Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 04:39 AM JST

PDB ID	:	6KR3
Title	:	Crystal structure of Dengue virus nonstructural protein NS5 (form 2)
Authors	:	Wu, J.; Lu, G.; Ye, H.Q.; Gong, P.
Deposited on	:	2019-08-20
Resolution	:	2.93 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 (i) 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 (i)) were used in the production of this report:

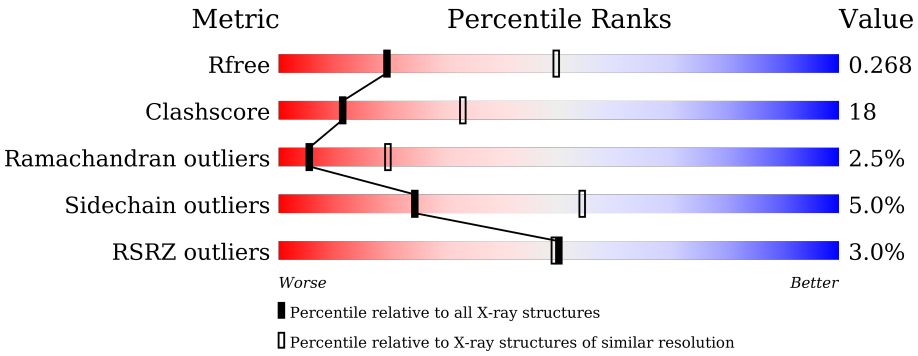
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

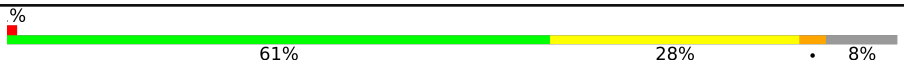
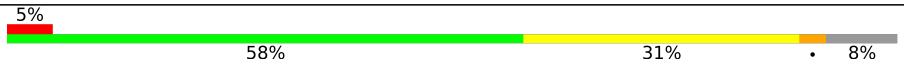
The reported resolution of this entry is 2.93 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	911	
1	B	911	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	1009	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12957 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total 6452	C 4064	N 1149	O 1197	S 42	0	0	0
1	B	836	Total 6305	C 3968	N 1123	O 1170	S 44	0	0	0

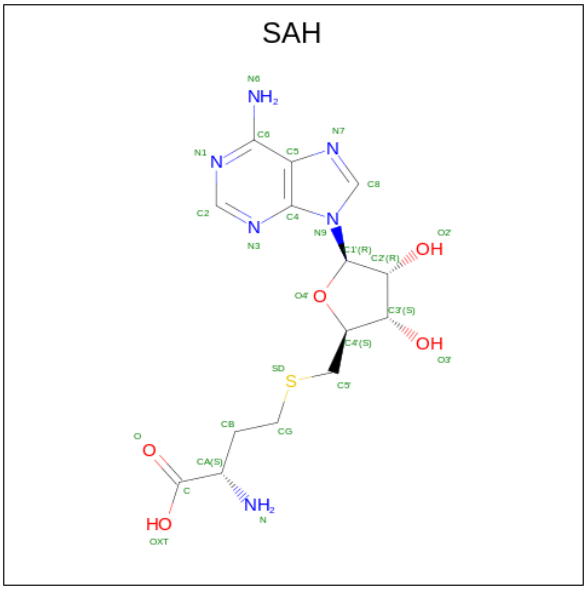
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q91H74
A	901	GLY	-	expression tag	UNP Q91H74
A	902	SER	-	expression tag	UNP Q91H74
A	903	SER	-	expression tag	UNP Q91H74
A	904	SER	-	expression tag	UNP Q91H74
A	905	HIS	-	expression tag	UNP Q91H74
A	906	HIS	-	expression tag	UNP Q91H74
A	907	HIS	-	expression tag	UNP Q91H74
A	908	HIS	-	expression tag	UNP Q91H74
A	909	HIS	-	expression tag	UNP Q91H74
A	910	HIS	-	expression tag	UNP Q91H74
B	0	MET	-	initiating methionine	UNP Q91H74
B	901	GLY	-	expression tag	UNP Q91H74
B	902	SER	-	expression tag	UNP Q91H74
B	903	SER	-	expression tag	UNP Q91H74
B	904	SER	-	expression tag	UNP Q91H74
B	905	HIS	-	expression tag	UNP Q91H74
B	906	HIS	-	expression tag	UNP Q91H74
B	907	HIS	-	expression tag	UNP Q91H74
B	908	HIS	-	expression tag	UNP Q91H74
B	909	HIS	-	expression tag	UNP Q91H74
B	910	HIS	-	expression tag	UNP Q91H74

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total I 12 12	0	0
2	B	3	Total I 3 3	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

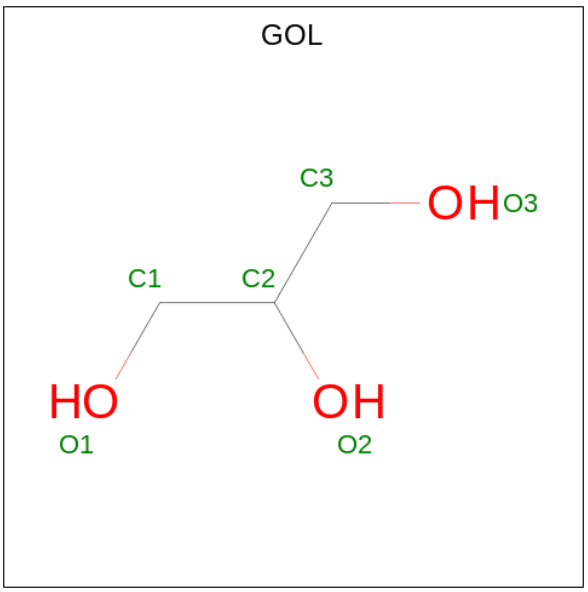


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 26 14 6 5 1	0	0
3	A	1	Total C N O S 26 14 6 5 1	0	0
3	B	1	Total C N O S 26 14 6 5 1	0	0
3	B	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

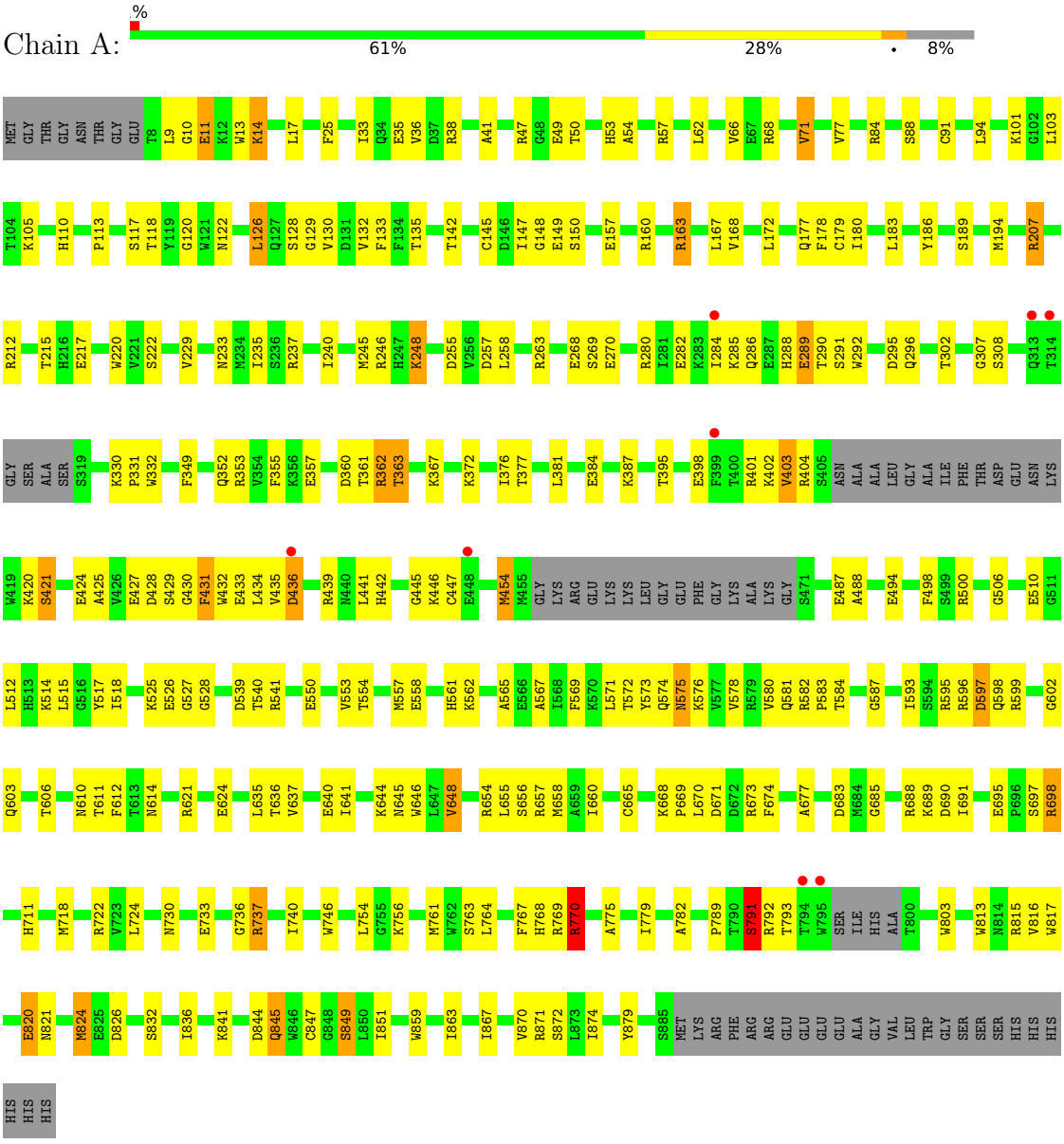
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	31	Total O 31 31	0	0
6	B	16	Total O 16 16	0	0

3 Residue-property plots (i)

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

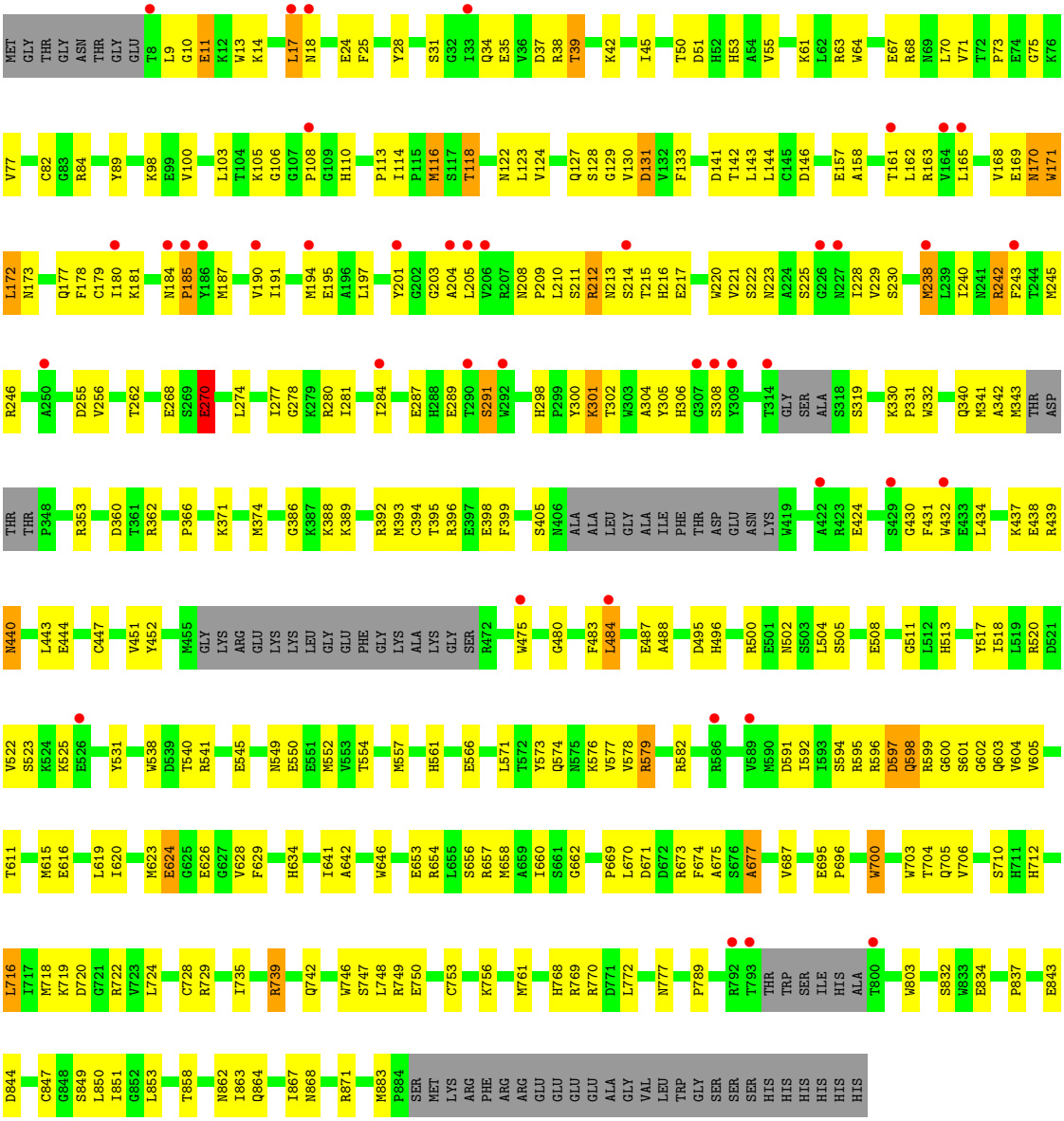
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein

Chain B:


5%
58%
31%
8%


MET GLY THR GLY ASN THR GLY GLU T8 L9 G10 E11 K12 W13 K14 L17 N18 E24 F25 Y28 S31 G32 I33 Q34 E35 V36 D37 R38 T39 K42 I45 T50 D51 H52 H53 A54 V55 K61 L62 R63 W64 E67 R68 N69 L70 V71 T72 P73 E74 G75 K76
V77 C82 G83 R84 Y89 K98 E99 V100 L103 T104 K105 G106 G107 P108 G109 H110 P113 I114 P115 M116 S117 T118 N122 L123 V124 Q127 S128 G129 V130 D131 V132 F133 D141 T142 L143 L144 C145 D146 E157 A158 T161 L162 R163 V164 L165 V168 E169 N170 W171
L172 N173 Q177 F178 C179 I180 K181 N184 P185 Y186 M187 V190 I191 M194 E195 A196 L197 Y201 G202 G203 A204 L205 V206 R207 N208 P209 L210 S211 R212 N213 S214 T215 H216 E217 W220 V221 S222 N223 A224 S225 G226 N227 I228 V229 S230 M238 L239 I240 N241 R242 F243 T244 M245
R246 A250 D255 V256 T262 E268 S269 E270 L274 I277 G278 K279 R280 I281 I284 E287 H288 E289 T290 S291 W292 H298 P299 Y300 K301 T302 W303 A304 Y305 H306 G307 S308 Y309 T314 GLY SER ALA S318 S319 K330 P331 W332 Q340 M341 A342 M343 THR ASP
THR THR P348 R353 D360 T361 R362 P366 K371 M374 G386 K387 K388 K389 R392 M393 C394 T395 R396 E397 E398 F399 S405 N406 ALA ALA LEU GLY ALA ILE PHE THR ASP GLU ASN LYS W419 A422 R423 E424 S429 G430 F431 W432 E433 L434 K437 E438 R439
N440 L443 E444 C447 V451 Y452 M455 GLY LYS ARG GLU LYS LYS LEU GLY GLU PHE GLY LYS ALA LYS GLY SER R472 W475 G480 F483 L484 E487 A488 D495 H496 R500 E501 N502 S503 L504 S505 E508 G511 L512 H513 Y517 I518 L519 R520 D521
V522 S523 K524 K525 E526 Y531 W538 D539 T540 R541 E545 N549 E550 E551 M552 V553 T554 M557 H561 E566 L571 T572 Y573 Q574 N575 K576 V577 V578 R579 R582 R586 V589 M590 D591 I592 I593 S594 R595 R596 D597 Q598 R599 G600 S601 G602 Q603 V604 V605
T611 M615 E616 L619 I620 M623 E624 G625 E626 G627 V628 F629 H634 I641 A642 W646 E653 R654 L655 S656 R657 M658 A659 I660 S661 G662 P669 L670 D671 D672 R673 F674 A675 S676 A677 V687 E695 P696 W700 W703 T704 Q705 V706 S710 H711 H712
L716 I717 M718 K719 D720 G721 R722 V723 L724 C728 R729 I735 R739 Q742 W746 S747 L748 R749 E750 C753 K756 M761 H768 R769 R770 D771 L772 N777 P789 R792 T793 THR TRP SER ILE HIS ALA T800 W803 S832 W833 E834 P837 E843
D844 C847 G848 S849 L850 I851 G852 L853 T858 N862 I863 Q864 I867 N868 R871 M883 P884 SER MET LYS ARG PHE ARG ARG GLU GLU GLU GLU GLU ALA GLY VAL LEU TRP GLY SER SER SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	178.84Å 209.97Å 157.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.93 49.81 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.81-2.93) 99.9 (49.81-2.93)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.233 , 0.268 0.234 , 0.268	Depositor DCC
R_{free} test set	3164 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12957	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, IOD, GOL, ZN

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	0.61	9/6601 (0.1%)	0.70	5/8968 (0.1%)
1	B	0.63	14/6453 (0.2%)	0.68	4/8787 (0.0%)
All	All	0.62	23/13054 (0.2%)	0.69	9/17755 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	ARG	CZ-NH2	-11.11	1.18	1.33
1	B	212	ARG	NE-CZ	-10.86	1.19	1.33
1	A	698	ARG	NE-CZ	-9.75	1.20	1.33
1	A	68	ARG	CZ-NH1	-9.16	1.21	1.33
1	A	698	ARG	CZ-NH1	-9.04	1.21	1.33
1	B	212	ARG	CZ-NH1	-8.71	1.21	1.33
1	B	82	CYS	CB-SG	8.48	1.96	1.82
1	B	242	ARG	NE-CZ	-7.58	1.23	1.33
1	A	68	ARG	NE-CZ	-7.48	1.23	1.33
1	B	212	ARG	CD-NE	-7.40	1.33	1.46
1	B	242	ARG	CZ-NH2	-7.38	1.23	1.33
1	A	698	ARG	CZ-NH2	-7.28	1.23	1.33
1	B	35	GLU	CD-OE2	6.88	1.33	1.25
1	A	698	ARG	CD-NE	-6.42	1.35	1.46
1	B	438	GLU	CD-OE2	6.08	1.32	1.25
1	B	287	GLU	CD-OE1	5.83	1.32	1.25
1	A	847	CYS	CB-SG	5.75	1.92	1.82
1	A	68	ARG	CZ-NH2	-5.46	1.25	1.33
1	B	270	GLU	CD-OE1	-5.25	1.19	1.25
1	B	753	CYS	CB-SG	-5.20	1.73	1.81
1	A	68	ARG	CD-NE	-5.13	1.37	1.46
1	B	287	GLU	CD-OE2	5.10	1.31	1.25
1	B	35	GLU	CD-OE1	5.06	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	820	GLU	C-N-CA	-6.69	104.97	121.70
1	A	770	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	B	600	GLY	N-CA-C	-5.61	99.08	113.10
1	B	131	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	698	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	B	670	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	246	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	716	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	A	434	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6452	0	5986	214	1
1	B	6305	0	5713	224	0
2	A	12	0	0	2	0
2	B	3	0	0	0	0
3	A	52	0	38	1	0
3	B	52	0	38	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	12	0	16	3	0
5	B	18	0	24	5	0
6	A	31	0	0	2	0
6	B	16	0	0	1	0
All	All	12957	0	11815	438	1

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 18.

All (438) 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:A:57:ARG:NH1	1:A:212:ARG:NH1	1.93	1.16
1:A:57:ARG:HH11	1:A:212:ARG:NH1	1.41	1.16
1:B:165:LEU:HD21	1:B:197:LEU:HD12	1.26	1.14
1:B:238:MET:HE3	1:B:242:ARG:NH1	1.77	0.99
1:B:165:LEU:HD21	1:B:197:LEU:CD1	1.93	0.99
1:B:238:MET:CE	1:B:242:ARG:NH1	2.28	0.96
1:A:525:LYS:NZ	1:A:656:SER:OG	2.00	0.94
1:A:57:ARG:NH1	1:A:212:ARG:CZ	2.31	0.92
1:B:165:LEU:CD2	1:B:197:LEU:HD12	1.99	0.91
1:A:35:GLU:OE2	1:A:212:ARG:NH1	2.04	0.90
1:B:392:ARG:NH2	1:B:495:ASP:OD1	2.11	0.84
1:B:71:VAL:HG13	1:B:221:VAL:HG23	1.57	0.84
1:A:817:TRP:O	1:A:821:ASN:ND2	2.12	0.82
1:B:624:GLU:HB3	1:B:677:ALA:HB1	1.61	0.82
1:A:764:LEU:HD11	1:A:816:VAL:HG21	1.61	0.81
1:B:756:LYS:HG2	1:B:789:PRO:HG3	1.65	0.79
1:B:579:ARG:HB3	1:B:592:ILE:HG22	1.66	0.78
1:A:101:LYS:HD3	1:A:103:LEU:HD21	1.67	0.77
1:B:864:GLN:O	1:B:868:ASN:ND2	2.18	0.76
1:B:133:PHE:CE1	1:B:163:ARG:HG2	2.21	0.75
1:B:440:ASN:HA	1:B:443:LEU:HD23	1.69	0.74
1:A:212:ARG:HH21	1:A:212:ARG:HG3	1.52	0.74
1:A:35:GLU:CD	1:A:212:ARG:HH11	1.91	0.74
1:B:394:CYS:HB2	1:B:487:GLU:HA	1.70	0.73
1:B:769:ARG:NH2	1:B:844:ASP:OD1	2.22	0.73
1:A:756:LYS:HD3	1:A:789:PRO:HG3	1.70	0.73
1:A:57:ARG:HH12	1:A:212:ARG:CZ	2.01	0.73
1:A:611:THR:HG23	1:A:660:ILE:HG22	1.71	0.73
1:A:574:GLN:C	1:A:575:ASN:HD22	1.92	0.72
1:A:35:GLU:OE2	1:A:57:ARG:NH1	2.23	0.72
1:A:595:ARG:HE	1:A:597:ASP:HB2	1.55	0.71
1:B:695:GLU:OE1	1:B:696:PRO:HD2	1.91	0.71
1:A:428:ASP:O	1:A:430:GLY:N	2.23	0.71
1:B:165:LEU:CD2	1:B:197:LEU:CD1	2.64	0.71
1:B:452:TYR:HB2	1:B:578:VAL:HG22	1.74	0.69
1:B:278:GLY:HA2	1:B:281:ILE:HD12	1.74	0.69
1:A:38:ARG:NH1	1:A:54:ALA:O	2.19	0.69
1:B:177:GLN:OE1	1:B:223:ASN:ND2	2.25	0.69
1:B:9:LEU:H	1:B:11:GLU:HG3	1.57	0.69
1:B:70:LEU:HB3	1:B:221:VAL:HG21	1.75	0.69
1:A:526:GLU:O	1:A:657:ARG:NH2	2.25	0.69
1:B:238:MET:HE3	1:B:242:ARG:HH12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ARG:HD3	1:A:685:GLY:O	1.93	0.68
1:A:145:CYS:SG	1:A:147:ILE:HD12	2.32	0.68
1:A:421:SER:O	1:A:424:GLU:N	2.27	0.68
1:A:432:TRP:HA	1:A:435:VAL:HG12	1.75	0.68
1:A:207:ARG:NH1	1:A:215:THR:O	2.27	0.68
1:A:599:ARG:NH1	1:A:610:ASN:OD1	2.22	0.67
1:B:157:GLU:O	1:B:161:THR:HG22	1.94	0.67
1:A:872:SER:HB3	1:B:746:TRP:O	1.95	0.67
1:B:340:GLN:O	1:B:342:ALA:N	2.27	0.67
1:B:850:LEU:HD22	1:B:853:LEU:HD12	1.76	0.67
1:A:599:ARG:HD3	1:A:606:THR:HB	1.77	0.67
1:A:737:ARG:HD2	2:A:1012:IOD:I	2.64	0.67
1:A:149:GLU:HB3	1:A:160:ARG:NH2	2.09	0.67
1:A:50:THR:O	1:A:117:SER:N	2.23	0.66
1:A:282:GLU:O	1:A:286:GLN:HG3	1.95	0.66
1:B:304:ALA:HB3	1:B:594:SER:HB2	1.76	0.66
1:B:14:LYS:O	1:B:18:ASN:ND2	2.29	0.66
1:A:229:VAL:O	1:A:233:ASN:ND2	2.29	0.66
1:A:189:SER:OG	2:A:1011:IOD:I	2.84	0.66
1:B:439:ARG:HH22	1:B:487:GLU:CD	2.00	0.65
1:A:355:PHE:CD2	1:A:454:MET:HE1	2.32	0.65
1:A:245:MET:O	1:A:248:LYS:HE3	1.97	0.65
1:A:576:LYS:NZ	1:A:597:ASP:O	2.29	0.65
1:B:302:THR:OG1	1:B:595:ARG:NH1	2.29	0.65
1:A:722:ARG:HD2	1:A:824:MET:SD	2.37	0.64
1:B:169:GLU:OE1	1:B:197:LEU:HD21	1.96	0.64
1:B:451:VAL:HG12	1:B:577:VAL:HG13	1.78	0.64
1:B:37:ASP:OD2	1:B:39:THR:OG1	2.06	0.64
1:A:355:PHE:HD2	1:A:454:MET:HE1	1.63	0.64
1:B:63:ARG:CZ	1:B:256:VAL:HG22	2.28	0.64
1:A:101:LYS:NZ	6:A:1101:HOH:O	2.26	0.64
1:A:730:ASN:HB3	1:A:733:GLU:HG3	1.80	0.63
1:B:277:ILE:HD12	1:B:281:ILE:HD11	1.79	0.63
1:A:295:ASP:OD1	1:A:296:GLN:N	2.31	0.63
1:A:851:ILE:HD12	1:A:851:ILE:H	1.63	0.63
1:B:146:ASP:HB3	3:B:1005:SAH:HN1	1.64	0.63
1:A:432:TRP:O	1:A:436:ASP:HB2	1.99	0.62
1:B:573:TYR:O	1:B:576:LYS:NZ	2.32	0.62
1:A:349:PHE:O	1:A:353:ARG:HG3	1.98	0.62
1:A:770:ARG:HD2	1:A:844:ASP:OD2	2.00	0.62
1:B:671:ASP:OD2	1:B:673:ARG:NE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:O	1:B:172:LEU:N	2.32	0.61
1:B:280:ARG:HE	1:B:447:CYS:HB2	1.64	0.61
1:A:867:ILE:HG22	1:A:871:ARG:HD2	1.82	0.61
1:A:381:LEU:HD23	1:A:612:PHE:CE1	2.36	0.61
1:B:735:ILE:O	1:B:739:ARG:HG2	2.00	0.61
1:A:77:VAL:HG22	1:A:142:THR:CG2	2.31	0.61
1:B:110:HIS:HB3	3:B:1005:SAH:O2'	2.00	0.61
1:B:305:TYR:O	1:B:306:HIS:ND1	2.33	0.61
1:A:215:THR:OG1	1:A:217:GLU:HG3	2.00	0.61
1:B:500:ARG:NH2	1:B:658:MET:O	2.34	0.60
1:A:569:PHE:O	1:A:574:GLN:HG3	2.02	0.60
1:A:567:ALA:O	1:A:571:LEU:HB2	2.02	0.60
1:B:430:GLY:O	1:B:434:LEU:HD12	2.02	0.60
1:A:128:SER:OG	1:A:129:GLY:N	2.33	0.60
1:A:550:GLU:CD	1:A:599:ARG:HH22	2.05	0.60
1:B:61:LYS:HA	1:B:208:ASN:HD21	1.66	0.60
1:B:268:GLU:O	1:B:362:ARG:NH2	2.35	0.60
1:B:238:MET:HE2	1:B:242:ARG:NH1	2.16	0.60
1:B:611:THR:CG2	1:B:662:GLY:H	2.15	0.60
1:A:177:GLN:OE1	1:A:222:SER:OG	2.21	0.59
1:B:284:ILE:HD11	1:B:592:ILE:HG12	1.85	0.59
1:B:484:LEU:HD12	1:B:484:LEU:H	1.67	0.59
1:B:611:THR:HG23	1:B:662:GLY:H	1.67	0.59
1:B:371:LYS:HD3	1:B:545:GLU:HG3	1.84	0.59
1:B:274:LEU:HD23	1:B:274:LEU:H	1.67	0.59
1:A:290:THR:OG1	1:A:291:SER:N	2.35	0.59
1:A:280:ARG:HH21	1:A:447:CYS:HB2	1.67	0.59
1:A:439:ARG:NH1	1:A:487:GLU:OE1	2.35	0.59
1:B:602:GLY:O	1:B:604:VAL:N	2.36	0.59
1:B:280:ARG:NH1	1:B:571:LEU:O	2.36	0.58
1:A:574:GLN:O	1:A:575:ASN:ND2	2.32	0.58
1:B:122:ASN:HD22	1:B:262:THR:HB	1.68	0.58
1:A:770:ARG:HB2	1:A:851:ILE:HD11	1.86	0.58
1:A:527:GLY:HA2	1:A:670:LEU:O	2.03	0.58
1:A:567:ALA:HA	1:A:571:LEU:HD23	1.84	0.58
1:B:165:LEU:CG	1:B:197:LEU:HD12	2.34	0.58
1:A:688:ARG:NH1	1:A:697:SER:OG	2.37	0.58
1:A:57:ARG:NH1	1:A:212:ARG:HH11	1.98	0.57
1:A:240:ILE:HD13	5:A:1017:GOL:H2	1.87	0.57
1:A:167:LEU:HD11	6:A:1108:HOH:O	2.05	0.57
1:B:280:ARG:HE	1:B:447:CYS:CB	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:CD1	1:A:167:LEU:HD22	2.39	0.57
1:B:716:LEU:HD11	1:B:837:PRO:HG2	1.87	0.57
1:A:157:GLU:HB3	1:A:183:LEU:CD1	2.35	0.56
1:A:331:PRO:HG2	1:A:332:TRP:CE3	2.40	0.56
1:A:33:ILE:HD13	1:A:212:ARG:HD3	1.86	0.56
1:A:35:GLU:HG3	1:A:36:VAL:H	1.70	0.56
1:B:31:SER:HB3	1:B:245:MET:HE3	1.87	0.56
1:A:157:GLU:HB3	1:A:183:LEU:HD12	1.87	0.56
1:B:554:THR:HA	1:B:557:MET:SD	2.46	0.56
1:B:84:ARG:HB3	1:B:114:ILE:HG13	1.86	0.56
1:B:396:ARG:HG2	1:B:483:PHE:CZ	2.41	0.56
1:B:770:ARG:HD2	1:B:851:ILE:HD13	1.87	0.56
1:B:89:TYR:HB3	1:B:118:THR:HG21	1.86	0.55
1:B:366:PRO:O	1:B:371:LYS:NZ	2.31	0.55
1:B:270:GLU:HG2	1:B:362:ARG:HH12	1.70	0.55
1:B:51:ASP:O	1:B:53:HIS:N	2.37	0.55
1:B:500:ARG:HH11	1:B:518:ILE:HG23	1.72	0.55
1:B:641:ILE:HD12	1:B:642:ALA:N	2.21	0.55
1:A:212:ARG:HH21	1:A:212:ARG:CG	2.19	0.55
1:B:389:LYS:HE3	1:B:502:ASN:HD22	1.71	0.55
1:A:330:LYS:HB3	5:B:1009:GOL:H32	1.89	0.55
1:B:242:ARG:HG3	1:B:245:MET:HE2	1.89	0.55
1:A:602:GLY:O	1:A:606:THR:HG23	2.06	0.55
1:A:775:ALA:O	1:A:779:ILE:HG13	2.07	0.55
1:A:782:ALA:HB2	1:A:867:ILE:HG23	1.88	0.55
1:A:871:ARG:HG2	1:A:879:TYR:CE2	2.42	0.55
1:A:384:GLU:HA	1:A:387:LYS:HD2	1.88	0.54
1:B:143:LEU:HD13	1:B:171:TRP:HB3	1.89	0.54
1:B:626:GLU:CD	1:B:654:ARG:HH21	2.11	0.54
1:A:512:LEU:HD23	1:A:515:LEU:HD12	1.90	0.54
1:B:343:MET:CE	5:B:1009:GOL:O1	2.55	0.54
1:A:550:GLU:OE1	1:A:599:ARG:NH2	2.41	0.54
1:B:128:SER:O	1:B:130:VAL:HG23	2.07	0.54
1:B:146:ASP:HA	1:B:181:LYS:HB2	1.90	0.54
1:A:84:ARG:HA	1:A:113:PRO:HA	1.89	0.54
1:B:331:PRO:HG2	1:B:332:TRP:CZ3	2.43	0.54
1:B:194:MET:CE	1:B:205:LEU:HD21	2.37	0.54
1:B:710:SER:HB3	1:B:729:ARG:HH21	1.73	0.54
1:A:557:MET:HE3	1:A:561:HIS:CD2	2.42	0.54
1:B:17:LEU:HD11	1:B:25:PHE:HE1	1.72	0.53
1:B:158:ALA:HB2	1:B:187:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:SER:OG	1:B:750:GLU:HG3	2.08	0.53
1:B:832:SER:OG	1:B:834:GLU:HG3	2.08	0.53
1:A:133:PHE:HD1	1:A:167:LEU:HD22	1.74	0.53
1:B:172:LEU:HD13	1:B:201:TYR:CD1	2.43	0.53
1:B:191:ILE:O	1:B:195:GLU:HG3	2.07	0.53
1:A:41:ALA:HA	1:A:53:HIS:ND1	2.24	0.53
1:B:574:GLN:O	1:B:596:ARG:HB3	2.09	0.53
1:A:282:GLU:OE1	1:A:286:GLN:NE2	2.39	0.53
1:B:179:CYS:HA	1:B:220:TRP:O	2.09	0.53
1:A:103:LEU:HB3	1:A:130:VAL:HG11	1.91	0.53
1:A:126:LEU:HB2	5:A:1018:GOL:H31	1.91	0.53
1:A:292:TRP:CH2	1:A:307:GLY:HA3	2.44	0.53
1:B:747:SER:O	1:B:749:ARG:N	2.38	0.53
1:B:215:THR:OG1	1:B:217:GLU:HG3	2.09	0.52
1:B:716:LEU:HD11	1:B:837:PRO:CG	2.39	0.52
1:A:94:LEU:O	1:A:263:ARG:NH2	2.42	0.52
1:B:843:GLU:OE1	1:B:843:GLU:N	2.35	0.52
1:A:36:VAL:HG21	1:A:255:ASP:HA	1.91	0.52
1:A:454:MET:HG3	1:A:578:VAL:CG1	2.40	0.52
1:B:240:ILE:HA	1:B:243:PHE:CD2	2.45	0.52
1:A:331:PRO:HG2	1:A:332:TRP:CZ3	2.45	0.52
1:A:718:MET:HG2	1:A:724:LEU:HD11	1.92	0.52
1:A:257:ASP:HB3	1:A:357:GLU:HB3	1.92	0.52
1:B:270:GLU:OE1	1:B:596:ARG:HG3	2.09	0.52
1:B:500:ARG:NH1	1:B:518:ILE:HG23	2.25	0.51
1:A:133:PHE:CE1	1:A:163:ARG:HD2	2.45	0.51
1:B:213:ASN:O	1:B:215:THR:N	2.41	0.51
1:B:184:ASN:O	1:B:190:VAL:HG21	2.11	0.51
1:A:500:ARG:NH2	1:A:658:MET:O	2.44	0.51
1:A:718:MET:HE1	1:A:724:LEU:HD21	1.91	0.51
1:A:761:MET:SD	1:A:793:THR:HG21	2.51	0.51
1:B:488:ALA:O	1:B:561:HIS:HE1	1.93	0.51
1:B:343:MET:HE3	5:B:1009:GOL:O1	2.11	0.51
1:B:868:ASN:HA	1:B:871:ARG:HB2	1.93	0.51
1:A:863:ILE:O	1:A:867:ILE:HG13	2.11	0.51
1:B:185:PRO:HA	1:B:190:VAL:HG11	1.91	0.51
1:A:14:LYS:HD2	1:A:186:TYR:OH	2.11	0.51
1:B:143:LEU:O	1:B:178:PHE:HA	2.10	0.51
1:A:688:ARG:NH2	1:A:695:GLU:O	2.38	0.51
1:B:582:ARG:HH11	1:B:591:ASP:CG	2.13	0.51
1:A:36:VAL:CG2	1:A:255:ASP:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLY:O	1:B:13:TRP:HB3	2.11	0.51
1:A:105:LYS:HD3	1:A:110:HIS:CE1	2.47	0.50
1:A:817:TRP:C	1:A:821:ASN:ND2	2.63	0.50
1:A:813:TRP:CZ2	1:A:836:ILE:HG12	2.47	0.50
1:B:475:TRP:HZ3	1:B:576:LYS:HD2	1.75	0.50
1:B:255:ASP:OD2	1:B:256:VAL:N	2.37	0.50
1:A:288:HIS:C	1:A:290:THR:H	2.15	0.50
1:A:870:VAL:O	1:A:874:ILE:HG13	2.11	0.50
1:B:863:ILE:O	1:B:867:ILE:HG13	2.11	0.50
1:A:736:GLY:O	1:A:740:ILE:HD13	2.12	0.50
1:B:61:LYS:NZ	6:B:1104:HOH:O	2.44	0.50
1:B:496:HIS:ND1	1:B:508:GLU:OE1	2.44	0.50
1:B:703:TRP:C	1:B:705:GLN:H	2.15	0.50
1:A:292:TRP:CD1	1:A:292:TRP:C	2.85	0.49
1:B:63:ARG:NH1	1:B:256:VAL:HG22	2.27	0.49
1:B:505:SER:HB2	1:B:615:MET:SD	2.52	0.49
1:A:280:ARG:O	1:A:284:ILE:HD12	2.13	0.49
1:B:238:MET:CE	1:B:242:ARG:HH11	2.18	0.49
1:B:300:TYR:OH	1:B:591:ASP:OD1	2.27	0.49
1:A:168:VAL:HG11	1:A:180:ILE:HG12	1.94	0.49
1:A:35:GLU:HG3	1:A:36:VAL:N	2.27	0.49
1:A:302:THR:OG1	1:A:360:ASP:OD1	2.27	0.49
1:A:512:LEU:HD11	1:A:711:HIS:CE1	2.48	0.49
1:A:270:GLU:OE1	1:A:362:ARG:NH2	2.46	0.49
1:A:441:LEU:O	1:A:445:GLY:N	2.41	0.49
1:B:624:GLU:HG3	1:B:629:PHE:CZ	2.48	0.49
1:B:654:ARG:HA	1:B:657:ARG:HG3	1.95	0.49
1:B:858:THR:O	1:B:862:ASN:ND2	2.37	0.49
1:A:10:GLY:O	1:A:13:TRP:HB3	2.13	0.49
1:A:237:ARG:NH2	5:A:1017:GOL:O3	2.45	0.49
1:A:510:GLU:OE1	1:A:514:LYS:HD3	2.13	0.49
1:B:616:GLU:O	1:B:620:ILE:HG13	2.13	0.49
1:B:849:SER:OG	1:B:850:LEU:N	2.46	0.49
1:B:25:PHE:O	1:B:28:TYR:N	2.46	0.48
1:A:573:TYR:O	1:A:576:LYS:HD2	2.14	0.48
1:B:522:VAL:O	1:B:525:LYS:HB2	2.13	0.48
1:B:646:TRP:CH2	1:B:654:ARG:HG3	2.48	0.48
1:A:557:MET:O	1:A:558:GLU:HB3	2.11	0.48
1:A:167:LEU:HD12	1:A:167:LEU:O	2.14	0.48
1:A:614:ASN:HD21	1:A:665:CYS:HB3	1.79	0.48
1:A:402:LYS:C	1:A:404:ARG:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:PRO:HG2	1:B:332:TRP:CE3	2.49	0.48
1:B:626:GLU:OE1	1:B:654:ARG:NH2	2.44	0.48
1:A:71:VAL:HG21	1:A:179:CYS:HB2	1.95	0.47
1:A:285:LYS:O	1:A:289:GLU:N	2.47	0.47
1:B:280:ARG:NH2	1:B:577:VAL:HG12	2.29	0.47
1:A:454:MET:HG3	1:A:578:VAL:HG11	1.95	0.47
1:A:690:ASP:O	1:A:691:ILE:HG23	2.15	0.47
1:B:540:THR:HA	1:B:598:GLN:HG3	1.95	0.47
1:A:47:ARG:NH1	1:A:49:GLU:OE2	2.47	0.47
1:A:168:VAL:O	1:A:172:LEU:HG	2.15	0.47
1:A:292:TRP:CZ2	1:A:307:GLY:HA3	2.48	0.47
1:B:240:ILE:HA	1:B:243:PHE:HD2	1.78	0.47
1:B:451:VAL:HG12	1:B:577:VAL:CG1	2.42	0.47
1:A:582:ARG:HG2	1:A:583:PRO:HD2	1.97	0.47
1:B:64:TRP:CE2	1:B:209:PRO:HD2	2.49	0.47
1:A:38:ARG:HD2	1:A:57:ARG:HG2	1.96	0.47
1:A:558:GLU:HA	1:A:562:LYS:HB2	1.96	0.47
1:A:645:ASN:O	1:A:648:VAL:N	2.48	0.47
1:B:161:THR:HG23	1:B:162:LEU:N	2.30	0.47
1:B:735:ILE:HG22	1:B:739:ARG:HD3	1.96	0.47
1:A:57:ARG:HH11	1:A:212:ARG:HH12	1.50	0.47
1:A:207:ARG:HD2	1:A:235:ILE:HD12	1.97	0.47
1:B:37:ASP:O	1:B:38:ARG:HB2	2.14	0.47
1:B:144:LEU:HD22	1:B:179:CYS:HB3	1.96	0.47
1:A:498:PHE:O	1:A:506:GLY:HA3	2.15	0.46
1:B:17:LEU:HD11	1:B:25:PHE:CE1	2.49	0.46
1:A:671:ASP:CG	1:A:673:ARG:HE	2.18	0.46
1:A:859:TRP:HB2	5:B:1009:GOL:H31	1.96	0.46
1:B:50:THR:HA	1:B:116:MET:CE	2.45	0.46
1:B:212:ARG:H	1:B:212:ARG:HG2	1.52	0.46
1:B:742:GLN:O	1:B:746:TRP:NE1	2.31	0.46
1:B:777:ASN:HB3	1:B:883:MET:SD	2.55	0.46
1:A:361:THR:O	1:A:595:ARG:NH1	2.44	0.46
1:A:763:SER:O	1:A:767:PHE:HB3	2.14	0.46
1:B:280:ARG:NE	1:B:447:CYS:HB2	2.29	0.46
1:B:289:GLU:C	1:B:291:SER:H	2.18	0.46
1:B:669:PRO:HG3	1:B:674:PHE:CB	2.44	0.46
1:A:500:ARG:NH1	1:A:518:ILE:HG23	2.29	0.46
1:B:100:VAL:HG13	1:B:124:VAL:HA	1.96	0.46
1:B:194:MET:HE1	1:B:205:LEU:HD21	1.98	0.46
1:B:538:TRP:CD1	1:B:538:TRP:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:THR:HA	1:A:557:MET:SD	2.56	0.46
1:B:541:ARG:HH21	1:B:687:VAL:HG11	1.81	0.46
1:B:619:LEU:HD23	1:B:619:LEU:HA	1.71	0.46
1:B:277:ILE:HD13	1:B:594:SER:OG	2.15	0.46
1:B:576:LYS:HG3	1:B:595:ARG:O	2.16	0.46
1:A:268:GLU:HA	1:A:362:ARG:HD2	1.98	0.46
1:A:849:SER:HB3	1:A:851:ILE:HD12	1.98	0.46
1:B:362:ARG:HA	1:B:595:ARG:HH22	1.81	0.46
1:A:57:ARG:HH11	1:A:212:ARG:CZ	2.04	0.45
1:A:132:VAL:HG22	3:A:1013:SAH:N1	2.31	0.45
1:A:442:HIS:CD2	1:A:447:CYS:SG	3.07	0.45
1:B:42:LYS:HA	1:B:45:ILE:HG22	1.99	0.45
1:B:51:ASP:C	1:B:53:HIS:H	2.20	0.45
1:A:167:LEU:HD12	1:A:167:LEU:C	2.37	0.45
1:B:73:PRO:HA	1:B:142:THR:HG21	1.99	0.45
1:B:768:HIS:CD2	1:B:768:HIS:H	2.33	0.45
1:A:120:GLY:HA2	1:A:263:ARG:HG3	1.98	0.45
1:A:595:ARG:CZ	1:A:598:GLN:HE21	2.29	0.45
1:B:68:ARG:HD3	3:B:1004:SAH:HG1	1.98	0.45
1:B:394:CYS:O	1:B:487:GLU:HG3	2.15	0.45
1:A:815:ARG:O	1:A:820:GLU:HB2	2.16	0.45
1:B:146:ASP:HB3	3:B:1005:SAH:HB2	1.97	0.45
1:A:352:GLN:NE2	1:A:582:ARG:HG3	2.32	0.45
1:A:553:VAL:O	1:A:557:MET:HG3	2.17	0.45
1:A:57:ARG:HH12	1:A:212:ARG:NE	2.13	0.45
1:B:213:ASN:C	1:B:215:THR:H	2.20	0.45
1:A:402:LYS:HE3	1:A:494:GLU:OE1	2.16	0.45
1:B:14:LYS:HA	1:B:17:LEU:HB3	1.99	0.45
1:B:615:MET:HG3	1:B:660:ILE:HD12	1.98	0.45
1:B:768:HIS:ND1	1:B:769:ARG:HD3	2.31	0.45
1:A:768:HIS:CD2	1:A:768:HIS:H	2.34	0.45
1:B:208:ASN:OD1	1:B:210:LEU:HB2	2.17	0.45
1:B:242:ARG:HD2	1:B:245:MET:HE1	1.98	0.45
1:B:768:HIS:CE1	1:B:769:ARG:HD3	2.51	0.45
1:B:205:LEU:HD22	1:B:220:TRP:HA	1.99	0.45
1:B:284:ILE:CD1	1:B:592:ILE:HG21	2.45	0.45
1:A:280:ARG:NH1	1:A:571:LEU:O	2.45	0.44
1:A:584:THR:OG1	1:A:587:GLY:O	2.34	0.44
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.52	0.44
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.78	0.44
1:A:367:LYS:HG2	1:A:683:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LYS:N	1:B:331:PRO:HD2	2.32	0.44
1:B:550:GLU:OE1	1:B:599:ARG:NH2	2.48	0.44
1:A:288:HIS:O	1:A:290:THR:HG23	2.17	0.44
1:A:372:LYS:HE3	1:A:640:GLU:OE1	2.17	0.44
1:B:55:VAL:CG1	1:B:84:ARG:HB2	2.47	0.44
1:B:389:LYS:HG3	1:B:502:ASN:ND2	2.32	0.44
1:B:602:GLY:O	1:B:605:VAL:N	2.51	0.44
1:A:178:PHE:HB2	1:A:180:ILE:CD1	2.46	0.44
1:A:330:LYS:N	1:A:331:PRO:HD2	2.33	0.44
1:B:77:VAL:HB	1:B:100:VAL:HG23	1.98	0.44
1:B:187:MET:HB2	1:B:187:MET:HE2	1.73	0.44
1:B:844:ASP:OD1	1:B:849:SER:HB2	2.18	0.44
3:B:1005:SAH:H4'	3:B:1005:SAH:HG1	1.76	0.44
1:A:441:LEU:HD22	1:A:446:LYS:CB	2.47	0.44
1:B:68:ARG:HB2	1:B:70:LEU:HG	1.98	0.44
1:B:511:GLY:HA3	1:B:513:HIS:CE1	2.53	0.44
1:B:13:TRP:CZ2	1:B:17:LEU:HD22	2.52	0.44
1:B:392:ARG:HD2	1:B:393:MET:O	2.18	0.44
1:A:816:VAL:HG23	1:A:817:TRP:N	2.33	0.44
1:B:168:VAL:HG21	1:B:180:ILE:HG12	1.99	0.44
1:B:386:GLY:HA2	1:B:389:LYS:HB2	1.99	0.44
1:B:105:LYS:O	1:B:129:GLY:HA2	2.18	0.44
1:B:161:THR:HG23	1:B:162:LEU:H	1.83	0.44
1:B:374:MET:HB3	1:B:616:GLU:OE2	2.17	0.44
1:B:480:GLY:O	1:B:484:LEU:HD12	2.17	0.44
1:A:194:MET:HE1	1:A:220:TRP:CG	2.53	0.43
1:B:653:GLU:O	1:B:656:SER:OG	2.28	0.43
1:A:133:PHE:CD1	1:A:167:LEU:CD2	3.02	0.43
1:A:689:LYS:O	1:A:690:ASP:HB2	2.17	0.43
1:A:764:LEU:HD11	1:A:816:VAL:CG2	2.42	0.43
1:B:178:PHE:HB2	1:B:180:ILE:HD11	2.01	0.43
1:B:178:PHE:HB2	1:B:180:ILE:CD1	2.48	0.43
1:B:439:ARG:NH2	1:B:487:GLU:OE2	2.51	0.43
1:A:363:THR:HG23	1:A:541:ARG:CZ	2.47	0.43
1:B:343:MET:HE1	5:B:1009:GOL:O1	2.18	0.43
1:B:720:ASP:OD1	1:B:722:ARG:HG3	2.19	0.43
1:A:381:LEU:HD23	1:A:612:PHE:CD1	2.52	0.43
1:A:572:THR:O	1:A:576:LYS:HG3	2.18	0.43
1:A:599:ARG:HD2	1:A:610:ASN:OD1	2.19	0.43
1:B:431:PHE:O	1:B:434:LEU:N	2.51	0.43
1:B:84:ARG:HA	1:B:113:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:PHE:O	1:B:487:GLU:N	2.49	0.43
1:A:376:ILE:HG13	1:A:377:THR:N	2.33	0.43
1:A:11:GLU:H	1:A:11:GLU:HG3	1.60	0.43
1:B:712:HIS:CD2	1:B:728:CYS:HB3	2.54	0.43
1:A:624:GLU:HB3	1:A:677:ALA:HB1	2.01	0.42
1:B:395:THR:OG1	1:B:398:GLU:HG3	2.19	0.42
1:A:454:MET:HE3	1:A:454:MET:HB3	1.93	0.42
1:A:637:VAL:O	1:A:641:ILE:HG13	2.19	0.42
1:A:640:GLU:O	1:A:644:LYS:HG3	2.19	0.42
1:B:165:LEU:CD2	1:B:197:LEU:HD11	2.48	0.42
1:A:288:HIS:O	1:A:290:THR:N	2.49	0.42
1:A:761:MET:HB2	1:A:803:TRP:CD1	2.53	0.42
1:A:841:LYS:O	1:A:845:GLN:HG2	2.19	0.42
1:B:240:ILE:O	1:B:243:PHE:HB2	2.19	0.42
1:A:621:ARG:HG2	1:A:674:PHE:CE2	2.54	0.42
1:B:557:MET:HE3	1:B:561:HIS:CG	2.55	0.42
1:A:54:ALA:HA	1:A:258:LEU:HD12	2.01	0.42
1:B:517:TYR:OH	1:B:724:LEU:HA	2.20	0.42
1:A:395:THR:O	1:A:398:GLU:HB3	2.19	0.42
1:A:431:PHE:C	1:A:431:PHE:CD2	2.93	0.42
1:B:541:ARG:HH21	1:B:687:VAL:CG1	2.32	0.42
1:B:761:MET:HB2	1:B:803:TRP:CE2	2.54	0.42
1:A:500:ARG:HD2	1:A:518:ILE:HD13	2.01	0.42
1:B:531:TYR:CE2	1:B:675:ALA:HB2	2.55	0.42
1:B:623:MET:HB3	1:B:628:VAL:HG22	2.00	0.42
1:B:203:GLY:O	1:B:225:SER:HA	2.19	0.42
1:B:399:PHE:HD2	1:B:432:TRP:HH2	1.68	0.42
1:A:77:VAL:HG13	1:A:142:THR:HG23	2.02	0.42
1:B:28:TYR:O	1:B:213:ASN:ND2	2.40	0.42
1:A:17:LEU:HD11	1:A:25:PHE:CE1	2.54	0.42
1:A:540:THR:HA	1:A:598:GLN:HG2	2.02	0.42
1:A:754:LEU:HD13	1:A:791:SER:CB	2.50	0.41
1:A:122:ASN:OD1	1:A:122:ASN:N	2.53	0.41
1:A:57:ARG:HE	1:A:57:ARG:HB3	1.38	0.41
1:A:488:ALA:HB1	1:A:565:ALA:HB2	2.01	0.41
1:B:13:TRP:CE3	1:B:216:HIS:HD2	2.37	0.41
1:A:33:ILE:CD1	1:A:212:ARG:HD3	2.49	0.41
1:A:372:LYS:O	1:A:376:ILE:HG23	2.21	0.41
1:A:669:PRO:HG3	1:A:674:PHE:CG	2.56	0.41
1:A:718:MET:HG3	1:A:722:ARG:O	2.20	0.41
1:B:98:LYS:O	1:B:123:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:772:LEU:HD23	1:B:772:LEU:HA	1.87	0.41
1:B:554:THR:HG21	1:B:566:GLU:HG2	2.02	0.41
1:A:528:GLY:O	1:A:668:LYS:HE2	2.21	0.41
1:A:580:VAL:HG22	1:A:581:GLN:O	2.20	0.41
1:A:655:LEU:HA	1:A:658:MET:HE2	2.03	0.41
1:B:55:VAL:HG11	1:B:84:ARG:HB2	2.01	0.41
1:B:298:HIS:CD2	1:B:305:TYR:CD2	3.09	0.41
1:B:440:ASN:CA	1:B:443:LEU:HD23	2.45	0.41
1:B:700:TRP:CB	1:B:706:VAL:HG12	2.51	0.41
1:A:401:ARG:C	1:A:403:VAL:H	2.24	0.41
1:A:430:GLY:O	1:A:433:GLU:N	2.53	0.41
1:A:782:ALA:HA	1:A:871:ARG:HG3	2.03	0.41
1:B:75:GLY:HA3	1:B:141:ASP:OD1	2.21	0.41
1:B:103:LEU:HD22	1:B:127:GLN:NE2	2.35	0.41
1:B:388:LYS:O	1:B:389:LYS:HG2	2.21	0.41
1:B:393:MET:HE3	1:B:393:MET:HB3	1.95	0.41
1:A:770:ARG:HD2	1:A:770:ARG:HH11	1.69	0.40
1:B:170:ASN:C	1:B:172:LEU:H	2.25	0.40
1:A:91:CYS:HA	1:A:94:LEU:HD12	2.03	0.40
1:B:301:LYS:HG3	1:B:360:ASP:OD1	2.21	0.40
1:A:62:LEU:O	1:A:66:VAL:HG23	2.22	0.40
1:A:517:TYR:OH	1:A:724:LEU:HA	2.22	0.40
1:B:749:ARG:HH11	1:B:749:ARG:HD2	1.74	0.40
1:A:844:ASP:C	1:A:849:SER:HB2	2.42	0.40
1:B:178:PHE:CZ	1:B:222:SER:HA	2.57	0.40
1:A:425:ALA:C	1:A:427:GLU:H	2.25	0.40
1:A:688:ARG:NH1	1:A:691:ILE:HD11	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:NH1	1:A:826:ASP:OD2[6_445]	2.11	0.09

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	832/911 (91%)	738 (89%)	81 (10%)	13 (2%)	9 30
1	B	824/911 (90%)	703 (85%)	92 (11%)	29 (4%)	3 13
All	All	1656/1822 (91%)	1441 (87%)	173 (10%)	42 (2%)	5 19

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	ASP
1	A	791	SER
1	A	792	ARG
1	B	171	TRP
1	B	214	SER
1	B	341	MET
1	B	405	SER
1	B	603	GLN
1	A	9	LEU
1	A	403	VAL
1	A	421	SER
1	B	24	GLU
1	B	131	ASP
1	B	173	ASN
1	B	229	VAL
1	B	424	GLU
1	B	597	ASP
1	B	847	CYS
1	A	429	SER
1	A	431	PHE
1	A	603	GLN
1	B	170	ASN
1	B	172	LEU
1	B	204	ALA
1	B	228	ILE
1	B	437	LYS
1	B	440	ASN
1	B	601	SER
1	A	420	LYS
1	B	39	THR
1	B	291	SER

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Mol	Chain	Res	Type
1	B	552	MET
1	A	269	SER
1	A	289	GLU
1	B	17	LEU
1	B	106	GLY
1	B	185	PRO
1	B	504	LEU
1	B	677	ALA
1	B	704	THR
1	A	148	GLY
1	B	108	PRO

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	638/790 (81%)	605 (95%)	33 (5%)	23 53
1	B	605/790 (77%)	576 (95%)	29 (5%)	25 56
All	All	1243/1580 (79%)	1181 (95%)	62 (5%)	24 54

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	LYS
1	A	71	VAL
1	A	88	SER
1	A	118	THR
1	A	126	LEU
1	A	135	THR
1	A	150	SER
1	A	163	ARG
1	A	207	ARG
1	A	248	LYS
1	A	308	SER

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Mol	Chain	Res	Type
1	A	362	ARG
1	A	363	THR
1	A	436	ASP
1	A	454	MET
1	A	539	ASP
1	A	575	ASN
1	A	593	ILE
1	A	596	ARG
1	A	635	LEU
1	A	636	THR
1	A	648	VAL
1	A	698	ARG
1	A	737	ARG
1	A	746	TRP
1	A	769	ARG
1	A	770	ARG
1	A	791	SER
1	A	824	MET
1	A	832	SER
1	A	845	GLN
1	A	849	SER
1	B	11	GLU
1	B	34	GLN
1	B	67	GLU
1	B	116	MET
1	B	118	THR
1	B	211	SER
1	B	230	SER
1	B	238	MET
1	B	246	ARG
1	B	270	GLU
1	B	301	LYS
1	B	308	SER
1	B	319	SER
1	B	353	ARG
1	B	444	GLU
1	B	484	LEU
1	B	520	ARG
1	B	523	SER
1	B	549	ASN
1	B	579	ARG
1	B	597	ASP

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Mol	Chain	Res	Type
1	B	598	GLN
1	B	624	GLU
1	B	634	HIS
1	B	700	TRP
1	B	718	MET
1	B	719	LYS
1	B	739	ARG
1	B	748	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	166	ASN
1	A	306	HIS
1	A	440	ASN
1	A	502	ASN
1	A	561	HIS
1	A	575	ASN
1	A	622	GLN
1	A	868	ASN
1	B	18	ASN
1	B	127	GLN
1	B	177	GLN
1	B	223	ASN
1	B	502	ASN
1	B	561	HIS
1	B	711	HIS
1	B	869	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 19 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	SAH	B	1005	-	24,28,28	1.25	2 (8%)	25,40,40	2.08	5 (20%)
5	GOL	A	1018	-	5,5,5	0.45	0	5,5,5	0.42	0
5	GOL	B	1010	-	5,5,5	0.57	0	5,5,5	0.40	0
3	SAH	A	1013	-	24,28,28	1.24	3 (12%)	25,40,40	1.93	5 (20%)
3	SAH	A	1014	-	24,28,28	1.25	1 (4%)	25,40,40	2.39	11 (44%)
5	GOL	B	1008	-	5,5,5	0.56	0	5,5,5	0.83	0
5	GOL	B	1009	-	5,5,5	0.52	0	5,5,5	0.85	0
5	GOL	A	1017	-	5,5,5	0.50	0	5,5,5	0.85	0
3	SAH	B	1004	-	24,28,28	1.40	2 (8%)	25,40,40	1.99	7 (28%)

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
3	SAH	B	1005	-	-	4/11/31/31	0/3/3/3
5	GOL	A	1018	-	-	2/4/4/4	-
5	GOL	B	1010	-	-	4/4/4/4	-
3	SAH	A	1013	-	-	3/11/31/31	0/3/3/3
3	SAH	A	1014	-	-	1/11/31/31	0/3/3/3
5	GOL	B	1008	-	-	4/4/4/4	-
5	GOL	B	1009	-	-	2/4/4/4	-
5	GOL	A	1017	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	B	1004	-	-	7/11/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	SAH	C2-N3	5.22	1.40	1.32
3	A	1014	SAH	C2-N3	3.93	1.38	1.32
3	B	1005	SAH	C2-N3	3.66	1.38	1.32
3	A	1013	SAH	C2-N3	3.31	1.37	1.32
3	B	1005	SAH	C2-N1	3.11	1.39	1.33
3	B	1004	SAH	C2-N1	3.10	1.39	1.33
3	A	1013	SAH	C2'-C1'	-2.40	1.50	1.53
3	A	1013	SAH	O4'-C4'	-2.00	1.40	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1014	SAH	N3-C2-N1	-6.22	118.96	128.68
3	A	1013	SAH	C5'-SD-CG	-5.59	85.50	102.27
3	A	1013	SAH	N3-C2-N1	-5.31	120.38	128.68
3	B	1005	SAH	N3-C2-N1	-5.30	120.40	128.68
3	B	1004	SAH	N3-C2-N1	-4.74	121.27	128.68
3	B	1004	SAH	C5'-SD-CG	-4.71	88.14	102.27
3	B	1005	SAH	C5'-SD-CG	-4.42	89.01	102.27
3	B	1005	SAH	N6-C6-N1	4.12	127.13	118.57
3	A	1014	SAH	OXT-C-O	-3.67	115.75	124.09
3	B	1005	SAH	C5-C6-N6	-3.59	114.90	120.35
3	A	1014	SAH	CB-CA-C	3.54	118.73	110.30
3	A	1014	SAH	C4'-C5'-SD	-3.54	101.07	113.78
3	A	1014	SAH	C5-C6-N6	-3.32	115.31	120.35
3	B	1004	SAH	O4'-C1'-C2'	-3.30	102.11	106.93
3	A	1014	SAH	O3'-C3'-C2'	-2.92	102.36	111.82
3	A	1014	SAH	OXT-C-CA	2.70	122.59	113.38
3	B	1004	SAH	OXT-C-CA	2.52	121.96	113.38
3	B	1004	SAH	C3'-C2'-C1'	2.48	104.71	100.98
3	A	1013	SAH	OXT-C-CA	2.48	121.82	113.38
3	A	1014	SAH	N6-C6-N1	2.37	123.50	118.57
3	B	1005	SAH	C3'-C2'-C1'	2.37	104.54	100.98
3	A	1014	SAH	O4'-C1'-C2'	2.26	110.22	106.93
3	A	1013	SAH	OXT-C-O	-2.23	119.02	124.09
3	B	1004	SAH	OXT-C-O	-2.20	119.09	124.09
3	A	1014	SAH	CB-CG-SD	-2.19	108.39	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1013	SAH	C2'-C3'-C4'	2.19	106.89	102.64
3	A	1014	SAH	C3'-C2'-C1'	2.18	104.27	100.98
3	B	1004	SAH	C4'-C5'-SD	-2.06	106.40	113.78

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1004	SAH	CA-CB-CG-SD
3	B	1004	SAH	O4'-C4'-C5'-SD
3	B	1004	SAH	C3'-C4'-C5'-SD
5	A	1017	GOL	O1-C1-C2-C3
5	A	1018	GOL	O1-C1-C2-C3
5	B	1008	GOL	O1-C1-C2-C3
5	B	1009	GOL	C1-C2-C3-O3
5	B	1010	GOL	O1-C1-C2-C3
5	A	1017	GOL	C1-C2-C3-O3
5	B	1008	GOL	C1-C2-C3-O3
5	B	1010	GOL	O1-C1-C2-O2
3	B	1005	SAH	C-CA-CB-CG
5	A	1018	GOL	O1-C1-C2-O2
5	B	1008	GOL	O1-C1-C2-O2
5	B	1009	GOL	O2-C2-C3-O3
5	A	1017	GOL	O1-C1-C2-O2
3	B	1005	SAH	N-CA-CB-CG
5	B	1010	GOL	O2-C2-C3-O3
3	B	1004	SAH	O-C-CA-CB
3	B	1004	SAH	OXT-C-CA-CB
5	A	1017	GOL	O2-C2-C3-O3
3	A	1013	SAH	CA-CB-CG-SD
3	A	1013	SAH	C-CA-CB-CG
3	A	1014	SAH	C-CA-CB-CG
5	B	1010	GOL	C1-C2-C3-O3
3	B	1004	SAH	CB-CG-SD-C5'
3	B	1005	SAH	OXT-C-CA-N
3	B	1004	SAH	N-CA-CB-CG
5	B	1008	GOL	O2-C2-C3-O3
3	A	1013	SAH	OXT-C-CA-CB
3	B	1005	SAH	CB-CG-SD-C5'

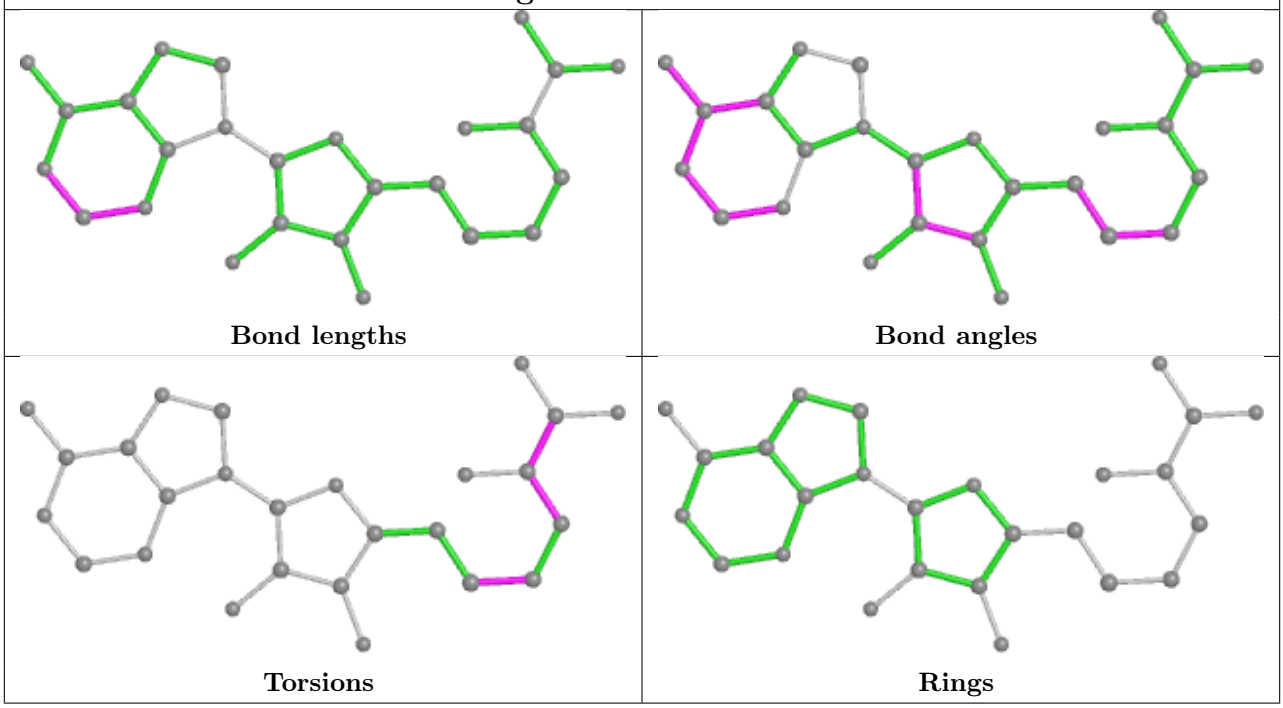
There are no ring outliers.

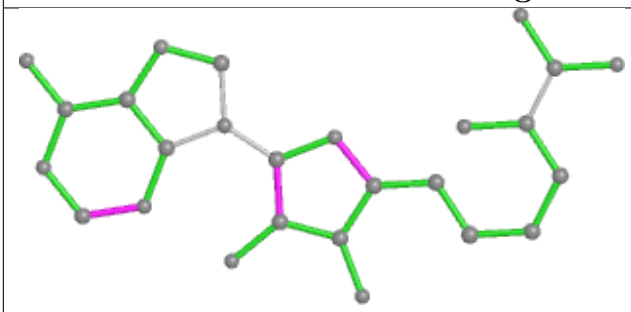
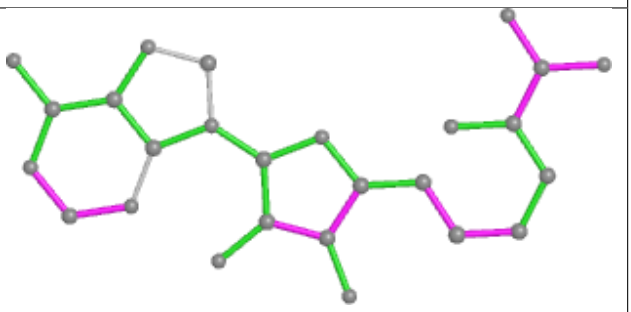
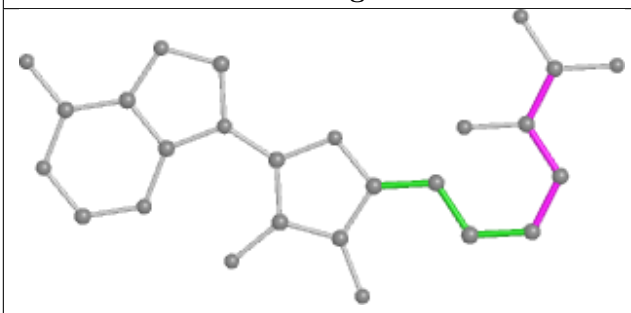
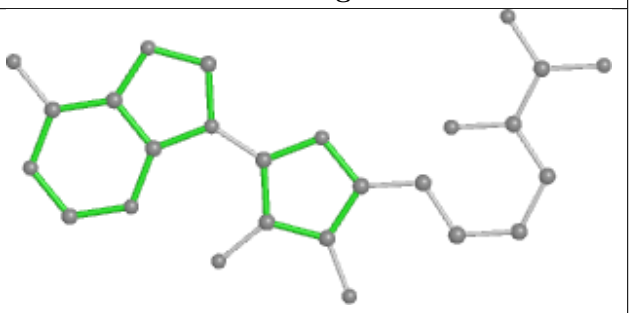
6 monomers are involved in 14 short contacts:

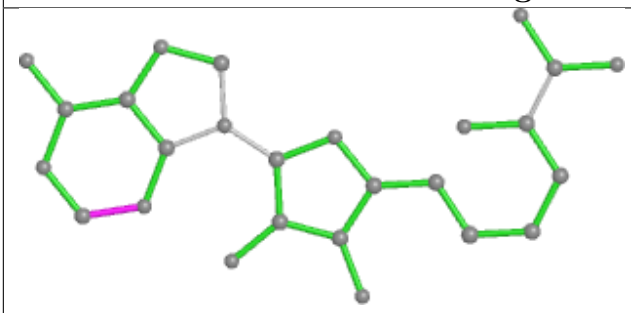
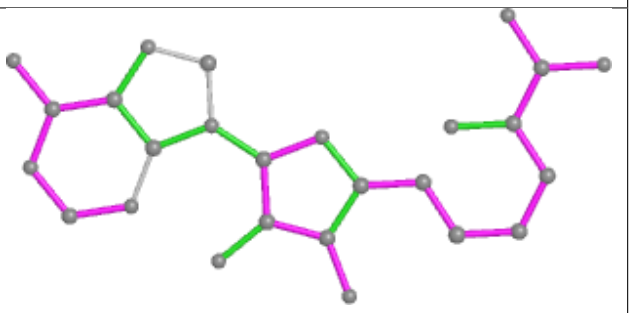
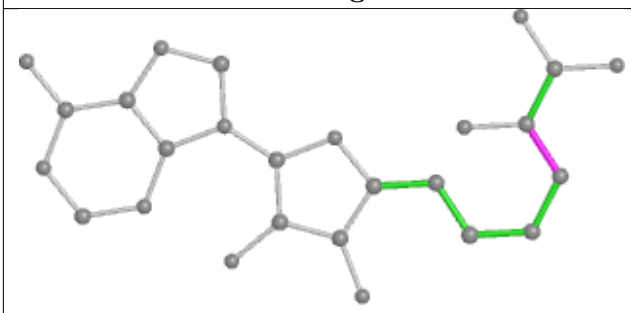
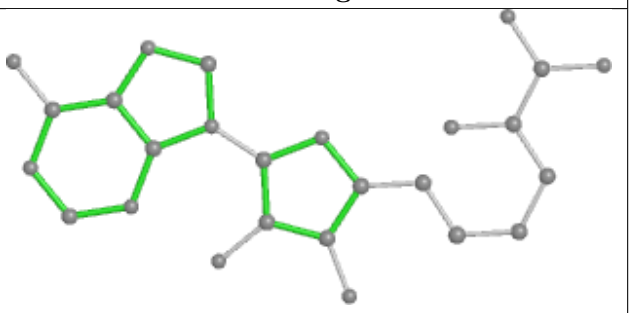
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1005	SAH	4	0
5	A	1018	GOL	1	0
3	A	1013	SAH	1	0
5	B	1009	GOL	5	0
5	A	1017	GOL	2	0
3	B	1004	SAH	1	0

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

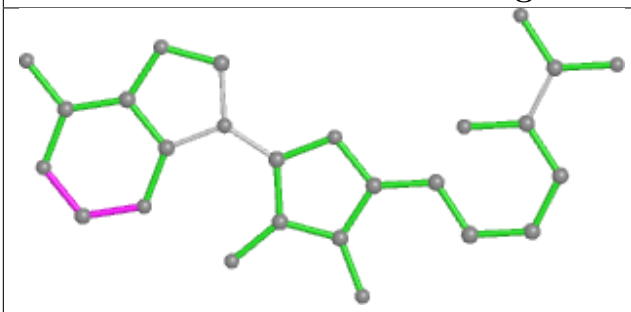
Ligand SAH B 1005



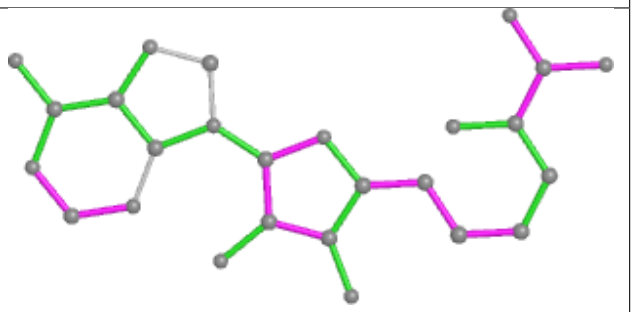
Ligand SAH A 1013	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH A 1014	
 Bond lengths	 Bond angles
 Torsions	 Rings

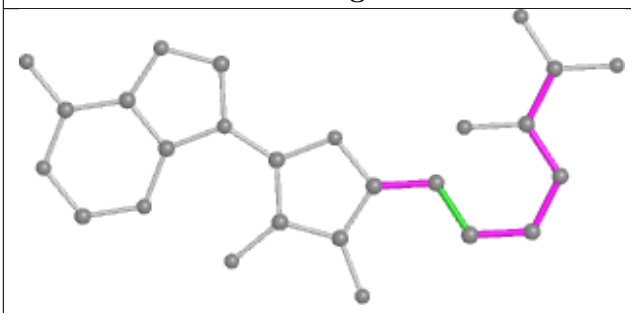
Ligand SAH B 1004



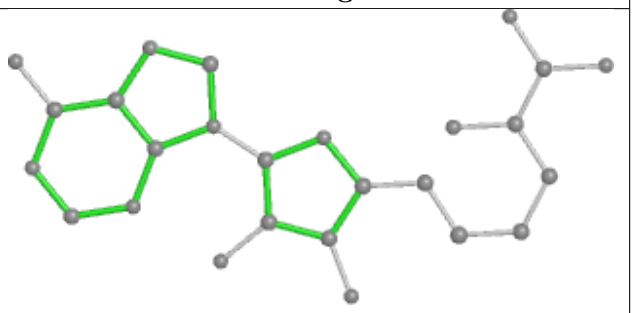
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	842/911 (92%)	-0.04	8 (0%)	82	83	33, 51, 78, 97	0
1	B	836/911 (91%)	0.28	42 (5%)	28	28	37, 69, 88, 104	0
All	All	1678/1822 (92%)	0.12	50 (2%)	50	49	33, 59, 85, 104	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	LEU	5.6
1	A	795	TRP	5.6
1	A	794	THR	3.6
1	A	313	GLN	3.4
1	B	586	ARG	3.4
1	A	314	THR	3.2
1	B	309	TYR	3.2
1	B	108	PRO	3.0
1	B	314	THR	3.0
1	B	307	GLY	3.0
1	B	284	ILE	2.9
1	B	201	TYR	2.9
1	B	164	VAL	2.8
1	B	432	TRP	2.7
1	B	214	SER	2.6
1	B	238	MET	2.6
1	B	194	MET	2.6
1	B	526	GLU	2.6
1	B	792	ARG	2.6
1	B	308	SER	2.6
1	B	484	LEU	2.5
1	B	180	ILE	2.4
1	B	226	GLY	2.4
1	B	17	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	165	LEU	2.4
1	B	185	PRO	2.3
1	B	204	ALA	2.3
1	A	436	ASP	2.3
1	B	292	TRP	2.3
1	B	186	TYR	2.3
1	B	793	THR	2.3
1	B	243	PHE	2.2
1	A	448	GLU	2.2
1	B	190	VAL	2.2
1	B	422	ALA	2.2
1	B	429	SER	2.2
1	B	227	ASN	2.2
1	B	475	TRP	2.1
1	B	8	THR	2.1
1	B	206	VAL	2.1
1	A	399	PHE	2.1
1	B	290	THR	2.1
1	B	589	VAL	2.1
1	B	800	THR	2.1
1	B	33	ILE	2.1
1	A	284	ILE	2.0
1	B	161	THR	2.0
1	B	250	ALA	2.0
1	B	18	ASN	2.0
1	B	184	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

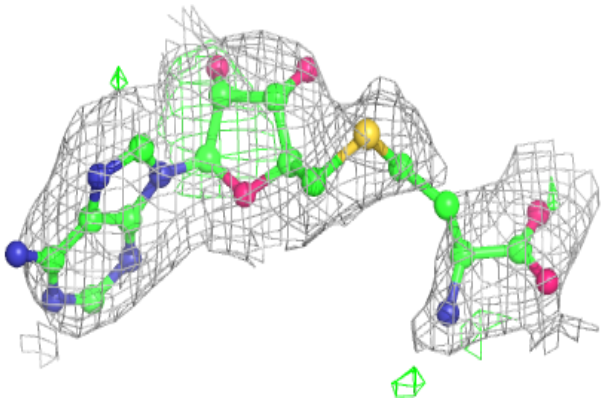
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

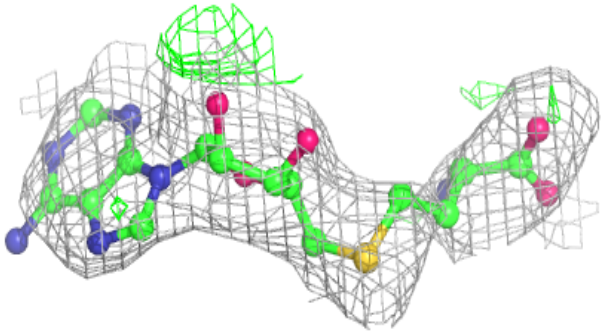
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SAH	B	1005	26/26	0.79	0.23	72,78,84,90	26
3	SAH	B	1004	26/26	0.82	0.21	52,64,74,79	0
3	SAH	A	1014	26/26	0.86	0.21	44,62,73,76	0
4	ZN	B	1006	1/1	0.87	0.13	121,121,121,121	0
5	GOL	A	1017	6/6	0.90	0.21	43,46,48,51	0
2	IOD	B	1003	1/1	0.93	0.18	113,113,113,113	1
5	GOL	A	1018	6/6	0.93	0.22	42,46,48,51	6
5	GOL	B	1010	6/6	0.93	0.25	44,46,48,53	6
2	IOD	B	1002	1/1	0.94	0.08	108,108,108,108	1
5	GOL	B	1008	6/6	0.94	0.20	46,48,50,53	0
4	ZN	A	1015	1/1	0.94	0.10	127,127,127,127	0
2	IOD	A	1012	1/1	0.95	0.16	91,91,91,91	1
2	IOD	A	1008	1/1	0.95	0.20	101,101,101,101	1
2	IOD	A	1007	1/1	0.96	0.07	109,109,109,109	1
2	IOD	A	1003	1/1	0.96	0.12	76,76,76,76	0
3	SAH	A	1013	26/26	0.96	0.20	41,44,54,64	0
2	IOD	A	1006	1/1	0.96	0.14	94,94,94,94	1
2	IOD	A	1011	1/1	0.97	0.08	91,91,91,91	1
2	IOD	B	1001	1/1	0.97	0.07	117,117,117,117	1
2	IOD	A	1010	1/1	0.98	0.07	91,91,91,91	1
4	ZN	A	1016	1/1	0.98	0.14	55,55,55,55	1
2	IOD	A	1009	1/1	0.98	0.11	103,103,103,103	1
5	GOL	B	1009	6/6	0.98	0.13	39,42,43,58	0
4	ZN	B	1007	1/1	0.98	0.13	62,62,62,62	1
2	IOD	A	1005	1/1	0.99	0.12	76,76,76,76	0
2	IOD	A	1002	1/1	0.99	0.17	76,76,76,76	0
2	IOD	A	1001	1/1	1.00	0.11	76,76,76,76	0
2	IOD	A	1004	1/1	1.00	0.27	76,76,76,76	0

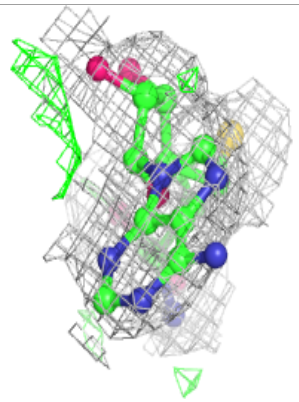
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH B 1005:

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







Electron density around SAH B 1004:

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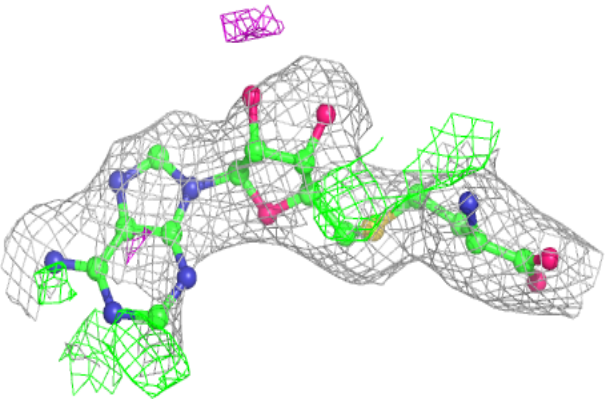
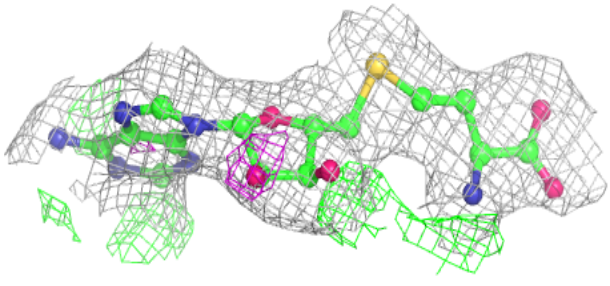
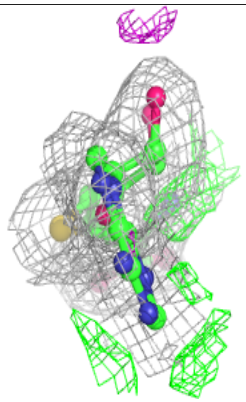
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

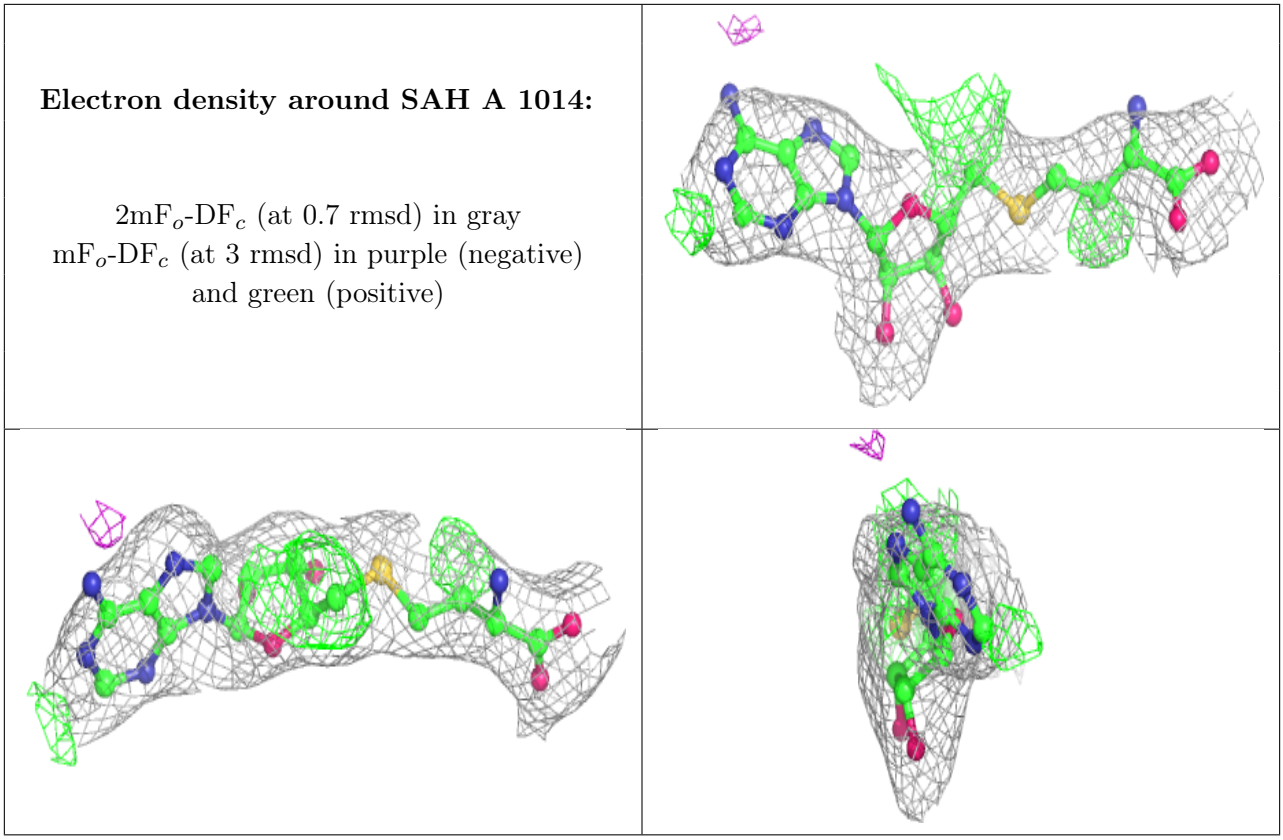






Electron density around SAH A 1014:

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



Electron density around ZN B 1006:

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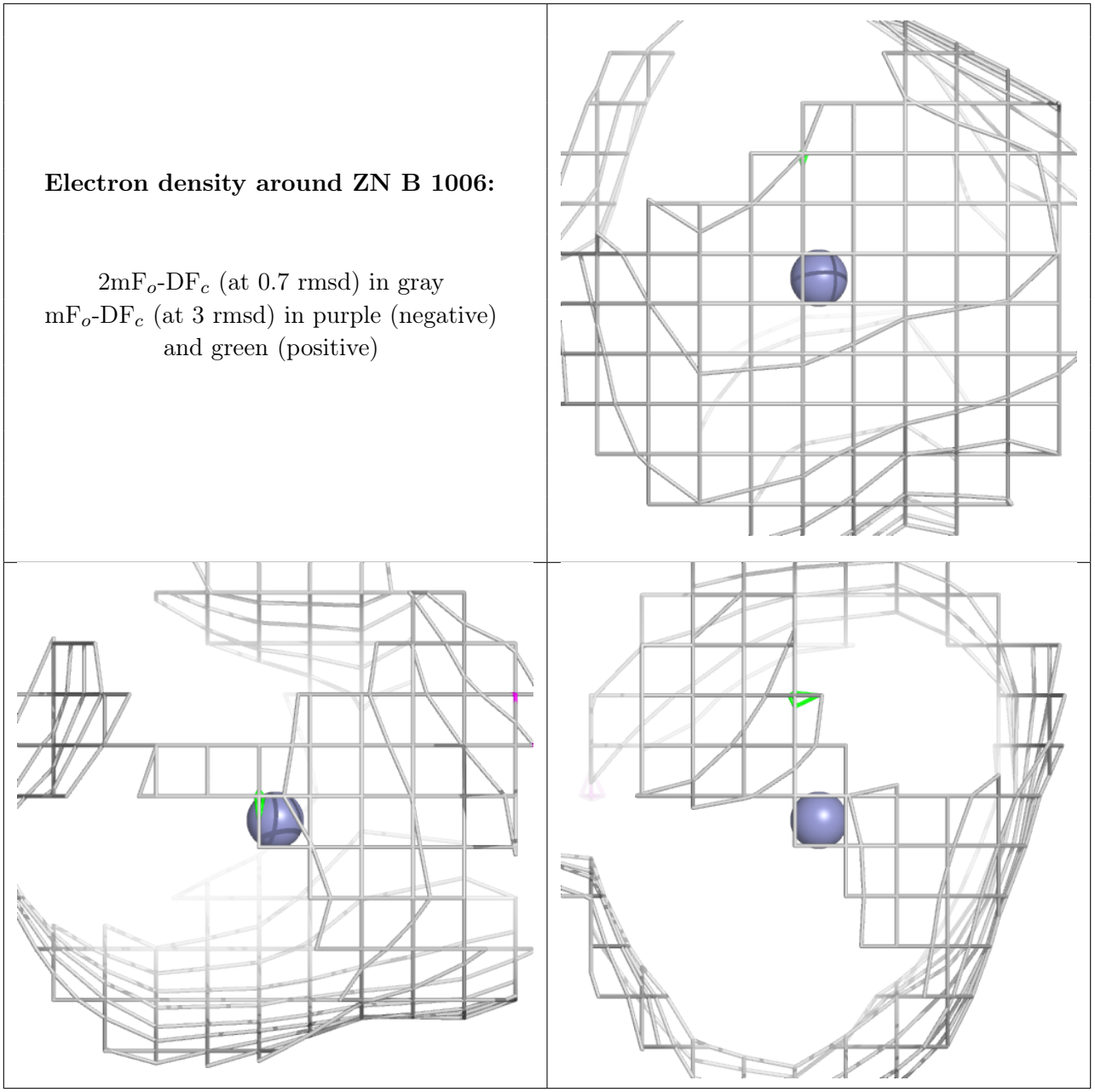

Electron density around ZN A 1015:

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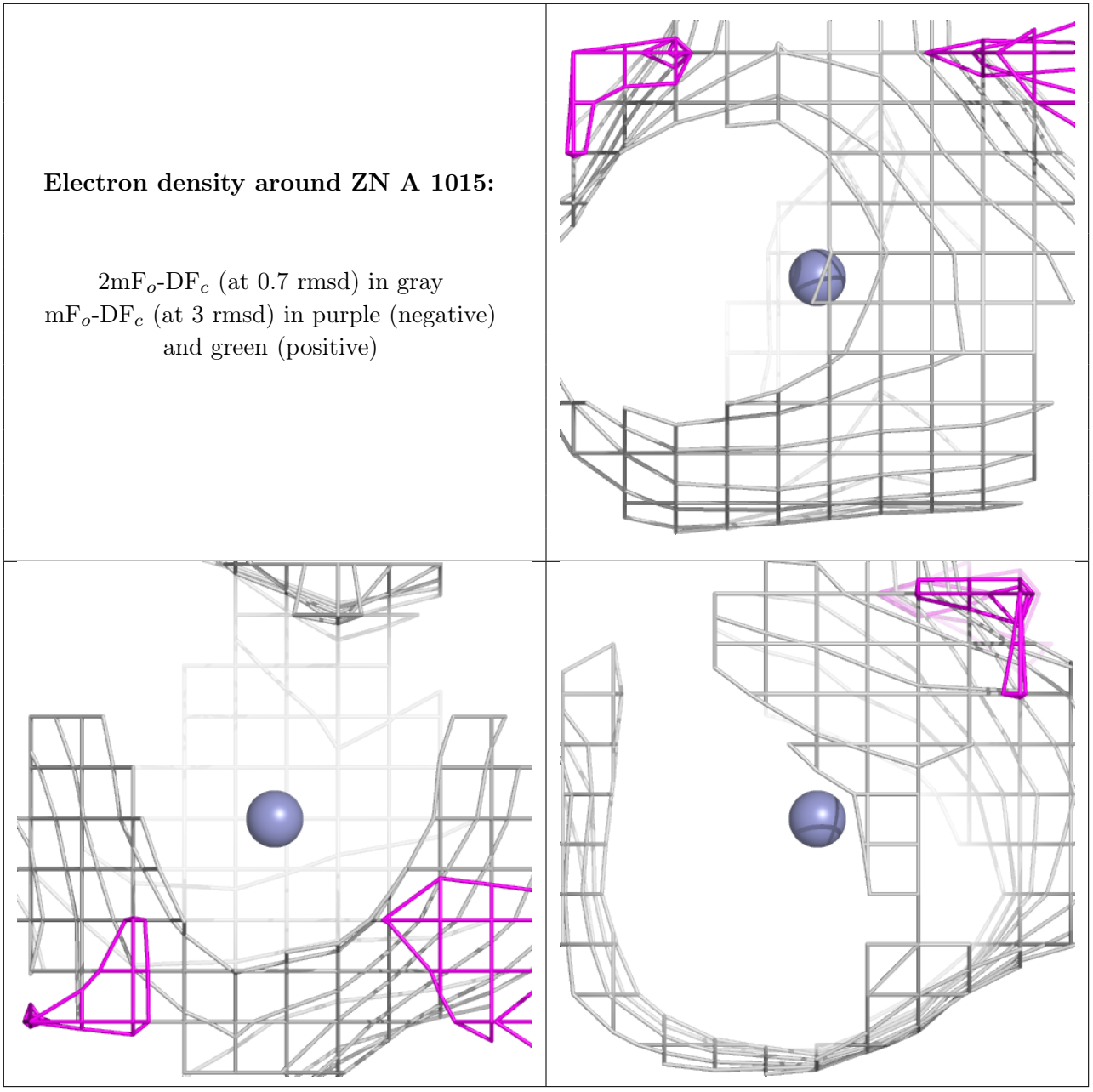
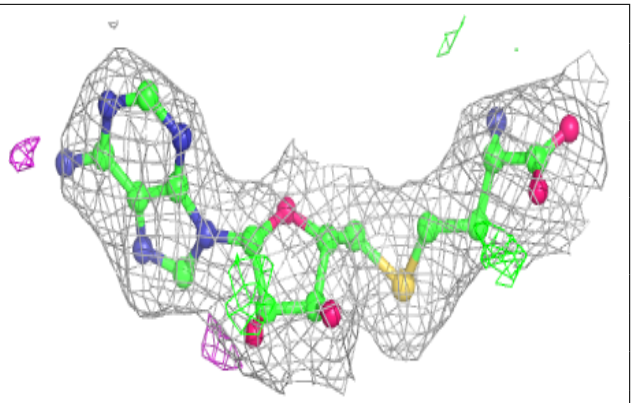
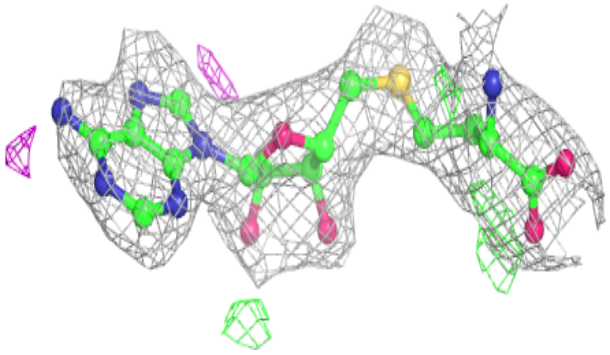
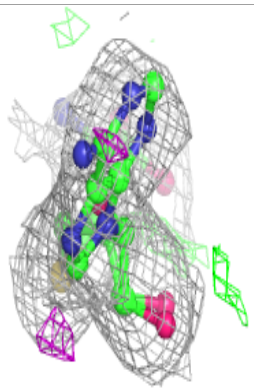


Electron density around SAH A 1013:

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







Electron density around ZN A 1016:

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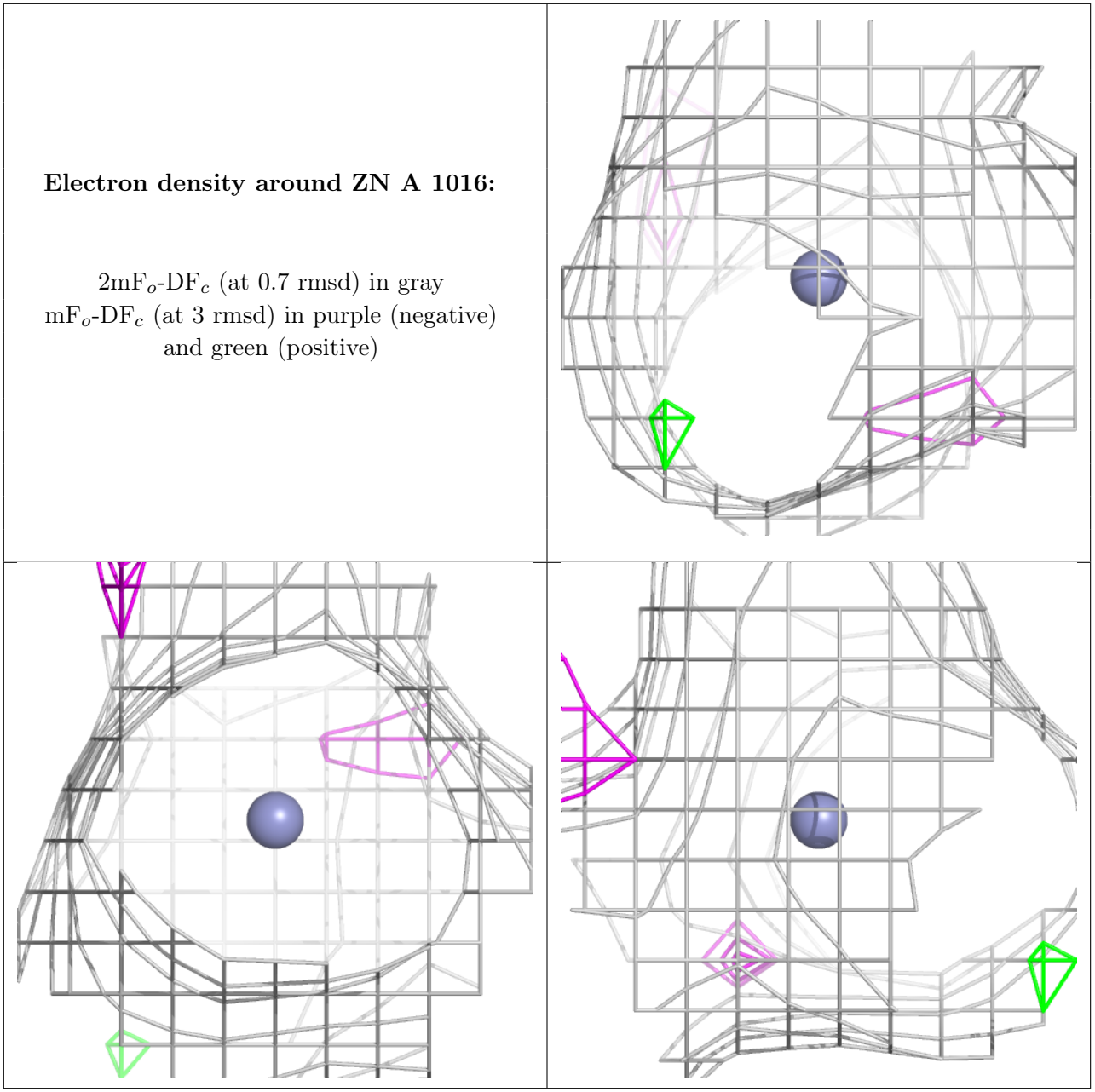
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZN B 1007:

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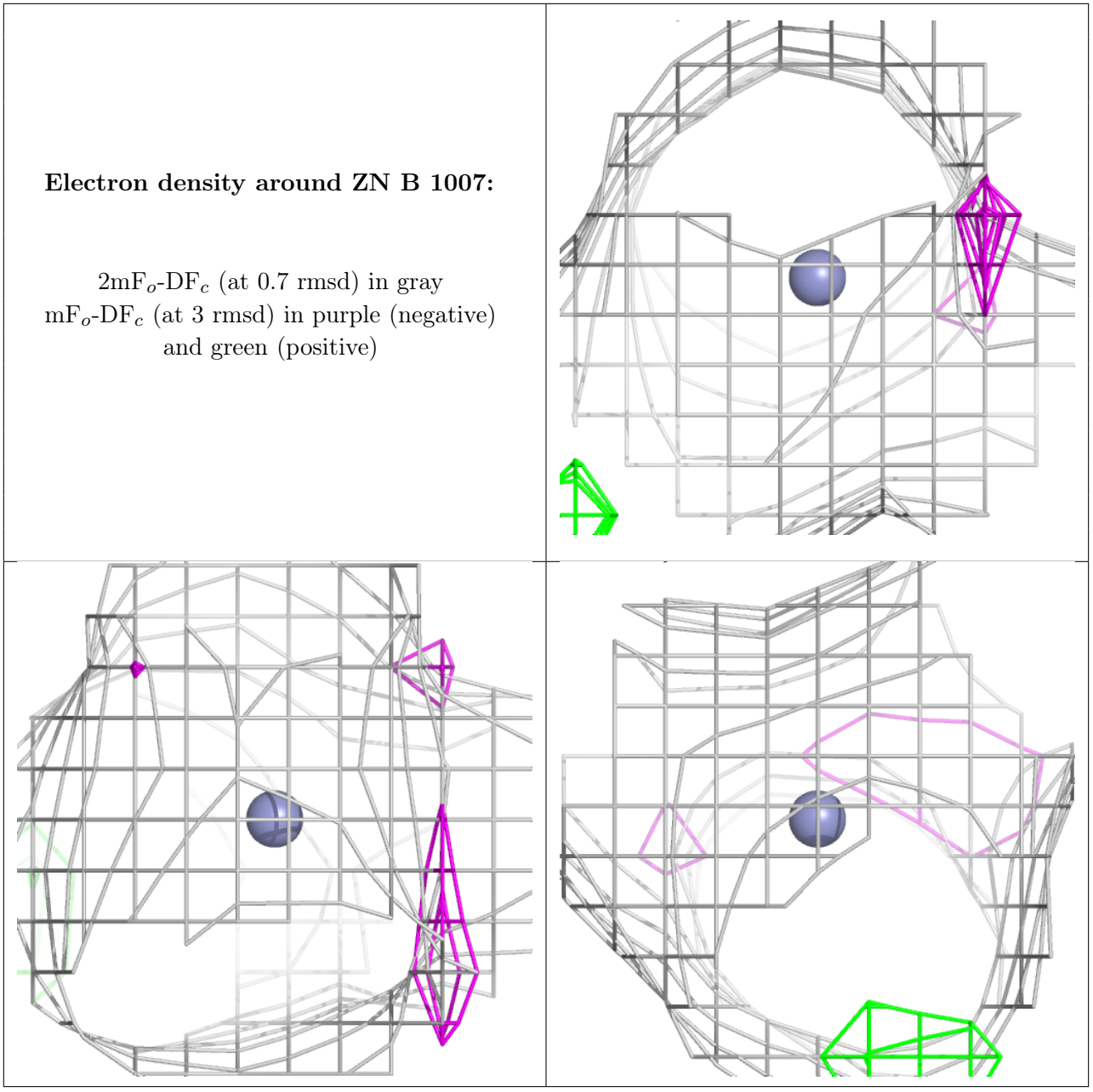

6.5 Other polymers (i)

There are no such residues in this entry.