



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:47 pm BST

PDB ID : 1PL0
Title : Crystal structure of human ATIC in complex with folate-based inhibitor, BW2315U89UC
Authors : Cheong, C.G.; Greasley, S.E.; Horton, P.A.; Beardsley, G.P.; Wilson, I.A.
Deposited on : 2003-06-06
Resolution : 2.60 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 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 : 2.11
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) : 2.11

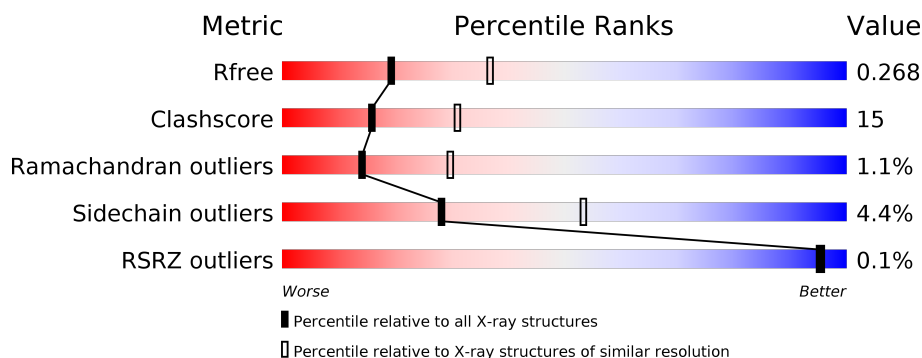
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	592	 69% 29% ..
1	B	592	 72% 25% ..
1	C	592	 68% 29% ..
1	D	592	 68% 28% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17953 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.

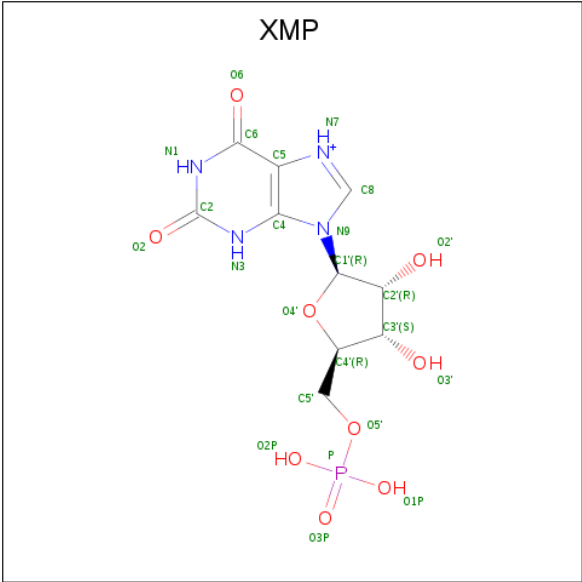
- Molecule 1 is a protein called Bifunctional purine biosynthesis protein PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4424	2801	776	829	18			
1	B	587	Total	C	N	O	S	0	0	0
			4405	2781	768	838	18			
1	C	585	Total	C	N	O	S	0	0	0
			4332	2736	763	815	18			
1	D	579	Total	C	N	O	S	0	0	0
			4236	2677	741	800	18			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

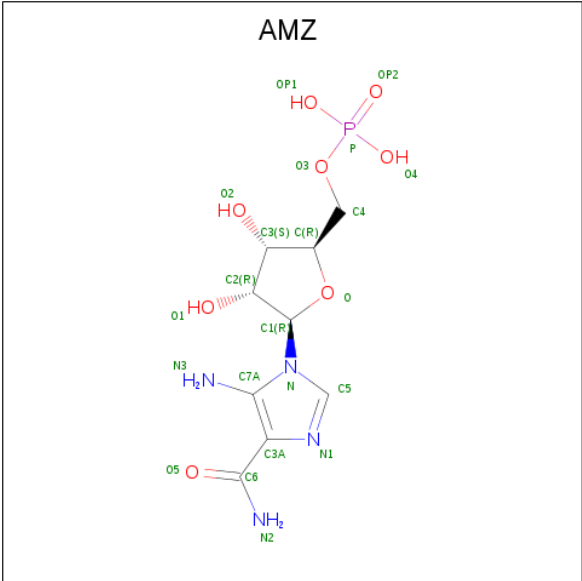
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

- Molecule 3 is XANTHOSINE-5'-MONOPHOSPHATE (three-letter code: XMP) (formula: C₁₀H₁₄N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	4	9	1		

- Molecule 4 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (three-letter code: AMZ) (formula: C₉H₁₅N₄O₈P).



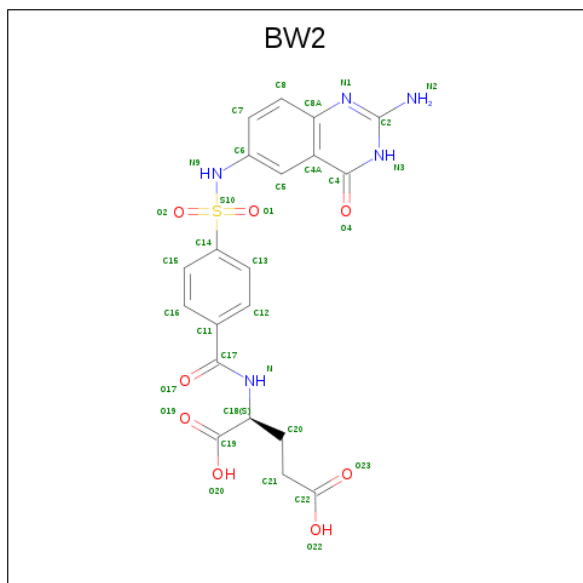
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			22	9	4	8	1		

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

- Molecule 5 is N-(4-[(2-AMINO-4-OXO-3,4-DIHYDROQUINAZOLIN-6-YL)AMINO]SULFONYL}BENZOYL)GLUTAMIC ACID (three-letter code: BW2) (formula: C₂₀H₁₉N₅O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			25	15	5	4	1		
5	D	1	Total	C	N	O	S	0	0
			25	15	5	4	1		

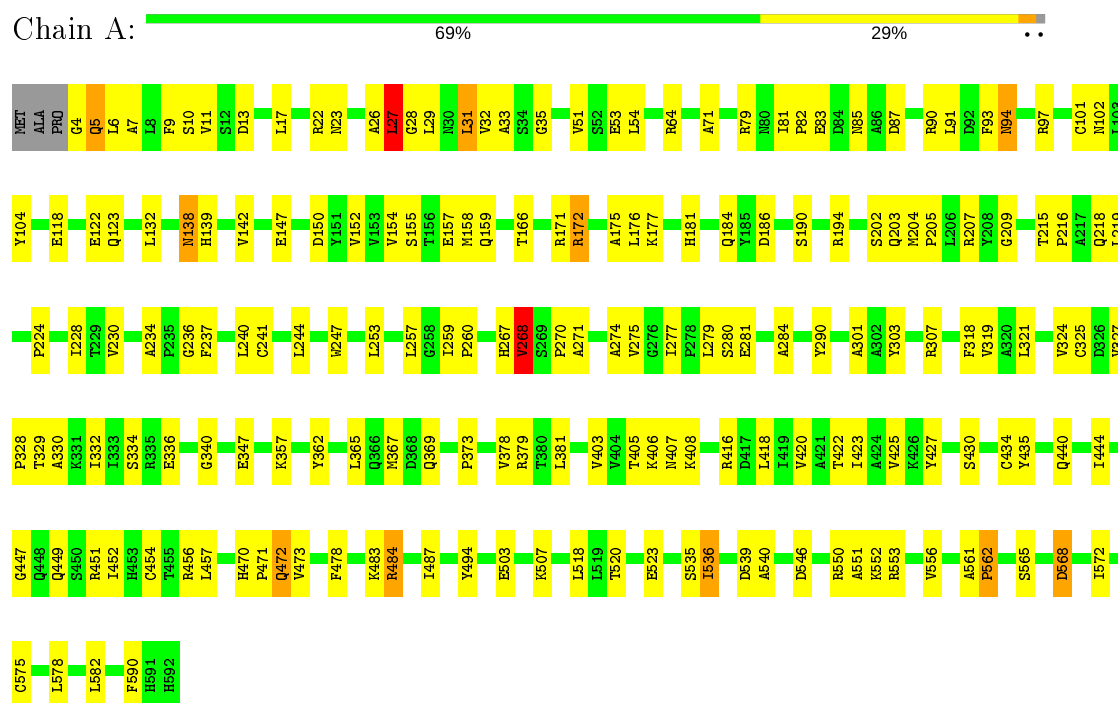
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		
6	B	124	Total	O	0	0
			124	124		
6	C	77	Total	O	0	0
			77	77		
6	D	97	Total	O	0	0
			97	97		

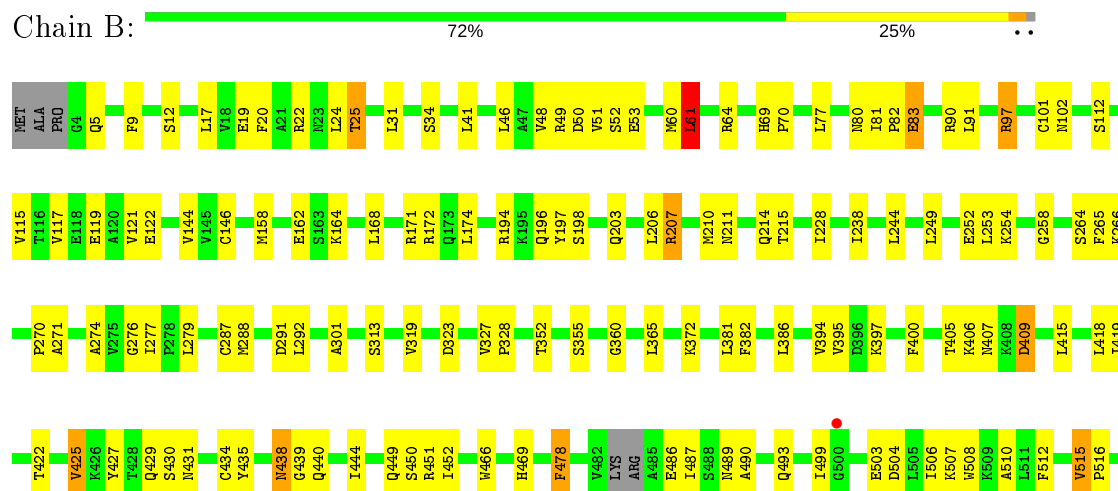
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Bifunctional purine biosynthesis protein PURH



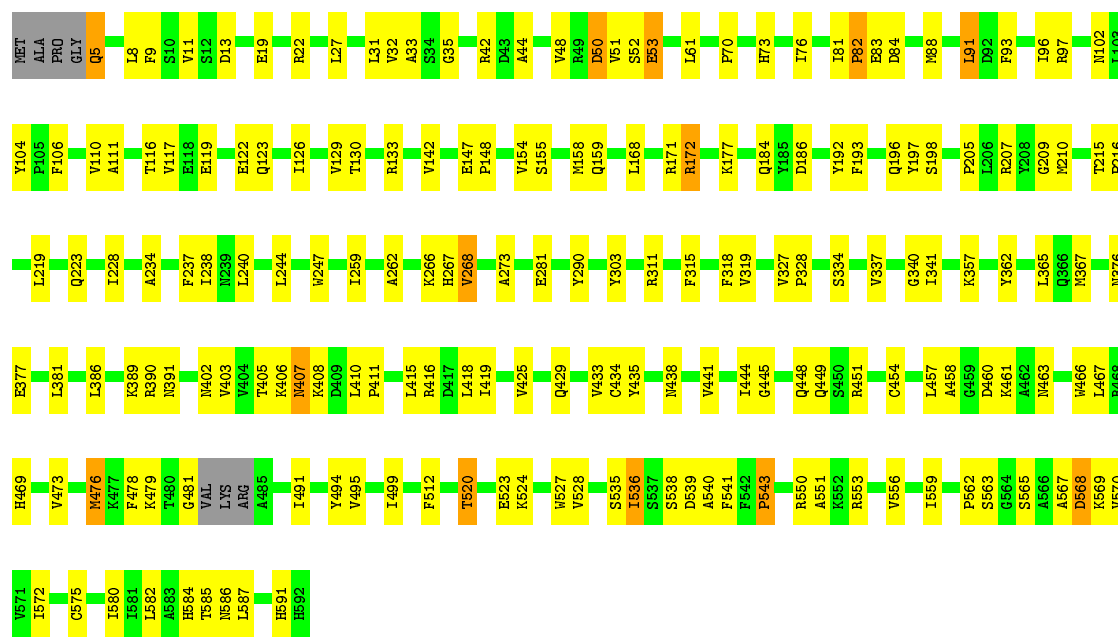
- Molecule 1: Bifunctional purine biosynthesis protein PURH





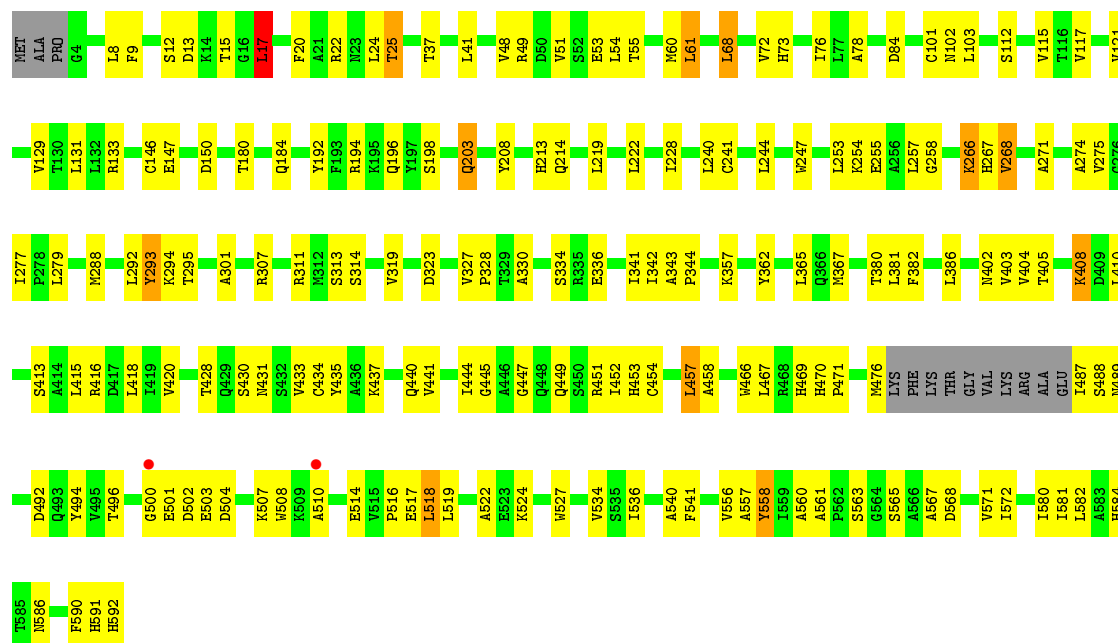
• Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain C: 68% 29% ..



• Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain D: 68% 28% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.12Å 92.97Å 178.49Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.96 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 86.5 (19.96-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.275 0.206 , 0.268	Depositor DCC
R_{free} test set	3594 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 9.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.157 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17953	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BW2, AMZ, XMP, K

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	0.42	0/4507	0.65	0/6131
1	B	0.45	0/4487	0.66	0/6104
1	C	0.43	0/4411	0.64	0/6002
1	D	0.46	0/4314	0.66	0/5882
All	All	0.44	0/17719	0.65	0/24119

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
1	C	303	TYR	Sidechain

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	4424	0	4391	137	0
1	B	4405	0	4320	130	0
1	C	4332	0	4227	144	0
1	D	4236	0	4090	136	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	12	3	0
3	C	24	0	12	0	0
4	B	22	0	13	1	0
4	D	44	0	26	1	0
5	B	25	0	11	2	0
5	D	25	0	11	6	0
6	A	90	0	0	6	0
6	B	124	0	0	9	0
6	C	77	0	0	3	0
6	D	97	0	0	2	0
All	All	17953	0	17113	507	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 15.

All (507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:GLU:HG2	1:C:290:TYR:HE1	1.30	0.94
1:C:435:TYR:CZ	1:C:536:ILE:HD11	2.06	0.91
1:A:13:ASP:H	1:A:102:ASN:HD22	1.19	0.86
1:A:552:LYS:HG2	1:A:578:LEU:HD22	1.59	0.84
1:C:244:LEU:HD12	1:D:381:LEU:HD23	1.60	0.84
1:C:11:VAL:HB	1:C:102:ASN:ND2	1.94	0.82
1:C:418:LEU:HD23	1:C:535:SER:HB3	1.61	0.82
1:B:194:ARG:HG2	1:B:203:GLN:HB2	1.62	0.81
1:A:155:SER:O	1:A:159:GLN:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:MET:HE3	1:B:238:ILE:HD11	1.63	0.78
1:D:228:ILE:HD11	1:D:365:LEU:HD13	1.66	0.78
1:C:155:SER:O	1:C:159:GLN:HG3	1.85	0.77
1:A:23:ASN:O	1:A:27:LEU:HD12	1.84	0.77
1:C:210:MET:HE1	1:D:592:HIS:HB2	1.65	0.77
1:A:11:VAL:HB	1:A:102:ASN:ND2	2.00	0.77
1:C:116:THR:OG1	1:C:119:GLU:HG3	1.85	0.77
1:D:445:GLY:H	1:D:458:ALA:HB2	1.50	0.76
1:B:22:ARG:O	1:B:25:THR:HG22	1.86	0.76
1:C:281:GLU:HG2	1:C:290:TYR:CE1	2.19	0.75
1:A:91:LEU:HD22	1:B:60:MET:SD	2.27	0.74
1:D:487:ILE:C	1:D:489:ASN:H	1.87	0.74
1:B:568:ASP:O	1:B:572:ILE:HG13	1.88	0.74
1:D:500:GLY:HA3	1:D:504:ASP:CB	2.16	0.74
1:C:403:VAL:HG11	1:C:408:LYS:HA	1.70	0.73
1:A:565:SER:HB3	1:A:568:ASP:OD1	1.88	0.73
1:B:478:PHE:CE2	1:B:487:ILE:HG23	2.23	0.72
1:D:430:SER:O	1:D:447:GLY:HA2	1.87	0.72
1:C:319:VAL:HG13	1:C:341:ILE:HG13	1.72	0.72
1:D:266:LYS:HG3	1:D:313:SER:O	1.90	0.72
1:D:403:VAL:HG11	1:D:408:LYS:HA	1.70	0.72
1:B:451:ARG:HB3	5:B:802:BW2:O4	1.90	0.71
1:B:49:ARG:HG2	1:B:53:GLU:OE2	1.90	0.70
1:A:422:THR:O	1:A:425:VAL:HG12	1.90	0.70
1:A:451:ARG:NH2	1:A:540:ALA:HB3	2.06	0.70
1:C:228:ILE:HD11	1:C:365:LEU:HD13	1.72	0.70
1:B:9:PHE:CD2	1:B:17:LEU:HD11	2.27	0.70
1:C:13:ASP:H	1:C:102:ASN:HD22	1.40	0.69
1:A:381:LEU:HD23	1:B:244:LEU:HD12	1.74	0.69
1:D:405:THR:HG23	1:D:582:LEU:HB3	1.74	0.69
1:C:565:SER:HB3	1:C:568:ASP:OD1	1.93	0.69
1:C:550:ARG:HD2	1:C:553:ARG:HD2	1.76	0.69
1:A:478:PHE:CE1	1:A:487:ILE:HG23	2.28	0.68
1:A:568:ASP:O	1:A:572:ILE:HG13	1.92	0.68
1:C:445:GLY:HA2	1:C:457:LEU:HD22	1.76	0.68
1:D:500:GLY:HA3	1:D:504:ASP:HB2	1.75	0.68
1:A:228:ILE:HD11	1:A:365:LEU:HD13	1.74	0.68
1:A:83:GLU:CD	1:A:83:GLU:H	1.98	0.67
1:D:466:TRP:O	1:D:469:HIS:HB2	1.94	0.67
1:B:81:ILE:HG13	1:B:83:GLU:HG2	1.75	0.66
1:D:503:GLU:O	1:D:507:LYS:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HG2	1:A:203:GLN:HB2	1.76	0.66
1:B:478:PHE:CZ	1:B:487:ILE:HG23	2.31	0.66
1:A:520:THR:HG23	1:A:523:GLU:H	1.62	0.65
1:C:210:MET:HE3	1:C:238:ILE:HG12	1.78	0.65
1:D:434:CYS:HB2	1:D:444:ILE:CD1	2.27	0.65
1:A:484:ARG:HG2	1:A:484:ARG:HH21	1.62	0.64
1:B:83:GLU:N	1:B:83:GLU:OE1	2.30	0.64
1:D:49:ARG:HG2	1:D:53:GLU:HB2	1.80	0.64
1:D:117:VAL:O	1:D:121:VAL:HG23	1.96	0.64
1:A:209:GLY:HA2	1:A:237:PHE:HB2	1.80	0.64
1:C:61:LEU:HD13	1:D:78:ALA:HA	1.80	0.63
1:D:428:THR:O	1:D:591:HIS:HB3	1.98	0.63
1:C:568:ASP:O	1:C:572:ILE:HG13	1.99	0.63
1:B:279:LEU:HD13	1:B:301:ALA:HB1	1.81	0.62
1:A:33:ALA:O	1:A:51:VAL:HG23	2.00	0.62
1:C:13:ASP:O	1:C:102:ASN:ND2	2.32	0.62
1:A:405:THR:C	1:A:407:ASN:H	2.03	0.62
1:B:406:LYS:N	1:B:576:ASP:OD1	2.24	0.62
1:C:381:LEU:HD23	1:D:244:LEU:HD12	1.82	0.62
1:D:541:PHE:CD1	1:D:565:SER:HB2	2.34	0.62
1:A:257:LEU:HD12	1:A:275:VAL:HG11	1.80	0.62
1:C:381:LEU:HD21	1:D:241:CYS:HA	1.81	0.62
1:A:321:LEU:HD11	1:A:329:THR:HG21	1.81	0.61
1:A:456:ARG:HD2	6:A:1089:HOH:O	2.00	0.61
1:A:503:GLU:O	1:A:507:LYS:HG3	2.01	0.61
1:D:101:CYS:O	1:D:146:CYS:HA	2.01	0.61
1:D:203:GLN:HG3	6:D:1090:HOH:O	2.00	0.61
1:D:501:GLU:HA	1:D:501:GLU:OE2	2.00	0.61
1:A:403:VAL:HG11	1:A:408:LYS:HA	1.83	0.60
1:B:466:TRP:O	1:B:469:HIS:HB2	2.00	0.60
1:C:425:VAL:CG1	1:C:539:ASP:HB3	2.32	0.60
1:C:536:ILE:HD12	1:C:556:VAL:HG21	1.83	0.60
1:D:434:CYS:HB2	1:D:444:ILE:HD13	1.82	0.60
1:C:5:GLN:OE1	1:C:97:ARG:HB2	2.01	0.60
1:A:494:TYR:CE1	1:A:518:LEU:HA	2.37	0.60
1:B:168:LEU:O	1:B:172:ARG:HG3	2.02	0.60
1:A:244:LEU:HD12	1:B:381:LEU:HD23	1.84	0.60
1:B:265:PHE:CE1	1:B:270:PRO:HB3	2.37	0.60
1:C:391:ASN:HB2	1:D:214:GLN:OE1	2.02	0.59
1:B:61:LEU:O	1:B:64:ARG:HD3	2.02	0.59
1:D:254:LYS:O	1:D:258:GLY:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ARG:HG2	1:D:53:GLU:CB	2.32	0.59
1:B:486:GLU:HA	1:B:489:ASN:HD22	1.66	0.59
1:C:33:ALA:O	1:C:51:VAL:HG23	2.02	0.59
1:D:500:GLY:HA3	1:D:504:ASP:HB3	1.84	0.59
1:A:435:TYR:CE1	1:A:536:ILE:HD11	2.38	0.59
1:C:457:LEU:CD2	1:C:461:LYS:HE3	2.33	0.59
1:A:6:LEU:HD22	1:A:32:VAL:HG23	1.85	0.59
1:C:467:LEU:HD23	1:C:527:TRP:HD1	1.66	0.59
1:A:147:GLU:OE1	1:A:177:LYS:HD3	2.03	0.59
5:D:804:BW2:H5	5:D:804:BW2:O2	2.02	0.58
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.68	0.58
1:B:115:VAL:HA	1:B:119:GLU:OE1	2.03	0.58
1:C:106:PHE:O	1:C:110:VAL:HG22	2.03	0.58
1:C:8:LEU:HD12	1:C:32:VAL:O	2.03	0.58
1:D:451:ARG:NH2	1:D:540:ALA:HB3	2.17	0.58
1:C:319:VAL:HG13	1:C:341:ILE:CG1	2.33	0.58
1:A:5:GLN:HG2	1:A:97:ARG:HB2	1.86	0.58
1:B:46:LEU:HD21	6:B:1030:HOH:O	2.03	0.58
1:D:487:ILE:C	1:D:489:ASN:N	2.55	0.58
1:B:435:TYR:CZ	1:B:536:ILE:HD11	2.39	0.58
1:B:478:PHE:N	1:B:478:PHE:CD1	2.72	0.57
1:B:69:HIS:ND1	1:B:70:PRO:HD2	2.19	0.57
1:D:476:MET:HE3	1:D:494:TYR:CE2	2.39	0.57
1:B:434:CYS:HB2	1:B:444:ILE:CD1	2.33	0.57
1:A:53:GLU:HG2	1:A:53:GLU:O	2.05	0.57
1:B:541:PHE:CD1	1:B:565:SER:HB2	2.40	0.57
1:D:416:ARG:O	1:D:420:VAL:HG23	2.03	0.57
1:D:467:LEU:HD23	1:D:527:TRP:CD1	2.40	0.57
1:A:430:SER:O	1:A:447:GLY:HA2	2.05	0.57
1:B:112:SER:HB3	1:B:115:VAL:HG11	1.86	0.57
1:B:291:ASP:O	1:B:292:LEU:HD23	2.05	0.57
1:C:418:LEU:CD2	1:C:535:SER:HB3	2.32	0.57
1:B:9:PHE:HD2	1:B:17:LEU:HD11	1.69	0.57
1:B:551:ALA:HB1	1:B:556:VAL:HG21	1.87	0.57
1:C:524:LYS:O	1:C:528:VAL:HG23	2.05	0.56
1:D:267:HIS:C	1:D:268:VAL:HG23	2.25	0.56
1:B:557:ALA:HB2	6:B:1111:HOH:O	2.06	0.56
1:D:41:LEU:HB2	1:D:48:VAL:HG21	1.88	0.56
1:A:244:LEU:HB2	1:B:381:LEU:HD21	1.87	0.56
1:D:22:ARG:O	1:D:25:THR:HG22	2.05	0.56
1:D:180:THR:HG22	1:D:184:GLN:HE21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ALA:O	1:D:571:VAL:HG23	2.06	0.56
1:B:9:PHE:HE1	1:B:31:LEU:HD22	1.70	0.56
1:C:457:LEU:HD21	1:C:461:LYS:HE3	1.87	0.56
1:C:88:MET:HE3	1:C:93:PHE:O	2.06	0.56
1:A:90:ARG:HG3	1:A:91:LEU:HD12	1.88	0.55
1:A:5:GLN:HE21	1:A:97:ARG:HE	1.54	0.55
1:C:147:GLU:CD	1:C:177:LYS:HD3	2.27	0.55
1:B:117:VAL:CG2	1:B:196:GLN:HG2	2.36	0.55
1:A:247:TRP:CE2	1:A:367:MET:HG2	2.42	0.55
1:B:9:PHE:CE1	1:B:31:LEU:HD22	2.42	0.55
1:B:12:SER:H	1:B:102:ASN:HB2	1.71	0.55
1:C:147:GLU:OE2	1:C:177:LYS:HD3	2.07	0.55
1:C:42:ARG:C	1:C:44:ALA:H	2.10	0.55
1:A:215:THR:OG1	1:A:216:PRO:HA	2.06	0.55
1:B:451:ARG:NH2	1:B:540:ALA:HB3	2.22	0.55
1:A:451:ARG:HH21	1:A:540:ALA:HB3	1.71	0.55
1:D:445:GLY:N	1:D:458:ALA:HB2	2.20	0.55
1:A:520:THR:HG22	1:A:523:GLU:CD	2.27	0.54
1:B:162:GLU:HG2	1:B:162:GLU:O	2.06	0.54
1:B:82:PRO:HB2	1:B:83:GLU:OE1	2.07	0.54
1:C:357:LYS:NZ	1:C:357:LYS:HB3	2.22	0.54
1:B:507:LYS:O	1:B:510:ALA:HB3	2.07	0.54
1:C:551:ALA:HB1	1:C:556:VAL:HG21	1.90	0.54
1:A:328:PRO:O	1:A:332:ILE:HG13	2.08	0.54
1:A:253:LEU:HD23	1:A:423:ILE:HD12	1.89	0.54
1:A:325:CYS:O	1:A:347:GLU:HG3	2.08	0.54
1:A:484:ARG:HG2	1:A:484:ARG:NH2	2.23	0.54
1:A:104:TYR:CE1	3:A:901:XMP:H4'	2.42	0.54
1:A:157:GLU:OE1	1:A:166:THR:HG22	2.08	0.54
1:D:410:LEU:HD13	1:D:581:ILE:HG21	1.90	0.54
1:D:117:VAL:HA	1:D:192:TYR:OH	2.07	0.54
1:C:210:MET:CE	1:C:238:ILE:HG12	2.37	0.54
1:A:6:LEU:HD22	1:A:32:VAL:CG2	2.39	0.53
1:B:407:ASN:OD1	1:B:409:ASP:HB2	2.08	0.53
1:C:9:PHE:O	1:C:33:ALA:HA	2.08	0.53
1:C:81:ILE:HB	1:C:82:PRO:HD2	1.89	0.53
1:D:487:ILE:O	1:D:489:ASN:N	2.41	0.53
1:B:97:ARG:HD2	6:B:1062:HOH:O	2.07	0.53
1:C:541:PHE:CD1	1:C:565:SER:HB2	2.44	0.53
1:B:478:PHE:HD1	1:B:478:PHE:N	2.06	0.53
1:D:194:ARG:HG2	1:D:203:GLN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:MET:CE	1:B:238:ILE:HD11	2.38	0.53
1:B:101:CYS:O	1:B:146:CYS:HA	2.09	0.53
1:C:315:PHE:CE2	1:C:337:VAL:HG11	2.44	0.53
1:D:557:ALA:C	1:D:580:ILE:HG23	2.29	0.53
1:C:334:SER:HA	1:C:357:LYS:HD2	1.90	0.53
1:B:478:PHE:CD2	1:B:487:ILE:HG12	2.44	0.53
1:B:252:GLU:OE1	1:B:427:TYR:OH	2.26	0.52
1:D:466:TRP:O	1:D:469:HIS:N	2.39	0.52
1:B:327:VAL:HB	1:B:328:PRO:HD3	1.91	0.52
1:B:452:ILE:HA	1:B:547:ASN:OD1	2.08	0.52
1:A:434:CYS:HB2	1:A:444:ILE:HD12	1.89	0.52
1:B:434:CYS:HB2	1:B:444:ILE:HD13	1.91	0.52
1:C:559:ILE:HD12	1:C:580:ILE:HG21	1.91	0.52
1:A:575:CYS:SG	1:A:582:LEU:HD13	2.49	0.52
1:A:327:VAL:HB	1:A:328:PRO:HD3	1.92	0.52
1:C:133:ARG:HH12	1:D:129:VAL:HG21	1.75	0.52
1:C:550:ARG:O	1:C:553:ARG:HG2	2.10	0.52
1:D:288:MET:HG3	1:D:311:ARG:NE	2.25	0.52
1:B:520:THR:HG22	1:B:523:GLU:OE2	2.10	0.52
1:B:580:ILE:HG22	1:B:581:ILE:N	2.25	0.52
1:A:31:LEU:CD1	1:A:31:LEU:N	2.73	0.52
1:A:452:ILE:HD13	1:A:546:ASP:OD1	2.10	0.52
1:D:557:ALA:HB3	1:D:558:TYR:CE1	2.45	0.52
1:A:5:GLN:HB3	1:A:29:LEU:CD2	2.40	0.52
1:A:104:TYR:HB2	1:A:123:GLN:O	2.09	0.51
1:D:112:SER:O	1:D:115:VAL:HG22	2.11	0.51
1:C:267:HIS:C	1:C:268:VAL:HG23	2.29	0.51
1:C:478:PHE:HA	1:C:512:PHE:HA	1.91	0.51
1:C:184:GLN:NE2	1:D:222:LEU:HD13	2.25	0.51
1:D:274:ALA:HB2	1:D:440:GLN:HB2	1.90	0.51
1:A:150:ASP:O	1:A:154:VAL:HG23	2.11	0.51
1:A:181:HIS:CE1	6:A:1030:HOH:O	2.63	0.51
1:B:503:GLU:O	1:B:506:ILE:N	2.35	0.51
1:A:81:ILE:HB	1:A:82:PRO:HD2	1.91	0.51
6:A:1035:HOH:O	1:B:429:GLN:HG3	2.10	0.51
1:C:327:VAL:HB	1:C:328:PRO:HD3	1.92	0.51
1:B:466:TRP:HD1	1:B:528:VAL:HA	1.75	0.51
1:D:219:LEU:HD22	1:D:240:LEU:HD13	1.93	0.51
1:D:319:VAL:HG13	1:D:341:ILE:HG13	1.91	0.51
1:A:87:ASP:OD1	1:A:90:ARG:NH1	2.44	0.51
1:B:466:TRP:CD1	1:B:528:VAL:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:GLU:HA	1:B:489:ASN:ND2	2.25	0.51
1:D:342:ILE:HD11	1:D:367:MET:HB2	1.93	0.51
1:A:172:ARG:HD2	1:B:197:TYR:CD1	2.46	0.50
1:C:73:HIS:CE1	1:C:130:THR:HG22	2.45	0.50
1:C:133:ARG:NH1	1:D:129:VAL:HG21	2.26	0.50
1:D:492:ASP:O	1:D:496:THR:CB	2.58	0.50
1:B:203:GLN:HG3	6:B:1003:HOH:O	2.12	0.50
1:C:142:VAL:O	1:C:171:ARG:HD2	2.11	0.50
1:D:433:VAL:O	1:D:444:ILE:HD12	2.11	0.50
1:C:104:TYR:HB3	1:C:123:GLN:OE1	2.11	0.50
1:D:73:HIS:CE1	1:D:131:LEU:HD23	2.46	0.50
1:D:444:ILE:HG23	1:D:444:ILE:O	2.11	0.50
1:A:236:GLY:HA3	6:B:1004:HOH:O	2.11	0.50
1:A:494:TYR:HE1	1:A:518:LEU:HA	1.76	0.50
1:A:551:ALA:HB1	1:A:556:VAL:HG21	1.93	0.50
1:B:489:ASN:O	1:B:493:GLN:HG3	2.11	0.50
1:C:193:PHE:HD1	1:C:197:TYR:CE2	2.30	0.50
1:C:520:THR:H	1:C:523:GLU:CB	2.25	0.50
1:A:22:ARG:NH1	1:A:22:ARG:HG2	2.26	0.50
1:B:567:ALA:O	1:B:571:VAL:HG23	2.12	0.50
1:A:10:SER:OG	3:A:901:XMP:H8	2.12	0.50
1:D:522:ALA:HA	6:D:1078:HOH:O	2.12	0.50
1:B:117:VAL:HG21	1:B:196:GLN:CG	2.42	0.49
1:C:111:ALA:HB2	6:C:1058:HOH:O	2.12	0.49
1:C:154:VAL:O	1:C:158:MET:HG3	2.12	0.49
1:C:247:TRP:CE2	1:C:367:MET:HG2	2.47	0.49
1:C:445:GLY:N	1:C:458:ALA:HB2	2.27	0.49
1:C:444:ILE:HG23	1:C:444:ILE:O	2.12	0.49
1:C:543:PRO:O	1:C:567:ALA:HB3	2.12	0.49
1:A:26:ALA:C	1:A:28:GLY:H	2.16	0.49
1:B:266:LYS:HG3	1:B:313:SER:O	2.12	0.49
5:B:802:BW2:O2	5:B:802:BW2:H5	2.12	0.49
1:D:568:ASP:O	1:D:572:ILE:HG13	2.12	0.49
1:B:274:ALA:HB2	1:B:440:GLN:HB2	1.93	0.49
1:D:17:LEU:CD2	1:D:41:LEU:HD21	2.42	0.49
1:D:557:ALA:O	1:D:580:ILE:HG23	2.12	0.49
1:A:259:ILE:HG22	1:A:260:PRO:HD2	1.95	0.49
1:A:277:ILE:HD11	1:A:416:ARG:NH1	2.28	0.49
1:D:343:ALA:HB1	1:D:344:PRO:HD2	1.94	0.49
1:D:434:CYS:SG	1:D:441:VAL:HG13	2.52	0.49
1:B:397:LYS:CB	1:B:415:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:MET:CE	1:D:592:HIS:HB2	2.41	0.49
1:A:142:VAL:O	1:A:171:ARG:HD2	2.12	0.49
1:C:585:THR:HG23	1:C:587:LEU:H	1.77	0.49
1:C:61:LEU:HA	1:D:84:ASP:OD1	2.13	0.49
1:C:91:LEU:HD22	1:C:93:PHE:CZ	2.48	0.49
1:A:425:VAL:HG22	1:A:539:ASP:HB3	1.94	0.48
1:B:158:MET:O	1:B:164:LYS:HA	2.12	0.48
1:B:144:VAL:O	1:B:174:LEU:HB3	2.12	0.48
1:C:582:LEU:HD21	1:C:584:HIS:NE2	2.28	0.48
1:B:102:ASN:HB3	6:B:1052:HOH:O	2.13	0.48
1:D:327:VAL:HB	1:D:328:PRO:HD3	1.95	0.48
1:A:176:LEU:O	1:A:176:LEU:HD12	2.13	0.48
1:A:284:ALA:HB1	1:A:290:TYR:HA	1.96	0.48
1:B:287:CYS:O	1:B:288:MET:HB2	2.14	0.48
1:B:41:LEU:HB2	1:B:48:VAL:HG21	1.95	0.48
1:A:219:LEU:HD13	1:A:240:LEU:HD13	1.94	0.48
1:A:81:ILE:O	1:A:85:ASN:ND2	2.47	0.48
1:A:244:LEU:HD12	1:B:381:LEU:CD2	2.43	0.48
1:C:82:PRO:HG2	1:C:83:GLU:OE2	2.14	0.48
1:C:207:ARG:HD3	1:C:234:ALA:O	2.14	0.48
1:A:267:HIS:HB3	1:B:592:HIS:CE1	2.49	0.48
1:A:202:SER:HB3	1:A:224:PRO:O	2.14	0.48
1:A:378:VAL:HG22	1:A:379:ARG:N	2.29	0.48
1:A:418:LEU:HD23	1:A:535:SER:HB3	1.95	0.48
1:D:277:ILE:HD11	1:D:416:ARG:HD2	1.95	0.48
1:D:563:SER:HB3	1:D:584:HIS:CG	2.48	0.48
1:C:386:LEU:CD2	1:D:219:LEU:HD13	2.44	0.47
1:C:540:ALA:HA	1:C:562:PRO:HG2	1.95	0.47
1:D:435:TYR:CZ	1:D:536:ILE:HD11	2.48	0.47
1:C:367:MET:HE3	1:D:382:PHE:HE2	1.79	0.47
1:A:101:CYS:HB3	1:A:132:LEU:HD21	1.96	0.47
1:B:279:LEU:CD1	1:B:301:ALA:HB1	2.44	0.47
1:D:257:LEU:HD12	1:D:275:VAL:HG11	1.95	0.47
1:D:292:LEU:O	1:D:293:TYR:C	2.53	0.47
1:A:330:ALA:O	1:A:334:SER:HB2	2.14	0.47
1:B:400:PHE:CE1	1:B:418:LEU:HB3	2.49	0.47
1:A:219:LEU:HD13	1:B:386:LEU:HD21	1.96	0.47
1:C:435:TYR:CE2	1:C:536:ILE:HD11	2.50	0.47
1:A:64:ARG:NH1	1:B:77:LEU:O	2.42	0.47
1:C:434:CYS:O	1:C:536:ILE:HA	2.14	0.47
1:C:215:THR:OG1	1:C:216:PRO:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LEU:HD23	1:D:54:LEU:O	2.14	0.47
1:B:490:ALA:HB1	1:B:512:PHE:CE1	2.50	0.47
1:B:541:PHE:CE1	1:B:565:SER:HB2	2.49	0.47
1:C:473:VAL:HA	1:C:476:MET:HG3	1.97	0.46
1:C:91:LEU:HD22	1:C:93:PHE:CE2	2.50	0.46
1:A:279:LEU:CD1	1:A:301:ALA:HB1	2.46	0.46
1:A:336:GLU:OE1	1:A:336:GLU:HA	2.15	0.46
1:A:207:ARG:NH1	6:A:1054:HOH:O	2.47	0.46
1:C:466:TRP:O	1:C:469:HIS:HB2	2.16	0.46
1:C:425:VAL:HG13	1:C:539:ASP:HB3	1.95	0.46
1:D:453:HIS:O	1:D:457:LEU:HB2	2.16	0.46
1:D:418:LEU:HD22	1:D:560:ALA:HB2	1.96	0.46
1:D:72:VAL:O	1:D:76:ILE:HG13	2.14	0.46
1:D:20:PHE:CE2	1:D:24:LEU:HD11	2.51	0.46
1:A:307:ARG:O	1:A:307:ARG:HG2	2.15	0.46
1:A:4:GLY:O	1:A:94:ASN:ND2	2.48	0.46
1:C:467:LEU:HD23	1:C:527:TRP:CD1	2.48	0.46
1:B:277:ILE:HD12	1:B:439:GLY:HA3	1.98	0.46
1:A:271:ALA:HA	1:B:449:GLN:HG2	1.97	0.46
1:C:318:PHE:CE2	1:C:340:GLY:HA3	2.51	0.46
1:C:491:ILE:O	1:C:495:VAL:HG22	2.16	0.46
1:C:449:GLN:HE21	1:D:271:ALA:HA	1.80	0.46
1:D:307:ARG:HG2	1:D:307:ARG:O	2.16	0.46
1:A:104:TYR:HE1	3:A:901:XMP:H4'	1.80	0.46
1:A:5:GLN:NE2	1:A:97:ARG:HE	2.13	0.46
1:A:172:ARG:HD2	1:B:197:TYR:CG	2.50	0.46
1:C:129:VAL:HG21	1:D:133:ARG:NH2	2.31	0.46
1:D:307:ARG:NH1	1:D:314:SER:HB3	2.29	0.46
1:C:429:GLN:HA	1:C:591:HIS:O	2.15	0.46
1:D:404:VAL:O	1:D:404:VAL:HG22	2.16	0.46
1:D:451:ARG:H	5:D:804:BW2:H5	1.81	0.46
1:A:253:LEU:HD21	1:A:420:VAL:HA	1.98	0.46
1:C:405:THR:HG21	1:C:575:CYS:HB3	1.98	0.46
1:D:41:LEU:CB	1:D:48:VAL:HG21	2.45	0.46
1:D:563:SER:HB3	1:D:584:HIS:ND1	2.30	0.46
1:C:207:ARG:HB2	1:C:207:ARG:HE	1.57	0.45
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.81	0.45
1:B:90:ARG:HH21	1:B:91:LEU:HD21	1.81	0.45
1:C:377:GLU:HB2	1:D:380:THR:HB	1.98	0.45
1:B:117:VAL:O	1:B:121:VAL:HG23	2.15	0.45
1:B:34:SER:OG	1:B:51:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:TRP:C	1:D:510:ALA:N	2.69	0.45
1:B:394:VAL:HA	6:B:1061:HOH:O	2.15	0.45
1:C:209:GLY:HA2	1:C:237:PHE:HB2	1.98	0.45
1:C:357:LYS:HZ2	1:C:357:LYS:HB3	1.82	0.45
1:C:415:LEU:O	1:C:419:ILE:HG13	2.16	0.45
1:C:416:ARG:NH2	1:C:438:ASN:HA	2.31	0.45
1:A:184:GLN:OE1	1:A:184:GLN:HA	2.16	0.45
1:A:87:ASP:HA	1:A:90:ARG:HH11	1.81	0.45
1:B:372:LYS:HD2	6:B:1025:HOH:O	2.16	0.45
1:B:415:LEU:O	1:B:419:ILE:HG13	2.17	0.45
1:D:279:LEU:HD13	1:D:301:ALA:HB1	1.99	0.45
1:B:520:THR:HG23	1:B:523:GLU:H	1.81	0.45
1:C:205:PRO:HG3	6:C:1016:HOH:O	2.17	0.45
1:A:267:HIS:C	1:A:268:VAL:HG23	2.36	0.45
1:B:264:SER:O	1:B:271:ALA:N	2.40	0.45
1:D:247:TRP:CE2	1:D:367:MET:HG2	2.51	0.45
1:A:405:THR:C	1:A:407:ASN:N	2.70	0.45
1:B:61:LEU:CD1	1:B:61:LEU:H	2.30	0.44
1:C:50:ASP:O	1:C:53:GLU:HG3	2.17	0.44
1:A:13:ASP:N	1:A:102:ASN:HD22	2.01	0.44
1:B:61:LEU:CD1	1:B:61:LEU:N	2.80	0.44
1:A:590:PHE:HB2	1:B:211:ASN:OD1	2.18	0.44
1:C:126:ILE:HA	1:D:133:ARG:HH12	1.82	0.44
1:D:470:HIS:ND1	1:D:471:PRO:HD2	2.32	0.44
1:A:241:CYS:HA	1:B:381:LEU:CD2	2.48	0.44
1:A:471:PRO:C	1:A:473:VAL:H	2.20	0.44
1:B:117:VAL:HG21	1:B:196:GLN:HG2	1.99	0.44
1:D:357:LYS:HB2	1:D:362:TYR:HB2	2.00	0.44
1:D:452:ILE:HG23	1:D:453:HIS:N	2.33	0.44
1:A:449:GLN:HE21	1:B:271:ALA:HA	1.82	0.44
1:A:150:ASP:OD2	1:A:177:LYS:NZ	2.41	0.44
1:B:355:SER:O	1:B:360:GLY:HA2	2.17	0.44
1:B:228:ILE:HD11	1:B:365:LEU:HD13	1.98	0.44
1:A:207:ARG:NH2	4:B:702:AMZ:O4	2.48	0.44
1:B:50:ASP:OD2	1:B:52:SER:HB3	2.17	0.44
1:C:210:MET:HE3	1:C:238:ILE:CG1	2.48	0.44
1:C:520:THR:HB	1:C:523:GLU:H	1.83	0.44
1:A:270:PRO:HD3	1:A:427:TYR:O	2.17	0.44
1:B:430:SER:HA	1:B:431:ASN:C	2.37	0.44
1:D:8:LEU:HD23	1:D:9:PHE:N	2.32	0.44
1:A:274:ALA:HB2	1:A:440:GLN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:MET:HE1	1:B:382:PHE:HE2	1.83	0.43
1:B:5:GLN:OE1	1:B:97:ARG:HD3	2.18	0.43
1:C:13:ASP:OD2	1:C:148:PRO:HG2	2.18	0.43
1:C:391:ASN:OD1	1:D:213:HIS:NE2	2.44	0.43
1:C:425:VAL:HG23	1:C:434:CYS:HB2	1.99	0.43
1:C:460:ASP:HA	1:C:463:ASN:HD22	1.83	0.43
1:D:430:SER:HB3	1:D:431:ASN:HA	1.99	0.43
1:D:494:TYR:CE1	1:D:518:LEU:HA	2.53	0.43
1:D:534:VAL:O	1:D:556:VAL:HA	2.18	0.43
1:C:266:LYS:HZ1	5:D:804:BW2:HN9	1.64	0.43
1:B:249:LEU:C	1:B:249:LEU:HD23	2.39	0.43
1:B:546:ASP:HA	1:B:549:ASP:OD2	2.18	0.43
1:D:51:VAL:O	1:D:55:THR:HG23	2.17	0.43
1:B:499:ILE:HD13	1:B:508:TRP:CD2	2.53	0.43
1:D:20:PHE:O	1:D:24:LEU:HG	2.18	0.43
1:A:79:ARG:NH1	1:B:122:GLU:OE2	2.50	0.43
1:B:503:GLU:O	1:B:504:ASP:C	2.57	0.43
1:B:69:HIS:CE1	1:B:70:PRO:HD2	2.53	0.43
1:C:389:LYS:HG2	1:C:390:ARG:N	2.34	0.43
1:C:406:LYS:O	1:C:407:ASN:HB2	2.19	0.43
1:C:479:LYS:C	1:C:481:GLY:H	2.20	0.43
1:B:438:ASN:HA	1:B:438:ASN:HD22	1.58	0.43
1:B:444:ILE:HG23	1:B:444:ILE:O	2.18	0.43
1:C:386:LEU:HD21	1:D:219:LEU:HD13	1.99	0.43
1:D:253:LEU:HD21	1:D:420:VAL:HA	1.99	0.43
1:A:203:GLN:HE21	1:A:218:GLN:HB2	1.83	0.43
1:C:433:VAL:O	1:C:444:ILE:HD12	2.18	0.43
1:C:536:ILE:HD12	1:C:551:ALA:HB1	2.01	0.43
1:A:204:MET:HA	1:A:205:PRO:HD3	1.92	0.43
1:A:565:SER:HA	6:A:1087:HOH:O	2.17	0.43
1:D:147:GLU:HB2	1:D:150:ASP:OD2	2.19	0.43
1:A:9:PHE:HD2	1:A:17:LEU:CD1	2.32	0.43
1:A:381:LEU:CD2	1:B:244:LEU:HD12	2.46	0.43
1:C:192:TYR:O	1:C:196:GLN:HG2	2.19	0.43
1:C:451:ARG:NH1	1:C:538:SER:OG	2.52	0.43
1:D:536:ILE:CD1	1:D:556:VAL:HG21	2.48	0.43
1:D:208:TYR:OH	4:D:703:AMZ:OP2	2.35	0.43
1:A:470:HIS:HE1	1:A:472:GLN:NE2	2.17	0.43
1:C:31:LEU:HB3	1:C:48:VAL:HG23	2.00	0.43
1:C:61:LEU:HD22	1:D:84:ASP:OD2	2.19	0.43
1:B:22:ARG:HG3	1:B:22:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PHE:CZ	1:B:24:LEU:HD11	2.54	0.43
1:B:20:PHE:O	1:B:24:LEU:HG	2.19	0.43
1:A:373:PRO:HD3	1:B:382:PHE:CE1	2.54	0.43
1:A:138:ASN:HA	6:A:1036:HOH:O	2.19	0.42
1:A:357:LYS:HB2	1:A:362:TYR:HB2	2.01	0.42
1:A:590:PHE:HA	1:A:590:PHE:HD1	1.76	0.42
1:C:27:LEU:HD21	1:C:158:MET:HB3	2.01	0.42
1:D:540:ALA:HB2	1:D:590:PHE:CE1	2.54	0.42
1:D:452:ILE:HB	5:D:804:BW2:N3	2.34	0.42
1:A:483:LYS:O	1:A:487:ILE:HG13	2.19	0.42
1:B:12:SER:H	1:B:102:ASN:CB	2.32	0.42
1:B:19:GLU:OE2	1:B:19:GLU:HA	2.18	0.42
1:B:41:LEU:CB	1:B:48:VAL:HG21	2.48	0.42
1:D:13:ASP:OD2	1:D:15:THR:HG22	2.19	0.42
1:D:37:THR:O	1:D:41:LEU:HG	2.18	0.42
1:D:430:SER:HA	1:D:431:ASN:C	2.39	0.42
1:C:512:PHE:N	1:C:512:PHE:CD1	2.87	0.42
1:D:12:SER:N	1:D:102:ASN:OD1	2.51	0.42
1:C:244:LEU:HB2	1:D:381:LEU:HD21	2.01	0.42
1:C:76:ILE:HG13	1:C:96:ILE:HD12	2.02	0.42
1:B:210:MET:HB3	1:B:214:GLN:OE1	2.19	0.42
1:A:405:THR:O	1:A:407:ASN:N	2.51	0.42
1:A:71:ALA:HB2	1:A:93:PHE:CE1	2.55	0.42
1:B:544:PHE:HD1	6:B:1112:HOH:O	2.02	0.42
1:D:437:LYS:HD2	1:D:534:VAL:HG22	2.01	0.42
1:C:223:GLN:HA	1:C:223:GLN:OE1	2.19	0.42
1:C:563:SER:HB3	1:C:584:HIS:CG	2.55	0.42
1:D:293:TYR:O	1:D:295:THR:N	2.52	0.42
1:D:561:ALA:O	1:D:584:HIS:HA	2.20	0.42
1:A:281:GLU:O	1:A:284:ALA:HB3	2.20	0.42
1:B:422:THR:O	1:B:425:VAL:HG12	2.19	0.42
1:D:102:ASN:OD1	1:D:102:ASN:O	2.37	0.42
1:D:203:GLN:HE21	1:D:203:GLN:HB3	1.65	0.42
1:C:70:PRO:HD3	1:D:68:LEU:O	2.20	0.42
1:B:20:PHE:CE2	1:B:24:LEU:HD11	2.55	0.42
1:C:567:ALA:C	1:C:569:LYS:N	2.73	0.42
1:C:244:LEU:HD12	1:D:381:LEU:CD2	2.40	0.41
1:D:558:TYR:CD1	1:D:558:TYR:N	2.87	0.41
1:B:515:VAL:HA	1:B:516:PRO:HD2	1.93	0.41
1:A:154:VAL:O	1:A:158:MET:HG3	2.20	0.41
1:A:5:GLN:HB3	1:A:29:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:VAL:HG11	1:C:197:TYR:OH	2.21	0.41
1:C:448:GLN:HB2	1:C:454:CYS:SG	2.60	0.41
1:A:139:HIS:HB3	1:A:175:ALA:HB2	2.02	0.41
1:A:230:VAL:HG22	1:A:365:LEU:CD2	2.51	0.41
1:C:168:LEU:O	1:C:172:ARG:HG2	2.21	0.41
1:C:237:PHE:CE2	1:D:386:LEU:HB3	2.56	0.41
1:C:184:GLN:NE2	6:C:1024:HOH:O	2.53	0.41
1:B:206:LEU:O	1:B:207:ARG:C	2.58	0.41
1:B:405:THR:C	1:B:407:ASN:H	2.24	0.41
1:C:357:LYS:HB2	1:C:362:TYR:HB2	2.02	0.41
1:D:467:LEU:HD23	1:D:527:TRP:HD1	1.84	0.41
1:A:207:ARG:HE	1:A:207:ARG:HB2	1.50	0.41
1:C:402:ASN:HB3	1:C:584:HIS:O	2.20	0.41
1:C:457:LEU:HD23	1:C:461:LYS:HE3	2.01	0.41
1:D:519:LEU:HB2	1:D:524:LYS:HE3	2.02	0.41
1:B:254:LYS:O	1:B:258:GLY:N	2.50	0.41
1:C:19:GLU:O	1:C:22:ARG:HB2	2.20	0.41
1:D:253:LEU:HA	1:D:253:LEU:HD23	1.94	0.41
1:A:444:ILE:HG23	1:A:444:ILE:O	2.20	0.41
1:C:219:LEU:HD22	1:C:240:LEU:CD1	2.51	0.41
1:C:219:LEU:HD22	1:C:240:LEU:HD13	2.03	0.41
1:D:117:VAL:CG1	1:D:196:GLN:HG2	2.51	0.41
1:D:330:ALA:O	1:D:334:SER:HB2	2.21	0.41
1:A:9:PHE:O	1:A:33:ALA:HA	2.21	0.41
1:B:253:LEU:HD23	1:B:253:LEU:HA	1.86	0.41
1:C:273:ALA:O	1:C:441:VAL:HG23	2.21	0.41
1:D:451:ARG:HB3	5:D:804:BW2:O4	2.21	0.41
1:A:13:ASP:HB3	1:A:102:ASN:ND2	2.35	0.40
1:A:561:ALA:C	1:A:562:PRO:O	2.58	0.40
1:B:61:LEU:HD12	1:B:61:LEU:H	1.86	0.40
1:D:408:LYS:HG2	1:D:408:LYS:H	1.45	0.40
1:A:7:ALA:HB2	1:A:29:LEU:HD13	2.03	0.40
1:A:87:ASP:HA	1:A:90:ARG:NH1	2.37	0.40
1:C:262:ALA:O	1:C:273:ALA:HA	2.21	0.40
1:C:50:ASP:C	1:C:52:SER:N	2.75	0.40
1:D:336:GLU:OE1	1:D:336:GLU:HA	2.21	0.40
1:A:32:VAL:HG12	1:A:51:VAL:HG22	2.03	0.40
1:C:494:TYR:HA	1:C:499:ILE:HD11	2.03	0.40
1:C:575:CYS:HB3	1:C:580:ILE:O	2.22	0.40
1:D:405:THR:CG2	1:D:582:LEU:H	2.35	0.40
1:D:49:ARG:HG3	1:D:53:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LEU:HA	1:C:411:PRO:HD3	1.91	0.40
1:C:567:ALA:O	1:C:570:VAL:N	2.54	0.40
1:A:207:ARG:HD3	1:A:234:ALA:O	2.22	0.40
1:A:318:PHE:CE2	1:A:340:GLY:HA3	2.56	0.40
1:A:550:ARG:O	1:A:553:ARG:HG2	2.21	0.40
1:C:266:LYS:NZ	5:D:804:BW2:HN9	2.20	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	587/592 (99%)	541 (92%)	39 (7%)	7 (1%)	13	27
1	B	583/592 (98%)	543 (93%)	36 (6%)	4 (1%)	22	43
1	C	581/592 (98%)	540 (93%)	36 (6%)	5 (1%)	17	35
1	D	575/592 (97%)	514 (89%)	52 (9%)	9 (2%)	9	19
All	All	2326/2368 (98%)	2138 (92%)	163 (7%)	25 (1%)	14	30

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	82	PRO
1	C	407	ASN
1	A	35	GLY
1	B	61	LEU
1	B	276	GLY
1	C	35	GLY
1	C	476	MET
1	D	61	LEU
1	D	294	LYS

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Mol	Chain	Res	Type
1	D	488	SER
1	D	518	LEU
1	A	27	LEU
1	A	406	LYS
1	B	515	VAL
1	A	472	GLN
1	B	409	ASP
1	D	17	LEU
1	D	293	TYR
1	C	543	PRO
1	D	502	ASP
1	D	514	GLU
1	A	562	PRO
1	D	402	ASN
1	A	324	VAL
1	A	268	VAL

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	460/488 (94%)	439 (95%)	21 (5%)	27	51
1	B	456/488 (93%)	438 (96%)	18 (4%)	32	58
1	C	436/488 (89%)	419 (96%)	17 (4%)	32	58
1	D	423/488 (87%)	401 (95%)	22 (5%)	23	46
All	All	1775/1952 (91%)	1697 (96%)	78 (4%)	28	53

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	27	LEU
1	A	31	LEU
1	A	54	LEU
1	A	94	ASN

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Mol	Chain	Res	Type
1	A	118	GLU
1	A	122	GLU
1	A	138	ASN
1	A	152	VAL
1	A	172	ARG
1	A	186	ASP
1	A	190	SER
1	A	268	VAL
1	A	280	SER
1	A	319	VAL
1	A	369	GLN
1	A	454	CYS
1	A	457	LEU
1	A	484	ARG
1	A	536	ILE
1	A	568	ASP
1	B	25	THR
1	B	61	LEU
1	B	80	ASN
1	B	83	GLU
1	B	97	ARG
1	B	198	SER
1	B	207	ARG
1	B	215	THR
1	B	319	VAL
1	B	323	ASP
1	B	352	THR
1	B	395	VAL
1	B	425	VAL
1	B	438	ASN
1	B	450	SER
1	B	478	PHE
1	B	520	THR
1	B	536	ILE
1	C	5	GLN
1	C	50	ASP
1	C	53	GLU
1	C	84	ASP
1	C	91	LEU
1	C	122	GLU
1	C	172	ARG
1	C	186	ASP

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Mol	Chain	Res	Type
1	C	198	SER
1	C	259	ILE
1	C	268	VAL
1	C	311	ARG
1	C	376	ASN
1	C	520	THR
1	C	536	ILE
1	C	568	ASP
1	C	586	ASN
1	D	17	LEU
1	D	25	THR
1	D	60	MET
1	D	61	LEU
1	D	68	LEU
1	D	103	LEU
1	D	198	SER
1	D	203	GLN
1	D	255	GLU
1	D	266	LYS
1	D	268	VAL
1	D	323	ASP
1	D	408	LYS
1	D	413	SER
1	D	415	LEU
1	D	449	GLN
1	D	454	CYS
1	D	457	LEU
1	D	516	PRO
1	D	517	GLU
1	D	558	TYR
1	D	586	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	85	ASN
1	A	102	ASN
1	A	138	ASN
1	A	181	HIS
1	A	453	HIS
1	A	472	GLN

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Mol	Chain	Res	Type
1	A	547	ASN
1	B	23	ASN
1	B	73	HIS
1	B	80	ASN
1	B	85	ASN
1	B	239	ASN
1	B	438	ASN
1	B	489	ASN
1	B	584	HIS
1	C	102	ASN
1	C	184	GLN
1	C	245	ASN
1	C	429	GLN
1	C	438	ASN
1	C	448	GLN
1	C	449	GLN
1	C	463	ASN
1	C	472	GLN
1	D	23	ASN
1	D	73	HIS
1	D	85	ASN
1	D	184	GLN
1	D	203	GLN
1	D	449	GLN
1	D	453	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
4	AMZ	D	703	-	18,23,23	2.88	5 (27%)	22,35,35	1.87	6 (27%)
3	XMP	A	901	-	21,26,26	2.94	5 (23%)	23,40,40	2.36	6 (26%)
5	BW2	B	802	-	26,27,36	4.67	15 (57%)	36,40,52	2.88	11 (30%)
5	BW2	D	804	-	26,27,36	4.64	15 (57%)	36,40,52	2.77	12 (33%)
4	AMZ	B	702	-	18,23,23	2.62	5 (27%)	22,35,35	1.79	7 (31%)
3	XMP	C	903	-	21,26,26	2.97	6 (28%)	23,40,40	2.42	6 (26%)
4	AMZ	D	704	-	18,23,23	2.59	5 (27%)	22,35,35	1.77	8 (36%)

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
4	AMZ	D	703	-	-	0/6/30/30	0/2/2/2
3	XMP	A	901	-	-	5/6/26/26	0/3/3/3
5	BW2	B	802	-	-	0/15/15/28	0/3/3/3
5	BW2	D	804	-	-	0/15/15/28	0/3/3/3
4	AMZ	B	702	-	-	0/6/30/30	0/2/2/2
3	XMP	C	903	-	-	5/6/26/26	0/3/3/3
4	AMZ	D	704	-	-	0/6/30/30	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	804	BW2	O1-S10	14.27	1.59	1.43
5	B	802	BW2	O2-S10	13.79	1.59	1.43
5	B	802	BW2	O1-S10	13.46	1.58	1.43
5	D	804	BW2	O2-S10	12.40	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	XMP	C4-N3	8.86	1.44	1.33
4	D	703	AMZ	C6-N2	8.73	1.49	1.33
3	A	901	XMP	C4-N3	8.68	1.44	1.33
4	D	704	AMZ	C6-N2	8.30	1.48	1.33
4	B	702	AMZ	C6-N2	7.88	1.48	1.33
3	A	901	XMP	C6-N1	7.38	1.45	1.33
3	C	903	XMP	C6-N1	7.04	1.45	1.33
5	D	804	BW2	C2-N3	6.26	1.46	1.35
5	B	802	BW2	C8A-N1	6.12	1.47	1.37
5	B	802	BW2	C11-C17	-5.50	1.42	1.50
5	D	804	BW2	C11-C17	-5.48	1.42	1.50
5	B	802	BW2	C2-N3	5.40	1.45	1.35
5	D	804	BW2	C8A-N1	5.14	1.46	1.37
4	D	703	AMZ	C7A-N3	5.09	1.49	1.33
5	B	802	BW2	S10-N9	5.09	1.72	1.63
4	B	702	AMZ	C7A-N3	4.90	1.48	1.33
4	D	704	AMZ	C7A-N3	4.77	1.48	1.33
5	D	804	BW2	S10-N9	4.71	1.71	1.63
4	B	702	AMZ	O-C1	4.07	1.46	1.41
4	D	703	AMZ	O-C1	3.99	1.46	1.41
3	A	901	XMP	C2-N1	3.64	1.45	1.38
4	D	703	AMZ	C5-N1	3.62	1.41	1.35
5	D	804	BW2	C12-C11	3.55	1.45	1.39
3	C	903	XMP	P-O3P	3.53	1.61	1.50
3	C	903	XMP	C2-N1	3.49	1.45	1.38
5	D	804	BW2	C16-C11	3.41	1.45	1.39
4	D	703	AMZ	P-OP2	3.36	1.61	1.50
5	B	802	BW2	C16-C11	3.25	1.44	1.39
5	B	802	BW2	C12-C11	3.22	1.44	1.39
5	D	804	BW2	C5-C6	3.08	1.44	1.37
3	A	901	XMP	C2-N3	3.04	1.44	1.38
4	D	704	AMZ	P-OP2	2.97	1.60	1.50
4	B	702	AMZ	P-OP2	2.90	1.59	1.50
3	A	901	XMP	P-O3P	2.89	1.59	1.50
4	D	704	AMZ	O-C1	2.75	1.44	1.41
5	D	804	BW2	C4-N3	2.74	1.37	1.33
3	C	903	XMP	O4'-C1'	2.71	1.44	1.41
5	D	804	BW2	C8-C7	2.67	1.42	1.36
4	D	704	AMZ	C5-N1	2.62	1.39	1.35
5	B	802	BW2	C8-C7	2.59	1.42	1.36
3	C	903	XMP	C2-N3	2.51	1.43	1.38
5	D	804	BW2	C13-C12	2.50	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	AMZ	C5-N1	2.34	1.39	1.35
5	B	802	BW2	C4-N3	2.33	1.37	1.33
5	B	802	BW2	C2-N2	2.29	1.38	1.33
5	D	804	BW2	C13-C14	2.28	1.42	1.38
5	B	802	BW2	C4A-C8A	2.26	1.45	1.41
5	D	804	BW2	C4A-C8A	2.22	1.45	1.41
5	B	802	BW2	C5-C6	2.20	1.42	1.37
5	B	802	BW2	C13-C12	2.19	1.42	1.38
5	D	804	BW2	C7-C6	2.15	1.42	1.39
5	B	802	BW2	C13-C14	2.11	1.42	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	804	BW2	C4A-C4-N3	-8.61	118.40	124.40
5	B	802	BW2	C4A-C4-N3	-7.84	118.94	124.40
5	B	802	BW2	O1-S10-O2	-7.66	110.14	119.55
5	B	802	BW2	C4A-C8A-N1	-6.97	119.81	123.60
5	D	804	BW2	C4A-C8A-N1	-6.86	119.87	123.60
3	C	903	XMP	O4'-C1'-C2'	-6.75	97.06	106.93
3	A	901	XMP	O4'-C1'-C2'	-6.49	97.44	106.93
3	C	903	XMP	C6-N1-C2	6.27	120.44	115.14
3	A	901	XMP	C6-N1-C2	6.24	120.41	115.14
5	D	804	BW2	O1-S10-O2	-5.93	112.26	119.55
5	B	802	BW2	O1-S10-C14	4.69	113.75	107.97
5	B	802	BW2	N1-C2-N3	-4.38	121.38	127.22
4	D	703	AMZ	C3-C2-C1	4.20	107.31	100.98
5	D	804	BW2	O2-S10-C14	4.16	113.09	107.97
5	D	804	BW2	O1-S10-C14	4.10	113.02	107.97
5	D	804	BW2	N1-C2-N3	-4.08	121.77	127.22
4	B	702	AMZ	O5-C6-N2	-4.00	116.89	122.58
5	B	802	BW2	C4-N3-C2	4.00	122.28	115.93
4	D	703	AMZ	O5-C6-N2	-3.95	116.96	122.58
4	D	704	AMZ	O5-C6-N2	-3.94	116.97	122.58
4	D	704	AMZ	C3-C2-C1	3.74	106.60	100.98
5	B	802	BW2	O2-S10-C14	3.73	112.56	107.97
5	D	804	BW2	C4-N3-C2	3.51	121.50	115.93
5	B	802	BW2	C4-C4A-C8A	-3.42	115.61	118.59
5	D	804	BW2	O17-C17-N	-3.28	117.92	122.58
4	B	702	AMZ	C3-C2-C1	3.24	105.86	100.98
5	B	802	BW2	O17-C17-N	-3.19	118.05	122.58
3	C	903	XMP	O3'-C3'-C4'	-3.09	102.12	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	804	BW2	C4-C4A-C8A	-2.97	116.00	118.59
3	A	901	XMP	O3'-C3'-C2'	2.95	121.36	111.82
5	D	804	BW2	O2-S10-N9	-2.92	99.42	106.73
3	A	901	XMP	O3'-C3'-C4'	-2.92	102.61	111.05
4	B	702	AMZ	OP1-P-O3	2.89	114.43	106.73
3	C	903	XMP	O3'-C3'-C2'	2.89	121.18	111.82
3	A	901	XMP	C3'-C2'-C1'	2.86	105.29	100.98
4	D	703	AMZ	C3A-C6-N2	2.76	120.10	115.75
4	D	703	AMZ	OP1-P-O3	2.71	113.95	106.73
4	B	702	AMZ	C2-C3-C	-2.65	97.50	102.64
3	C	903	XMP	C3'-C2'-C1'	2.64	104.95	100.98
4	D	704	AMZ	C3A-C6-N2	2.57	119.81	115.75
5	D	804	BW2	C2-N1-C8A	2.47	122.45	116.33
4	B	702	AMZ	C3A-C6-N2	2.45	119.61	115.75
4	B	702	AMZ	C5-N1-C3A	2.42	107.60	102.99
3	C	903	XMP	C5-C6-N1	-2.41	120.14	123.43
4	D	704	AMZ	C5-N1-C3A	2.35	107.47	102.99
4	D	703	AMZ	P-O3-C4	-2.32	111.89	118.30
4	D	703	AMZ	C5-N1-C3A	2.32	107.42	102.99
4	D	704	AMZ	C2-C3-C	-2.29	98.19	102.64
5	B	802	BW2	O17-C17-C11	2.29	122.37	119.63
5	B	802	BW2	C2-N1-C8A	2.28	121.96	116.33
4	B	702	AMZ	O-C1-C2	-2.25	103.63	106.93
4	D	704	AMZ	OP1-P-O3	2.25	112.71	106.73
4	D	704	AMZ	O-C1-C2	-2.18	103.73	106.93
3	A	901	XMP	C5-C6-N1	-2.15	120.50	123.43
4	D	704	AMZ	P-O3-C4	-2.05	112.65	118.30
5	D	804	BW2	C11-C17-N	2.00	120.16	117.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	XMP	C5'-O5'-P-O1P
3	A	901	XMP	C5'-O5'-P-O2P
3	A	901	XMP	C5'-O5'-P-O3P
3	A	901	XMP	O4'-C4'-C5'-O5'
3	A	901	XMP	C3'-C4'-C5'-O5'
3	C	903	XMP	C5'-O5'-P-O1P
3	C	903	XMP	C5'-O5'-P-O2P
3	C	903	XMP	C5'-O5'-P-O3P
3	C	903	XMP	O4'-C4'-C5'-O5'

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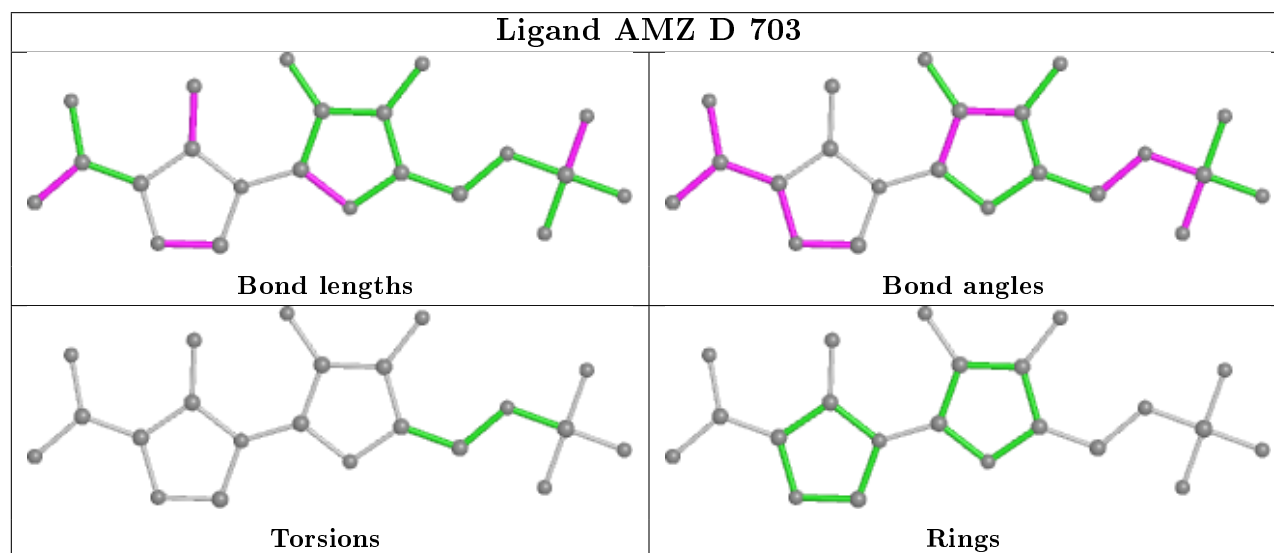
Mol	Chain	Res	Type	Atoms
3	C	903	XMP	C3'-C4'-C5'-O5'

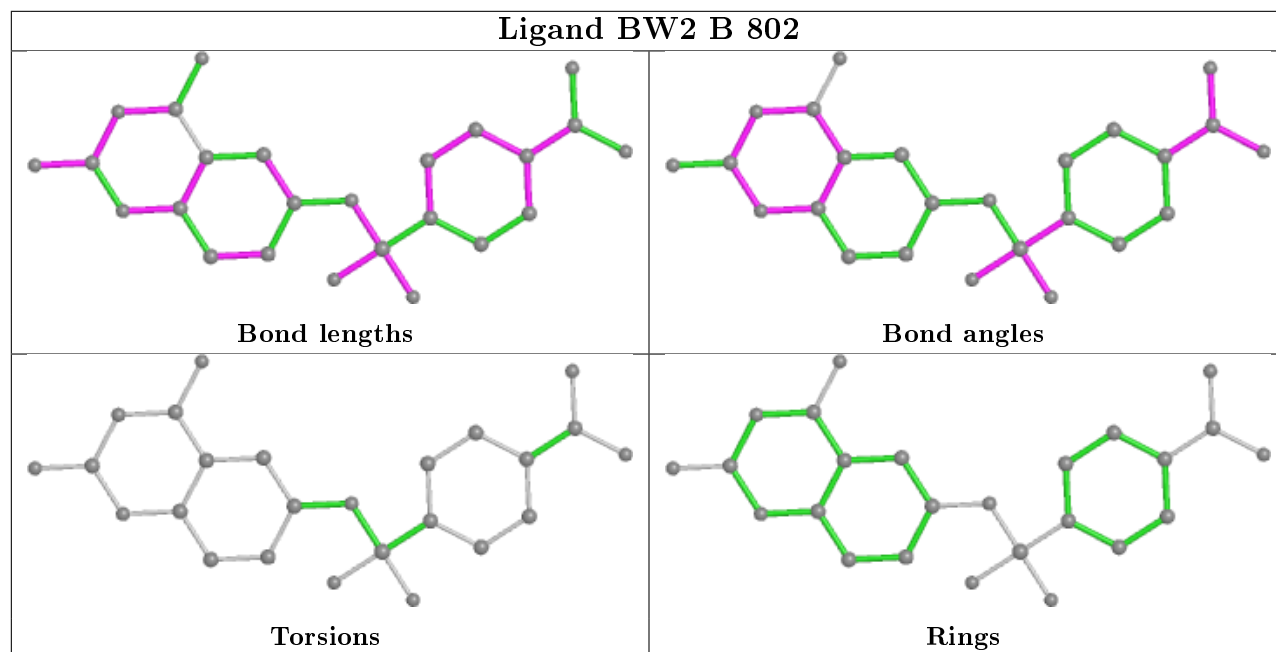
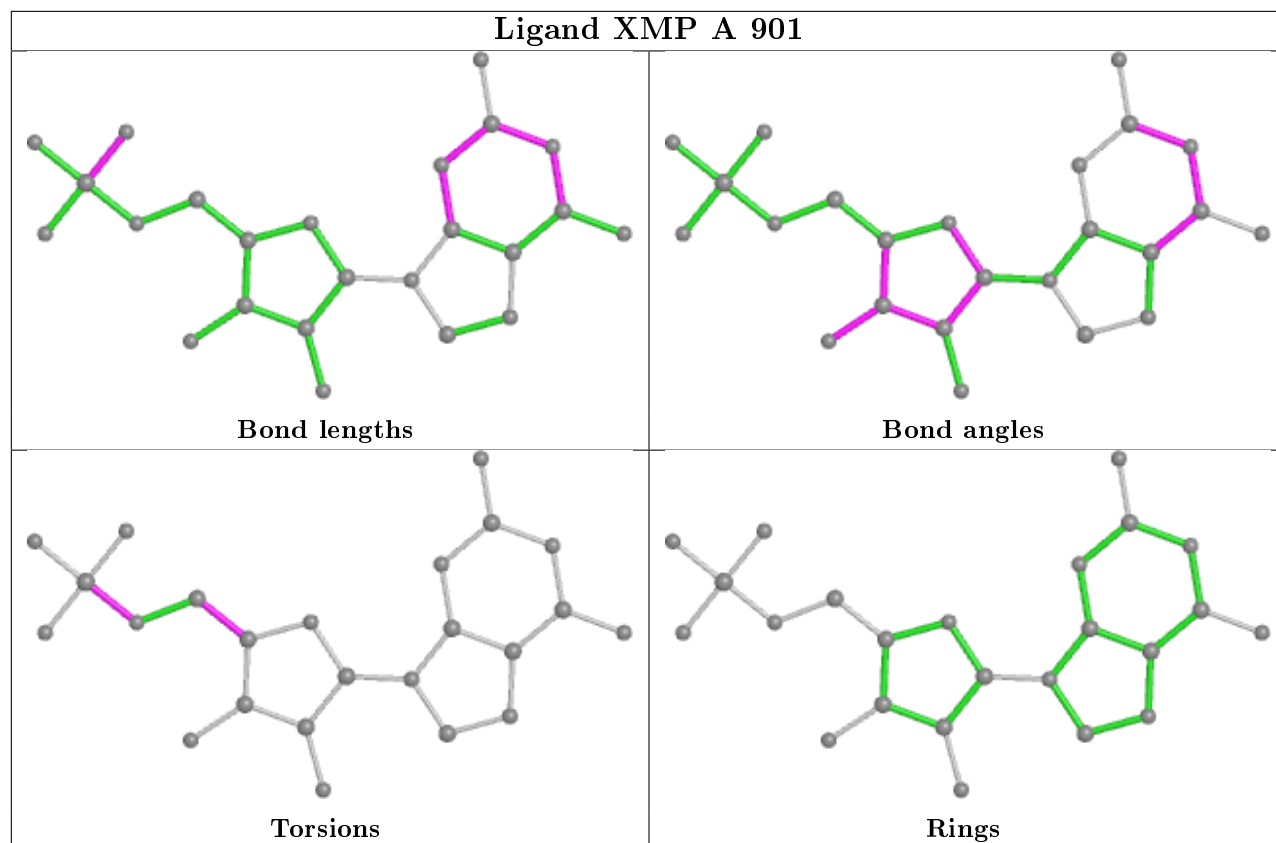
There are no ring outliers.

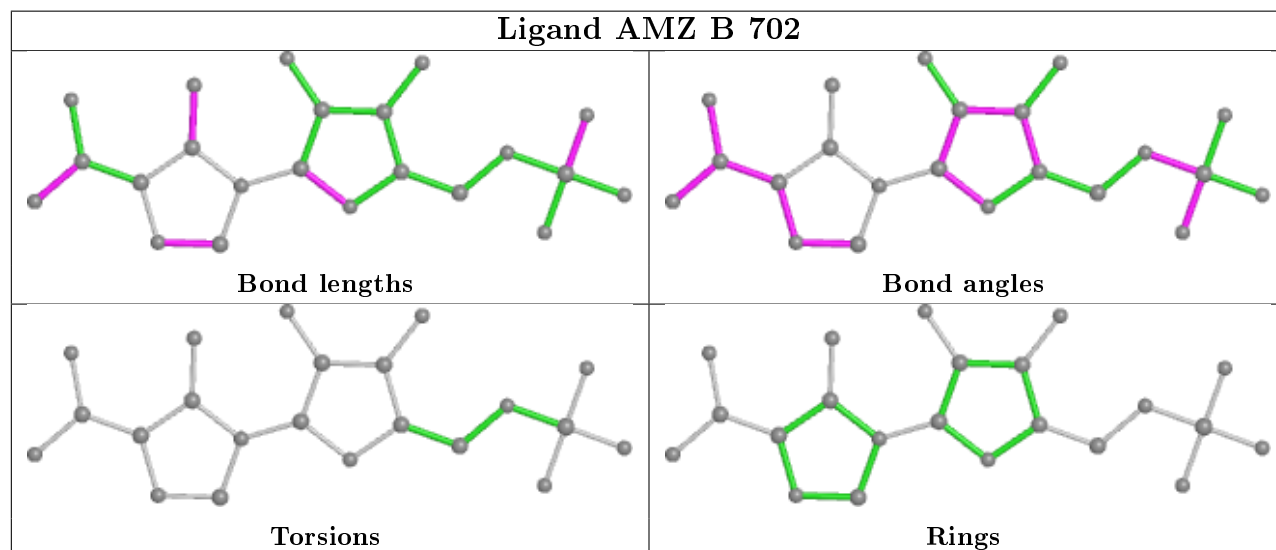
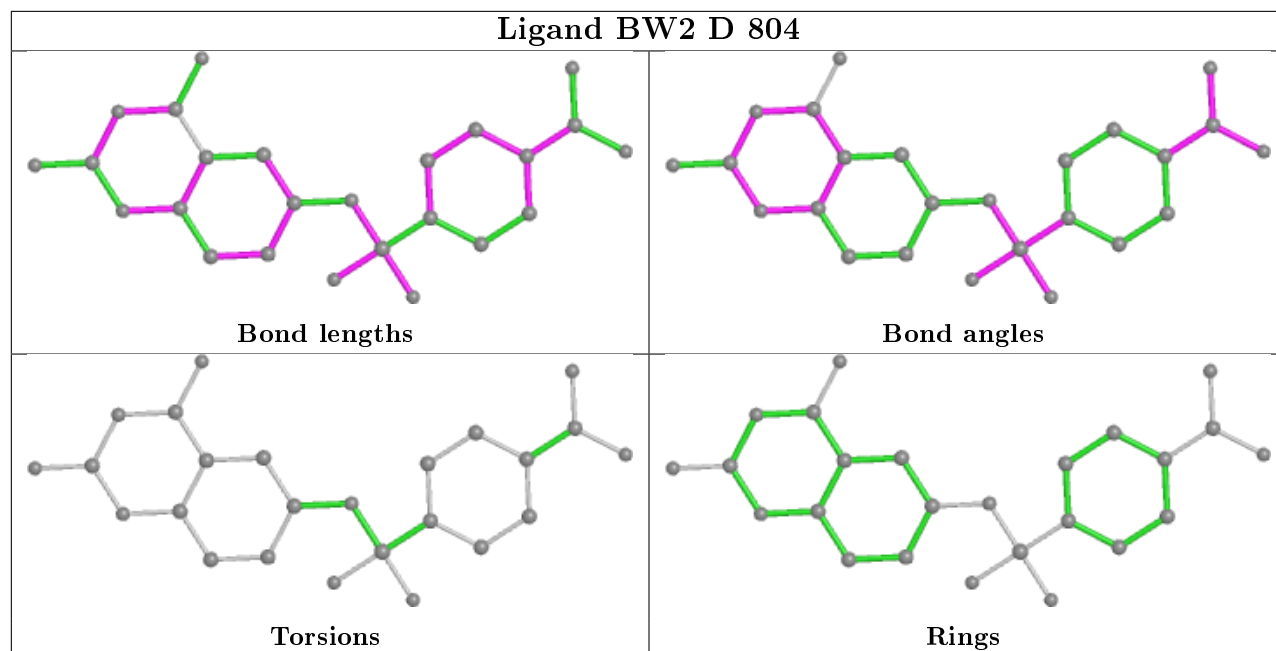
5 monomers are involved in 13 short contacts:

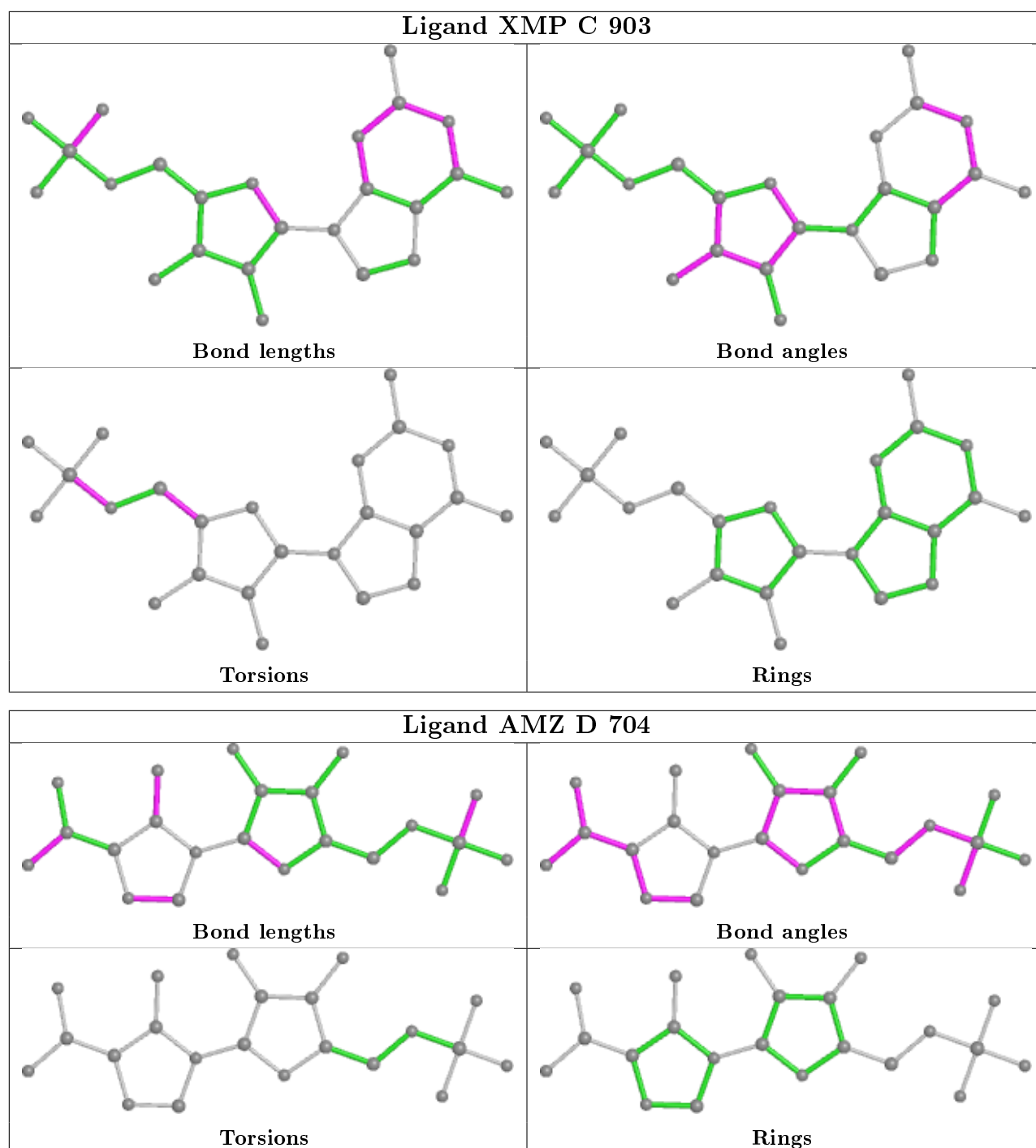
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	703	AMZ	1	0
3	A	901	XMP	3	0
5	B	802	BW2	2	0
5	D	804	BW2	6	0
4	B	702	AMZ	1	0

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 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	589/592 (99%)	-0.75	0 100 100	6, 26, 51, 64	0
1	B	587/592 (99%)	-0.78	1 (0%) 95 95	3, 22, 51, 74	0
1	C	585/592 (98%)	-0.71	0 100 100	8, 29, 54, 66	0
1	D	579/592 (97%)	-0.75	2 (0%) 94 93	4, 25, 54, 75	0
All	All	2340/2368 (98%)	-0.75	3 (0%) 95 95	3, 25, 53, 75	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	510	ALA	2.4
1	B	500	GLY	2.3
1	D	500	GLY	2.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

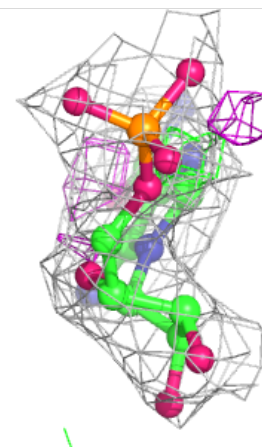
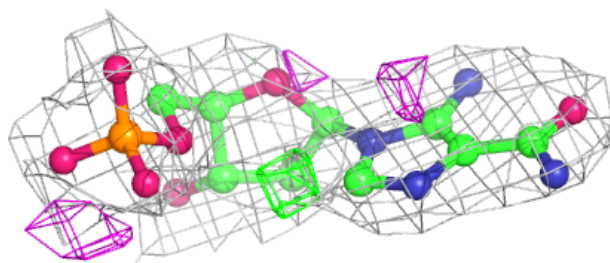
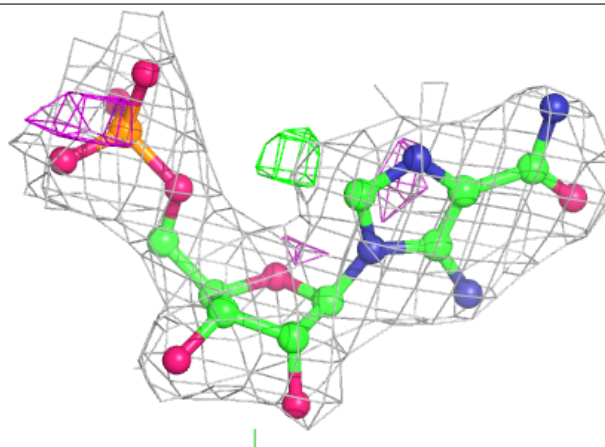
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	AMZ	D	703	22/22	0.95	0.15	34,39,40,41	0
5	BW2	D	804	25/34	0.96	0.13	27,31,33,34	0
4	AMZ	B	702	22/22	0.97	0.13	27,30,32,33	0
5	BW2	B	802	25/34	0.97	0.12	21,25,32,33	0
3	XMP	A	901	24/24	0.97	0.11	19,21,26,31	0
4	AMZ	D	704	22/22	0.97	0.12	20,22,25,27	0
3	XMP	C	903	24/24	0.98	0.09	17,21,28,30	0
2	K	B	1002	1/1	0.99	0.07	12,12,12,12	0
2	K	C	1003	1/1	0.99	0.06	17,17,17,17	0
2	K	A	1001	1/1	0.99	0.06	16,16,16,16	0
2	K	D	1004	1/1	0.99	0.07	17,17,17,17	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.

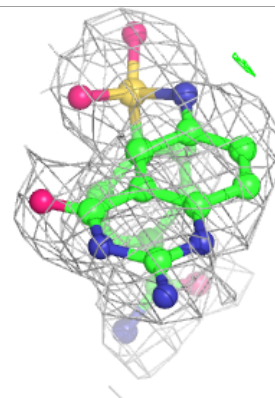
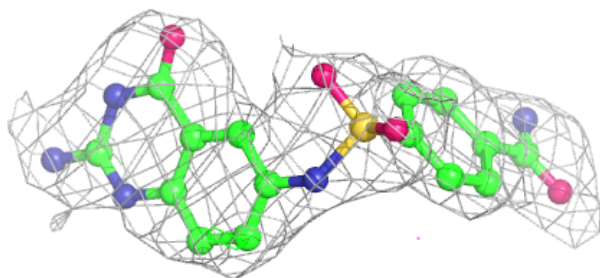
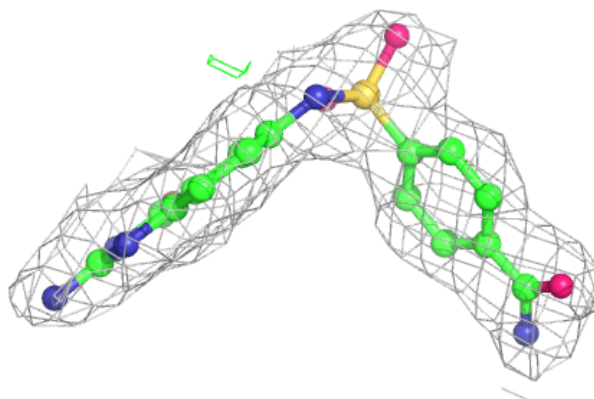
Electron density around AMZ D 703:

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



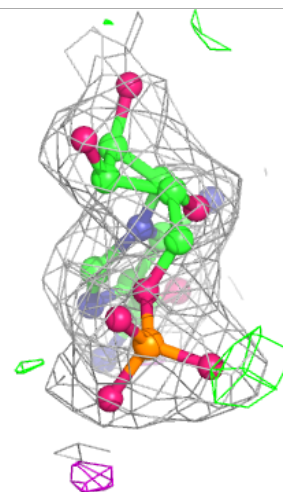
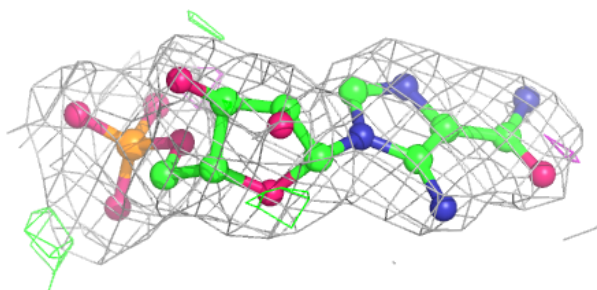
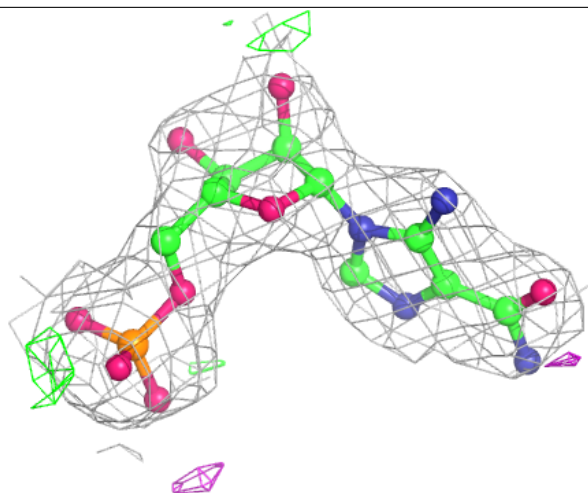
Electron density around BW2 D 804:

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



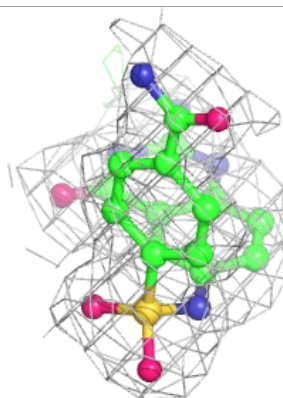
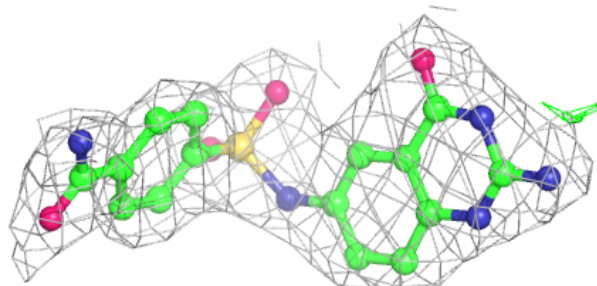
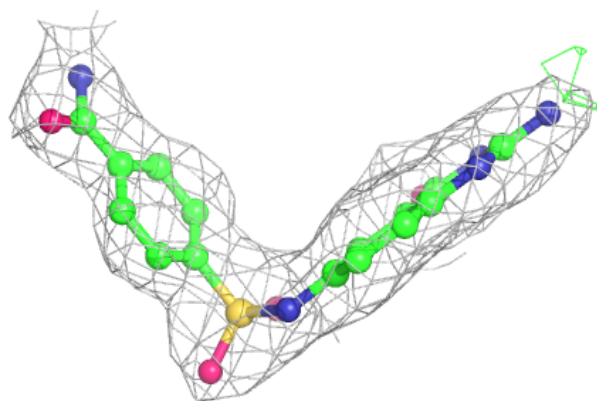
Electron density around AMZ B 702:

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

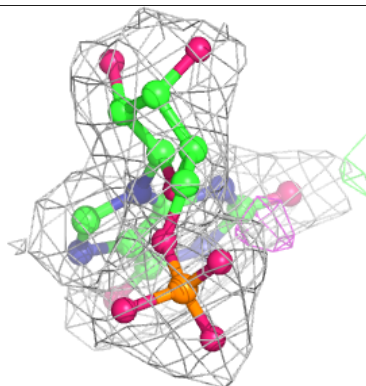
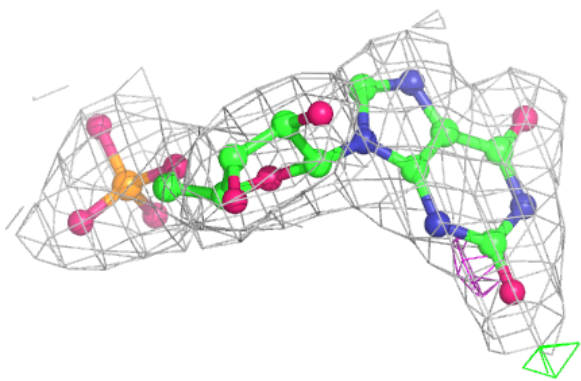
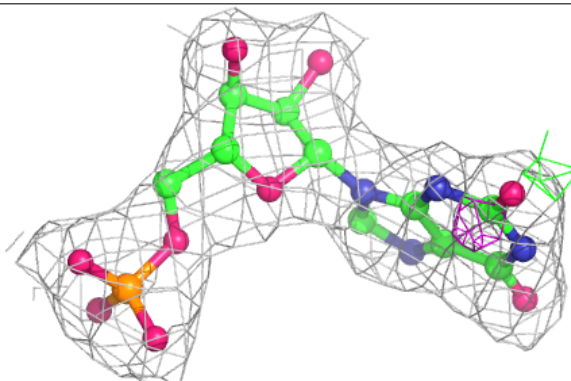


Electron density around BW2 B 802:

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

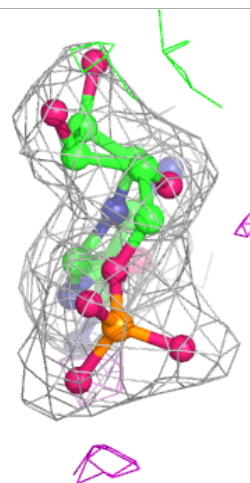
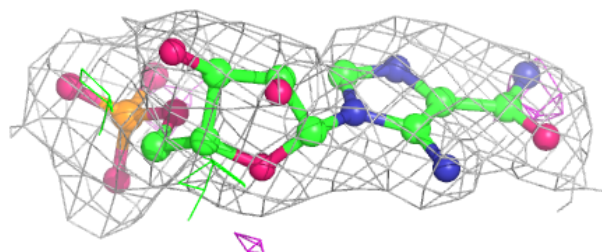
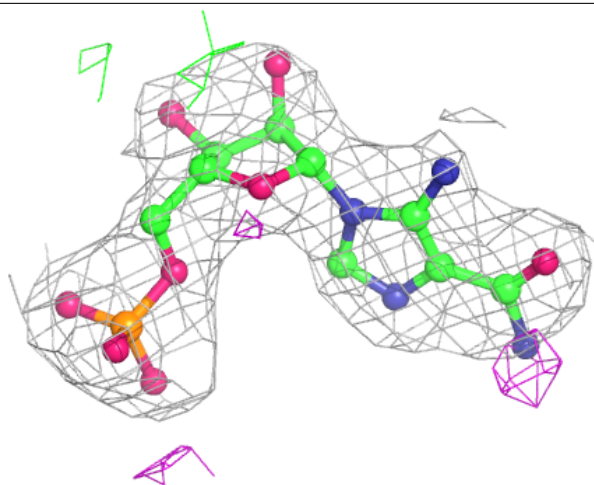
**Electron density around XMP A 901:**

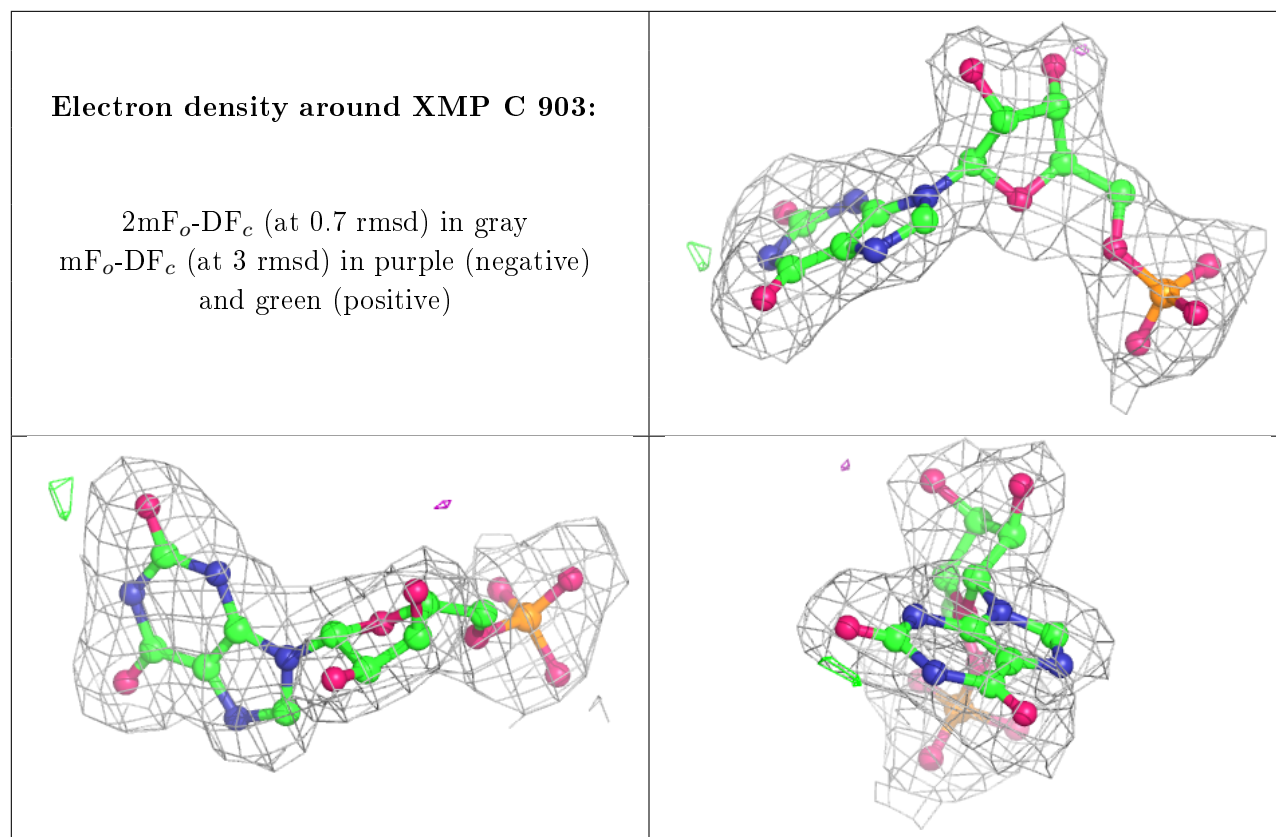
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMZ D 704:

$2mF_o-DF_c$ (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.