



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 AM UTC

PDB ID : 8H5Z / pdb_00008h5z
Title : Crystal structure of RadD/ATP analogue complex
Authors : Yan, X.X.; Tian, L.F.
Deposited on : 2022-10-14
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

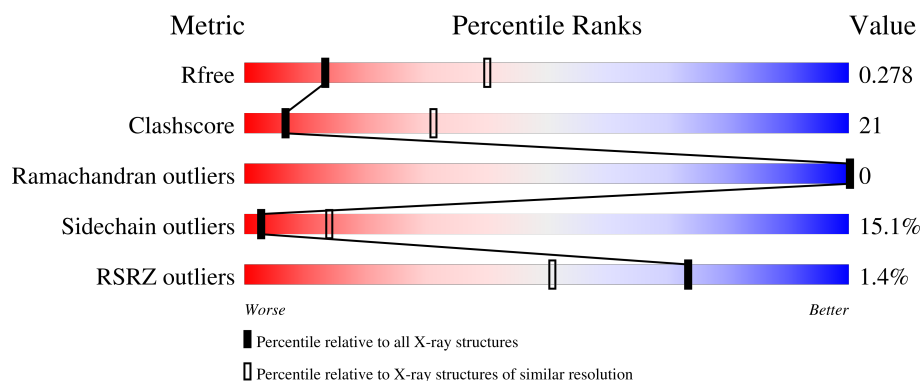
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	586	0% 56% 31% 8% 5%
1	B	586	2% 57% 31% 7% 5%

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
2	AGS	A	601	-	-	X	-
2	AGS	B	601	-	-	X	-

2 Entry composition [i](#)

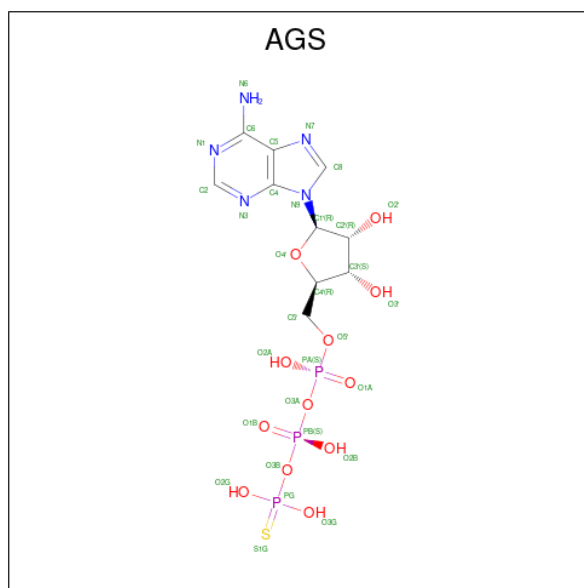
There are 3 unique types of molecules in this entry. The entry contains 8670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative DNA repair helicase RadD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	555	Total	C	N	O	S	0	0	0
			4299	2737	775	770	17			
1	A	559	Total	C	N	O	S	0	0	0
			4307	2742	775	774	16			

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

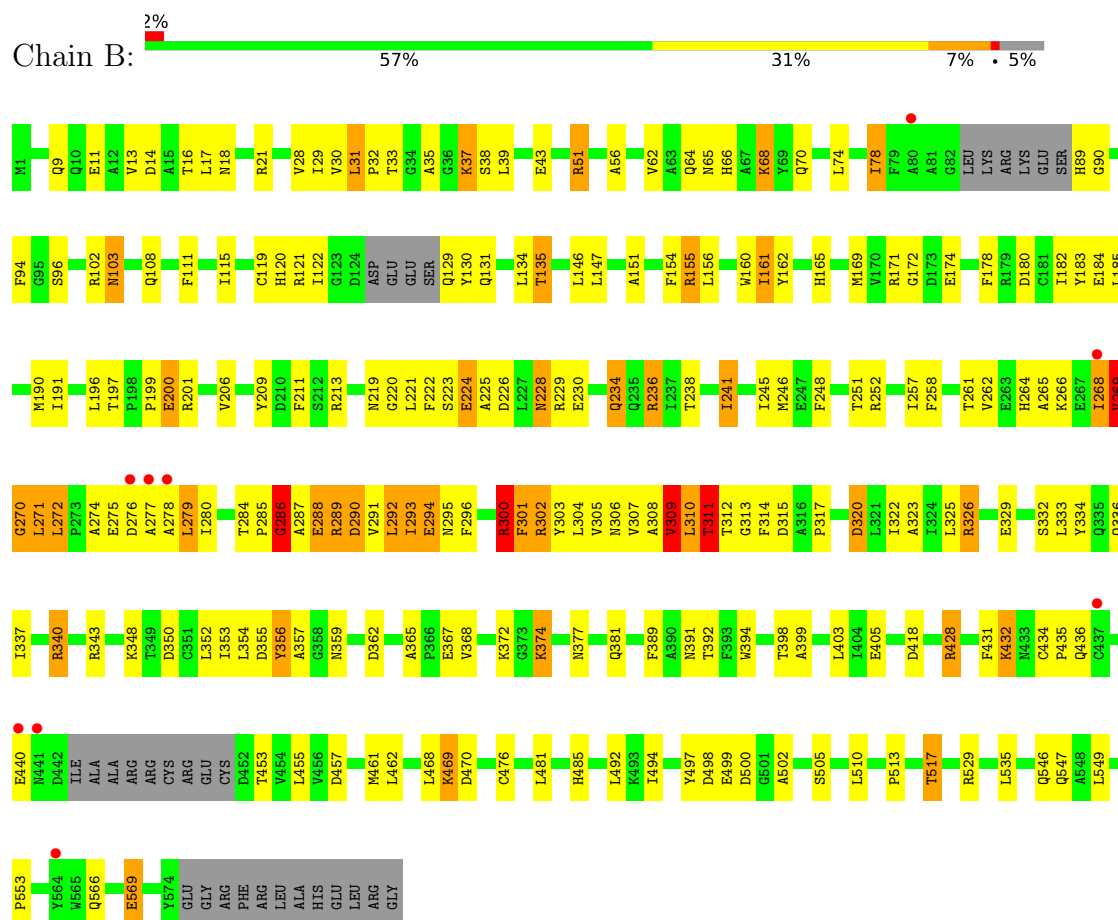
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0

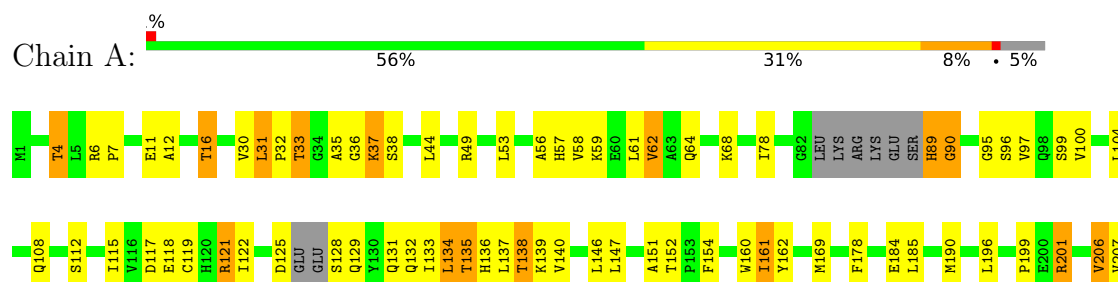
3 Residue-property plots

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

• Molecule 1: Putative DNA repair helicase RadD



• Molecule 1: Putative DNA repair helicase RadD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.59Å 79.17Å 109.82Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.98-3.00) 99.2 (19.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.98Å)	Xtriage
Refinement program	PHENIX 1.12-2829_1692	Depositor
R, R_{free}	0.239 , 0.281 0.239 , 0.278	Depositor DCC
R_{free} test set	1488 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8670	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4004e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 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	0.50	2/4408 (0.0%)	0.95	27/5991 (0.5%)
1	B	0.51	2/4400 (0.0%)	1.00	25/5977 (0.4%)
All	All	0.50	4/8808 (0.0%)	0.98	52/11968 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	VAL	C-N	10.26	1.47	1.33
1	A	439	ALA	C-N	-9.05	1.26	1.33
1	B	300	ARG	C-N	7.24	1.43	1.33
1	A	453	THR	CA-C	-6.80	1.44	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	GLY	CA-C-N	17.13	148.19	121.98
1	B	286	GLY	C-N-CA	17.13	148.19	121.98
1	B	268	ILE	CB-CA-C	-13.30	89.48	111.29
1	B	432	LYS	CB-CA-C	13.00	136.30	110.42
1	A	437	CYS	CA-C-N	11.23	139.05	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	CYS	C-N-CA	11.23	139.05	121.19
1	B	270	GLY	N-CA-C	-10.95	87.24	113.18
1	B	432	LYS	N-CA-C	-10.75	87.89	110.80
1	A	440	GLU	CB-CA-C	-10.52	98.99	114.87
1	B	271	LEU	N-CA-C	10.17	139.49	111.00
1	A	455	LEU	N-CA-C	10.15	124.87	108.63
1	B	271	LEU	N-CA-CB	-10.09	93.35	110.50
1	A	440	GLU	N-CA-CB	-10.04	99.27	109.51
1	A	441	ASN	N-CA-C	9.82	131.71	110.80
1	B	310	LEU	N-CA-CB	-9.53	94.31	110.50
1	B	300	ARG	CA-C-N	9.40	138.62	121.70
1	B	300	ARG	C-N-CA	9.40	138.62	121.70
1	B	277	ALA	CA-C-N	9.35	139.40	121.54
1	B	277	ALA	C-N-CA	9.35	139.40	121.54
1	A	433	ASN	CB-CA-C	-8.73	93.05	110.42
1	B	269	VAL	CB-CA-C	8.66	131.44	111.77
1	A	133	ILE	N-CA-C	-8.36	100.76	110.21
1	A	90	GLY	N-CA-C	7.96	136.39	113.30
1	A	432	LYS	CB-CA-C	-7.68	96.68	111.97
1	A	244	GLN	N-CA-C	7.24	131.28	111.00
1	A	454	VAL	N-CA-C	-6.70	98.78	108.36
1	A	243	SER	N-CA-C	6.51	118.53	110.91
1	A	210	ASP	CA-C-N	6.23	132.92	121.70
1	A	210	ASP	C-N-CA	6.23	132.92	121.70
1	A	442	ASP	CA-C-N	6.23	132.92	121.70
1	A	442	ASP	C-N-CA	6.23	132.92	121.70
1	B	272	LEU	CA-C-N	-5.98	112.36	119.84
1	B	272	LEU	C-N-CA	-5.98	112.36	119.84
1	B	311	THR	CA-C-N	5.76	132.06	121.70
1	B	311	THR	C-N-CA	5.76	132.06	121.70
1	B	313	GLY	N-CA-C	-5.76	101.11	110.55
1	A	285	PRO	N-CA-C	5.58	120.88	113.40
1	B	172	GLY	CA-C-N	-5.54	110.95	121.54
1	B	172	GLY	C-N-CA	-5.54	110.95	121.54
1	A	439	ALA	CB-CA-C	-5.47	99.53	110.42
1	A	283	ASP	N-CA-C	5.46	119.03	111.71
1	A	432	LYS	N-CA-C	-5.34	102.42	110.06
1	A	439	ALA	N-CA-C	5.30	122.09	110.80
1	A	293	ILE	N-CA-C	5.27	125.77	111.00
1	B	300	ARG	N-CA-C	5.23	119.14	111.04
1	B	356	TYR	N-CA-C	-5.22	103.02	110.59
1	A	432	LYS	CA-C-N	5.17	131.42	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	LYS	C-N-CA	5.17	131.42	121.54
1	A	437	CYS	CB-CA-C	5.17	126.72	114.11
1	B	289	ARG	N-CA-C	-5.15	105.15	111.75
1	B	301	PHE	N-CA-CB	-5.08	101.86	110.50
1	A	210	ASP	N-CA-C	-5.01	100.10	108.32

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	LEU	Peptide
1	A	243	SER	Peptide
1	A	292	LEU	Peptide
1	B	286	GLY	Peptide
1	B	292	LEU	Peptide
1	B	300	ARG	Peptide
1	B	309	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4307	0	4103	170	0
1	B	4299	0	4128	189	0
2	A	31	0	12	13	0
2	B	31	0	12	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	8670	0	8255	362	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 21.

All (362) 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:B:37:LYS:HB3	2:B:601:AGS:S1G	1.50	1.51
1:A:36:GLY:HA2	2:A:601:AGS:O1B	1.44	1.17
1:B:37:LYS:CB	2:B:601:AGS:S1G	2.32	1.16
1:A:37:LYS:HE3	2:A:601:AGS:S1G	1.88	1.13
1:B:64:GLN:NE2	1:B:68:LYS:HZ1	1.46	1.13
1:B:268:ILE:HG22	1:B:268:ILE:O	1.48	1.12
1:B:308:ALA:HB1	1:B:310:LEU:HB2	1.34	1.08
1:A:36:GLY:CA	2:A:601:AGS:O1B	2.06	1.03
1:B:290:ASP:HA	1:B:293:ILE:HG22	1.41	1.02
1:B:37:LYS:N	2:B:601:AGS:S1G	2.34	1.01
1:B:37:LYS:HD2	2:B:601:AGS:S1G	2.03	0.98
1:B:39:LEU:HG	2:B:601:AGS:N6	1.83	0.93
1:A:210:ASP:OD1	1:A:212:SER:N	2.04	0.90
1:A:89:HIS:O	1:A:89:HIS:ND1	2.05	0.90
1:B:266:LYS:HA	1:B:269:VAL:CG1	2.04	0.88
1:B:265:ALA:O	1:B:269:VAL:HG12	1.74	0.87
1:A:210:ASP:HA	1:A:211:PHE:HB2	1.56	0.87
1:A:249:ALA:O	1:A:302:ARG:NH2	2.07	0.87
1:B:285:PRO:HB2	1:B:287:ALA:H	1.39	0.87
1:A:428:ARG:HE	1:A:435:PRO:HG3	1.41	0.86
1:B:16:THR:HG23	1:B:29:ILE:HD11	1.58	0.86
1:B:224:GLU:O	1:B:228:ASN:ND2	2.09	0.86
1:A:265:ALA:HB1	1:A:279:LEU:HD21	1.58	0.85
1:A:432:LYS:O	1:A:432:LYS:HG3	1.73	0.85
1:B:268:ILE:O	1:B:268:ILE:CG2	2.24	0.85
1:B:64:GLN:HE21	1:B:68:LYS:HZ1	1.22	0.85
1:B:16:THR:CG2	1:B:29:ILE:HD11	2.07	0.83
1:B:307:VAL:HB	1:B:308:ALA:HA	1.61	0.83
1:A:441:ASN:O	1:A:451:CYS:N	2.12	0.82
1:B:201:ARG:NH1	1:B:334:TYR:OH	2.14	0.80
1:A:243:SER:O	1:A:243:SER:OG	1.96	0.79
1:B:428:ARG:HD3	1:B:434:CYS:HA	1.66	0.78
1:B:332:SER:OG	1:B:367:GLU:OE1	2.01	0.77
1:A:152:THR:HG21	1:A:336:GLN:HG3	1.66	0.76
1:B:252:ARG:O	1:B:302:ARG:NH1	2.18	0.76
1:A:33:THR:HA	2:A:601:AGS:O3G	1.87	0.75
1:A:131:GLN:O	1:A:135:THR:OG1	2.04	0.75
1:A:317:PRO:O	1:A:348:LYS:NZ	2.18	0.75
1:B:51:ARG:NH1	1:B:90:GLY:O	2.20	0.75
1:B:257:ILE:HG23	1:B:323:ALA:HB3	1.66	0.75
1:B:306:ASN:HB3	1:B:308:ALA:HB2	1.69	0.75
1:B:320:ASP:OD1	1:B:320:ASP:N	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:PRO:HD3	1:B:185:LEU:HB3	1.70	0.74
1:B:315:ASP:O	1:B:343:ARG:NH2	2.21	0.73
1:A:432:LYS:O	1:A:432:LYS:CG	2.28	0.73
1:B:274:ALA:C	1:B:276:ASP:HA	2.14	0.73
1:B:64:GLN:O	1:B:68:LYS:HG2	1.89	0.73
1:B:300:ARG:HB2	1:B:301:PHE:HB3	1.69	0.72
1:A:118:GLU:OE2	1:A:121:ARG:NH1	2.23	0.72
1:A:33:THR:C	2:A:601:AGS:O3G	2.32	0.72
1:B:64:GLN:O	1:B:68:LYS:CG	2.38	0.71
1:B:64:GLN:NE2	1:B:68:LYS:NZ	2.32	0.71
1:B:266:LYS:HA	1:B:269:VAL:HG11	1.71	0.71
1:B:131:GLN:O	1:B:135:THR:OG1	2.09	0.70
1:B:405:GLU:HG3	1:B:529:ARG:HB3	1.72	0.70
1:A:536:ARG:O	1:A:546:GLN:NE2	2.25	0.70
1:B:230:GLU:O	1:B:234:GLN:NE2	2.21	0.70
1:A:506:GLU:OE1	1:A:570:LYS:NZ	2.25	0.69
1:B:39:LEU:HG	2:B:601:AGS:HN61	1.55	0.69
1:A:470:ASP:O	1:A:560:MET:N	2.26	0.69
1:B:434:CYS:SG	1:B:440:GLU:HB2	2.33	0.69
1:B:278:ALA:HB3	1:B:301:PHE:CE1	2.28	0.68
1:A:146:LEU:HD22	1:A:178:PHE:HE1	1.59	0.68
1:B:37:LYS:CD	2:B:601:AGS:S1G	2.79	0.68
1:B:37:LYS:CA	2:B:601:AGS:S1G	2.82	0.68
1:B:266:LYS:CA	1:B:269:VAL:HG12	2.25	0.67
1:B:372:LYS:HG2	1:B:377:ASN:HB2	1.75	0.67
1:A:64:GLN:O	1:A:68:LYS:HG3	1.95	0.67
1:A:206:VAL:HG13	1:A:207:VAL:H	1.60	0.67
1:A:37:LYS:CE	2:A:601:AGS:S1G	2.78	0.66
1:A:37:LYS:N	2:A:601:AGS:O1B	2.28	0.66
1:A:219:ASN:OD1	1:A:220:GLY:N	2.28	0.66
1:A:296:PHE:HB2	1:A:301:PHE:CZ	2.30	0.66
1:B:311:THR:HB	1:B:312:THR:HA	1.78	0.66
1:B:498:ASP:HB2	1:B:502:ALA:HB3	1.77	0.65
1:A:439:ALA:HA	1:A:455:LEU:HD22	1.78	0.65
1:A:442:ASP:OD1	1:A:443:ILE:N	2.30	0.64
1:A:557:VAL:HB	1:A:569:GLU:HB3	1.78	0.64
1:B:64:GLN:CD	1:B:68:LYS:HZ1	2.04	0.64
1:B:68:LYS:HD2	2:B:601:AGS:O1B	1.96	0.64
1:B:295:ASN:HB2	1:B:301:PHE:HD2	1.62	0.64
1:B:329:GLU:OE2	1:B:329:GLU:N	2.26	0.64
1:A:418:ASP:OD1	1:A:418:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLU:OE1	1:B:234:GLN:NE2	2.30	0.64
1:A:32:PRO:HD3	1:A:185:LEU:HB3	1.79	0.64
1:B:279:LEU:CD2	1:B:305:VAL:HB	2.27	0.64
1:A:308:ALA:HB3	1:A:310:LEU:HB2	1.80	0.64
1:A:292:LEU:H	1:A:295:ASN:H	1.46	0.64
1:B:285:PRO:O	1:B:289:ARG:N	2.28	0.64
1:B:461:MET:HE2	1:B:569:GLU:HG2	1.79	0.63
1:A:296:PHE:HB2	1:A:301:PHE:CE1	2.34	0.63
1:A:405:GLU:HG3	1:A:529:ARG:HB3	1.81	0.63
2:B:601:AGS:PA	2:B:601:AGS:H3'	2.39	0.63
1:A:162:TYR:HA	1:A:178:PHE:O	1.98	0.63
1:B:155:ARG:HG3	1:B:155:ARG:HH11	1.64	0.62
1:B:165:HIS:NE2	1:B:184:GLU:OE2	2.28	0.62
1:B:266:LYS:CA	1:B:269:VAL:CG1	2.77	0.62
1:A:59:LYS:O	1:A:62:VAL:HG23	1.98	0.62
1:A:329:GLU:N	1:A:329:GLU:OE2	2.29	0.62
1:B:285:PRO:C	1:B:289:ARG:H	2.06	0.62
1:B:35:ALA:N	2:B:601:AGS:O2G	2.32	0.62
1:B:64:GLN:HG2	1:B:68:LYS:HE2	1.81	0.62
1:A:232:LYS:O	1:A:233:LYS:HB3	1.98	0.62
1:B:197:THR:OG1	1:B:343:ARG:O	2.19	0.61
1:A:321:LEU:HD21	1:A:354:LEU:HD12	1.80	0.61
1:B:317:PRO:O	1:B:348:LYS:NZ	2.33	0.61
1:A:468:LEU:HD12	1:A:469:LYS:H	1.65	0.61
1:A:4:THR:O	2:A:601:AGS:N6	2.24	0.60
1:B:306:ASN:CB	1:B:308:ALA:HB2	2.31	0.60
1:B:272:LEU:O	1:B:274:ALA:N	2.35	0.60
1:A:440:GLU:H	1:A:455:LEU:HD22	1.66	0.60
1:A:33:THR:CA	2:A:601:AGS:O3G	2.48	0.60
1:A:37:LYS:HE2	1:A:117:ASP:OD2	2.02	0.59
1:A:59:LYS:HA	1:A:62:VAL:HG23	1.84	0.59
1:A:221:LEU:HA	1:A:329:GLU:HG2	1.84	0.59
1:B:279:LEU:HD21	1:B:305:VAL:HB	1.84	0.59
1:A:233:LYS:O	1:A:233:LYS:HG2	2.01	0.59
1:A:245:ILE:HG22	1:A:356:TYR:OH	2.03	0.59
1:A:280:ILE:HD11	1:A:304:LEU:HD21	1.84	0.59
1:B:190:MET:HE3	1:B:196:LEU:HG	1.84	0.58
1:B:270:GLY:HA2	1:B:271:LEU:CB	2.32	0.58
1:A:286:GLY:HA3	1:A:288:GLU:H	1.68	0.58
1:A:555:PHE:HB2	1:A:571:VAL:HB	1.85	0.58
1:A:30:VAL:HB	1:A:184:GLU:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASP:OD2	1:B:359:ASN:HB2	2.03	0.58
1:A:498:ASP:HB2	1:A:502:ALA:HB3	1.85	0.58
1:B:64:GLN:HG2	1:B:68:LYS:CE	2.33	0.58
1:A:306:ASN:HB2	1:A:310:LEU:HD22	1.85	0.57
1:B:368:VAL:HG22	1:B:392:THR:HG22	1.86	0.57
1:A:400:ASP:OD1	1:A:402:THR:OG1	2.20	0.57
1:A:527:HIS:HE1	1:A:553:PRO:HD3	1.68	0.57
1:A:309:VAL:N	1:A:310:LEU:HA	2.19	0.57
1:B:154:PHE:HB2	1:B:160:TRP:CE3	2.39	0.57
1:B:219:ASN:OD1	1:B:220:GLY:N	2.38	0.57
1:A:255:VAL:HG22	1:A:321:LEU:HB3	1.86	0.57
1:B:246:MET:HE1	1:B:272:LEU:CB	2.35	0.56
1:B:264:HIS:O	1:B:268:ILE:HG12	2.05	0.56
1:B:362:ASP:HB2	1:B:365:ALA:HB2	1.88	0.56
1:A:96:SER:OG	1:A:99:SER:HB3	2.06	0.56
1:A:310:LEU:HD12	1:A:311:THR:C	2.30	0.56
1:B:14:ASP:O	1:B:18:ASN:ND2	2.29	0.56
1:B:64:GLN:O	1:B:68:LYS:HG3	2.06	0.56
1:B:209:TYR:HD2	1:B:211:PHE:CZ	2.23	0.56
1:B:309:VAL:H	1:B:310:LEU:HD13	1.70	0.56
1:A:428:ARG:HE	1:A:435:PRO:CG	2.17	0.55
1:B:213:ARG:HB2	1:B:230:GLU:OE2	2.06	0.55
1:B:228:ASN:ND2	1:B:228:ASN:H	2.04	0.55
1:A:492:LEU:HD23	1:A:494:ILE:HD11	1.88	0.55
1:A:432:LYS:HD3	1:A:436:GLN:HA	1.89	0.55
1:B:270:GLY:CA	1:B:271:LEU:CB	2.84	0.55
1:A:433:ASN:C	1:A:434:CYS:SG	2.89	0.55
1:B:285:PRO:CB	1:B:287:ALA:H	2.15	0.55
2:B:601:AGS:H3'	2:B:601:AGS:O1A	2.07	0.55
1:B:225:ALA:O	1:B:229:ARG:HD3	2.06	0.55
1:B:32:PRO:HG2	1:B:190:MET:HG3	1.89	0.55
1:A:230:GLU:O	1:A:234:GLN:HG3	2.07	0.55
1:B:266:LYS:C	1:B:269:VAL:HG12	2.32	0.54
2:B:601:AGS:S1G	2:B:601:AGS:O2B	2.65	0.54
1:B:64:GLN:CD	1:B:68:LYS:NZ	2.65	0.54
1:A:235:GLN:O	1:A:239:PRO:HD3	2.07	0.54
1:A:261:THR:O	1:A:307:VAL:HG11	2.07	0.54
1:B:311:THR:CB	1:B:312:THR:HA	2.37	0.54
1:B:431:PHE:HD1	1:B:432:LYS:O	1.90	0.54
1:B:9:GLN:OE1	2:B:601:AGS:N6	2.40	0.54
1:B:368:VAL:HG13	1:B:392:THR:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:O	1:A:269:VAL:HG22	2.08	0.54
1:B:352:LEU:HD21	1:B:354:LEU:HD21	1.90	0.53
1:B:16:THR:HG22	1:B:182:ILE:HD11	1.90	0.53
1:B:258:PHE:HE1	1:B:322:ILE:HG23	1.73	0.53
1:A:58:VAL:O	1:A:61:LEU:HB3	2.08	0.53
1:B:275:GLU:N	1:B:276:ASP:HA	2.23	0.53
1:A:284:THR:HG22	1:A:286:GLY:CA	2.38	0.53
1:B:311:THR:HG21	1:B:340:ARG:HD3	1.91	0.53
1:A:161:ILE:HG23	1:A:178:PHE:HD2	1.73	0.53
1:A:241:ILE:HG23	1:A:356:TYR:CD2	2.44	0.53
1:B:293:ILE:O	1:B:294:GLU:HB2	2.09	0.53
1:A:36:GLY:C	2:A:601:AGS:O1B	2.51	0.52
1:B:265:ALA:O	1:B:269:VAL:N	2.42	0.52
1:B:285:PRO:HB2	1:B:287:ALA:N	2.18	0.52
1:A:295:ASN:HB3	1:A:300:ARG:CB	2.38	0.52
1:B:265:ALA:C	1:B:269:VAL:HG12	2.34	0.52
1:B:146:LEU:HD22	1:B:178:PHE:HE1	1.75	0.52
1:B:372:LYS:HA	1:B:394:TRP:CE2	2.45	0.52
1:A:211:PHE:CZ	1:A:231:LEU:HD21	2.45	0.52
1:B:197:THR:HG22	1:B:350:ASP:HA	1.92	0.52
1:A:89:HIS:HD1	1:A:89:HIS:C	2.17	0.52
1:B:245:ILE:HD11	1:B:356:TYR:HE2	1.75	0.51
1:A:265:ALA:O	1:A:269:VAL:HG13	2.10	0.51
1:A:53:LEU:HD23	1:A:137:LEU:HD11	1.93	0.51
1:A:276:ASP:C	1:A:301:PHE:HB2	2.35	0.51
1:B:468:LEU:HD23	1:B:469:LYS:O	2.10	0.51
1:B:296:PHE:HB2	1:B:301:PHE:CE2	2.46	0.51
1:A:68:LYS:NZ	1:A:343:ARG:HH22	2.09	0.51
1:B:258:PHE:CE1	1:B:337:ILE:HG23	2.45	0.51
1:B:257:ILE:O	1:B:305:VAL:HA	2.11	0.51
1:A:284:THR:HG22	1:A:286:GLY:HA2	1.92	0.51
1:B:209:TYR:HB2	1:B:211:PHE:CE1	2.46	0.51
1:A:433:ASN:O	1:A:434:CYS:SG	2.66	0.51
1:B:322:ILE:HB	1:B:353:ILE:HD12	1.93	0.51
1:A:368:VAL:HG22	1:A:392:THR:HG22	1.92	0.51
1:B:28:VAL:HG12	1:B:180:ASP:O	2.10	0.50
1:B:257:ILE:HB	1:B:305:VAL:HG13	1.94	0.50
1:A:244:GLN:HG3	1:A:245:ILE:N	2.26	0.50
1:A:264:HIS:O	1:A:268:ILE:HG13	2.11	0.50
1:A:292:LEU:CB	1:A:301:PHE:HE1	2.25	0.50
1:A:368:VAL:HG13	1:A:392:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ASN:CB	1:B:301:PHE:HD2	2.24	0.50
1:A:210:ASP:OD1	1:A:211:PHE:C	2.54	0.50
1:B:31:LEU:O	1:B:151:ALA:HA	2.12	0.50
1:B:70:GLN:HG2	1:B:74:LEU:O	2.12	0.50
1:B:129:GLN:HG3	1:B:130:TYR:H	1.77	0.50
1:B:497:TYR:HA	1:B:502:ALA:O	2.12	0.50
1:A:211:PHE:HZ	1:A:231:LEU:HD21	1.77	0.50
1:A:244:GLN:O	1:A:247:GLU:HB2	2.12	0.50
1:B:295:ASN:HB2	1:B:301:PHE:CD2	2.46	0.50
1:B:51:ARG:HB2	1:B:111:PHE:CE2	2.46	0.50
1:A:119:CYS:O	1:A:122:ILE:HG13	2.12	0.50
1:B:332:SER:O	1:B:336:GLN:HB2	2.12	0.49
1:A:56:ALA:HB1	1:A:61:LEU:HD23	1.94	0.49
1:A:154:PHE:HB2	1:A:160:TRP:CE3	2.47	0.49
1:A:292:LEU:CB	1:A:301:PHE:CE1	2.95	0.49
1:B:222:PHE:CE2	1:B:329:GLU:HG3	2.47	0.49
1:A:535:LEU:HD23	1:A:537:TRP:HD1	1.77	0.49
1:A:169:MET:SD	1:A:169:MET:N	2.84	0.49
1:A:57:HIS:CE1	1:A:97:VAL:HG21	2.48	0.49
1:A:136:HIS:O	1:A:139:LYS:HB3	2.13	0.49
1:B:428:ARG:HG2	1:B:428:ARG:HH11	1.78	0.49
1:B:288:GLU:C	1:B:290:ASP:N	2.71	0.48
1:A:219:ASN:O	1:A:371:PRO:HG3	2.13	0.48
1:B:209:TYR:CE1	1:B:241:ILE:HD12	2.48	0.48
1:A:190:MET:HE3	1:A:196:LEU:HG	1.95	0.48
1:B:37:LYS:CG	2:B:601:AGS:S1G	3.02	0.48
1:B:156:LEU:HB3	1:B:221:LEU:HD21	1.94	0.48
1:A:95:GLY:HA3	1:A:100:VAL:CG2	2.44	0.48
1:A:258:PHE:HE1	1:A:322:ILE:HG23	1.79	0.48
1:A:95:GLY:HA3	1:A:100:VAL:HG21	1.96	0.48
1:A:199:PRO:HB3	1:A:342:LEU:HD21	1.96	0.47
1:B:17:LEU:O	1:B:21:ARG:HG3	2.14	0.47
1:A:476:CYS:HB3	1:A:553:PRO:O	2.14	0.47
1:A:68:LYS:NZ	2:A:601:AGS:O2B	2.36	0.47
1:A:211:PHE:HD1	1:A:214:LEU:HD11	1.78	0.47
1:A:225:ALA:O	1:A:226:ASP:HB2	2.13	0.47
1:A:115:ILE:HA	1:A:147:LEU:O	2.14	0.47
1:B:285:PRO:C	1:B:288:GLU:H	2.23	0.47
1:B:428:ARG:NH1	1:B:435:PRO:HD3	2.30	0.47
1:A:279:LEU:CD2	1:A:305:VAL:HB	2.45	0.47
1:B:160:TRP:CD1	1:B:171:ARG:O	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:TYR:HA	1:B:178:PHE:O	2.15	0.47
1:B:261:THR:OG1	1:B:262:VAL:N	2.48	0.47
1:B:261:THR:H	1:B:264:HIS:HB3	1.78	0.47
1:A:210:ASP:CA	1:A:211:PHE:HB2	2.38	0.47
1:B:29:ILE:HG13	1:B:147:LEU:HD11	1.97	0.47
1:A:236:ARG:HG2	1:A:236:ARG:O	2.12	0.47
1:A:432:LYS:O	1:A:433:ASN:HB2	2.14	0.47
1:B:276:ASP:CB	1:B:278:ALA:HB2	2.45	0.46
1:A:89:HIS:HA	1:A:90:GLY:HA2	1.31	0.46
1:B:11:GLU:OE1	1:B:183:TYR:OH	2.24	0.46
1:B:103:ASN:OD1	1:B:103:ASN:N	2.48	0.46
1:B:236:ARG:HH11	1:B:236:ARG:HG3	1.80	0.46
1:A:201:ARG:HG2	1:A:353:ILE:O	2.16	0.46
1:A:498:ASP:HB3	1:A:500:ASP:H	1.79	0.46
1:B:481:LEU:HD11	1:B:547:GLN:HG3	1.97	0.46
1:A:231:LEU:C	1:A:232:LYS:O	2.57	0.46
1:B:428:ARG:HH11	1:B:428:ARG:CG	2.29	0.45
1:A:328:THR:HG22	1:A:333:LEU:HD23	1.98	0.45
1:B:64:GLN:HG2	1:B:68:LYS:NZ	2.32	0.45
1:A:223:SER:O	1:A:227:LEU:HB2	2.16	0.45
1:B:340:ARG:HE	1:B:340:ARG:HA	1.81	0.45
1:A:285:PRO:N	1:A:286:GLY:HA2	2.32	0.45
1:A:286:GLY:HA2	1:A:287:ALA:HB3	1.98	0.45
1:B:64:GLN:CG	1:B:68:LYS:NZ	2.80	0.45
1:A:440:GLU:H	1:A:455:LEU:CD2	2.30	0.45
1:B:286:GLY:N	1:B:289:ARG:H	2.14	0.45
1:B:492:LEU:HD23	1:B:494:ILE:HD11	1.98	0.45
1:A:134:LEU:O	1:A:138:THR:OG1	2.33	0.45
1:A:249:ALA:HB3	1:A:303:TYR:OH	2.17	0.45
1:A:468:LEU:HD12	1:A:469:LYS:N	2.31	0.45
1:B:476:CYS:HB3	1:B:553:PRO:O	2.17	0.45
1:A:16:THR:HG23	1:A:147:LEU:HD13	1.97	0.45
1:A:518:ALA:HB1	1:A:522:LEU:HD12	1.99	0.45
1:B:13:VAL:HG11	1:B:43:GLU:HG2	1.99	0.45
1:A:7:PRO:O	1:A:11:GLU:HG3	2.17	0.45
1:A:12:ALA:O	1:A:16:THR:OG1	2.33	0.45
1:B:279:LEU:HD23	1:B:305:VAL:HB	1.98	0.44
1:B:498:ASP:HB3	1:B:500:ASP:H	1.82	0.44
1:A:59:LYS:HA	1:A:62:VAL:CG2	2.47	0.44
1:B:200:GLU:O	1:B:352:LEU:HA	2.17	0.44
1:B:32:PRO:HD2	1:B:185:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HZ3	1:A:343:ARG:HH22	1.66	0.44
1:B:356:TYR:O	1:B:357:ALA:HB3	2.17	0.44
1:B:16:THR:HG22	1:B:147:LEU:HD13	1.99	0.44
1:B:306:ASN:HB3	1:B:308:ALA:CB	2.45	0.44
1:B:65:ASN:HB3	1:B:94:PHE:CE2	2.53	0.44
1:B:201:ARG:CD	1:B:353:ILE:HB	2.47	0.44
1:A:330:SER:HB2	1:A:367:GLU:OE1	2.17	0.44
1:B:309:VAL:CB	1:B:310:LEU:HA	2.48	0.44
1:A:524:ILE:HD13	1:A:535:LEU:HD22	2.00	0.44
1:B:381:GLN:HA	1:B:391:ASN:O	2.18	0.44
1:A:535:LEU:HD23	1:A:537:TRP:CD1	2.52	0.43
1:B:251:THR:C	1:B:252:ARG:HG2	2.42	0.43
1:B:513:PRO:O	1:B:517:THR:HB	2.18	0.43
1:A:49:ARG:O	1:A:112:SER:OG	2.32	0.43
1:B:398:THR:OG1	1:B:399:ALA:N	2.51	0.43
1:A:468:LEU:HD13	1:A:468:LEU:HA	1.86	0.43
1:B:300:ARG:HB2	1:B:301:PHE:CB	2.45	0.43
1:A:31:LEU:O	1:A:151:ALA:HA	2.18	0.43
1:A:417:ASP:OD1	1:A:421:HIS:N	2.51	0.43
1:B:326:ARG:HE	1:B:333:LEU:HD21	1.84	0.43
1:B:115:ILE:HA	1:B:147:LEU:O	2.18	0.43
1:B:169:MET:HB3	1:B:389:PHE:CZ	2.54	0.43
1:B:301:PHE:CD1	1:B:301:PHE:C	2.97	0.43
1:B:340:ARG:HE	1:B:340:ARG:CA	2.32	0.43
1:B:161:ILE:HG23	1:B:178:PHE:HD2	1.84	0.43
1:B:209:TYR:HE1	1:B:241:ILE:HD12	1.84	0.43
1:B:291:VAL:O	1:B:295:ASN:ND2	2.52	0.43
1:A:59:LYS:O	1:A:62:VAL:N	2.51	0.43
1:A:258:PHE:CE1	1:A:337:ILE:HG23	2.53	0.43
1:B:326:ARG:NE	1:B:333:LEU:HD21	2.34	0.42
1:B:280:ILE:CG1	1:B:304:LEU:HD11	2.49	0.42
1:A:403:LEU:HD23	1:A:533:ILE:CD1	2.48	0.42
1:A:284:THR:HG22	1:A:286:GLY:HA3	2.01	0.42
1:B:120:HIS:HA	1:B:161:ILE:HG12	2.00	0.42
1:B:238:THR:O	1:B:241:ILE:HB	2.20	0.42
1:A:33:THR:OG1	1:A:340:ARG:NH2	2.52	0.42
1:A:238:THR:N	1:A:239:PRO:CD	2.83	0.42
1:A:62:VAL:HG21	1:A:96:SER:HB3	2.00	0.42
1:A:233:LYS:O	1:A:233:LYS:CG	2.66	0.42
1:B:9:GLN:HE22	2:B:601:AGS:HN61	1.67	0.42
1:A:36:GLY:N	2:A:601:AGS:O1B	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HB	1:B:184:GLU:HG3	2.02	0.42
1:A:331:VAL:HG12	1:A:362:ASP:OD2	2.20	0.42
1:A:549:LEU:HA	1:A:549:LEU:HD12	1.79	0.42
1:B:13:VAL:O	1:B:17:LEU:HG	2.19	0.41
1:B:295:ASN:O	1:B:300:ARG:HG3	2.20	0.41
1:B:310:LEU:HB3	1:B:311:THR:H	1.61	0.41
1:B:191:ILE:HD13	1:B:199:PRO:HD3	2.02	0.41
1:A:393:PHE:CG	1:A:408:GLY:HA3	2.56	0.41
1:B:372:LYS:HG3	1:B:394:TRP:CH2	2.55	0.41
1:A:129:GLN:H	1:A:129:GLN:CD	2.29	0.41
1:A:398:THR:HG22	1:A:402:THR:O	2.21	0.41
1:A:35:ALA:HA	1:A:190:MET:HE1	2.03	0.41
1:A:308:ALA:HB3	1:A:310:LEU:CB	2.49	0.41
1:A:396:LYS:O	1:A:404:ILE:HB	2.20	0.41
1:B:56:ALA:HB3	1:B:62:VAL:HG22	2.02	0.41
1:B:374:LYS:HB3	1:B:374:LYS:HE2	1.79	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.91	0.41
1:B:16:THR:HG21	1:B:29:ILE:HD11	1.98	0.41
1:A:33:THR:O	2:A:601:AGS:O3G	2.38	0.41
1:A:245:ILE:HG12	1:A:246:MET:N	2.35	0.41
1:A:262:VAL:HG22	1:A:281:THR:HG21	2.03	0.41
1:A:527:HIS:CE1	1:A:553:PRO:HD3	2.51	0.41
1:A:289:ARG:CZ	1:A:289:ARG:HB2	2.51	0.41
1:B:119:CYS:O	1:B:122:ILE:HG13	2.21	0.40
1:B:246:MET:SD	1:B:303:TYR:OH	2.65	0.40
1:B:290:ASP:HA	1:B:293:ILE:CG2	2.31	0.40
1:A:56:ALA:O	1:A:96:SER:HA	2.20	0.40
1:A:280:ILE:HD11	1:A:304:LEU:HD11	2.02	0.40
1:B:56:ALA:O	1:B:96:SER:HA	2.22	0.40
1:B:66:HIS:ND1	1:B:78:ILE:HD11	2.37	0.40
1:A:129:GLN:HA	1:A:132:GLN:OE1	2.20	0.40
1:A:213:ARG:O	1:A:214:LEU:HG	2.21	0.40
1:A:332:SER:OG	1:A:367:GLU:OE1	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/586 (94%)	494 (90%)	57 (10%)	0	100	100
1	B	547/586 (93%)	490 (90%)	57 (10%)	0	100	100
All	All	1098/1172 (94%)	984 (90%)	114 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/491 (86%)	357 (85%)	65 (15%)	2	13
1	B	426/491 (87%)	363 (85%)	63 (15%)	3	15
All	All	848/982 (86%)	720 (85%)	128 (15%)	3	14

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	LEU
1	B	33	THR
1	B	37	LYS
1	B	38	SER
1	B	51	ARG
1	B	68	LYS
1	B	78	ILE
1	B	89	HIS

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Mol	Chain	Res	Type
1	B	102	ARG
1	B	103	ASN
1	B	108	GLN
1	B	121	ARG
1	B	134	LEU
1	B	135	THR
1	B	155	ARG
1	B	161	ILE
1	B	174	GLU
1	B	200	GLU
1	B	206	VAL
1	B	223	SER
1	B	224	GLU
1	B	226	ASP
1	B	228	ASN
1	B	234	GLN
1	B	236	ARG
1	B	241	ILE
1	B	248	PHE
1	B	269	VAL
1	B	279	LEU
1	B	284	THR
1	B	288	GLU
1	B	290	ASP
1	B	292	LEU
1	B	293	ILE
1	B	294	GLU
1	B	302	ARG
1	B	311	THR
1	B	314	PHE
1	B	320	ASP
1	B	325	LEU
1	B	326	ARG
1	B	340	ARG
1	B	374	LYS
1	B	403	LEU
1	B	418	ASP
1	B	428	ARG
1	B	436	GLN
1	B	453	THR
1	B	455	LEU
1	B	457	ASP

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Mol	Chain	Res	Type
1	B	462	LEU
1	B	469	LYS
1	B	470	ASP
1	B	485	HIS
1	B	499	GLU
1	B	505	SER
1	B	510	LEU
1	B	517	THR
1	B	535	LEU
1	B	546	GLN
1	B	549	LEU
1	B	566	GLN
1	B	569	GLU
1	A	4	THR
1	A	6	ARG
1	A	16	THR
1	A	31	LEU
1	A	33	THR
1	A	37	LYS
1	A	38	SER
1	A	62	VAL
1	A	78	ILE
1	A	89	HIS
1	A	104	LEU
1	A	108	GLN
1	A	121	ARG
1	A	125	ASP
1	A	128	SER
1	A	134	LEU
1	A	135	THR
1	A	138	THR
1	A	140	VAL
1	A	161	ILE
1	A	201	ARG
1	A	206	VAL
1	A	208	GLN
1	A	221	LEU
1	A	224	GLU
1	A	226	ASP
1	A	240	HIS
1	A	243	SER
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	245	ILE
1	A	246	MET
1	A	256	MET
1	A	269	VAL
1	A	275	GLU
1	A	276	ASP
1	A	279	LEU
1	A	280	ILE
1	A	281	THR
1	A	289	ARG
1	A	302	ARG
1	A	306	ASN
1	A	372	LYS
1	A	375	SER
1	A	402	THR
1	A	403	LEU
1	A	418	ASP
1	A	433	ASN
1	A	434	CYS
1	A	440	GLU
1	A	443	ILE
1	A	453	THR
1	A	455	LEU
1	A	457	ASP
1	A	462	LEU
1	A	468	LEU
1	A	475	ARG
1	A	499	GLU
1	A	505	SER
1	A	510	LEU
1	A	520	GLU
1	A	535	LEU
1	A	546	GLN
1	A	549	LEU
1	A	566	GLN
1	A	570	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	GLN
1	B	19	HIS

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Mol	Chain	Res	Type
1	B	23	HIS
1	B	64	GLN
1	B	66	HIS
1	B	193	HIS
1	A	208	GLN
1	A	244	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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$
2	AGS	A	601	-	32,33,33	2.04	6 (18%)	45,52,52	1.90	10 (22%)
2	AGS	B	601	-	32,33,33	2.04	6 (18%)	45,52,52	1.90	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	601	-	-	5/21/38/38	0/3/3/3
2	AGS	B	601	-	-	4/21/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	AGS	PG-S1G	7.98	2.08	1.90
2	A	601	AGS	PG-S1G	7.96	2.07	1.90
2	A	601	AGS	C5-C4	4.76	1.47	1.39
2	B	601	AGS	C5-C4	4.74	1.47	1.39
2	B	601	AGS	C5-C6	2.76	1.48	1.41
2	A	601	AGS	C5-C6	2.76	1.48	1.41
2	A	601	AGS	C8-N7	2.36	1.36	1.31
2	B	601	AGS	C8-N7	2.36	1.36	1.31
2	B	601	AGS	C5-N7	-2.22	1.35	1.39
2	A	601	AGS	C5-N7	-2.21	1.35	1.39
2	A	601	AGS	PG-O2G	2.08	1.61	1.54
2	B	601	AGS	PG-O2G	2.06	1.61	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	AGS	C5-C4-N3	-5.86	118.64	126.72
2	A	601	AGS	C5-C4-N3	-5.85	118.66	126.72
2	B	601	AGS	N3-C4-N9	4.64	135.05	127.17
2	A	601	AGS	N3-C4-N9	4.63	135.04	127.17
2	B	601	AGS	C2-N3-C4	3.72	120.93	111.83
2	A	601	AGS	C2-N3-C4	3.71	120.89	111.83
2	B	601	AGS	C4-C5-N7	-3.49	106.60	110.58
2	A	601	AGS	C4-C5-N7	-3.48	106.60	110.58
2	A	601	AGS	PB-O3B-PG	-3.45	120.53	133.17
2	B	601	AGS	PB-O3B-PG	-3.45	120.56	133.17
2	B	601	AGS	N3-C2-N1	-3.24	123.68	128.58
2	A	601	AGS	N3-C2-N1	-3.22	123.70	128.58
2	A	601	AGS	C4-N9-C8	2.63	108.50	105.74
2	B	601	AGS	C4-N9-C8	2.61	108.47	105.74
2	B	601	AGS	C3'-C2'-C1'	2.58	106.34	101.46
2	A	601	AGS	C3'-C2'-C1'	2.56	106.31	101.46
2	A	601	AGS	C5-N7-C8	2.54	107.45	103.45
2	B	601	AGS	C5-N7-C8	2.54	107.44	103.45
2	B	601	AGS	C6-C5-N7	2.07	136.08	132.09
2	A	601	AGS	C6-C5-N7	2.07	136.07	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

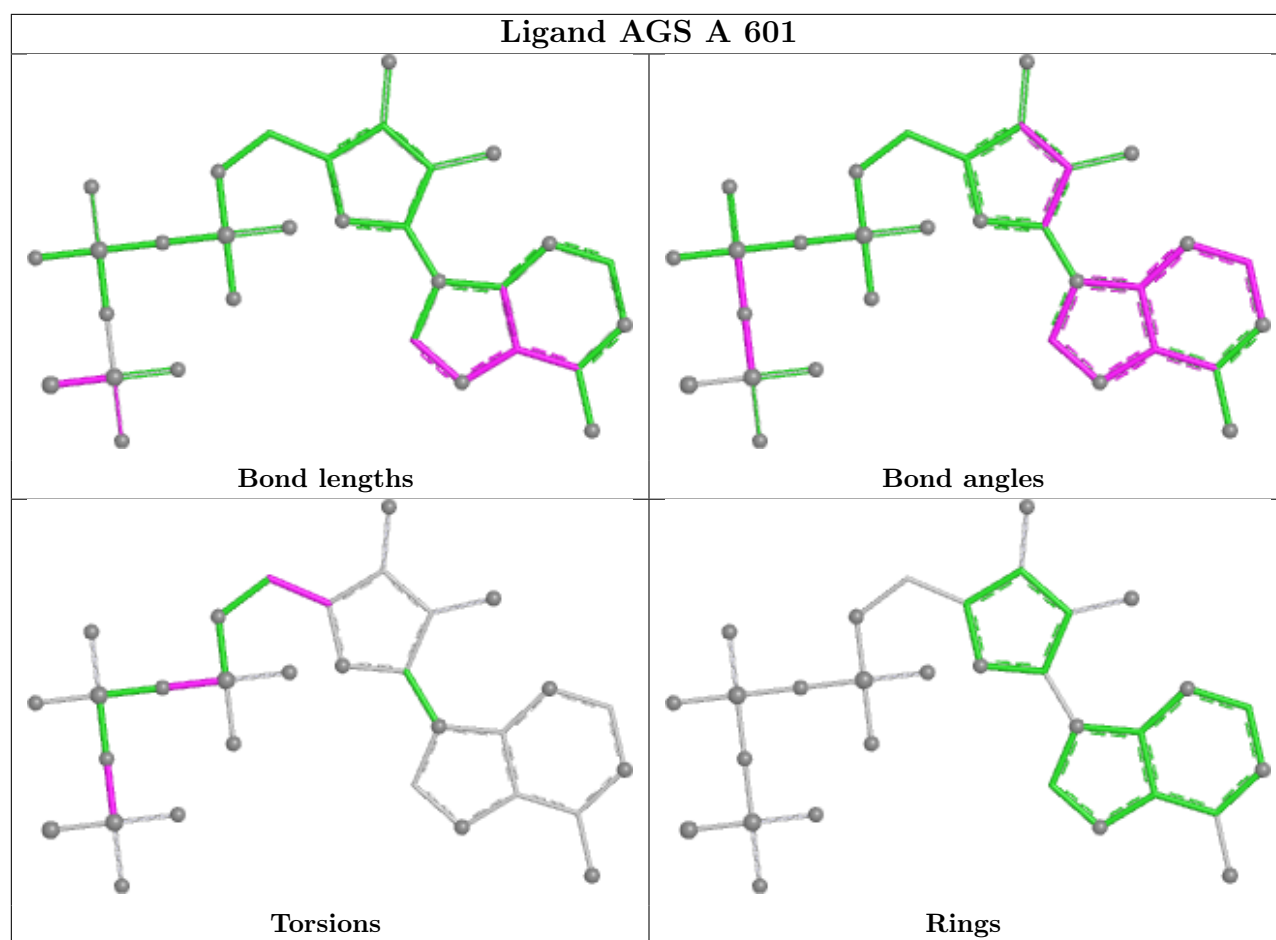
Mol	Chain	Res	Type	Atoms
2	B	601	AGS	C5'-O5'-PA-O1A
2	B	601	AGS	C5'-O5'-PA-O2A
2	B	601	AGS	C5'-O5'-PA-O3A
2	A	601	AGS	PB-O3B-PG-O2G
2	A	601	AGS	PB-O3B-PG-O3G
2	A	601	AGS	O4'-C4'-C5'-O5'
2	A	601	AGS	C3'-C4'-C5'-O5'
2	B	601	AGS	C4'-C5'-O5'-PA
2	A	601	AGS	PB-O3A-PA-O2A

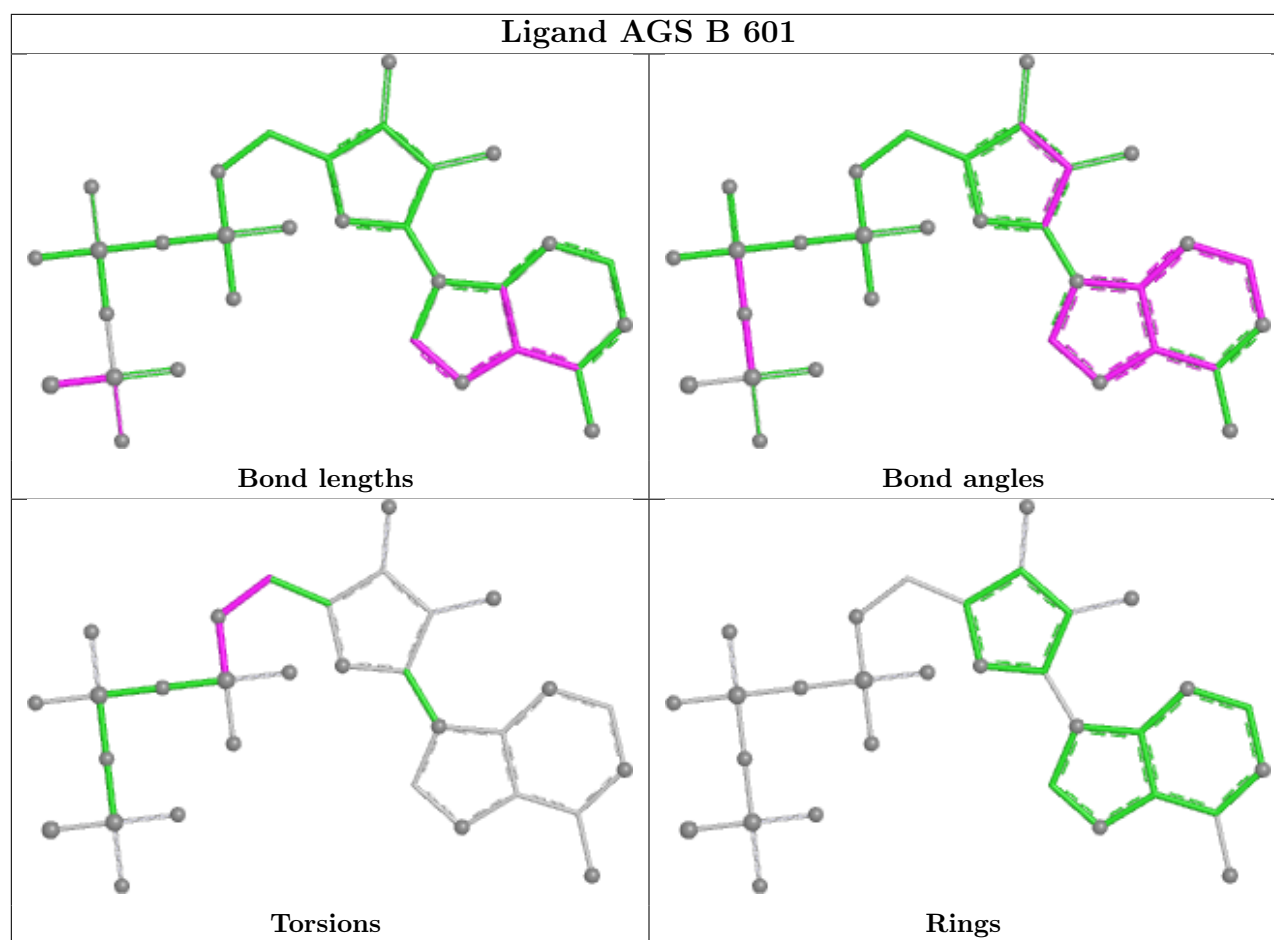
There are no ring outliers.

2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AGS	13	0
2	B	601	AGS	16	0

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





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	559/586 (95%)	-0.12	7 (1%) 75 53	31, 64, 101, 131	0
1	B	555/586 (94%)	-0.08	9 (1%) 70 47	32, 62, 108, 127	0
All	All	1114/1172 (95%)	-0.10	16 (1%) 73 51	31, 63, 105, 131	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	ALA	3.9
1	A	283	ASP	3.5
1	A	437	CYS	3.1
1	A	277	ALA	2.9
1	A	564	TYR	2.9
1	B	277	ALA	2.8
1	B	441	ASN	2.7
1	B	440	GLU	2.5
1	B	437	CYS	2.5
1	B	80	ALA	2.2
1	B	276	ASP	2.2
1	A	433	ASN	2.2
1	A	288	GLU	2.1
1	B	268	ILE	2.0
1	B	564	TYR	2.0
1	A	311	THR	2.0

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

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

6.3 Carbohydrates [i](#)

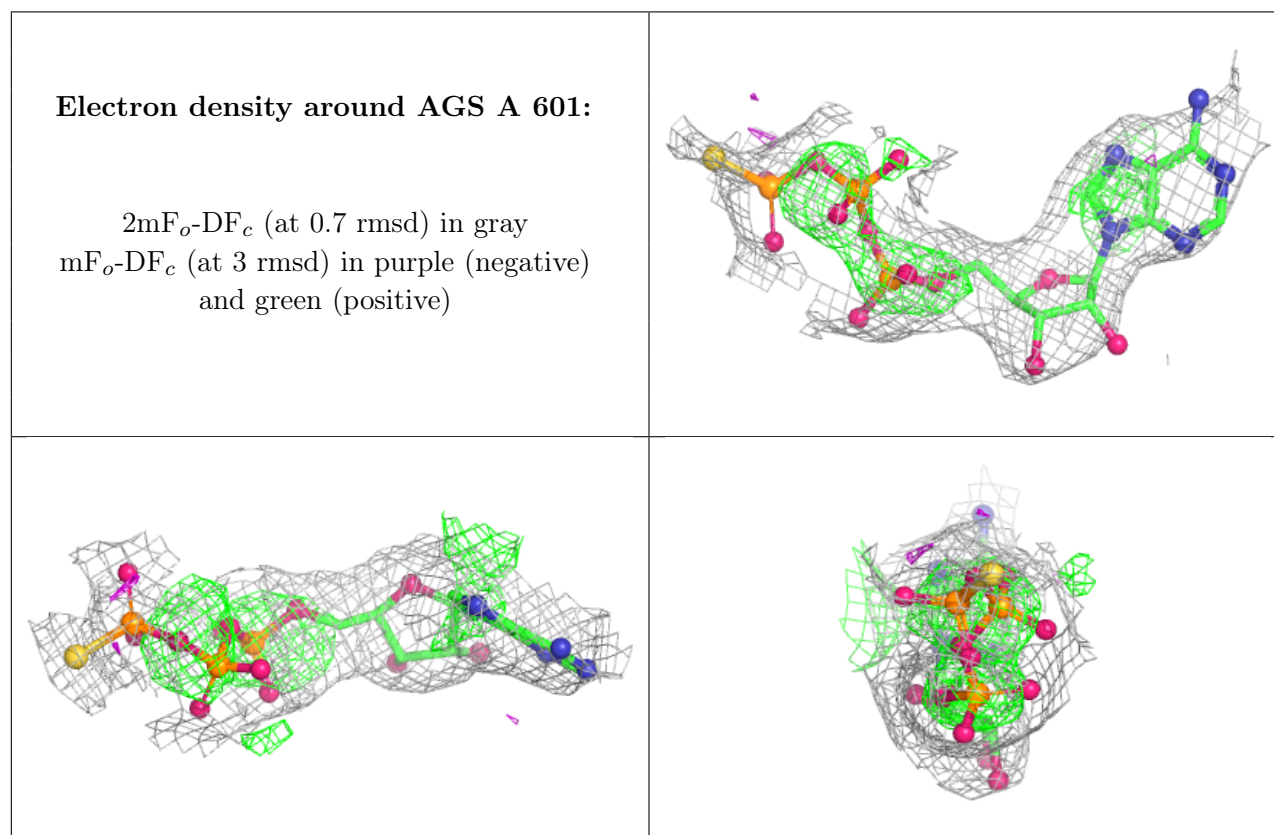
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

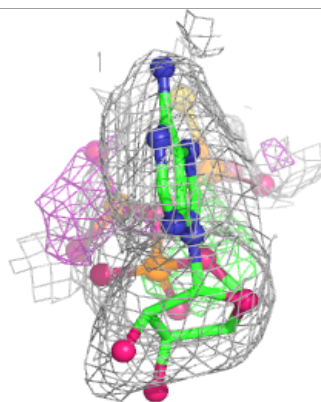
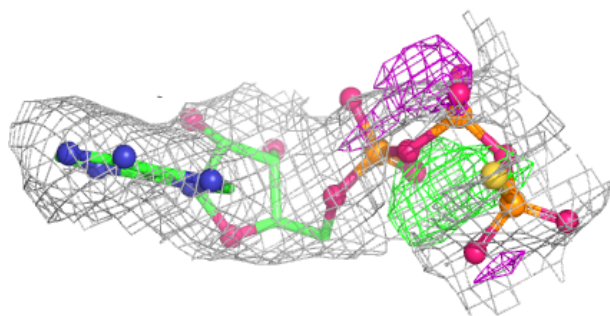
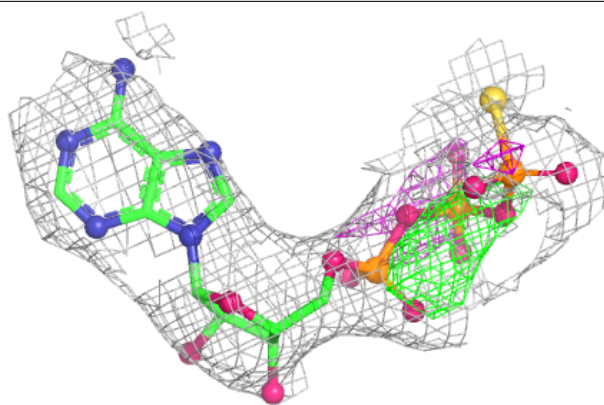
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AGS	A	601	31/31	0.74	0.19	80,103,169,202	0
2	AGS	B	601	31/31	0.77	0.14	62,89,120,146	0
3	ZN	B	602	1/1	0.99	0.04	42,42,42,42	0
3	ZN	A	602	1/1	1.00	0.05	47,47,47,47	0

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



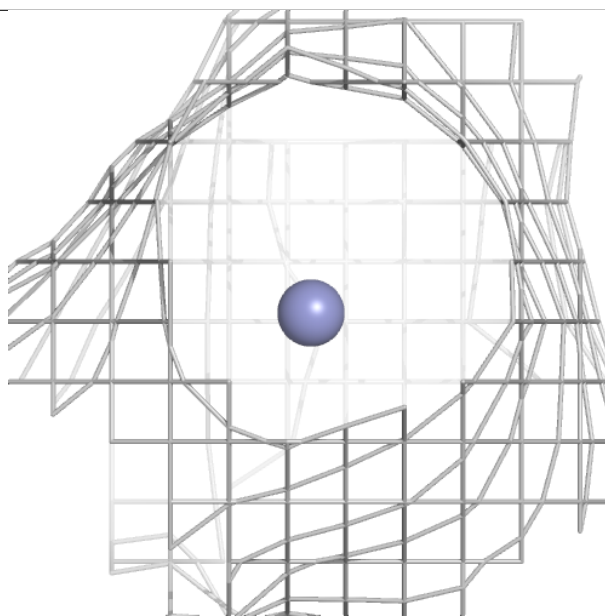
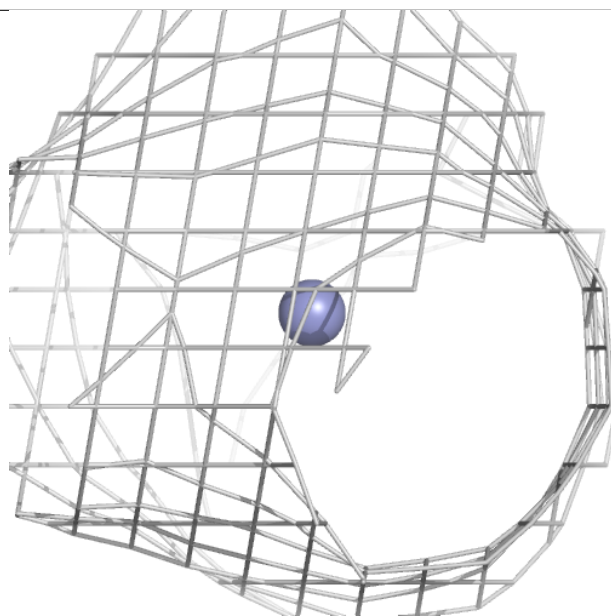
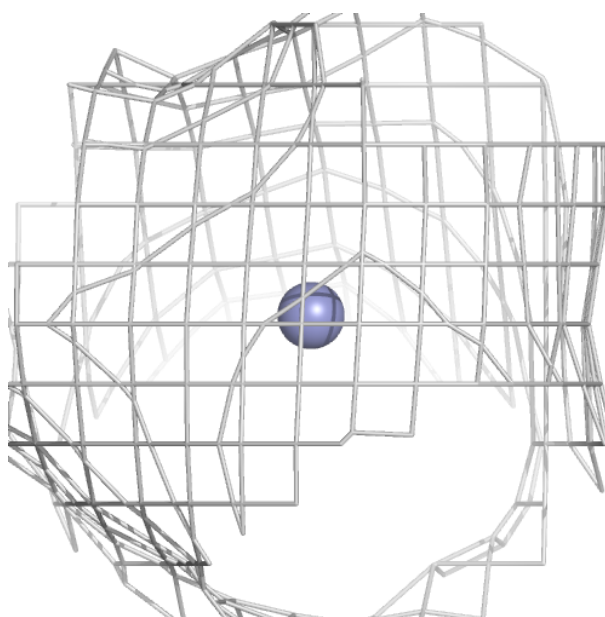
Electron density around AGS B 601:

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



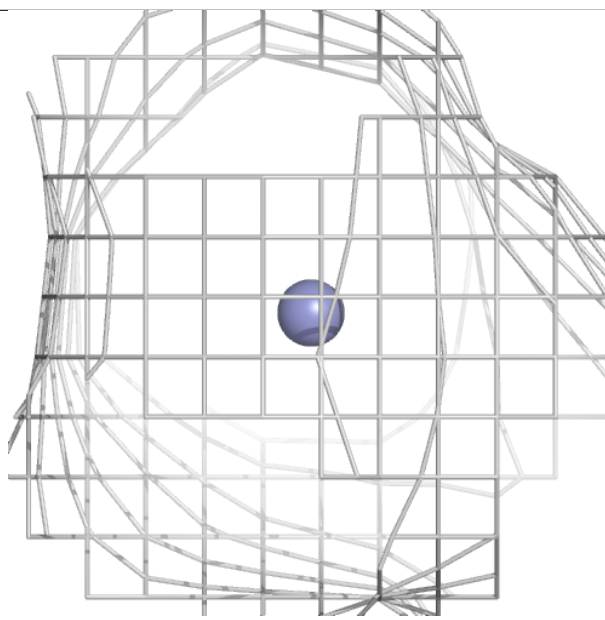
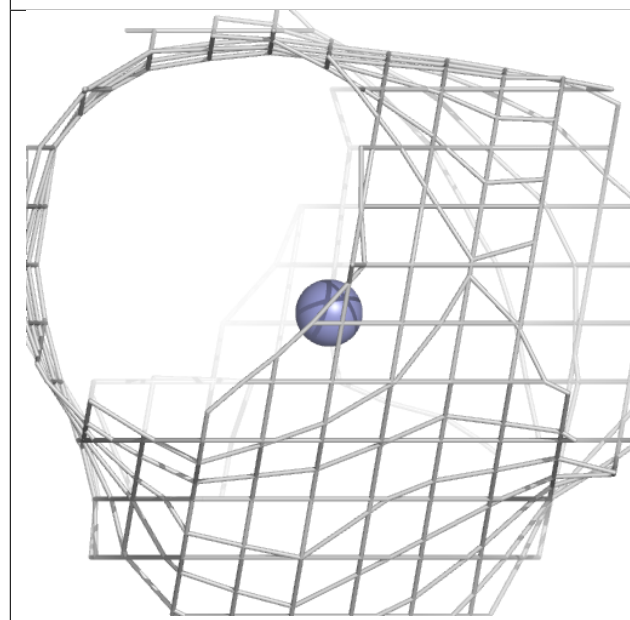
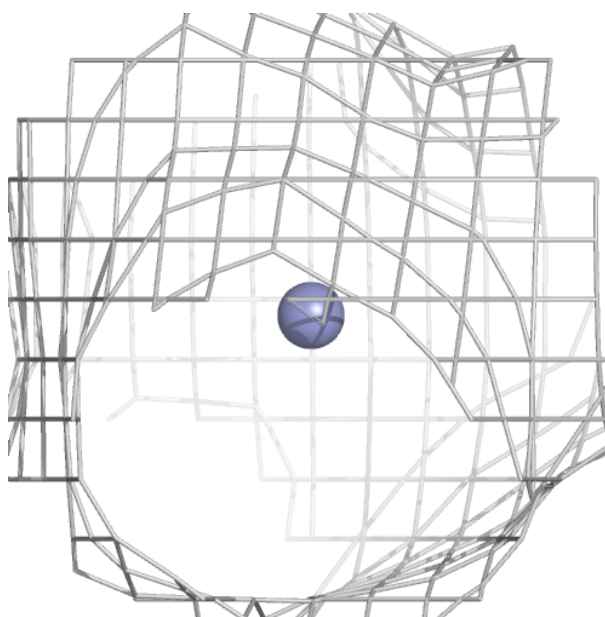
Electron density around ZN B 602:

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



Electron density around ZN A 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.