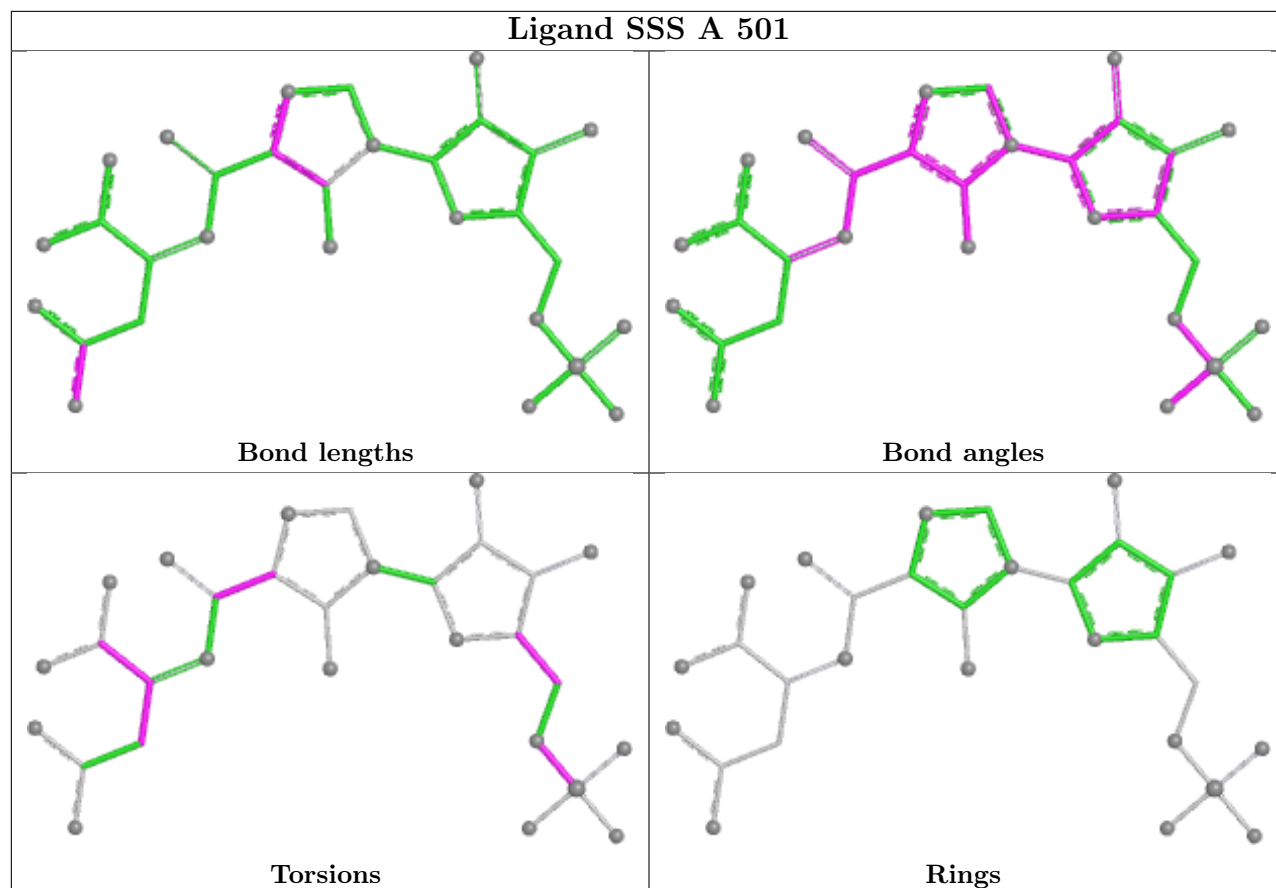


Ligand SSS D 502

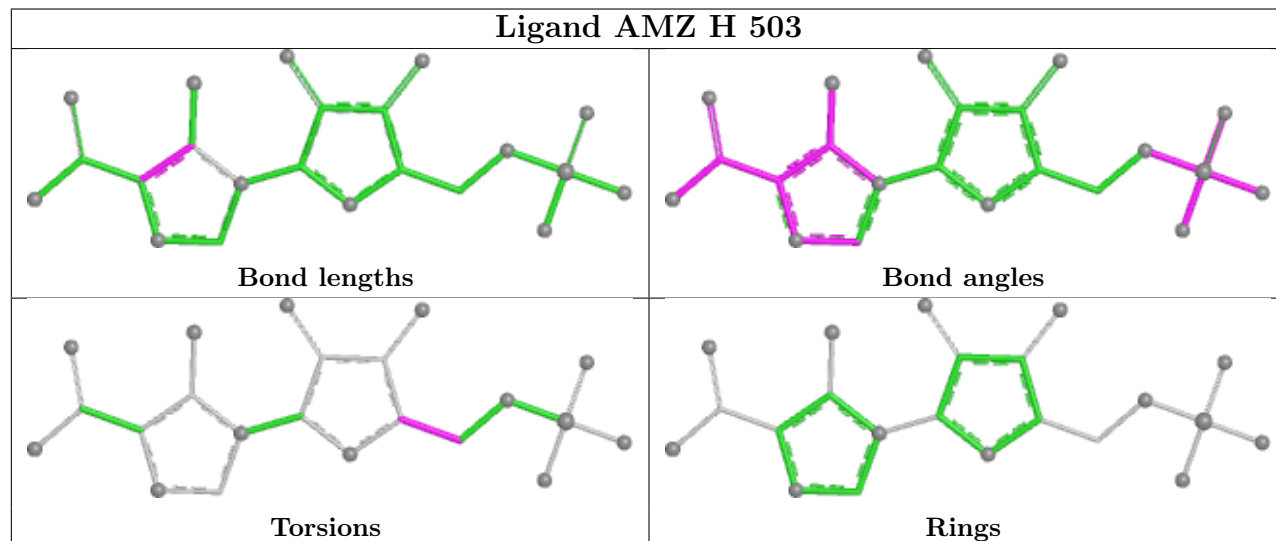


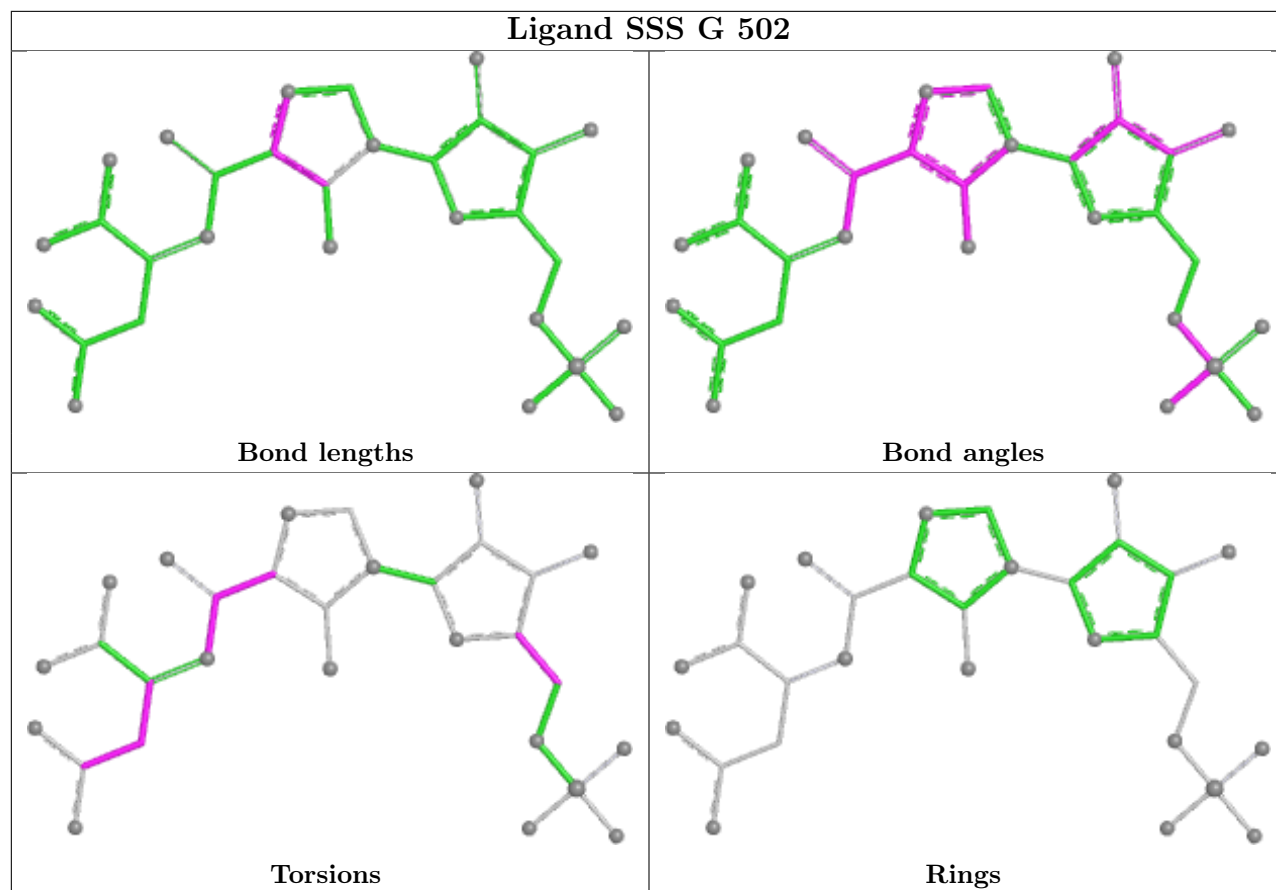


Ligand SSS A 501



Ligand AMZ H 503





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	464/487 (95%)	0.11	4 (0%) 81 78	35, 53, 81, 112	0
1	B	415/487 (85%)	0.20	6 (1%) 73 69	33, 52, 86, 108	0
1	C	418/487 (85%)	0.17	7 (1%) 69 65	35, 53, 95, 132	0
1	D	440/487 (90%)	0.08	6 (1%) 73 69	33, 51, 81, 138	0
1	E	466/487 (95%)	-0.02	9 (1%) 66 62	30, 45, 99, 131	0
1	F	466/487 (95%)	-0.02	4 (0%) 81 78	30, 48, 79, 110	0
1	G	463/487 (95%)	-0.09	1 (0%) 91 89	29, 47, 70, 92	0
1	H	477/487 (97%)	-0.14	1 (0%) 91 89	27, 41, 69, 100	0
All	All	3609/3896 (92%)	0.03	38 (1%) 78 74	27, 49, 81, 138	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	426	ARG	6.7
1	F	8	GLY	3.7
1	C	282	PHE	3.6
1	D	386	ILE	3.6
1	B	44	LEU	3.5
1	E	436	ILE	3.3
1	B	45	TRP	3.3
1	F	484	LEU	3.2
1	E	8	GLY	3.2
1	F	283	GLU	3.1
1	B	108	LEU	3.1
1	A	393	GLY	3.1
1	D	8	GLY	3.1
1	B	403	ILE	2.9
1	C	440	LEU	2.9
1	E	399	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	424	ILE	2.6
1	A	8	GLY	2.5
1	E	419	GLY	2.3
1	E	406	LEU	2.3
1	D	482	LEU	2.3
1	D	423	LEU	2.3
1	C	379	PHE	2.3
1	F	282	PHE	2.3
1	H	8	GLY	2.2
1	C	9	SER	2.2
1	E	385	ILE	2.2
1	E	379	PHE	2.2
1	G	9	SER	2.2
1	C	443	LEU	2.1
1	A	392	ALA	2.1
1	E	387	MET	2.1
1	B	405	VAL	2.1
1	C	390	VAL	2.1
1	E	403	ILE	2.1
1	A	382	THR	2.0
1	C	10	PRO	2.0
1	B	8	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SSS	B	502	30/30	0.87	0.11	49,68,75,76	0

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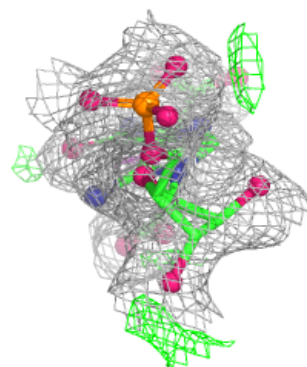
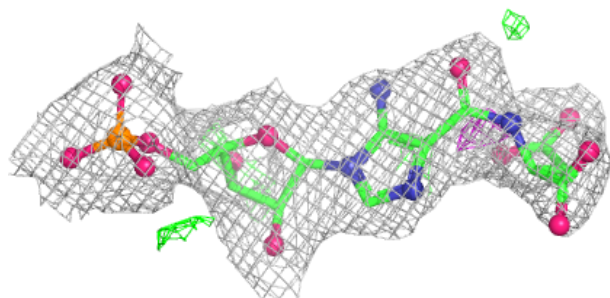
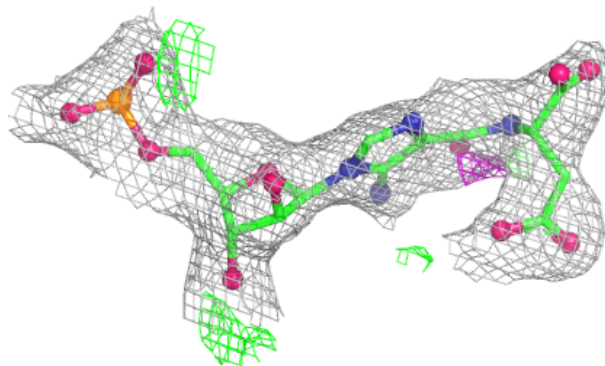
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SSS	A	501	30/30	0.93	0.09	47,57,70,76	0
2	SSS	D	502	30/30	0.95	0.08	34,54,67,70	0
4	FUM	B	503	8/8	0.95	0.06	48,52,53,54	0
2	SSS	G	502	30/30	0.96	0.07	34,40,62,68	0
3	CL	D	501	1/1	0.96	0.06	48,48,48,48	0
2	SSS	F	502	30/30	0.96	0.07	44,50,63,65	0
3	CL	C	501	1/1	0.97	0.06	51,51,51,51	0
2	SSS	H	501	30/30	0.97	0.06	35,39,42,44	0
3	CL	H	502	1/1	0.97	0.08	43,43,43,43	0
3	CL	B	501	1/1	0.97	0.06	61,61,61,61	0
5	AMZ	C	502	22/22	0.97	0.06	34,43,46,50	0
5	AMZ	H	503	22/22	0.97	0.06	31,36,38,40	0
3	CL	E	501	1/1	0.98	0.08	37,37,37,37	0
4	FUM	E	502	8/8	0.98	0.05	29,32,34,34	0
3	CL	G	501	1/1	0.98	0.07	39,39,39,39	0
3	CL	A	502	1/1	0.98	0.08	43,43,43,43	0
3	CL	F	501	1/1	0.99	0.03	48,48,48,48	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.

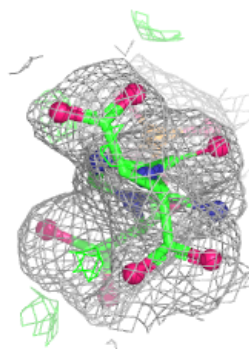
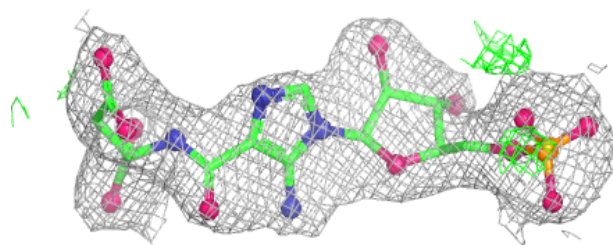
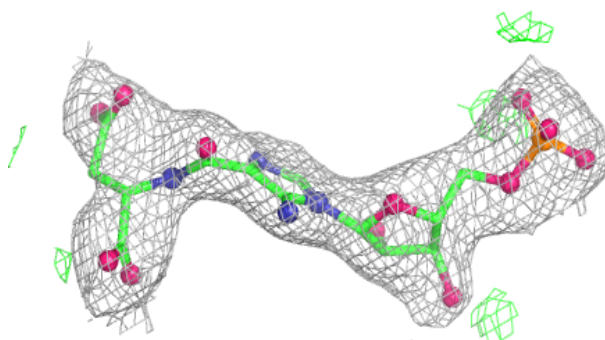
Electron density around SSS B 502:

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

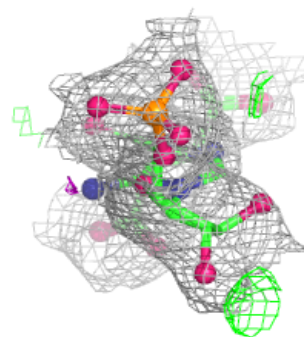
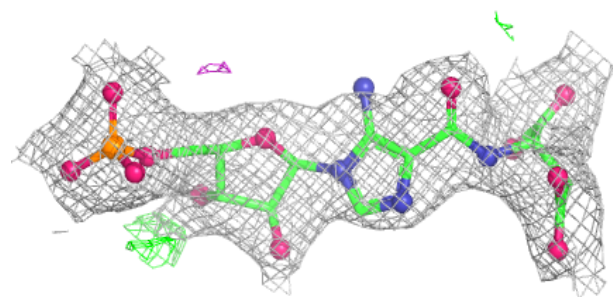
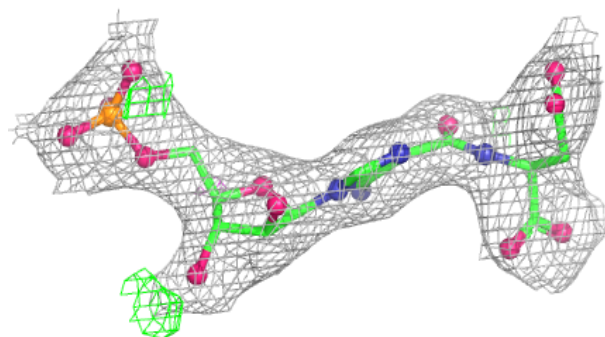


Electron density around SSS A 501:

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

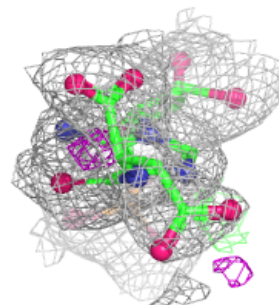
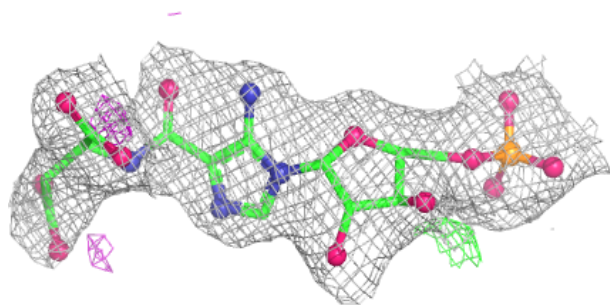
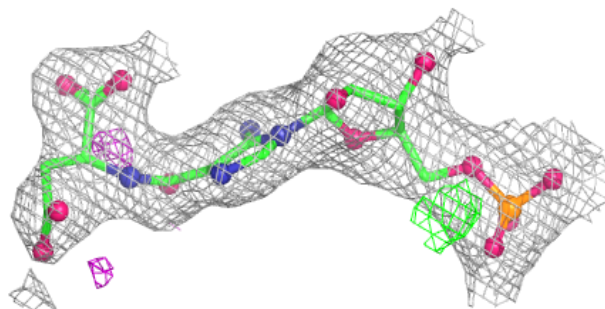
**Electron density around SSS D 502:**

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

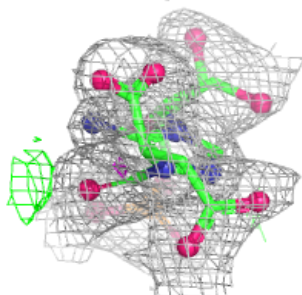
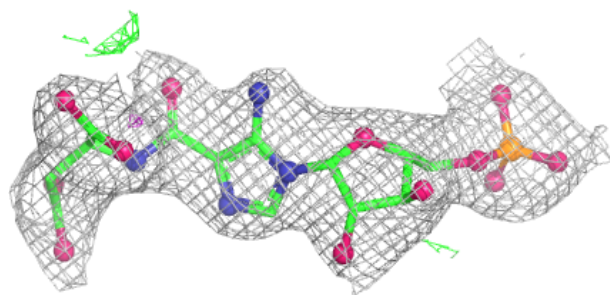
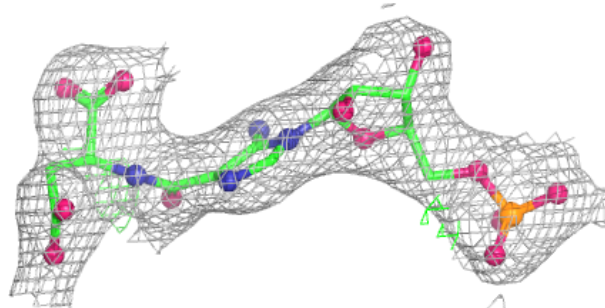


Electron density around SSS G 502:

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

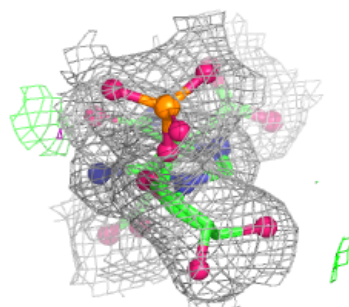
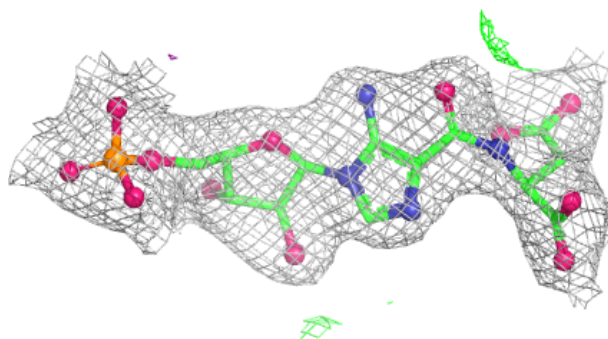
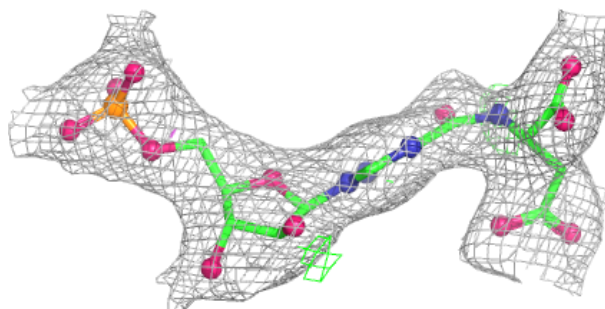
**Electron density around SSS F 502:**

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

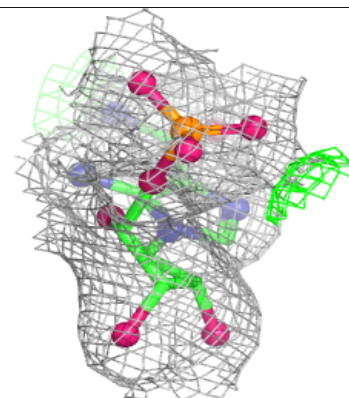
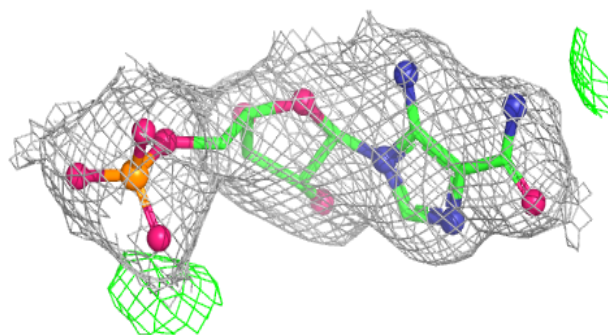
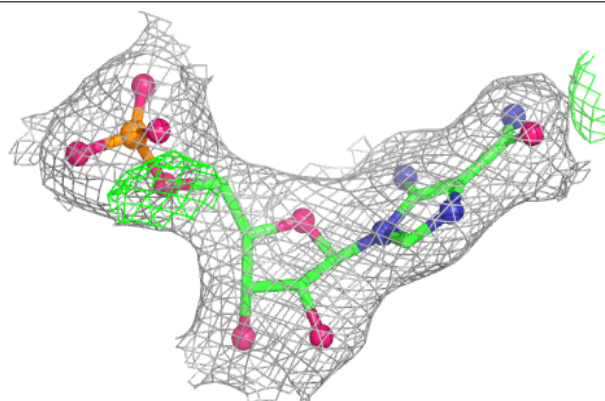


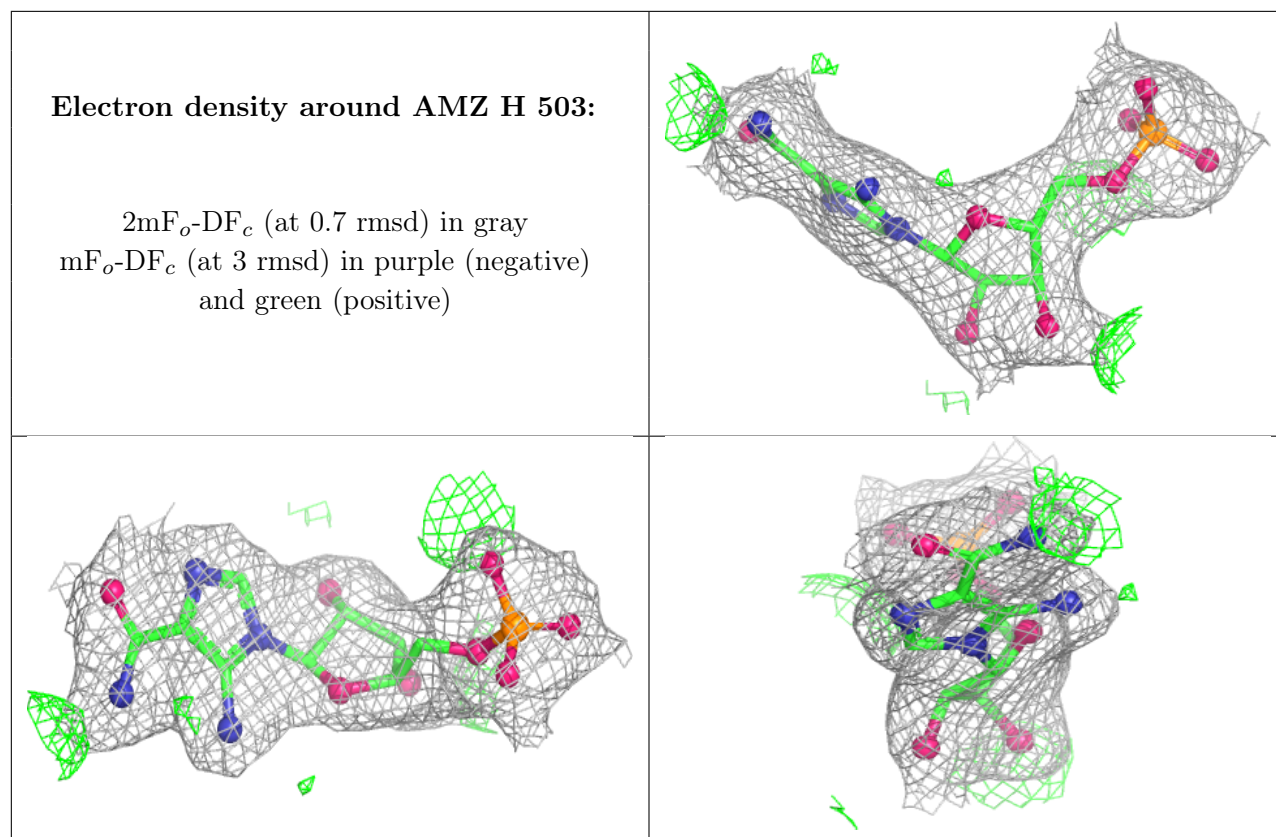
Electron density around SSS H 501:

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

**Electron density around AMZ C 502:**

$2mF_o-DF_c$ (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.