Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 03:47 AM JST

PDB ID	:	6KR2
Title	:	Crystal structure of Dengue virus nonstructural protein NS5 (form 1)
Authors	:	Wu, J.; Lu, G.; Ye, H.Q.; Gong, P.
Deposited on	:	2019-08-20
Resolution	:	3.06 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

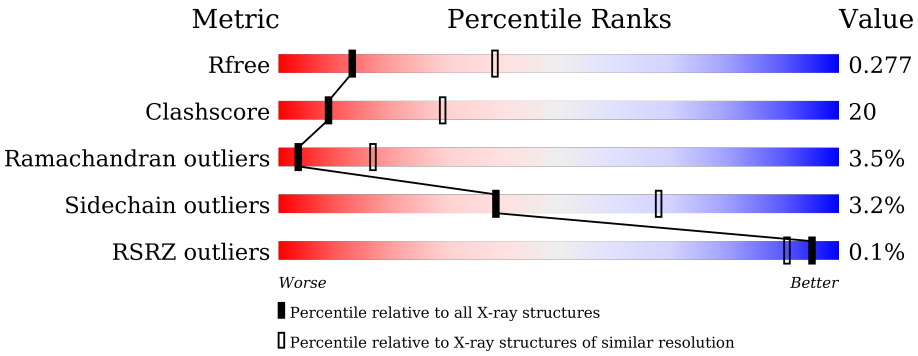
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	55% 36% · 6%
1	B	911	60% 31% · 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12727 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	857	Total	C	N	O	S	0	0	0
			6408	4026	1137	1203	42			
1	B	843	Total	C	N	O	S	0	0	0
			6230	3904	1103	1181	42			

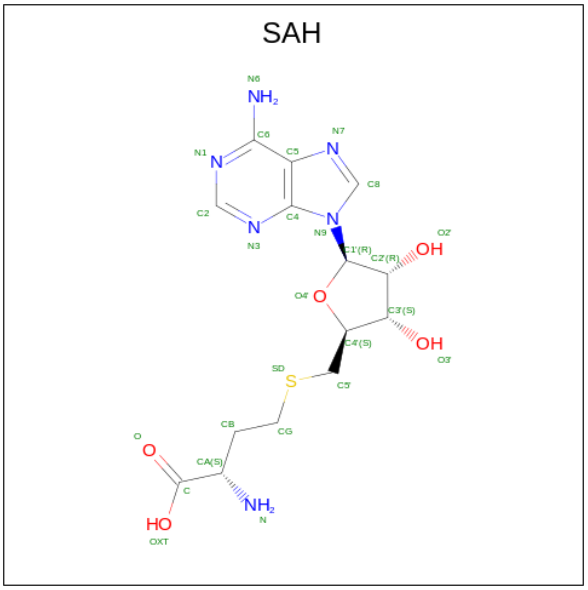
There are 22 discrepancies between the modelled and reference sequences:

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	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	B	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 4 is water.

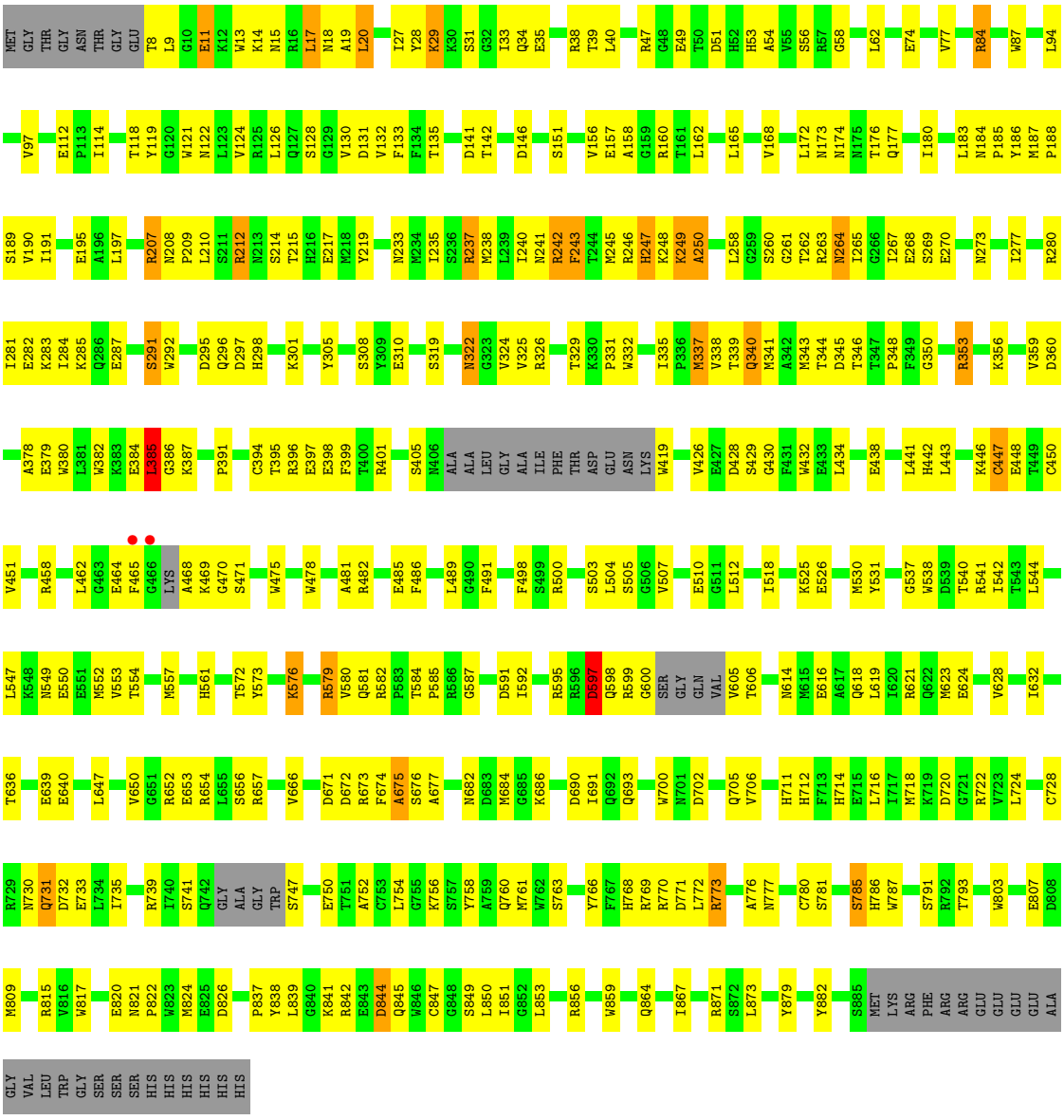
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	15	Total O 15 15	0	0

3 Residue-property plots (i)

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

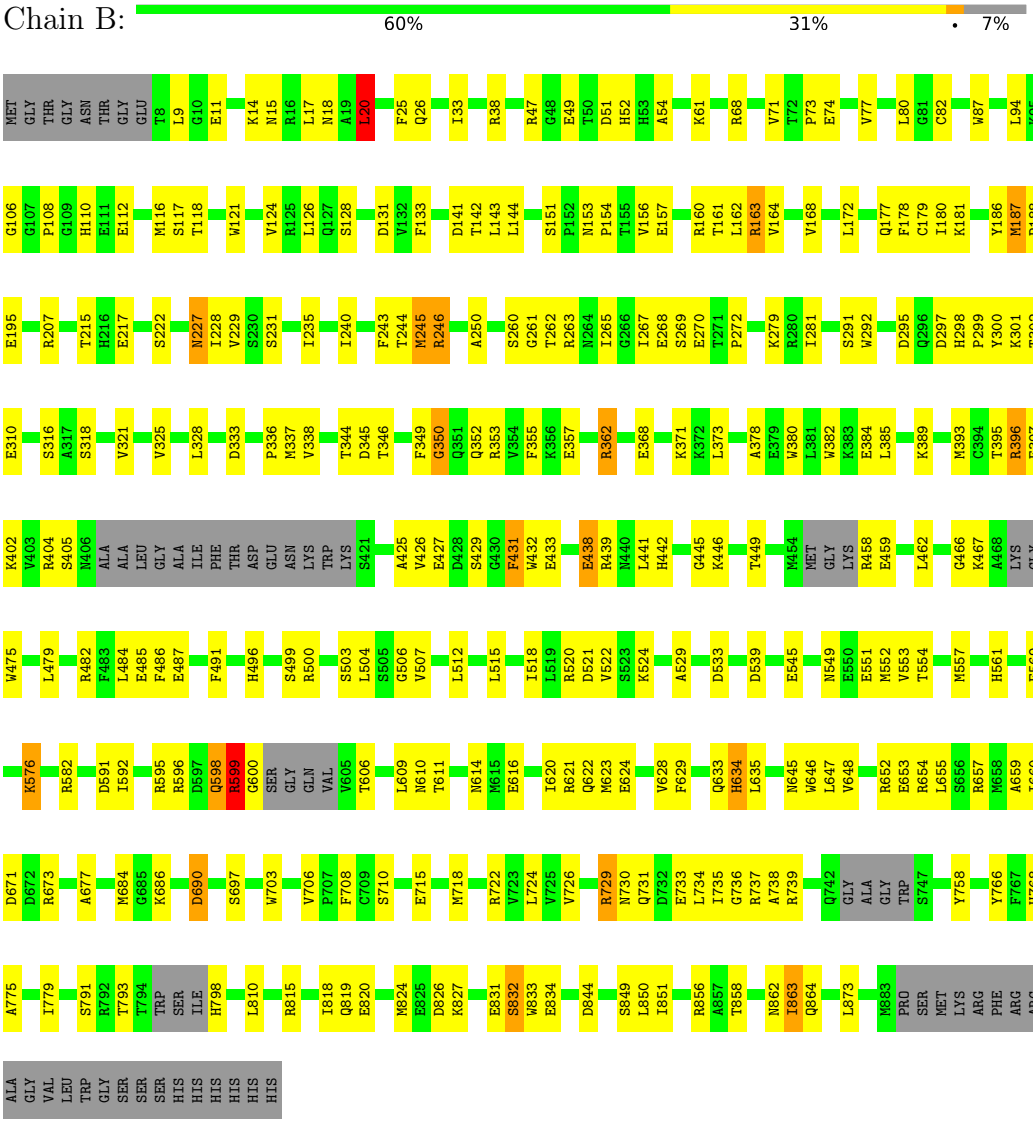
- Molecule 1: Genome polyprotein

Chain A:



• Molecule 1: Genome polyprotein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.22Å 146.42Å 98.39Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	44.82 – 3.06 44.82 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.82-3.06) 97.9 (44.82-3.05)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.224 , 0.275 0.226 , 0.277	Depositor DCC
R_{free} test set	2177 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12727	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: ZN, SAH

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	0.57	1/6558 (0.0%)	0.79	5/8932 (0.1%)
1	B	0.53	1/6372 (0.0%)	0.75	5/8683 (0.1%)
All	All	0.55	2/12930 (0.0%)	0.77	10/17615 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	CYS	CB-SG	-10.82	1.63	1.82
1	B	389	LYS	C-N	6.33	1.48	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	B	599	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	844	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	20	LEU	CB-CG-CD2	6.30	121.71	111.00
1	A	20	LEU	CA-CB-CG	6.22	129.61	115.30
1	B	68	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	A	360	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	850	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	207	ARG	NE-CZ-NH2	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	20	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	268	GLU	Peptide
1	B	279	LYS	Peptide
1	B	350	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6408	0	5754	275	0
1	B	6230	0	5502	219	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	26	0	19	4	0
3	B	26	0	19	0	0
4	A	18	0	0	1	0
4	B	15	0	0	0	0
All	All	12727	0	11294	488	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 20.

All (488) 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:785:SER:O	1:A:787:TRP:N	1.97	0.97
1:A:14:LYS:NZ	1:A:151:SER:O	1.97	0.96
1:A:233:ASN:O	1:A:237:ARG:HD3	1.70	0.92
1:A:305:TYR:HH	1:A:308:SER:HG	1.15	0.91
1:B:350:GLY:HA2	1:B:353:ARG:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:THR:HA	1:A:557:MET:HG3	1.57	0.86
1:B:195:GLU:HG2	1:B:228:ILE:HG21	1.60	0.83
1:A:654:ARG:HA	1:A:657:ARG:HG3	1.59	0.82
1:A:671:ASP:OD2	1:A:673:ARG:NE	2.12	0.82
1:A:741:SER:HB3	1:A:754:LEU:HD22	1.62	0.81
1:A:525:LYS:NZ	1:A:653:GLU:OE1	2.14	0.81
1:B:864:GLN:O	1:B:864:GLN:NE2	2.11	0.81
1:B:624:GLU:HB3	1:B:677:ALA:HB1	1.64	0.80
1:B:270:GLU:HG2	1:B:362:ARG:HH22	1.46	0.79
1:A:35:GLU:OE1	1:A:212:ARG:NH2	2.15	0.79
1:B:554:THR:HA	1:B:557:MET:HG3	1.63	0.78
1:B:151:SER:N	1:B:157:GLU:OE2	2.13	0.78
1:A:233:ASN:O	1:A:237:ARG:CD	2.32	0.78
1:B:862:ASN:O	1:B:864:GLN:N	2.16	0.78
1:B:599:ARG:HD2	1:B:606:THR:HG23	1.67	0.77
1:A:384:GLU:O	1:A:387:LYS:N	2.17	0.76
1:B:401:ARG:O	1:B:404:ARG:N	2.19	0.76
1:A:702:ASP:HB3	1:A:705:GLN:HG3	1.67	0.75
1:A:382:TRP:CZ2	1:A:553:VAL:HG22	2.21	0.74
1:B:485:GLU:OE1	1:B:573:TYR:OH	2.06	0.74
1:A:624:GLU:HB3	1:A:677:ALA:HB1	1.69	0.73
1:A:485:GLU:OE2	1:A:573:TYR:OH	2.06	0.73
1:B:302:THR:OG1	1:B:595:ARG:NH1	2.20	0.73
1:B:244:THR:OG1	1:B:245:MET:N	2.20	0.73
1:B:769:ARG:NH1	1:B:844:ASP:OD1	2.21	0.72
1:B:207:ARG:NH1	1:B:215:THR:O	2.23	0.71
1:A:673:ARG:CG	1:B:163:ARG:HG3	2.21	0.71
1:A:281:ILE:HD11	1:A:592:ILE:HG21	1.71	0.70
1:A:595:ARG:NH1	1:A:598:GLN:OE1	2.24	0.70
1:A:673:ARG:HG3	1:B:163:ARG:HG3	1.72	0.70
1:A:526:GLU:OE1	1:B:151:SER:OG	2.08	0.70
1:A:344:THR:HG22	1:A:345:ASP:H	1.58	0.69
1:B:344:THR:HG22	1:B:459:GLU:H	1.57	0.69
1:B:576:LYS:NZ	1:B:596:ARG:O	2.26	0.69
1:B:116:MET:HB3	1:B:118:THR:HG23	1.75	0.69
1:B:722:ARG:HD2	1:B:824:MET:SD	2.34	0.68
1:A:291:SER:OG	1:A:310:GLU:HG3	1.95	0.67
1:A:426:VAL:O	1:A:432:TRP:NE1	2.25	0.67
1:A:348:PRO:HG3	1:A:581:GLN:HE21	1.59	0.67
1:A:718:MET:HA	1:A:837:PRO:HG3	1.75	0.67
1:A:11:GLU:HB3	1:A:186:TYR:HE1	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:O	1:A:287:GLU:OE1	2.13	0.66
1:A:11:GLU:HB3	1:A:186:TYR:CE1	2.29	0.66
1:A:576:LYS:NZ	1:A:597:ASP:O	2.26	0.66
1:A:132:VAL:HG13	3:A:2003:SAH:H2	1.76	0.66
1:B:244:THR:O	1:B:246:ARG:N	2.29	0.66
1:B:382:TRP:CZ2	1:B:553:VAL:HG22	2.30	0.66
1:B:71:VAL:HG21	1:B:179:CYS:HB2	1.77	0.66
1:A:119:TYR:HB2	1:A:260:SER:H	1.60	0.65
1:B:654:ARG:HA	1:B:657:ARG:HG3	1.77	0.65
1:B:11:GLU:O	1:B:15:ASN:ND2	2.27	0.65
1:B:551:GLU:O	1:B:554:THR:HG23	1.97	0.65
1:A:769:ARG:HH22	1:A:844:ASP:HA	1.59	0.65
1:A:653:GLU:O	1:A:656:SER:OG	2.15	0.65
1:B:38:ARG:NH1	1:B:54:ALA:O	2.30	0.64
1:B:572:THR:O	1:B:576:LYS:HB3	1.97	0.64
1:A:722:ARG:HD3	1:A:826:ASP:HB3	1.78	0.64
1:B:281:ILE:HD13	1:B:592:ILE:HG21	1.78	0.64
1:B:399:PHE:HB2	1:B:486:PHE:CE2	2.32	0.64
1:A:191:ILE:O	1:A:195:GLU:HG3	1.97	0.64
1:A:295:ASP:OD2	1:A:582:ARG:NH2	2.30	0.64
1:B:94:LEU:O	1:B:263:ARG:NH2	2.30	0.64
1:B:684:MET:O	1:B:686:LYS:NZ	2.30	0.64
1:A:77:VAL:HG22	1:A:142:THR:CG2	2.28	0.64
1:A:337:MET:SD	1:A:462:LEU:HD13	2.38	0.64
1:A:871:ARG:NH1	1:A:879:TYR:HB3	2.13	0.64
1:A:770:ARG:NH2	1:A:844:ASP:OD2	2.31	0.64
1:B:291:SER:HB2	1:B:310:GLU:HG3	1.80	0.64
1:B:582:ARG:NH1	1:B:591:ASP:OD2	2.31	0.63
1:A:157:GLU:HB2	1:A:183:LEU:HD12	1.80	0.63
1:A:599:ARG:HD3	1:A:606:THR:HB	1.79	0.63
1:B:599:ARG:HH12	1:B:609:LEU:HB3	1.62	0.63
1:A:38:ARG:NH1	1:A:54:ALA:O	2.32	0.63
1:A:428:ASP:O	1:A:430:GLY:N	2.32	0.63
1:B:671:ASP:OD2	1:B:673:ARG:NE	2.31	0.63
1:A:344:THR:CG2	1:A:345:ASP:H	2.12	0.62
1:A:322:ASN:ND2	1:A:324:VAL:HG12	2.13	0.62
1:B:851:ILE:HA	1:B:856:ARG:HD2	1.82	0.62
1:A:13:TRP:CZ2	1:A:17:LEU:HD12	2.34	0.62
1:B:382:TRP:CE2	1:B:553:VAL:HG22	2.34	0.62
1:A:451:VAL:HG11	1:A:579:ARG:HD3	1.81	0.62
1:B:51:ASP:HB3	1:B:117:SER:OG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HA	1:B:670:LEU:HD21	1.80	0.62
1:A:550:GLU:O	1:A:553:VAL:HG23	2.00	0.62
1:A:768:HIS:H	1:A:768:HIS:CD2	2.17	0.62
1:B:299:PRO:HD2	1:B:300:TYR:CE2	2.34	0.62
1:B:151:SER:HB3	1:B:157:GLU:HG3	1.82	0.62
1:A:131:ASP:OD1	1:A:133:PHE:HB2	2.00	0.61
1:A:348:PRO:HG3	1:A:581:GLN:NE2	2.16	0.61
1:A:337:MET:HG3	1:A:732:ASP:HB3	1.83	0.61
1:A:248:LYS:HD3	1:A:249:LYS:HG2	1.84	0.60
1:A:332:TRP:HA	1:A:335:ILE:HD13	1.82	0.60
1:B:758:TYR:CD1	1:B:793:THR:HG23	2.37	0.60
1:B:74:GLU:H	1:B:142:THR:HG21	1.67	0.60
1:B:292:TRP:HZ3	1:B:592:ILE:HD12	1.65	0.59
1:B:624:GLU:HG3	1:B:629:PHE:CZ	2.37	0.59
1:B:228:ILE:HG23	1:B:229:VAL:H	1.66	0.59
1:A:475:TRP:CE3	1:A:600:GLY:HA2	2.37	0.59
1:A:718:MET:CE	1:A:724:LEU:HD21	2.32	0.59
1:B:316:SER:OG	1:B:318:SER:OG	2.04	0.59
1:B:646:TRP:CH2	1:B:654:ARG:HG3	2.37	0.59
1:A:871:ARG:HH11	1:A:879:TYR:HB3	1.68	0.58
1:B:653:GLU:OE2	1:B:654:ARG:NH1	2.36	0.58
1:A:845:GLN:NE2	1:A:851:ILE:O	2.37	0.58
1:B:442:HIS:HD2	1:B:446:LYS:O	1.86	0.58
1:B:646:TRP:CZ2	1:B:654:ARG:HG3	2.38	0.58
1:A:720:ASP:OD1	1:A:722:ARG:HG3	2.03	0.58
1:B:14:LYS:HG2	1:B:154:PRO:HG3	1.84	0.58
1:A:122:ASN:O	1:A:356:LYS:NZ	2.36	0.58
1:A:760:GLN:HG3	1:A:809:MET:SD	2.43	0.58
1:A:324:VAL:HG11	1:A:752:ALA:HA	1.84	0.57
1:A:156:VAL:HA	1:B:670:LEU:CD2	2.34	0.57
1:A:156:VAL:HG12	1:A:160:ARG:HE	1.70	0.57
1:A:215:THR:OG1	1:A:217:GLU:HG3	2.04	0.57
1:A:284:ILE:HG21	1:A:592:ILE:HD11	1.85	0.57
1:A:346:THR:HG21	4:A:2104:HOH:O	2.03	0.57
1:A:344:THR:HG22	1:A:345:ASP:N	2.18	0.57
1:B:439:ARG:NH2	1:B:487:GLU:OE2	2.38	0.57
1:B:595:ARG:HE	1:B:598:GLN:HG3	1.70	0.57
1:A:343:MET:HG2	1:A:458:ARG:NH2	2.19	0.56
1:A:584:THR:HB	1:A:585:PRO:HD2	1.87	0.56
1:B:124:VAL:HG12	1:B:126:LEU:HD13	1.86	0.56
1:B:616:GLU:O	1:B:620:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:HG22	1:A:332:TRP:HB2	1.88	0.56
1:B:599:ARG:HH12	1:B:609:LEU:CB	2.17	0.56
1:A:94:LEU:O	1:A:263:ARG:NH2	2.39	0.56
1:A:146:ASP:HB3	3:A:2003:SAH:HN1	1.70	0.56
1:A:807:GLU:OE2	1:A:815:ARG:NH1	2.38	0.56
1:B:47:ARG:NH1	1:B:49:GLU:OE2	2.39	0.56
1:A:29:LYS:HE3	1:A:212:ARG:HG2	1.87	0.56
1:A:544:LEU:HD12	1:A:547:LEU:HD12	1.87	0.56
1:B:438:GLU:HG3	1:B:449:THR:OG1	2.05	0.56
1:A:359:VAL:HG13	1:A:598:GLN:HE22	1.69	0.56
1:B:14:LYS:HD3	1:B:186:TYR:OH	2.06	0.56
1:B:858:THR:O	1:B:862:ASN:ND2	2.34	0.56
1:A:623:MET:HB3	1:A:628:VAL:CG1	2.36	0.56
1:B:557:MET:HB3	1:B:561:HIS:HD2	1.70	0.55
1:A:359:VAL:HG13	1:A:598:GLN:NE2	2.21	0.55
1:A:504:LEU:HD11	1:A:652:ARG:NH1	2.22	0.55
1:A:769:ARG:NH2	1:A:844:ASP:HA	2.21	0.55
1:A:537:GLY:O	1:A:541:ARG:HG2	2.07	0.55
1:A:208:ASN:OD1	1:A:210:LEU:HB2	2.07	0.54
1:B:771:ASP:OD1	1:B:856:ARG:NE	2.40	0.54
1:A:173:ASN:OD1	1:A:174:ASN:N	2.39	0.54
1:A:335:ILE:HG21	1:A:732:ASP:OD2	2.07	0.54
1:A:741:SER:HB3	1:A:754:LEU:CD2	2.33	0.54
1:B:533:ASP:OD2	1:B:697:SER:OG	2.23	0.54
1:B:121:TRP:HH2	1:B:352:GLN:HB3	1.72	0.54
1:A:382:TRP:CE2	1:A:553:VAL:HG22	2.43	0.54
1:A:769:ARG:NH2	1:A:844:ASP:OD1	2.41	0.54
1:A:17:LEU:O	1:A:20:LEU:HB3	2.08	0.54
1:A:507:VAL:O	1:A:510:GLU:HB2	2.08	0.54
1:A:864:GLN:HE22	1:A:871:ARG:NH2	2.06	0.54
1:B:80:LEU:HD22	1:B:143:LEU:HD11	1.88	0.53
1:A:51:ASP:O	1:A:53:HIS:N	2.33	0.53
1:A:142:THR:HB	1:A:177:GLN:HB2	1.89	0.53
1:A:119:TYR:HA	1:A:261:GLY:O	2.08	0.53
1:A:121:TRP:NE1	1:A:262:THR:HG22	2.24	0.53
1:B:395:THR:HB	1:B:398:GLU:H	1.74	0.53
1:B:576:LYS:H	1:B:576:LYS:HD3	1.72	0.53
1:A:674:PHE:O	1:A:676:SER:N	2.33	0.53
1:A:238:MET:O	1:A:242:ARG:HG3	2.09	0.53
1:A:538:TRP:NE1	1:A:542:ILE:HD11	2.24	0.53
1:B:775:ALA:O	1:B:779:ILE:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:LEU:HD21	1:B:831:GLU:HA	1.91	0.53
1:A:165:LEU:HD13	1:A:197:LEU:HD12	1.91	0.52
1:A:168:VAL:HG11	1:A:180:ILE:HD12	1.91	0.52
1:B:766:TYR:HA	1:B:768:HIS:CE1	2.44	0.52
1:A:157:GLU:HB2	1:A:183:LEU:CD1	2.39	0.52
1:A:530:MET:HE2	1:A:706:VAL:HG21	1.91	0.52
1:A:263:ARG:O	1:A:264:ASN:HB2	2.10	0.52
1:A:722:ARG:NH2	1:A:826:ASP:O	2.41	0.52
1:A:241:ASN:O	1:A:243:PHE:N	2.42	0.52
1:A:584:THR:OG1	1:A:587:GLY:O	2.23	0.52
1:B:611:THR:HG23	1:B:660:ILE:HG22	1.91	0.52
1:B:645:ASN:HA	1:B:648:VAL:HG12	1.91	0.52
1:A:38:ARG:C	1:A:40:LEU:H	2.13	0.52
1:A:262:THR:O	1:A:297:ASP:HB3	2.10	0.52
1:A:671:ASP:OD1	1:A:671:ASP:N	2.39	0.52
1:B:269:SER:HB2	1:B:362:ARG:NH1	2.24	0.52
1:B:380:TRP:CE3	1:B:647:LEU:HD22	2.44	0.52
1:B:735:ILE:O	1:B:738:ALA:N	2.42	0.52
1:A:132:VAL:HG22	3:A:2003:SAH:N1	2.25	0.52
1:A:395:THR:O	1:A:398:GLU:N	2.43	0.52
1:A:540:THR:HA	1:A:598:GLN:HG3	1.91	0.52
1:B:336:PRO:HD2	1:B:337:MET:SD	2.50	0.52
1:B:295:ASP:CG	1:B:582:ARG:HH22	2.14	0.51
1:B:512:LEU:O	1:B:515:LEU:HB2	2.11	0.51
1:B:178:PHE:H	1:B:222:SER:HB3	1.74	0.51
1:B:815:ARG:O	1:B:820:GLU:HG3	2.10	0.51
1:B:520:ARG:NH1	1:B:715:GLU:OE2	2.44	0.51
1:A:380:TRP:CD2	1:A:647:LEU:HD22	2.46	0.51
1:A:731:GLN:OE1	1:A:771:ASP:HB2	2.11	0.51
1:B:270:GLU:O	1:B:272:PRO:HD3	2.11	0.51
1:A:184:ASN:O	1:A:190:VAL:HG21	2.10	0.51
1:A:284:ILE:HD12	1:A:579:ARG:NH1	2.25	0.51
1:A:322:ASN:HD22	1:A:325:VAL:H	1.57	0.51
1:A:550:GLU:CD	1:A:599:ARG:HH22	2.14	0.51
1:A:761:MET:HB2	1:A:803:TRP:CD1	2.45	0.51
1:A:822:PRO:C	1:A:824:MET:H	2.14	0.51
1:B:142:THR:HA	1:B:177:GLN:O	2.11	0.51
1:B:263:ARG:HA	1:B:297:ASP:HB3	1.92	0.51
1:B:378:ALA:HB2	1:B:616:GLU:OE1	2.11	0.51
1:A:572:THR:O	1:A:576:LYS:HB3	2.11	0.51
1:A:295:ASP:CG	1:A:582:ARG:HH22	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:THR:CG2	1:A:345:ASP:N	2.74	0.50
1:A:442:HIS:HD2	1:A:446:LYS:O	1.93	0.50
1:A:851:ILE:HA	1:A:856:ARG:HD2	1.92	0.50
1:A:322:ASN:OD1	1:A:754:LEU:HD23	2.11	0.50
1:A:378:ALA:HB2	1:A:616:GLU:OE1	2.11	0.50
1:A:187:MET:C	1:A:189:SER:H	2.15	0.50
1:A:842:ARG:HA	1:A:845:GLN:HG3	1.92	0.50
1:A:84:ARG:HG2	1:A:114:ILE:HD12	1.93	0.50
1:B:554:THR:HG22	1:B:557:MET:HE3	1.93	0.50
1:A:185:PRO:HD2	1:A:186:TYR:HD2	1.77	0.50
1:B:281:ILE:HD11	1:B:292:TRP:HH2	1.77	0.50
1:A:77:VAL:HG13	1:A:142:THR:HG23	1.94	0.50
1:A:287:GLU:OE1	1:A:287:GLU:N	2.44	0.50
1:A:391:PRO:HB3	1:A:491:PHE:CE2	2.47	0.49
1:A:531:TYR:OH	1:A:672:ASP:OD1	2.24	0.49
1:B:228:ILE:O	1:B:231:SER:OG	2.30	0.49
1:A:730:ASN:O	1:A:732:ASP:N	2.45	0.49
1:B:51:ASP:O	1:B:52:HIS:HB2	2.12	0.49
1:B:121:TRP:CH2	1:B:352:GLN:HB3	2.47	0.49
1:A:240:ILE:O	1:A:243:PHE:HB2	2.12	0.49
1:B:549:ASN:O	1:B:552:MET:HB2	2.13	0.49
1:A:329:THR:HG22	1:A:329:THR:O	2.11	0.49
1:B:729:ARG:HH21	1:B:733:GLU:HB3	1.77	0.49
1:B:321:VAL:HA	1:B:739:ARG:O	2.13	0.49
1:A:249:LYS:HG3	1:A:250:ALA:H	1.78	0.49
1:B:17:LEU:O	1:B:20:LEU:HD22	2.12	0.49
1:B:670:LEU:HD22	1:B:670:LEU:O	2.13	0.49
1:A:112:GLU:OE1	1:A:128:SER:OG	2.12	0.49
1:A:38:ARG:O	1:A:40:LEU:N	2.39	0.49
1:B:325:VAL:O	1:B:328:LEU:N	2.44	0.49
1:B:395:THR:HG22	1:B:397:GLU:H	1.77	0.49
1:A:242:ARG:HA	1:A:245:MET:HB3	1.95	0.48
1:A:464:GLU:HA	1:A:468:ALA:HB3	1.95	0.48
1:B:718:MET:CE	1:B:722:ARG:HG3	2.42	0.48
1:A:557:MET:SD	1:A:561:HIS:CD2	3.06	0.48
1:A:718:MET:HE2	1:A:724:LEU:HD21	1.94	0.48
1:B:228:ILE:HG23	1:B:229:VAL:N	2.28	0.48
1:B:718:MET:HE2	1:B:722:ARG:HG3	1.95	0.48
1:A:712:HIS:CD2	1:A:728:CYS:HB3	2.48	0.48
1:B:371:LYS:HB3	1:B:545:GLU:HG2	1.95	0.48
1:A:766:TYR:O	1:A:769:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:HIS:HB3	1:B:499:SER:OG	2.13	0.48
1:A:684:MET:O	1:A:686:LYS:NZ	2.46	0.48
1:B:438:GLU:HA	1:B:441:LEU:HB2	1.95	0.48
1:A:281:ILE:CD1	1:A:592:ILE:HG21	2.41	0.48
1:A:673:ARG:HG2	1:B:163:ARG:HG3	1.96	0.48
1:B:14:LYS:O	1:B:18:ASN:OD1	2.32	0.48
1:B:133:PHE:CZ	1:B:163:ARG:HD3	2.48	0.48
1:A:447:CYS:HB3	1:A:450:CYS:HB2	1.96	0.48
1:B:504:LEU:CD1	1:B:652:ARG:HB3	2.44	0.48
1:A:758:TYR:CD1	1:A:793:THR:HG23	2.49	0.48
1:B:863:ILE:HG23	1:B:864:GLN:N	2.28	0.48
1:A:233:ASN:O	1:A:237:ARG:HD2	2.14	0.47
1:A:380:TRP:CE3	1:A:647:LEU:HD22	2.49	0.47
1:B:442:HIS:CE1	1:B:484:LEU:HD13	2.48	0.47
1:B:623:MET:O	1:B:628:VAL:HG12	2.14	0.47
1:A:331:PRO:HG3	1:A:859:TRP:HB2	1.96	0.47
1:A:844:ASP:OD1	1:A:849:SER:HB2	2.14	0.47
1:B:20:LEU:HD21	1:B:25:PHE:HB2	1.96	0.47
1:A:343:MET:HG3	1:A:344:THR:H	1.78	0.47
1:B:726:VAL:HG22	1:B:768:HIS:CE1	2.50	0.47
1:A:130:VAL:HG13	1:A:135:THR:HG21	1.97	0.47
1:A:173:ASN:HB3	1:A:176:THR:OG1	2.14	0.47
1:A:337:MET:CE	1:A:733:GLU:HG3	2.44	0.47
1:B:399:PHE:HB2	1:B:486:PHE:CD2	2.49	0.47
1:B:849:SER:OG	1:B:851:ILE:HG22	2.13	0.47
1:A:582:ARG:NH1	1:A:591:ASP:OD2	2.47	0.47
1:B:551:GLU:HG3	1:B:569:PHE:CG	2.50	0.47
1:A:282:GLU:OE2	1:A:285:LYS:HE3	2.14	0.47
1:A:344:THR:HG23	1:A:470:GLY:HA2	1.96	0.47
1:A:397:GLU:O	1:A:401:ARG:N	2.37	0.47
1:B:475:TRP:CD1	1:B:475:TRP:N	2.83	0.47
1:B:518:ILE:O	1:B:522:VAL:HG23	2.15	0.47
1:A:119:TYR:HB2	1:A:260:SER:N	2.29	0.46
1:A:187:MET:O	1:A:189:SER:N	2.49	0.46
1:B:77:VAL:HA	1:B:142:THR:HG23	1.97	0.46
1:B:633:GLN:O	1:B:634:HIS:HB3	2.15	0.46
1:A:118:THR:CG2	1:A:258:LEU:HB3	2.45	0.46
1:A:768:HIS:HB2	1:A:839:LEU:HG	1.97	0.46
1:B:373:LEU:HD11	1:B:635:LEU:HD13	1.96	0.46
1:B:703:TRP:HA	1:B:706:VAL:HG23	1.97	0.46
1:B:438:GLU:OE1	1:B:449:THR:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TRP:HH2	1:A:434:LEU:HD22	1.80	0.46
1:A:512:LEU:HD21	1:A:711:HIS:CE1	2.51	0.46
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.82	0.46
1:A:716:LEU:O	1:A:724:LEU:HB2	2.16	0.46
1:B:385:LEU:HD12	1:B:385:LEU:HA	1.80	0.46
1:B:730:ASN:O	1:B:733:GLU:HB2	2.15	0.46
1:B:504:LEU:HD13	1:B:652:ARG:HB3	1.98	0.46
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.64	0.46
1:A:341:MET:HA	1:A:462:LEU:HA	1.96	0.46
1:A:531:TYR:CE2	1:A:675:ALA:HB2	2.50	0.46
1:A:758:TYR:CE1	1:A:793:THR:HG23	2.50	0.46
1:B:557:MET:HB3	1:B:561:HIS:CD2	2.51	0.46
1:A:158:ALA:HB2	1:A:187:MET:HG2	1.96	0.46
1:B:393:MET:HG3	1:B:561:HIS:ND1	2.31	0.46
1:B:503:SER:O	1:B:504:LEU:HB2	2.16	0.46
1:B:333:ASP:OD1	1:B:739:ARG:NH1	2.37	0.46
1:B:832:SER:C	1:B:834:GLU:H	2.19	0.46
1:A:47:ARG:NE	1:A:49:GLU:OE2	2.38	0.45
1:B:824:MET:O	1:B:827:LYS:NZ	2.48	0.45
1:A:526:GLU:O	1:A:657:ARG:NH1	2.26	0.45
1:A:841:LYS:O	1:A:845:GLN:HG3	2.16	0.45
1:B:227:ASN:CG	1:B:228:ILE:H	2.19	0.45
1:B:355:PHE:C	1:B:357:GLU:H	2.19	0.45
1:B:475:TRP:CE3	1:B:600:GLY:HA2	2.51	0.45
1:A:549:ASN:O	1:A:552:MET:HE2	2.16	0.45
1:A:385:LEU:HD21	1:A:498:PHE:CE1	2.51	0.45
1:A:550:GLU:OE1	1:A:599:ARG:NH2	2.49	0.45
1:B:308:SER:OG	1:B:591:ASP:OD2	2.25	0.45
1:A:241:ASN:C	1:A:243:PHE:H	2.20	0.45
1:A:815:ARG:O	1:A:820:GLU:HG3	2.17	0.45
1:B:722:ARG:NH2	1:B:826:ASP:O	2.50	0.45
1:B:557:MET:SD	1:B:561:HIS:CD2	3.09	0.45
1:A:273:ASN:O	1:A:277:ILE:HG12	2.17	0.45
1:B:143:LEU:HD23	1:B:172:LEU:HD21	1.98	0.45
1:B:595:ARG:HG3	1:B:596:ARG:N	2.32	0.45
1:B:622:GLN:NE2	1:B:654:ARG:HD2	2.32	0.45
1:A:162:LEU:HD11	1:A:189:SER:HB3	1.98	0.45
1:A:345:ASP:OD1	1:A:350:GLY:HA3	2.17	0.45
1:B:188:PRO:HA	1:B:191:ILE:HG12	1.98	0.45
1:A:77:VAL:HG23	1:A:97:VAL:HG13	1.99	0.45
1:A:305:TYR:OH	1:A:308:SER:OG	2.01	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:SER:C	1:A:505:SER:H	2.20	0.45
1:B:207:ARG:HD2	1:B:235:ILE:HD12	1.99	0.45
1:B:302:THR:HG1	1:B:595:ARG:NH1	2.11	0.45
1:A:31:SER:HB2	1:A:248:LYS:H	1.82	0.44
1:A:284:ILE:H	1:A:284:ILE:HG12	1.51	0.44
1:A:650:VAL:O	1:A:654:ARG:HG2	2.17	0.44
1:A:29:LYS:HG3	1:A:214:SER:HB3	1.97	0.44
1:A:77:VAL:HG22	1:A:142:THR:HG23	1.97	0.44
1:A:132:VAL:HG13	3:A:2003:SAH:C2	2.45	0.44
1:A:339:THR:O	1:A:339:THR:HG22	2.17	0.44
1:B:77:VAL:HG22	1:B:142:THR:CG2	2.47	0.44
1:B:395:THR:HB	1:B:398:GLU:HB2	1.99	0.44
1:A:731:GLN:O	1:A:735:ILE:HG12	2.17	0.44
1:A:576:LYS:H	1:A:576:LYS:HD3	1.83	0.44
1:B:131:ASP:O	1:B:133:PHE:N	2.50	0.44
1:A:124:VAL:HG12	1:A:126:LEU:HD13	1.98	0.44
1:A:384:GLU:O	1:A:386:GLY:N	2.51	0.44
1:A:482:ARG:O	1:A:486:PHE:N	2.37	0.44
1:A:772:LEU:O	1:A:776:ALA:N	2.49	0.44
1:B:112:GLU:OE1	1:B:128:SER:OG	2.22	0.44
1:B:245:MET:O	1:B:245:MET:HG2	2.18	0.44
1:A:500:ARG:HE	1:A:518:ILE:HG23	1.82	0.44
1:B:292:TRP:CZ3	1:B:592:ILE:HD12	2.49	0.44
1:B:338:VAL:HG13	1:B:736:GLY:HA2	1.99	0.44
1:A:491:PHE:HZ	1:A:553:VAL:HG11	1.83	0.44
1:A:761:MET:O	1:A:761:MET:HG2	2.17	0.44
1:A:773:ARG:CZ	1:A:838:TYR:HE1	2.30	0.44
1:A:844:ASP:O	1:A:849:SER:N	2.41	0.44
1:A:478:TRP:O	1:A:481:ALA:N	2.51	0.43
1:A:817:TRP:O	1:A:821:ASN:HB3	2.18	0.43
1:B:299:PRO:HD2	1:B:300:TYR:CD2	2.52	0.43
1:B:539:ASP:OD1	1:B:599:ARG:HG2	2.18	0.43
1:A:337:MET:HE3	1:A:733:GLU:HG3	2.01	0.43
1:B:316:SER:H	1:B:346:THR:HB	1.83	0.43
1:A:621:ARG:HG2	1:A:674:PHE:CE2	2.54	0.43
1:A:712:HIS:CE1	1:A:847:CYS:SG	3.07	0.43
1:B:143:LEU:HD23	1:B:172:LEU:CD2	2.48	0.43
1:B:168:VAL:HG11	1:B:180:ILE:HD12	2.00	0.43
1:B:344:THR:OG1	1:B:345:ASP:N	2.51	0.43
1:A:27:ILE:HG22	1:A:28:TYR:N	2.32	0.43
1:A:118:THR:HG21	1:A:258:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:CG1	1:A:160:ARG:HE	2.30	0.43
1:A:632:ILE:HG21	1:A:632:ILE:HD13	1.72	0.43
1:A:636:THR:OG1	1:A:639:GLU:HB2	2.19	0.43
1:A:714:HIS:HD2	1:A:839:LEU:HD13	1.82	0.43
1:A:761:MET:HG3	1:A:803:TRP:CE2	2.54	0.43
1:A:781:SER:HB2	1:A:867:ILE:HD13	2.00	0.43
1:B:181:LYS:HE3	1:B:217:GLU:HG2	2.00	0.43
1:B:610:ASN:O	1:B:614:ASN:HB2	2.17	0.43
1:B:729:ARG:HD2	1:B:734:LEU:HG	2.01	0.43
1:B:344:THR:CG2	1:B:458:ARG:HA	2.49	0.43
1:B:521:ASP:O	1:B:524:LYS:HB2	2.18	0.43
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.67	0.43
1:B:368:GLU:OE1	1:B:371:LYS:NZ	2.51	0.43
1:A:246:ARG:O	1:A:247:HIS:C	2.57	0.43
1:B:260:SER:OG	1:B:261:GLY:N	2.52	0.43
1:B:295:ASP:OD2	1:B:582:ARG:NH2	2.52	0.43
1:B:431:PHE:O	1:B:433:GLU:N	2.52	0.43
1:B:491:PHE:HZ	1:B:553:VAL:HG11	1.82	0.43
1:B:652:ARG:HA	1:B:655:LEU:HD12	2.00	0.43
1:B:661:SER:HG	1:B:798:HIS:CD2	2.37	0.43
1:A:74:GLU:H	1:A:142:THR:HG21	1.83	0.42
1:B:529:ALA:O	1:B:669:PRO:HD2	2.19	0.42
1:B:690:ASP:OD1	1:B:690:ASP:N	2.52	0.42
1:A:573:TYR:OH	1:A:605:VAL:HG11	2.19	0.42
1:B:74:GLU:HA	1:B:96:ASN:O	2.19	0.42
1:B:500:ARG:HH22	1:B:659:ALA:HA	1.84	0.42
1:B:722:ARG:H	1:B:722:ARG:HG2	1.57	0.42
1:A:17:LEU:HB3	1:A:18:ASN:H	1.73	0.42
1:A:74:GLU:O	1:A:141:ASP:HB2	2.19	0.42
1:A:580:VAL:HG22	1:A:581:GLN:N	2.34	0.42
1:B:349:PHE:CZ	1:B:353:ARG:HD2	2.53	0.42
1:B:729:ARG:NH2	1:B:733:GLU:OE1	2.53	0.42
1:A:8:THR:HG23	1:A:11:GLU:HG3	2.00	0.42
1:A:777:ASN:O	1:A:781:SER:OG	2.27	0.42
1:B:73:PRO:HG2	1:B:94:LEU:HD13	2.01	0.42
1:B:262:THR:O	1:B:297:ASP:HB3	2.20	0.42
1:B:396:ARG:HH22	1:B:439:ARG:HE	1.67	0.42
1:B:161:THR:O	1:B:164:VAL:HG22	2.19	0.42
1:B:240:ILE:O	1:B:243:PHE:HB2	2.20	0.42
1:B:425:ALA:C	1:B:427:GLU:N	2.71	0.42
1:B:215:THR:OG1	1:B:217:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:LEU:HD23	1:B:484:LEU:HA	1.47	0.42
1:B:515:LEU:HD13	1:B:708:PHE:CE2	2.55	0.42
1:A:84:ARG:HG2	1:A:114:ILE:CD1	2.50	0.42
1:B:156:VAL:HG12	1:B:160:ARG:HE	1.84	0.42
1:B:599:ARG:HE	1:B:599:ARG:HB2	1.51	0.42
1:B:710:SER:HB3	1:B:729:ARG:HH11	1.84	0.42
1:A:248:LYS:NZ	1:A:249:LYS:HE3	2.35	0.42
1:A:747:SER:OG	1:A:750:GLU:HG3	2.19	0.42
1:B:832:SER:O	1:B:833:TRP:HB2	2.19	0.42
1:A:15:ASN:O	1:A:19:ALA:HB3	2.20	0.42
1:A:326:ARG:CB	1:A:739:ARG:HH11	2.33	0.42
1:A:623:MET:O	1:A:628:VAL:HG12	2.19	0.42
1:B:731:GLN:O	1:B:735:ILE:HG13	2.20	0.42
1:A:338:VAL:C	1:A:340:GLN:H	2.24	0.41
1:A:489:LEU:HA	1:A:491:PHE:CE1	2.55	0.41
1:B:355:PHE:O	1:B:357:GLU:N	2.53	0.41
1:B:380:TRP:CE2	1:B:384:GLU:HG3	2.55	0.41
1:B:500:ARG:HD2	1:B:506:GLY:O	2.20	0.41
1:B:595:ARG:NE	1:B:598:GLN:HG3	2.34	0.41
1:A:34:GLN:HB2	1:A:209:PRO:O	2.20	0.41
1:B:187:MET:HG3	1:B:188:PRO:HD2	2.02	0.41
1:B:479:LEU:O	1:B:482:ARG:N	2.53	0.41
1:A:280:ARG:HB2	1:A:448:GLU:HA	2.01	0.41
1:A:500:ARG:HG3	1:A:500:ARG:HH11	1.85	0.41
1:B:162:LEU:HD11	1:B:189:SER:HB2	2.03	0.41
1:A:207:ARG:HD2	1:A:235:ILE:HD12	2.02	0.41
1:B:82:CYS:SG	1:B:104:THR:HB	2.60	0.41
1:B:292:TRP:CZ2	1:B:307:GLY:HA3	2.55	0.41
1:B:551:GLU:O	1:B:551:GLU:HG2	2.20	0.41
1:B:551:GLU:OE2	1:B:570:LYS:HE3	2.21	0.41
1:A:121:TRP:HE1	1:A:262:THR:HG22	1.85	0.41
1:A:292:TRP:HA	1:A:308:SER:O	2.21	0.41
1:A:478:TRP:CD1	1:A:481:ALA:HB2	2.54	0.41
1:A:500:ARG:HD3	1:A:518:ILE:HD13	2.01	0.41
1:A:756:LYS:O	1:A:760:GLN:HB2	2.20	0.41
1:B:269:SER:HB2	1:B:362:ARG:HH11	1.84	0.41
1:B:818:ILE:HG22	1:B:819:GLN:N	2.35	0.41
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.55	0.41
1:A:552:MET:C	1:A:554:THR:N	2.72	0.41
1:B:507:VAL:HG23	1:B:798:HIS:CE1	2.56	0.41
1:B:653:GLU:OE1	1:B:657:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG21	1:A:592:ILE:CD1	2.50	0.41
1:A:636:THR:O	1:A:640:GLU:HG2	2.21	0.41
1:A:780:CYS:O	1:A:882:TYR:HE2	2.04	0.41
1:B:373:LEU:HD21	1:B:629:PHE:CE2	2.56	0.41
1:B:475:TRP:HZ3	1:B:576:LYS:HG3	1.85	0.41
1:B:673:ARG:HE	1:B:673:ARG:HB2	1.70	0.41
1:A:478:TRP:HD1	1:A:481:ALA:HB2	1.86	0.41
1:A:682:ASN:ND2	1:A:693:GLN:HG2	2.36	0.41
1:B:108:PRO:C	1:B:110:HIS:H	2.23	0.41
1:A:87:TRP:HH2	1:A:219:TYR:HE2	1.69	0.41
1:A:531:TYR:O	1:A:666:VAL:HA	2.21	0.41
1:A:614:ASN:O	1:A:618:GLN:HG2	2.21	0.41
1:A:853:LEU:N	1:A:853:LEU:HD23	2.36	0.41
1:A:62:LEU:HD22	1:A:87:TRP:CG	2.56	0.40
1:A:77:VAL:CG2	1:A:97:VAL:HG13	2.51	0.40
1:A:298:HIS:H	1:A:298:HIS:CD2	2.40	0.40
1:A:438:GLU:HA	1:A:441:LEU:HB2	2.02	0.40
1:A:761:MET:SD	1:A:793:THR:HG21	2.60	0.40
1:A:850:LEU:O	1:A:853:LEU:HG	2.21	0.40
1:A:56:SER:C	1:A:58:GLY:H	2.25	0.40
1:A:77:VAL:HA	1:A:142:THR:HG23	2.04	0.40
1:A:283:LYS:HD2	1:A:287:GLU:OE2	2.21	0.40
1:A:353:ARG:NH1	1:A:353:ARG:HG2	2.36	0.40
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.91	0.40
1:B:395:THR:HG22	1:B:397:GLU:N	2.36	0.40
1:B:87:TRP:CZ3	1:B:144:LEU:HB3	2.56	0.40
1:A:281:ILE:HA	1:A:281:ILE:HD12	1.64	0.40
1:B:395:THR:HG22	1:B:396:ARG:N	2.36	0.40
1:A:122:ASN:OD1	1:A:122:ASN:N	2.55	0.40
1:B:74:GLU:O	1:B:141:ASP:HB2	2.21	0.40
1:B:106:GLY:O	1:B:110:HIS:HB2	2.21	0.40
1:B:442:HIS:O	1:B:445:GLY:N	2.54	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	847/911 (93%)	698 (82%)	115 (14%)	34 (4%)	3 14
1	B	829/911 (91%)	698 (84%)	107 (13%)	24 (3%)	4 20
All	All	1676/1822 (92%)	1396 (83%)	222 (13%)	58 (4%)	3 17

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LYS
1	A	250	ALA
1	A	264	ASN
1	A	265	ILE
1	A	267	ILE
1	A	268	GLU
1	A	291	SER
1	A	385	LEU
1	A	429	SER
1	A	597	ASP
1	A	785	SER
1	A	786	HIS
1	A	791	SER
1	A	873	LEU
1	B	9	LEU
1	B	33	ILE
1	B	245	MET
1	B	246	ARG
1	B	267	ILE
1	B	401	ARG
1	B	402	LYS
1	B	405	SER
1	B	429	SER
1	B	432	TRP
1	B	467	LYS
1	B	863	ILE
1	A	9	LEU
1	A	17	LEU
1	A	212	ARG
1	A	242	ARG
1	A	405	SER

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Mol	Chain	Res	Type
1	A	465	PHE
1	A	675	ALA
1	B	265	ILE
1	B	598	GLN
1	A	269	SER
1	A	322	ASN
1	A	340	GLN
1	A	469	LYS
1	A	471	SER
1	B	227	ASN
1	B	462	LEU
1	B	466	GLY
1	B	791	SER
1	A	39	THR
1	A	319	SER
1	A	731	GLN
1	A	763	SER
1	B	431	PHE
1	B	832	SER
1	B	250	ALA
1	B	634	HIS
1	B	873	LEU
1	A	11	GLU
1	A	33	ILE
1	A	188	PRO
1	A	691	ILE
1	B	426	VAL

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	607/790 (77%)	587 (97%)	20 (3%)	38	67
1	B	582/790 (74%)	564 (97%)	18 (3%)	40	68
All	All	1189/1580 (75%)	1151 (97%)	38 (3%)	39	68

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	84	ARG
1	A	237	ARG
1	A	243	PHE
1	A	247	HIS
1	A	270	GLU
1	A	296	GLN
1	A	301	LYS
1	A	337	MET
1	A	353	ARG
1	A	379	GLU
1	A	385	LEU
1	A	396	ARG
1	A	399	PHE
1	A	576	LYS
1	A	579	ARG
1	A	597	ASP
1	A	690	ASP
1	A	700	TRP
1	A	773	ARG
1	B	20	LEU
1	B	26	GLN
1	B	61	LYS
1	B	153	ASN
1	B	163	ARG
1	B	187	MET
1	B	298	HIS
1	B	301	LYS
1	B	362	ARG
1	B	396	ARG
1	B	438	GLU
1	B	576	LYS
1	B	599	ARG
1	B	621	ARG
1	B	690	ASP
1	B	724	LEU
1	B	729	ARG
1	B	737	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	322	ASN
1	A	502	ASN
1	A	581	GLN
1	A	864	GLN
1	B	561	HIS
1	B	622	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	1003	-	24,28,28	1.13	3 (12%)	25,40,40	2.11	5 (20%)
3	SAH	A	2003	-	24,28,28	1.23	2 (8%)	25,40,40	1.87	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	B	1003	-	-	4/11/31/31	0/3/3/3
3	SAH	A	2003	-	-	4/11/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2003	SAH	C2-N3	2.94	1.36	1.32
3	B	1003	SAH	OXT-C	-2.56	1.22	1.30
3	A	2003	SAH	OXT-C	-2.47	1.22	1.30
3	B	1003	SAH	C2-N3	2.41	1.36	1.32
3	B	1003	SAH	C2-N1	2.17	1.37	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1003	SAH	N3-C2-N1	-6.55	118.44	128.68
3	A	2003	SAH	C5'-SD-CG	-5.32	86.32	102.27
3	A	2003	SAH	N3-C2-N1	-5.11	120.69	128.68
3	B	1003	SAH	C5'-SD-CG	-4.88	87.63	102.27
3	B	1003	SAH	C1'-N9-C4	-3.45	120.58	126.64
3	A	2003	SAH	OXT-C-O	-2.63	118.11	124.09
3	B	1003	SAH	OXT-C-O	-2.62	118.14	124.09
3	A	2003	SAH	OXT-C-CA	2.30	121.21	113.38
3	A	2003	SAH	C2'-C3'-C4'	2.24	106.99	102.64
3	B	1003	SAH	C2'-C3'-C4'	2.18	106.89	102.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	SAH	CA-CB-CG-SD
3	A	2003	SAH	CA-CB-CG-SD
3	A	2003	SAH	CB-CG-SD-C5'
3	B	1003	SAH	O-C-CA-CB
3	A	2003	SAH	OXT-C-CA-CB
3	B	1003	SAH	OXT-C-CA-CB
3	A	2003	SAH	O-C-CA-CB
3	B	1003	SAH	CB-CG-SD-C5'

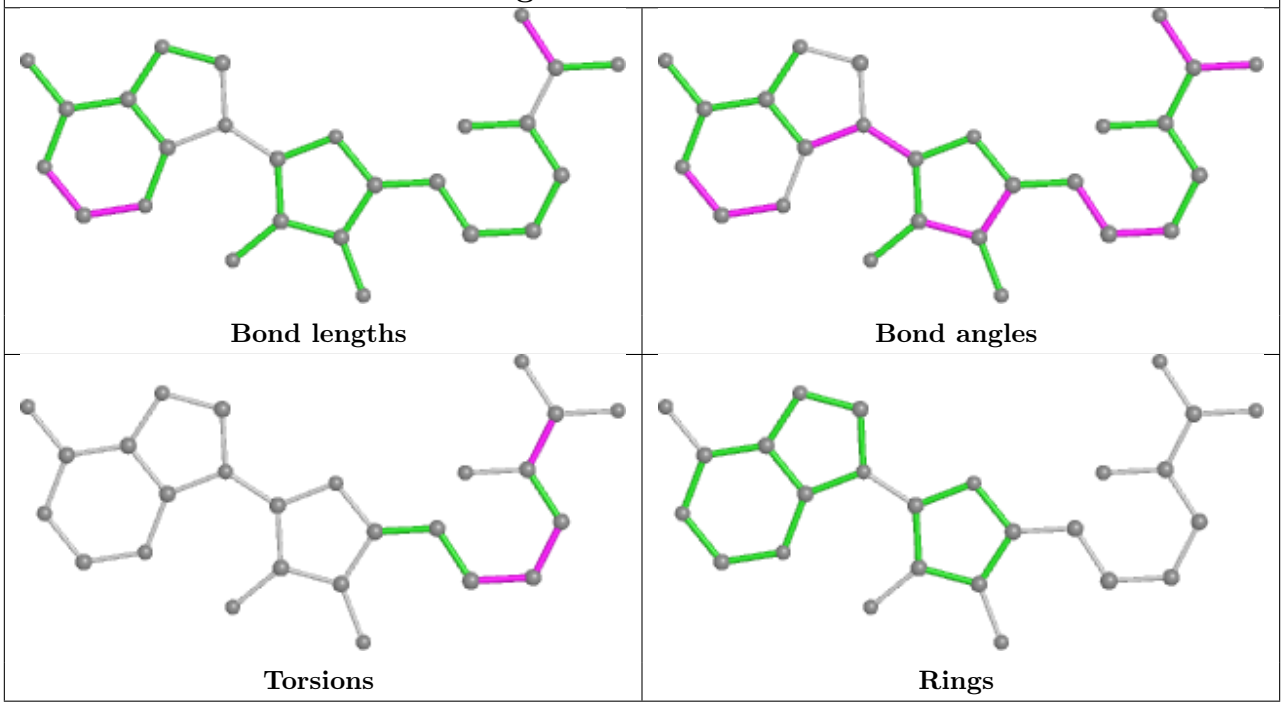
There are no ring outliers.

1 monomer is involved in 4 short contacts:

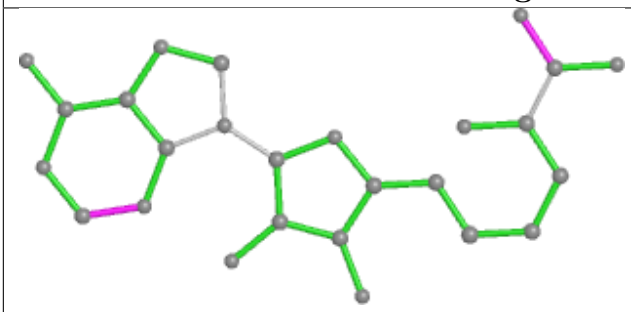
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2003	SAH	4	0

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.

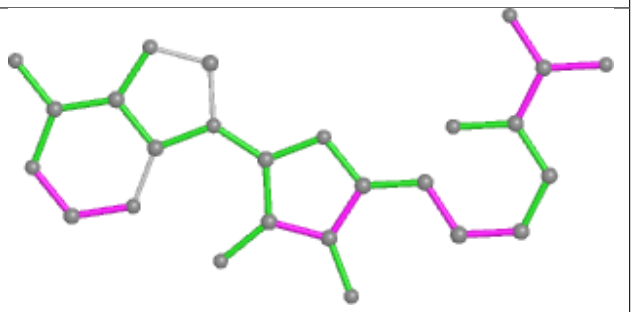
Ligand SAH B 1003



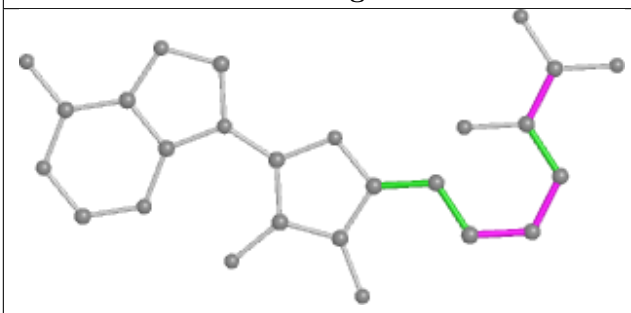
Ligand SAH A 2003



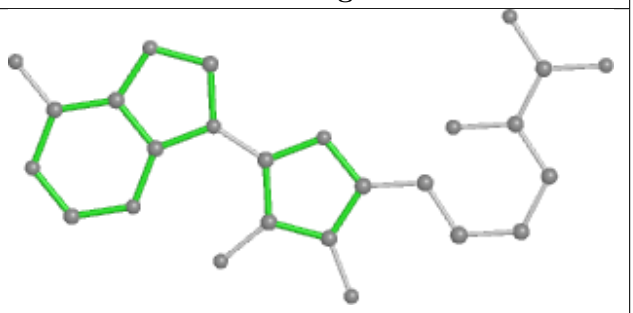
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	857/911 (94%)	-0.61	2 (0%) 95 89	9, 26, 47, 73	0
1	B	843/911 (92%)	-0.60	0 100 100	11, 27, 50, 87	0
All	All	1700/1822 (93%)	-0.60	2 (0%) 95 91	9, 26, 49, 87	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	PHE	3.5
1	A	466	GLY	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
2	ZN	A	2001	1/1	0.90	0.29	133,133,133,133	0
3	SAH	B	1003	26/26	0.91	0.24	37,51,57,79	0
3	SAH	A	2003	26/26	0.93	0.24	42,55,62,84	0

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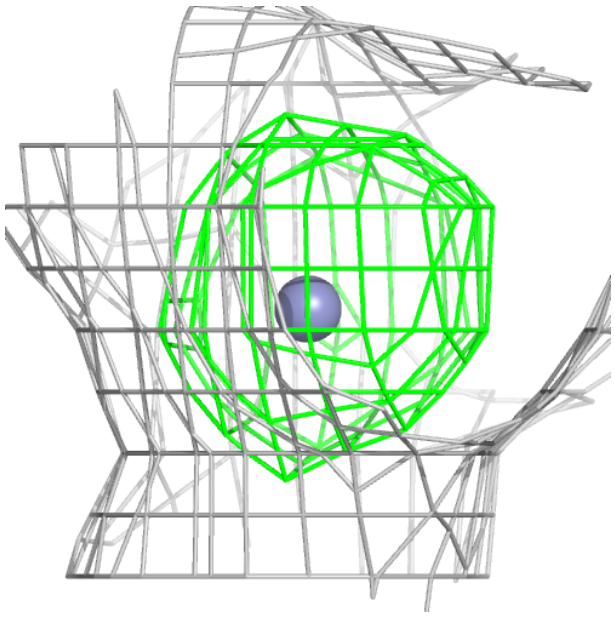
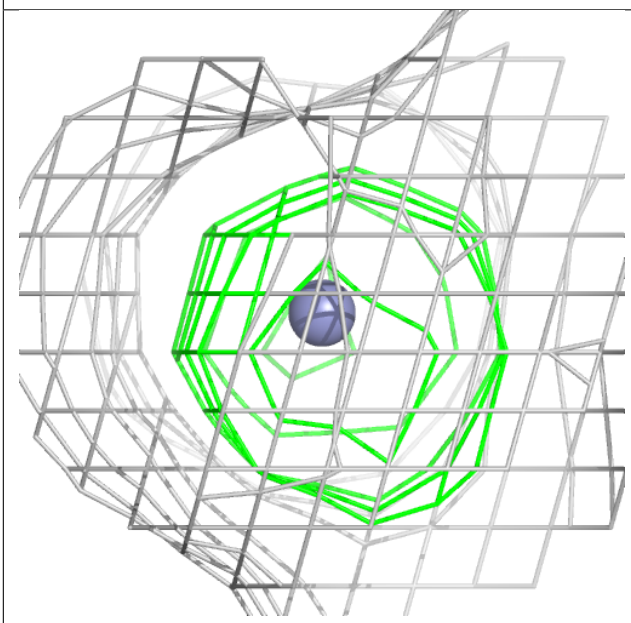
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	2002	1/1	0.94	0.26	128,128,128,128	0
2	ZN	B	1001	1/1	0.99	0.06	23,23,23,23	0
2	ZN	B	1002	1/1	1.00	0.10	20,20,20,20	0

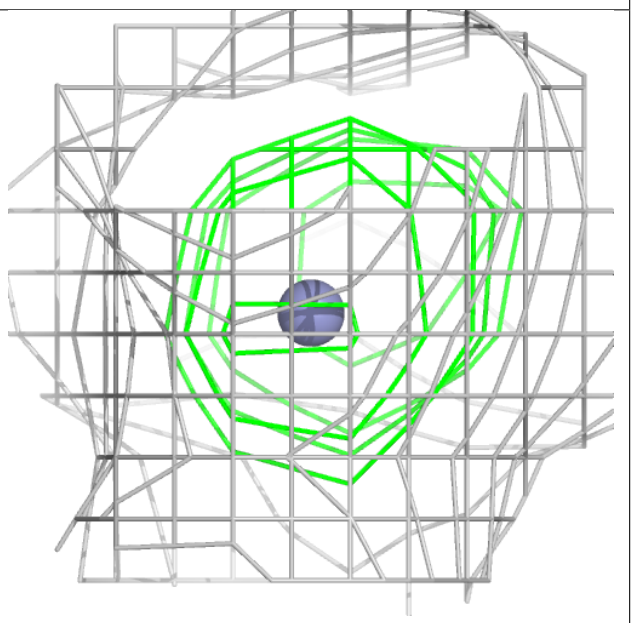
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN A 2001:

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

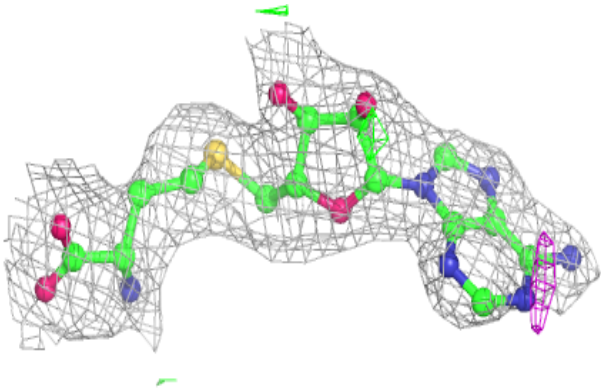


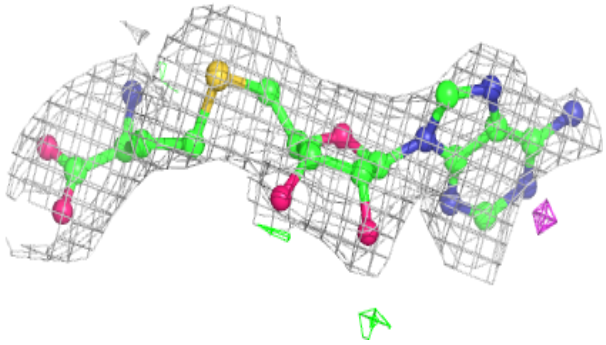


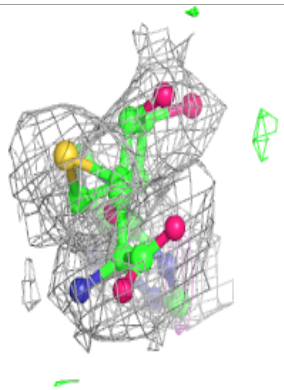


Electron density around SAH B 1003:

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

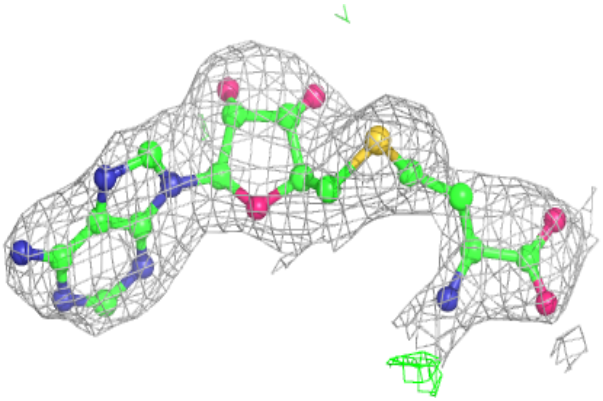


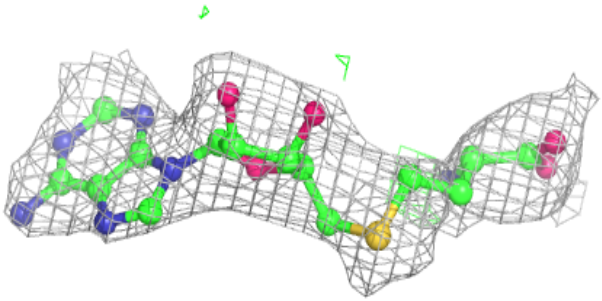


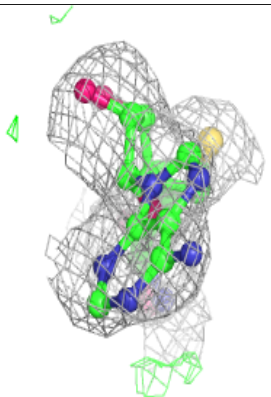


Electron density around SAH A 2003:

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

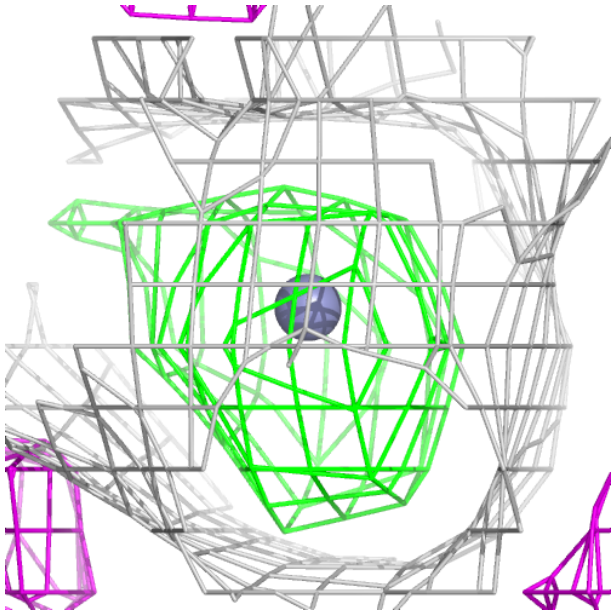


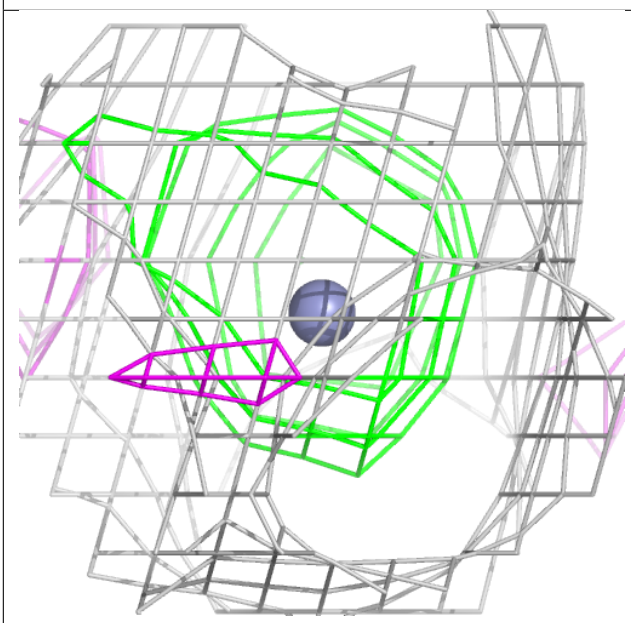


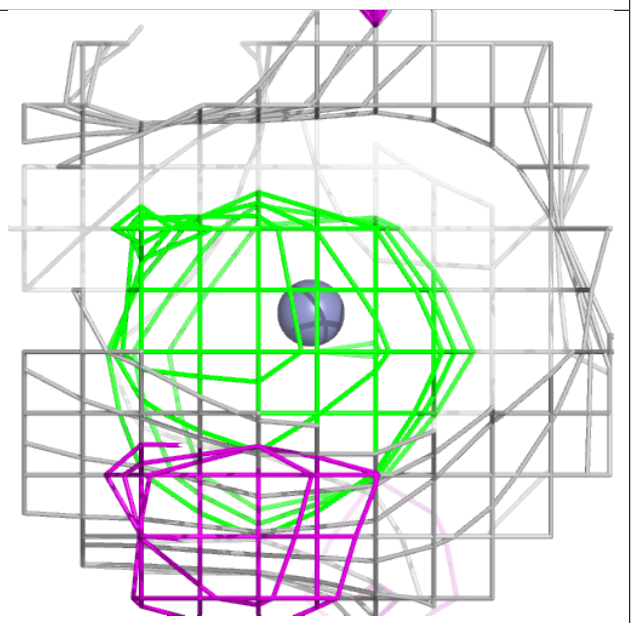


Electron density around ZN A 2002:

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

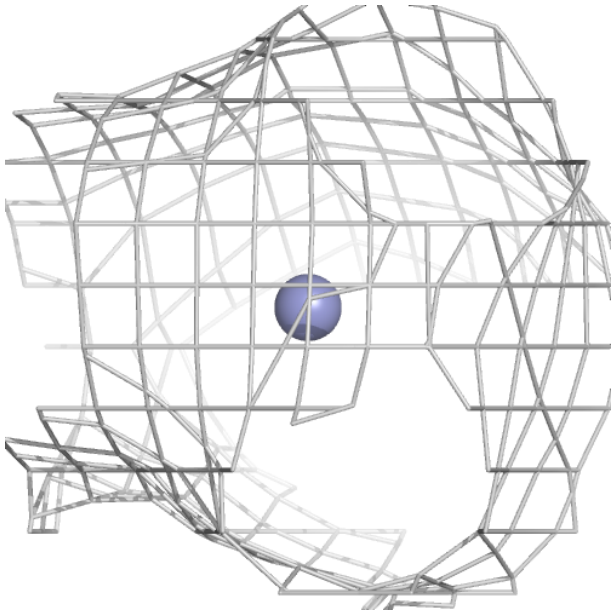


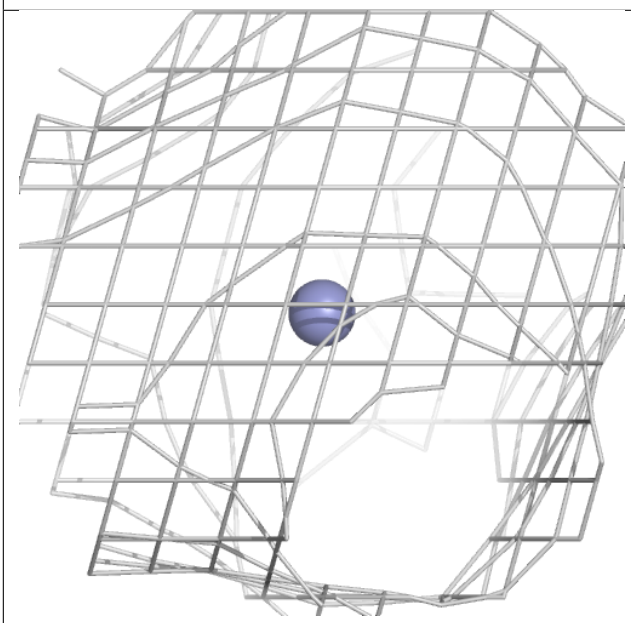


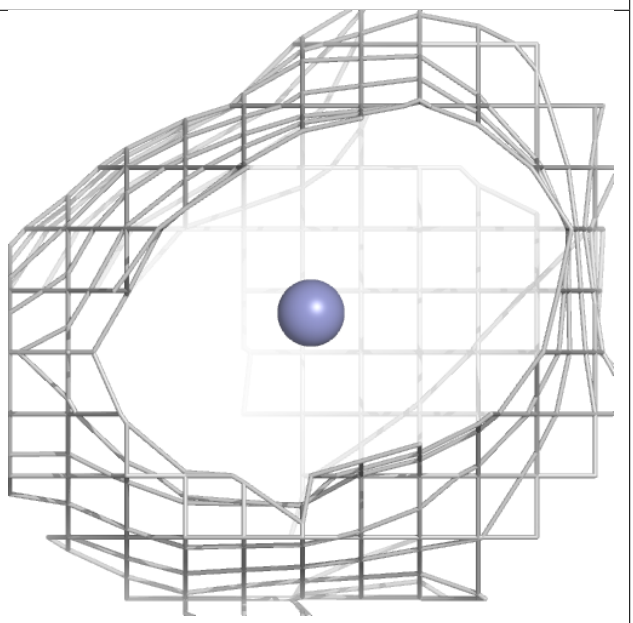


Electron density around ZN B 1001:

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

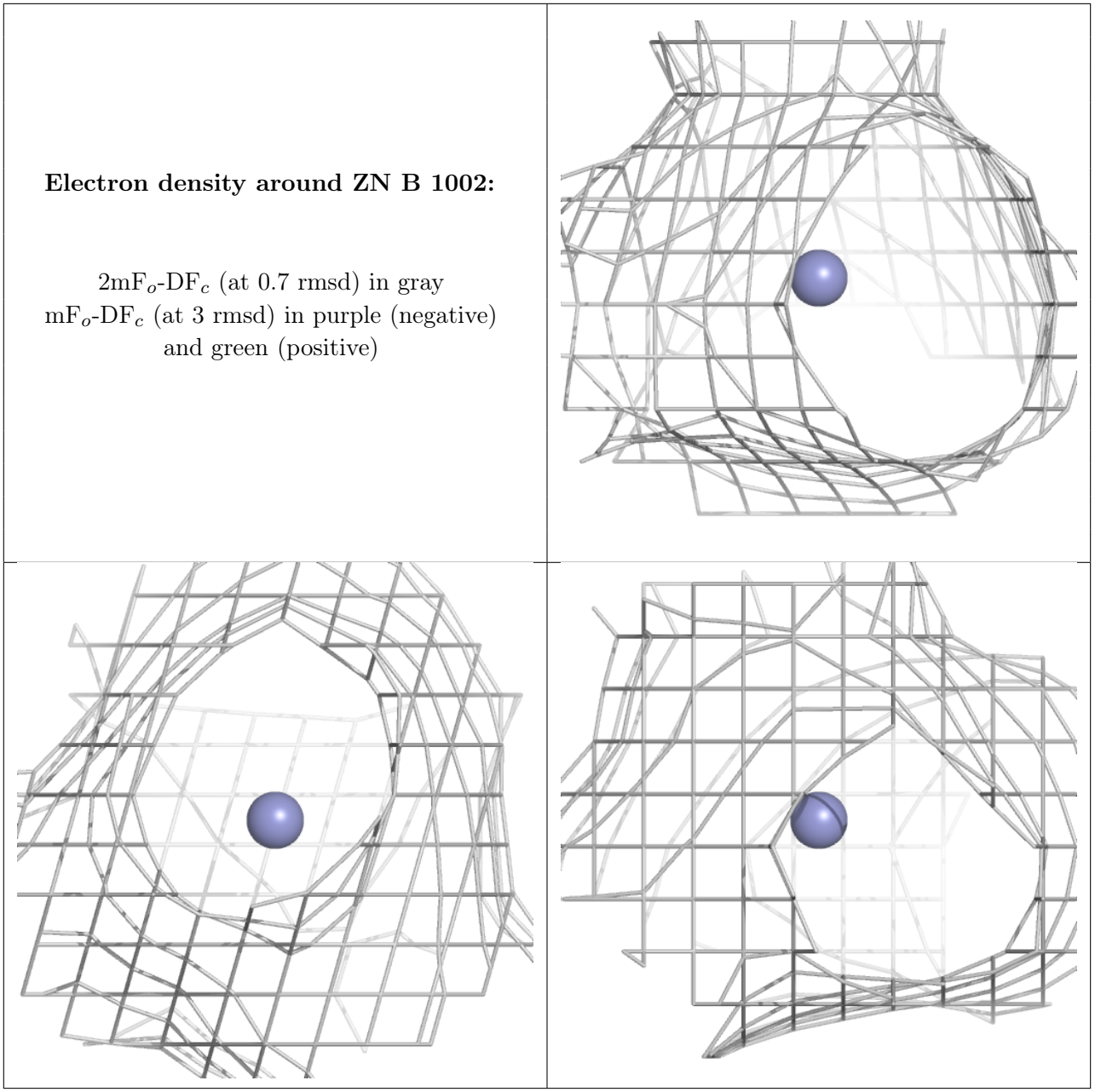






Electron density around ZN B 1002:

$2mF_o$-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

There are no such residues in this entry.