



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 06:18 AM EDT

PDB ID : 1PL0 / pdb_00001pl0
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 types of validation reports are described at

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

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

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

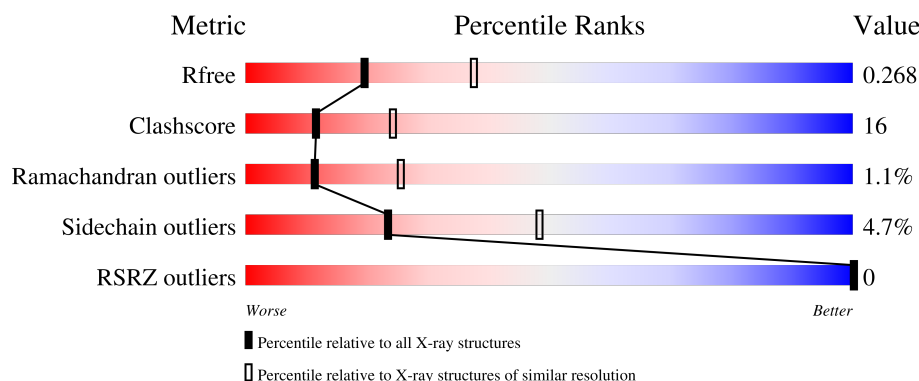
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	592	 65% 31% ..
1	B	592	 69% 27% ..
1	C	592	 64% 31% ..
1	D	592	 64% 31% ..

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.

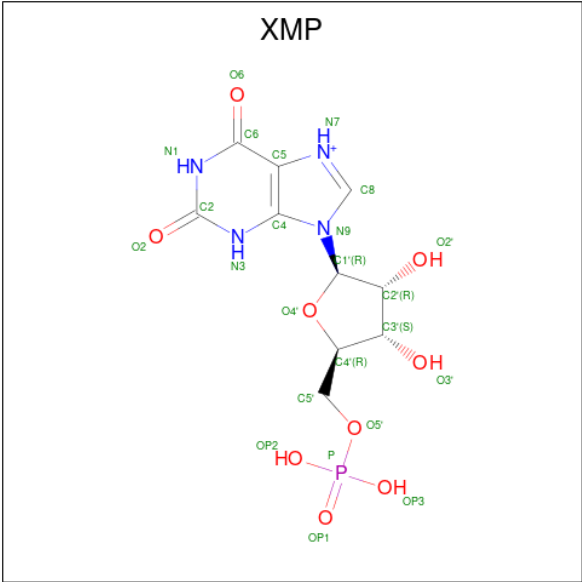
- Molecule 1 is a protein called Bifunctional purine biosynthesis protein PURH.

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 (CCD ID: K) (formula: K).

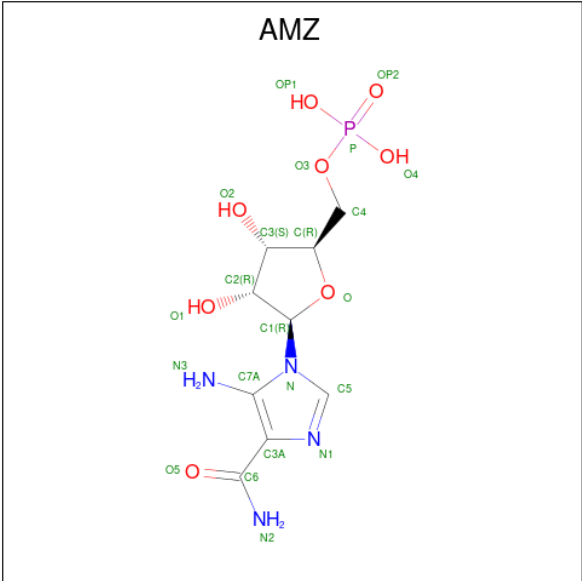
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		

- Molecule 3 is XANTHOSINE-5'-MONOPHOSPHATE (CCD ID: 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 (CCD ID: AMZ) (formula: C₉H₁₅N₄O₈P).



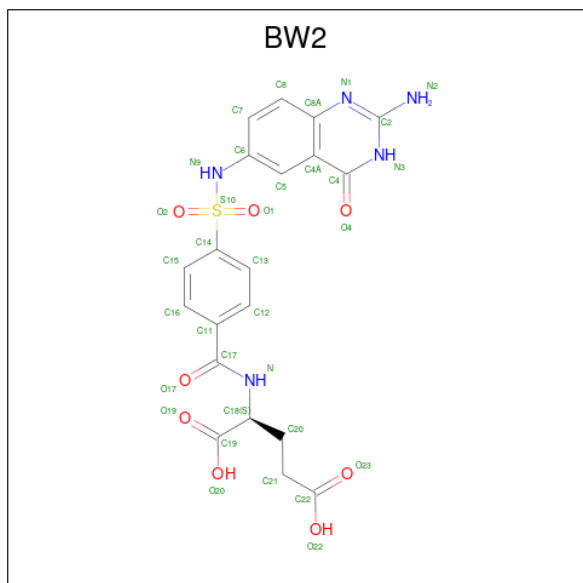
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			22	9	4	8	1		

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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 (CCD ID: 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		

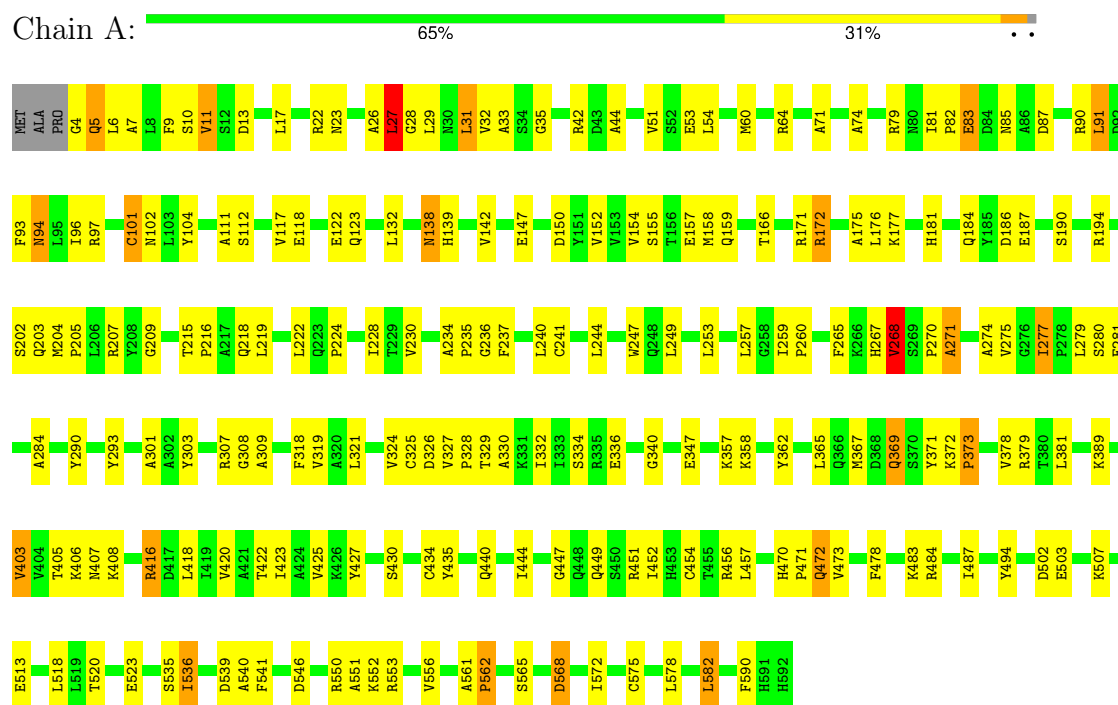
- Molecule 6 is water.

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		

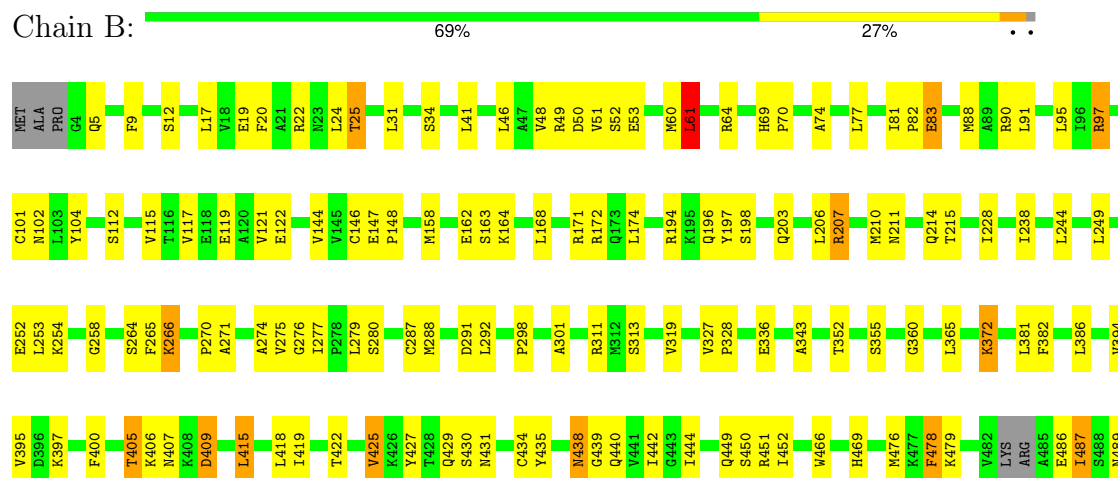
3 Residue-property plots

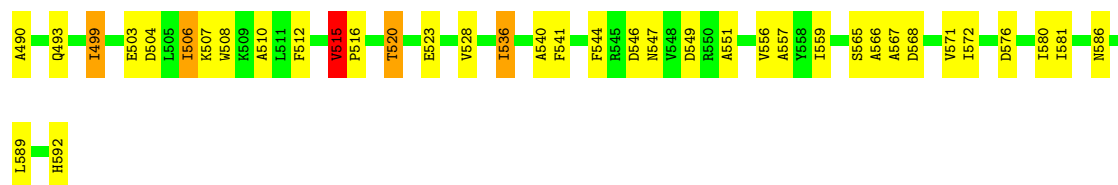
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bifunctional purine biosynthesis protein PURH



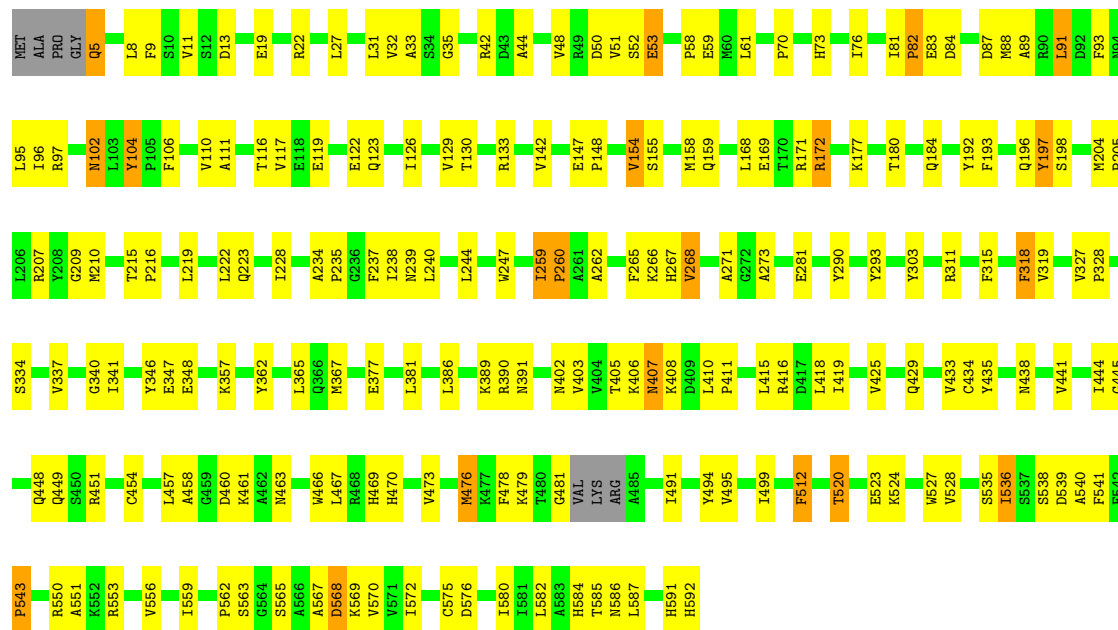
- Molecule 1: Bifunctional purine biosynthesis protein PURH





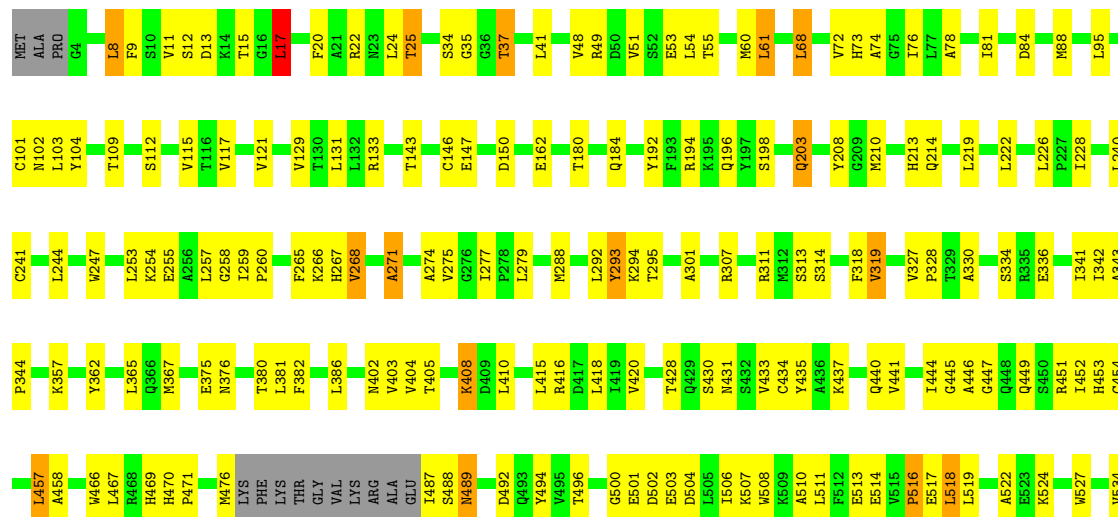
- Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain C: 64% 31% . .



- Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain D: 64% 31% . .



S535	I536		A540	F541	F542		V556	A557	Y558	I559	A560	A561	F562	S563	G564	S565	A566	A567	D568		V571	I572		I580	I581	L582	A583	H584	T585	N586		F590	H591	H592
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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 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 86.9 (20.00-2.60)	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 , 8.9	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	0.94	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, K, XMP, AMZ

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	0.55	0/4507	1.01	22/6131 (0.4%)
1	B	0.56	0/4487	1.03	18/6104 (0.3%)
1	C	0.53	0/4411	1.01	15/6002 (0.2%)
1	D	0.57	0/4314	1.05	23/5882 (0.4%)
All	All	0.55	0/17719	1.02	78/24119 (0.3%)

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.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	ALA	N-CA-C	-9.82	100.03	112.90
1	D	74	ALA	N-CA-C	-8.46	102.13	111.36
1	A	271	ALA	N-CA-C	-7.67	102.57	112.23
1	B	280	SER	N-CA-C	-7.17	101.06	110.53
1	B	343	ALA	N-CA-C	6.99	114.51	108.22
1	C	197	TYR	N-CA-C	6.93	121.86	113.41
1	B	163	SER	N-CA-C	-6.57	104.29	112.90
1	D	265	PHE	N-CA-C	6.53	119.88	109.24
1	A	265	PHE	N-CA-C	6.49	120.40	109.76
1	B	104	TYR	N-CA-C	-6.44	101.53	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	542	PHE	CA-C-N	6.35	125.92	119.19
1	D	542	PHE	C-N-CA	6.35	125.92	119.19
1	C	265	PHE	N-CA-C	6.32	120.36	110.32
1	D	511	LEU	N-CA-C	-6.29	105.50	113.43
1	A	293	TYR	N-CA-C	6.15	118.78	111.33
1	C	222	LEU	N-CA-C	-5.99	105.97	113.28
1	A	372	LYS	CA-C-N	5.98	125.95	120.21
1	A	372	LYS	C-N-CA	5.98	125.95	120.21
1	C	318	PHE	N-CA-C	-5.96	99.69	109.40
1	B	74	ALA	N-CA-C	-5.95	104.87	111.36
1	B	506	ILE	N-CA-C	-5.91	105.95	111.45
1	B	515	VAL	CA-C-N	5.87	126.36	120.14
1	B	515	VAL	C-N-CA	5.87	126.36	120.14
1	A	11	VAL	N-CA-C	5.86	116.92	108.48
1	A	222	LEU	N-CA-C	-5.86	106.17	113.38
1	D	566	ALA	N-CA-C	-5.84	105.41	112.54
1	B	372	LYS	CA-C-N	5.83	125.73	119.85
1	B	372	LYS	C-N-CA	5.83	125.73	119.85
1	D	271	ALA	N-CA-C	-5.80	105.30	112.90
1	D	162	GLU	N-CA-C	-5.79	106.17	113.18
1	A	416	ARG	N-CA-C	-5.74	104.66	111.03
1	A	74	ALA	N-CA-C	-5.71	105.04	112.23
1	D	104	TYR	N-CA-C	-5.70	102.59	109.72
1	C	180	THR	N-CA-C	-5.70	105.21	111.82
1	D	81	ILE	CA-C-N	5.65	126.91	119.84
1	D	81	ILE	C-N-CA	5.65	126.91	119.84
1	B	559	ILE	N-CA-C	5.62	116.21	108.12
1	D	319	VAL	N-CA-C	5.61	117.08	108.71
1	A	373	PRO	N-CA-C	5.58	119.04	111.22
1	A	403	VAL	N-CA-C	-5.55	101.64	109.63
1	D	376	ASN	N-CA-C	5.50	119.20	109.96
1	A	513	GLU	N-CA-C	-5.47	105.33	112.23
1	D	541	PHE	N-CA-C	5.46	117.37	110.33
1	A	101	CYS	N-CA-C	5.44	118.27	108.48
1	B	415	LEU	N-CA-C	-5.38	105.41	111.28
1	A	91	LEU	N-CA-C	-5.38	106.46	114.64
1	B	589	LEU	N-CA-C	5.37	116.89	110.44
1	A	96	ILE	N-CA-C	-5.36	100.73	108.87
1	C	102	ASN	N-CA-C	-5.35	102.27	110.14
1	D	513	GLU	N-CA-C	-5.34	105.59	113.61
1	D	586	ASN	N-CA-C	-5.28	105.54	112.41
1	B	442	ILE	N-CA-C	-5.26	108.00	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	LYS	N-CA-C	-5.25	102.75	110.52
1	D	11	VAL	N-CA-C	5.24	115.67	108.12
1	A	502	ASP	CB-CA-C	-5.24	110.51	116.54
1	C	154	VAL	N-CA-C	5.24	115.45	110.53
1	B	566	ALA	N-CA-C	-5.20	106.91	113.20
1	D	489	ASN	N-CA-C	-5.19	106.08	112.72
1	A	112	SER	CA-C-N	5.17	126.31	119.84
1	A	112	SER	C-N-CA	5.17	126.31	119.84
1	A	277	ILE	N-CA-C	-5.17	103.88	108.95
1	C	470	HIS	CA-C-N	5.17	126.31	119.84
1	C	470	HIS	C-N-CA	5.17	126.31	119.84
1	C	293	TYR	N-CA-C	5.16	117.64	111.71
1	A	111	ALA	N-CA-C	-5.14	106.16	112.90
1	B	487	ILE	N-CA-C	-5.14	105.50	113.16
1	D	506	ILE	N-CA-C	-5.14	98.65	109.34
1	D	37	THR	N-CA-C	-5.14	105.59	111.14
1	C	104	TYR	CA-C-N	5.12	126.24	119.84
1	C	104	TYR	C-N-CA	5.12	126.24	119.84
1	D	226	LEU	N-CA-C	-5.12	103.02	110.08
1	C	512	PHE	N-CA-C	5.11	117.84	110.28
1	A	187	GLU	N-CA-C	-5.04	105.88	112.23
1	C	576	ASP	N-CA-C	-5.04	105.87	111.36
1	D	446	ALA	N-CA-C	5.04	116.84	109.24
1	B	479	LYS	N-CA-C	5.01	118.26	108.18
1	D	318	PHE	N-CA-C	-5.00	101.01	109.07
1	B	499	ILE	N-CA-C	5.00	115.12	110.42

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	148	0
1	B	4405	0	4320	141	0
1	C	4332	0	4227	159	0
1	D	4236	0	4090	150	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	555	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 16.

All (555) 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:B:210:MET:HE3	1:B:238:ILE:HD11	1.63	0.80
1:D:88:MET:HE2	1:D:95:LEU:HD23	1.64	0.79
1:A:155:SER:O	1:A:159:GLN:HG3	1.83	0.79
1:D:487:ILE:C	1:D:489:ASN:H	1.87	0.79
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:A:11:VAL:HB	1:A:102:ASN:ND2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:83:GLU:CD	1:A:83:GLU:H	1.98	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:B:60:MET:HE2	1:B:61:LEU:HD13	1.73	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:88:MET:HE3	1:C:93:PHE:O	1.93	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:C:210:MET:HE3	1:C:238:ILE:HG12	1.75	0.67
1:D:466:TRP:O	1:D:469:HIS:HB2	1.94	0.67
1:A:405:THR:C	1:A:407:ASN:H	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:MET:HE2	1:C:95:LEU:HD23	1.79	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: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:D:267:HIS:C	1:D:268:VAL:HG23	2.25	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:OE2	1:D:501:GLU:HA	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:C:147:GLU:CD	1:C:177:LYS:HD3	2.27	0.60
1:A:244:LEU:HD12	1:B:381:LEU:HD23	1.84	0.60
1:B:168:LEU:O	1:B:172:ARG:HG3	2.02	0.60
1:B:265:PHE:CE1	1:B:270:PRO:HB3	2.37	0.60
1:C:210:MET:HE3	1:C:238:ILE:CG1	2.32	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:49:ARG:HG2	1:D:53:GLU:CB	2.32	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:C:42:ARG:C	1:C:44:ALA:H	2.10	0.59
1:B:486:GLU:HA	1:B:489:ASN:HD22	1.66	0.59
1:A:520:THR:HG22	1:A:523:GLU:CD	2.27	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:O2	5:D:804:BW2:H5	2.02	0.58
1:A:22:ARG:HH11	1:A:22:ARG:HG2	1.68	0.58
1:D:557:ALA:C	1:D:580:ILE:HG23	2.29	0.58
1:B:115:VAL:HA	1:B:119:GLU:OE1	2.03	0.58
1:C:8:LEU:HD12	1:C:32:VAL:O	2.03	0.58
1:C:106:PHE:O	1:C:110:VAL:HG22	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:B:435:TYR:CZ	1:B:536:ILE:HD11	2.39	0.58
1:B:69:HIS:ND1	1:B:70:PRO:HD2	2.19	0.57
1:B:478:PHE:CD1	1:B:478:PHE:N	2.72	0.57
1:B:83:GLU:CD	1:B:83:GLU:H	2.05	0.57
1:B:434:CYS:HB2	1:B:444:ILE:CD1	2.33	0.57
1:A:53:GLU:O	1:A:53:GLU:HG2	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: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:C:267:HIS:C	1:C:268:VAL:HG23	2.29	0.56
1:D:22:ARG:O	1:D:25:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:THR:HG22	1:D:184:GLN:HE21	1.71	0.56
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:A:5:GLN:HE21	1:A:97:ARG:HE	1.54	0.55
1:A:90:ARG:HG3	1:A:91:LEU:HD12	1.88	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: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:C:247:TRP:CD1	1:C:367:MET:HE3	2.42	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:B:82:PRO:HB2	1:B:83:GLU:OE1	2.07	0.54
1:B:162:GLU:O	1:B:162:GLU:HG2	2.06	0.54
1:A:367:MET:HE2	1:B:382:PHE:HE2	1.72	0.54
1:C:357:LYS:HB3	1:C:357:LYS:NZ	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:26:ALA:C	1:A:28:GLY:H	2.16	0.54
1:A:253:LEU:HD23	1:A:423:ILE:HD12	1.89	0.54
1:A:104:TYR:CE1	3:A:901:XMP:H4'	2.42	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: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:N	1:B:478:PHE:HD1	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: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:487:ILE:C	1:D:489:ASN:N	2.55	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:D:292:LEU:O	1:D:293:TYR:C	2.53	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:B:88:MET:HE2	1:B:95:LEU:HD23	1.90	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:B:476:MET:HE2	1:B:516:PRO:HG3	1.92	0.51
1:C:184:GLN:NE2	1:D:222:LEU:HD13	2.25	0.51
1:C:478:PHE:HA	1:C:512:PHE:HA	1.91	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:D:476:MET:HE2	1:D:516:PRO:HG3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:D:444:ILE:HG23	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:B:210:MET:CE	1:B:238:ILE:HD11	2.38	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:HG2	1:A:22:ARG:NH1	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:210:MET:CE	1:D:592:HIS:HB2	2.41	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:B:430:SER:HA	1:B:431:ASN:C	2.37	0.49
1:C:346:TYR:OH	1:C:365:LEU:O	2.30	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:267:HIS:C	1:A:268:VAL:HG23	2.36	0.49
1:B:210:MET:HE3	1:B:238:ILE:CD1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:471:PRO:C	1:A:473:VAL:H	2.20	0.49
1:B:397:LYS:CB	1:B:415:LEU:HD21	2.42	0.49
1:C:479:LYS:C	1:C:481:GLY:H	2.20	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:D:508:TRP:C	1:D:510:ALA:N	2.69	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:B:311:ARG:HH22	1:B:336:GLU:CD	2.21	0.48
1:D:327:VAL:HB	1:D:328:PRO:HD3	1.95	0.48
1:A:176:LEU:HD12	1:A:176:LEU:O	2.13	0.48
1:A:284:ALA:HB1	1:A:290:TYR:HA	1.96	0.48
1:B:41:LEU:HB2	1:B:48:VAL:HG21	1.95	0.48
1:B:249:LEU:C	1:B:249:LEU:HD23	2.39	0.48
1:B:287:CYS:O	1:B:288:MET:HB2	2.14	0.48
1:A:81:ILE:O	1:A:85:ASN:ND2	2.47	0.48
1:A:219:LEU:HD13	1:A:240:LEU:HD13	1.94	0.48
1:A:244:LEU:HD12	1:B:381:LEU:CD2	2.43	0.48
1:B:503:GLU:O	1:B:504:ASP:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:SER:HA	1:D:431:ASN:C	2.39	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: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
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:91:LEU:HD22	1:C:93:PHE:CE2	2.50	0.46
1:C:204:MET:HE3	1:C:235:PRO:HG2	1.98	0.46
1:C:473:VAL:HA	1:C:476:MET:HG3	1.97	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:425:VAL:HG13	1:C:539:ASP:HB3	1.95	0.46
1:C:466:TRP:O	1:C:469:HIS:HB2	2.16	0.46
1:D:72:VAL:O	1:D:76:ILE:HG13	2.14	0.46
1:D:418:LEU:HD22	1:D:560:ALA:HB2	1.96	0.46
1:D:453:HIS:O	1:D:457:LEU:HB2	2.16	0.46
1:D:20:PHE:CE2	1:D:24:LEU:HD11	2.51	0.46
1:A:4:GLY:O	1:A:94:ASN:ND2	2.48	0.46
1:A:307:ARG:HG2	1:A:307:ARG:O	2.15	0.46
1:C:467:LEU:HD23	1:C:527:TRP:CD1	2.48	0.46
1:A:271:ALA:HA	1:B:449:GLN:HG2	1.97	0.46
1:B:277:ILE:HD12	1:B:439:GLY:HA3	1.98	0.46
1:C:318:PHE:CE2	1:C:340:GLY:HA3	2.51	0.46
1:C:449:GLN:HE21	1:D:271:ALA:HA	1.80	0.46
1:C:491:ILE:O	1:C:495:VAL:HG22	2.16	0.46
1:A:5:GLN:NE2	1:A:97:ARG:HE	2.13	0.46
1:A:104:TYR:HE1	3:A:901:XMP:H4'	1.80	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:HG22	1:D:404:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:206:LEU:O	1:B:207:ARG:C	2.58	0.46
1:B:405:THR:C	1:B:407:ASN:H	2.24	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:HE	1:C:207:ARG:HB2	1.57	0.45
1:C:567:ALA:C	1:C:569:LYS:N	2.73	0.45
1:B:90:ARG:HH21	1:B:91:LEU:HD21	1.81	0.45
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.81	0.45
1:C:377:GLU:HB2	1:D:380:THR:HB	1.98	0.45
1:B:34:SER:OG	1:B:51:VAL:HG23	2.16	0.45
1:B:117:VAL:O	1:B:121:VAL:HG23	2.15	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: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:C:210:MET:HE2	1:D:592:HIS:CD2	2.52	0.45
1:A:87:ASP:HA	1:A:90:ARG:HH11	1.81	0.45
1:A:184:GLN:OE1	1:A:184:GLN:HA	2.16	0.45
1:A:204:MET:HE3	1:A:235:PRO:HG2	1.99	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:D:267:HIS:C	1:D:268:VAL:CG2	2.90	0.45
1:B:264:SER:O	1:B:271:ALA:N	2.40	0.45
1:C:61:LEU:HD22	1:D:84:ASP:CG	2.42	0.45
1:D:247:TRP:CE2	1:D:367:MET:HG2	2.51	0.45
1:D:307:ARG:O	1:D:307:ARG:HG2	2.16	0.45
1:B:61:LEU:H	1:B:61:LEU:CD1	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:B:147:GLU:O	1:B:148:PRO:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:ILE:HD11	1:B:365:LEU:HD13	1.98	0.44
1:B:355:SER:O	1:B:360:GLY:HA2	2.17	0.44
1:C:42:ARG:C	1:C:44:ALA:N	2.75	0.44
1:A:83:GLU:CD	1:A:83:GLU:N	2.73	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: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:C:357:LYS:HB3	1:C:357:LYS:HZ3	1.83	0.44
1:C:592:HIS:H	1:D:210:MET:HE3	1.82	0.44
1:D:8:LEU:HD23	1:D:9:PHE:N	2.32	0.44
1:A:42:ARG:C	1:A:44:ALA:H	2.26	0.44
1:D:508:TRP:C	1:D:510:ALA:H	2.26	0.44
1:A:249:LEU:C	1:A:249:LEU:HD23	2.43	0.43
1:A:274:ALA:HB2	1:A:440:GLN:HB2	1.99	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:266:LYS:HZ1	5:D:804:BW2:HN9	1.64	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:B:546:ASP:HA	1:B:549:ASP:OD2	2.18	0.43
1:C:50:ASP:C	1:C:52:SER:N	2.75	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:C:541:PHE:CD1	1:C:541:PHE:C	2.96	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:A:561:ALA:C	1:A:562:PRO:O	2.58	0.43
1:B:60:MET:O	1:B:61:LEU:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:PHE:CD1	1:D:541:PHE:C	2.96	0.43
1:B:438:ASN:HD22	1:B:438:ASN:HA	1.58	0.43
1:B:444:ILE:O	1:B:444:ILE:HG23	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:C:347:GLU:O	1:C:348:GLU:C	2.62	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:C:540:ALA:C	1:C:562:PRO:HD2	2.44	0.43
1:D:208:TYR:OH	4:D:703:AMZ:OP2	2.35	0.43
1:D:536:ILE:CD1	1:D:556:VAL:HG21	2.48	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:A:373:PRO:HD3	1:B:382:PHE:CE1	2.54	0.43
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:B:22:ARG:HG3	1:B:22:ARG:HH11	1.82	0.43
1:C:210:MET:HE2	1:D:592:HIS:HD2	1.84	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:HD1	1:A:590:PHE:HA	1.76	0.42
1:C:27:LEU:HD21	1:C:158:MET:HB3	2.01	0.42
1:D:452:ILE:HB	5:D:804:BW2:N3	2.34	0.42
1:D:540:ALA:HB2	1:D:590:PHE:CE1	2.54	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:259:ILE:O	1:D:260:PRO:C	2.61	0.42
1:C:244:LEU:HB2	1:D:381:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:PHE:CD1	1:C:512:PHE:N	2.87	0.42
1:D:12:SER:N	1:D:102:ASN:OD1	2.51	0.42
1:C:76:ILE:HG13	1:C:96:ILE:HD12	2.02	0.42
1:D:476:MET:HE1	1:D:494:TYR:CD2	2.55	0.42
1:B:210:MET:HB3	1:B:214:GLN:OE1	2.19	0.42
1:A:71:ALA:HB2	1:A:93:PHE:CE1	2.55	0.42
1:A:405:THR:O	1:A:407:ASN:N	2.51	0.42
1:B:544:PHE:HD1	6:B:1112:HOH:O	2.02	0.42
1:C:259:ILE:O	1:C:260:PRO:C	2.63	0.42
1:D:437:LYS:HD2	1:D:534:VAL:HG22	2.01	0.42
1:D:293:TYR:C	1:D:295:THR:H	2.27	0.42
1:C:223:GLN:OE1	1:C:223:GLN:HA	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:C:70:PRO:HD3	1:D:68:LEU:O	2.20	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:A:369:GLN:C	1:A:371:TYR:N	2.75	0.42
1:B:20:PHE:CE2	1:B:24:LEU:HD11	2.55	0.42
1:D:34:SER:O	1:D:35:GLY:C	2.63	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:C:238:ILE:O	1:C:239:ASN:C	2.63	0.41
1:A:5:GLN:HB3	1:A:29:LEU:HD21	2.01	0.41
1:A:154:VAL:O	1:A:158:MET:HG3	2.20	0.41
1:B:520:THR:HG22	1:B:523:GLU:CD	2.45	0.41
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:D:88:MET:HE2	1:D:95:LEU:CD2	2.43	0.41
1:A:326:ASP:CG	1:A:328:PRO:HD2	2.44	0.41
1:C:357:LYS:HB2	1:C:362:TYR:HB2	2.02	0.41
1:D:381:LEU:O	1:D:382:PHE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:357:LYS:O	1:A:358:LYS:C	2.63	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:A:60:MET:HE1	1:B:91:LEU:CD1	2.51	0.41
1:A:444:ILE:O	1:A:444:ILE:HG23	2.20	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: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:253:LEU:HD23	1:D:253:LEU:HA	1.94	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:A:541:PHE:CD1	1:A:541:PHE:C	2.98	0.41
1:B:253:LEU:HA	1:B:253:LEU:HD23	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:308:GLY:O	1:A:309:ALA:C	2.63	0.40
1:B:61:LEU:H	1:B:61:LEU:HD12	1.86	0.40
1:D:17:LEU:CD2	1:D:17:LEU:C	2.93	0.40
1:D:408:LYS:H	1:D:408:LYS:HG2	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:A:405:THR:C	1:A:407:ASN:N	2.70	0.40
1:C:262:ALA:O	1:C:273:ALA:HA	2.21	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:49:ARG:HG3	1:D:53:GLU:OE1	2.22	0.40
1:D:405:THR:CG2	1:D:582:LEU:H	2.35	0.40
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:369:GLN:C	1:A:371:TYR:H	2.29	0.40
1:A:550:ARG:O	1:A:553:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MET:HE2	1:B:61:LEU:CD1	2.47	0.40
1:C:58:PRO:O	1:C:59:GLU:C	2.64	0.40
1:C:87:ASP:C	1:C:89:ALA:N	2.78	0.40
1:C:88:MET:HE2	1:C:95:LEU:CD2	2.49	0.40
1:C:266:LYS:NZ	5:D:804:BW2:HN9	2.20	0.40
1:D:430:SER:C	1:D:447:GLY:HA2	2.45	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%)	10	23
1	B	583/592 (98%)	543 (93%)	36 (6%)	4 (1%)	18	38
1	C	581/592 (98%)	540 (93%)	36 (6%)	5 (1%)	14	30
1	D	575/592 (97%)	514 (89%)	52 (9%)	9 (2%)	7	16
All	All	2326/2368 (98%)	2138 (92%)	163 (7%)	25 (1%)	11	25

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%)	437 (95%)	23 (5%)	22	46
1	B	456/488 (93%)	435 (95%)	21 (5%)	24	49
1	C	436/488 (89%)	420 (96%)	16 (4%)	30	57
1	D	423/488 (87%)	400 (95%)	23 (5%)	20	42
All	All	1775/1952 (91%)	1692 (95%)	83 (5%)	23	48

All (83) 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	83	GLU

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Mol	Chain	Res	Type
1	A	94	ASN
1	A	117	VAL
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	536	ILE
1	A	568	ASP
1	A	582	LEU
1	B	25	THR
1	B	61	LEU
1	B	83	GLU
1	B	97	ARG
1	B	198	SER
1	B	207	ARG
1	B	215	THR
1	B	266	LYS
1	B	275	VAL
1	B	298	PRO
1	B	319	VAL
1	B	352	THR
1	B	395	VAL
1	B	405	THR
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	B	586	ASN
1	C	5	GLN
1	C	53	GLU
1	C	84	ASP

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Mol	Chain	Res	Type
1	C	91	LEU
1	C	122	GLU
1	C	169	GLU
1	C	172	ARG
1	C	198	SER
1	C	259	ILE
1	C	260	PRO
1	C	268	VAL
1	C	311	ARG
1	C	520	THR
1	C	536	ILE
1	C	568	ASP
1	C	586	ASN
1	D	8	LEU
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	109	THR
1	D	143	THR
1	D	198	SER
1	D	203	GLN
1	D	255	GLU
1	D	268	VAL
1	D	375	GLU
1	D	408	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	138	ASN
1	A	181	HIS
1	A	203	GLN
1	A	449	GLN
1	A	453	HIS
1	A	469	HIS
1	A	472	GLN
1	B	73	HIS
1	B	80	ASN
1	B	85	ASN
1	B	102	ASN
1	B	181	HIS
1	B	239	ASN
1	B	359	ASN
1	B	438	ASN
1	B	472	GLN
1	B	489	ASN
1	B	493	GLN
1	B	584	HIS
1	C	73	HIS
1	C	80	ASN
1	C	102	ASN
1	C	139	HIS
1	C	184	GLN
1	C	245	ASN
1	C	376	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	C	591	HIS
1	D	73	HIS
1	D	85	ASN
1	D	184	GLN
1	D	203	GLN
1	D	366	GLN
1	D	449	GLN
1	D	453	HIS
1	D	472	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 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$
3	XMP	A	901	-	26,26,26	1.99	5 (19%)	34,40,40	1.93	12 (35%)
5	BW2	B	802	-	27,27,36	4.48	14 (51%)	40,40,52	2.17	12 (30%)
4	AMZ	B	702	-	22,23,23	2.10	5 (22%)	32,35,35	2.19	8 (25%)
4	AMZ	D	704	-	22,23,23	2.11	5 (22%)	32,35,35	2.36	8 (25%)
5	BW2	D	804	-	27,27,36	4.49	16 (59%)	40,40,52	2.04	11 (27%)
4	AMZ	D	703	-	22,23,23	2.29	5 (22%)	32,35,35	2.39	7 (21%)
3	XMP	C	903	-	26,26,26	2.02	8 (30%)	34,40,40	1.98	12 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XMP	A	901	-	-	5/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BW2	B	802	-	-	0/15/15/28	0/3/3/3
4	AMZ	B	702	-	-	0/14/30/30	0/2/2/2
4	AMZ	D	704	-	-	0/14/30/30	0/2/2/2
5	BW2	D	804	-	-	0/15/15/28	0/3/3/3
4	AMZ	D	703	-	-	0/14/30/30	0/2/2/2
3	XMP	C	903	-	-	5/10/26/26	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	804	BW2	O1-S10	14.00	1.59	1.43
5	B	802	BW2	O2-S10	13.52	1.59	1.43
5	B	802	BW2	O1-S10	13.21	1.58	1.43
5	D	804	BW2	O2-S10	12.16	1.57	1.43
4	D	703	AMZ	C7A-N3	6.63	1.49	1.34
4	B	702	AMZ	C7A-N3	6.36	1.48	1.34
4	D	704	AMZ	C7A-N3	6.19	1.48	1.34
4	D	703	AMZ	C6-N2	5.61	1.49	1.33
5	B	802	BW2	C11-C17	-5.57	1.42	1.50
5	D	804	BW2	C11-C17	-5.54	1.42	1.50
5	B	802	BW2	S10-N9	5.37	1.72	1.63
4	D	704	AMZ	C6-N2	5.33	1.48	1.33
4	B	702	AMZ	C6-N2	5.05	1.48	1.33
5	D	804	BW2	S10-N9	4.97	1.71	1.63
5	D	804	BW2	C4A-C4	4.92	1.55	1.47
3	A	901	XMP	C2-N1	4.80	1.45	1.37
3	C	903	XMP	C2-N1	4.62	1.45	1.37
5	B	802	BW2	C8A-N1	4.44	1.47	1.39
3	C	903	XMP	C4-N3	4.21	1.44	1.37
3	A	901	XMP	C2-N3	4.08	1.44	1.37
3	A	901	XMP	C4-N3	4.07	1.44	1.37
5	B	802	BW2	C4A-C8A	4.03	1.45	1.40
5	D	804	BW2	C4A-C8A	3.98	1.45	1.40
5	D	804	BW2	C12-C11	3.93	1.45	1.39
5	B	802	BW2	C4A-C4	3.92	1.53	1.47
5	D	804	BW2	C16-C11	3.78	1.45	1.39
3	A	901	XMP	C6-N1	3.76	1.45	1.38
3	C	903	XMP	P-OP1	3.68	1.61	1.50
5	D	804	BW2	C2-N3	3.67	1.46	1.37
5	B	802	BW2	C16-C11	3.59	1.44	1.39
5	D	804	BW2	C8A-N1	3.57	1.46	1.39
5	B	802	BW2	C12-C11	3.56	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	703	AMZ	P-OP2	3.51	1.61	1.50
3	C	903	XMP	C6-N1	3.44	1.45	1.38
3	C	903	XMP	C2-N3	3.44	1.43	1.37
4	D	704	AMZ	P-OP2	3.11	1.60	1.50
4	D	703	AMZ	C5-N1	3.08	1.41	1.32
5	B	802	BW2	C2-N3	3.04	1.45	1.37
4	B	702	AMZ	P-OP2	3.03	1.59	1.50
3	A	901	XMP	P-OP1	3.02	1.59	1.50
5	D	804	BW2	C5-C6	2.92	1.44	1.39
5	D	804	BW2	C13-C12	2.78	1.43	1.38
3	C	903	XMP	C4-N9	2.62	1.39	1.37
4	D	704	AMZ	C5-N1	2.47	1.39	1.32
5	B	802	BW2	C13-C12	2.43	1.42	1.38
4	B	702	AMZ	C5-N1	2.30	1.39	1.32
5	D	804	BW2	C13-C14	2.27	1.42	1.38
4	D	704	AMZ	C3A-C6	2.21	1.53	1.47
5	D	804	BW2	C7-C6	2.14	1.42	1.39
5	D	804	BW2	C7-C8	2.11	1.42	1.38
5	B	802	BW2	C13-C14	2.10	1.42	1.38
5	D	804	BW2	C16-C15	2.07	1.42	1.38
4	B	702	AMZ	O-C1	2.06	1.46	1.42
3	C	903	XMP	C5'-C4'	2.03	1.57	1.51
3	C	903	XMP	C8-N7	2.03	1.38	1.32
4	D	703	AMZ	O-C1	2.01	1.46	1.42
5	B	802	BW2	C17-N	2.01	1.36	1.33
5	B	802	BW2	C7-C8	2.00	1.42	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	AMZ	C3A-C7A-N	9.89	109.80	105.75
4	D	704	AMZ	C3A-C7A-N	9.84	109.78	105.75
4	B	702	AMZ	C3A-C7A-N	8.26	109.13	105.75
5	B	802	BW2	O1-S10-O2	-7.73	110.14	119.52
5	D	804	BW2	O1-S10-O2	-5.98	112.26	119.52
5	B	802	BW2	O1-S10-C14	4.57	113.75	107.98
3	C	903	XMP	O4'-C1'-C2'	-4.46	97.06	106.62
3	A	901	XMP	C6-N1-C2	-4.33	120.41	126.37
3	C	903	XMP	C6-N1-C2	-4.31	120.44	126.37
3	A	901	XMP	O4'-C1'-C2'	-4.29	97.44	106.62
5	D	804	BW2	O2-S10-C14	4.05	113.09	107.98
4	D	704	AMZ	C7A-C3A-N1	-4.01	108.39	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	804	BW2	O1-S10-C14	4.00	113.02	107.98
4	B	702	AMZ	C7A-C3A-N1	-3.92	108.43	109.91
4	D	703	AMZ	C7A-C3A-N1	-3.91	108.43	109.91
5	B	802	BW2	C4A-C4-N3	3.80	118.94	114.93
5	B	802	BW2	O2-S10-C14	3.63	112.56	107.98
3	C	903	XMP	C2'-C1'-N9	3.38	122.66	113.25
3	A	901	XMP	C2'-C1'-N9	3.37	122.62	113.25
5	D	804	BW2	C8A-N1-C2	3.29	122.45	118.05
5	D	804	BW2	C4A-C4-N3	3.28	118.40	114.93
5	D	804	BW2	O17-C17-N	-3.25	117.92	122.62
4	B	702	AMZ	C6-C3A-C7A	3.23	128.55	125.92
5	B	802	BW2	O17-C17-N	-3.16	118.05	122.62
3	C	903	XMP	O3'-C3'-C4'	-3.12	102.12	111.08
4	D	703	AMZ	C3-C2-C1	3.09	107.31	101.46
3	A	901	XMP	O6-C6-C5	-3.01	118.58	126.53
5	D	804	BW2	O2-S10-N9	-3.00	99.42	106.74
5	D	804	BW2	O4-C4-N3	-2.98	117.08	120.62
5	B	802	BW2	O4-C4-N3	-2.98	117.08	120.62
3	A	901	XMP	O3'-C3'-C2'	2.98	121.36	111.82
4	B	702	AMZ	OP1-P-O3	2.98	114.43	106.67
3	A	901	XMP	O3'-C3'-C4'	-2.95	102.61	111.08
3	C	903	XMP	O3'-C3'-C2'	2.92	121.18	111.82
5	B	802	BW2	C8A-N1-C2	2.92	121.96	118.05
3	C	903	XMP	O6-C6-C5	-2.90	118.87	126.53
3	A	901	XMP	C5-C6-N1	2.85	120.50	113.25
4	D	703	AMZ	OP1-P-O3	2.79	113.95	106.67
5	D	804	BW2	C5-C4A-C4	2.75	125.23	120.09
3	C	903	XMP	N9-C8-N7	-2.73	108.34	113.40
4	D	704	AMZ	C3-C2-C1	2.72	106.60	101.46
3	C	903	XMP	C5-C6-N1	2.71	120.14	113.25
4	B	702	AMZ	O5-C6-N2	-2.68	116.89	122.89
4	D	703	AMZ	N-C5-N1	-2.66	108.46	113.40
3	A	901	XMP	N9-C8-N7	-2.65	108.49	113.40
4	D	703	AMZ	O5-C6-N2	-2.65	116.96	122.89
4	B	702	AMZ	C2-C3-C	-2.64	97.50	102.61
4	D	704	AMZ	O5-C6-N2	-2.64	116.97	122.89
4	D	704	AMZ	C3A-C7A-N3	-2.63	127.00	130.63
3	C	903	XMP	C4'-O4'-C1'	-2.62	103.67	109.47
5	B	802	BW2	C4A-C8A-N1	-2.58	119.81	122.41
5	D	804	BW2	C4A-C8A-N1	-2.53	119.87	122.41
5	B	802	BW2	C5-C4A-C4	2.47	124.69	120.09
4	D	703	AMZ	C3A-C7A-N3	-2.46	127.23	130.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	BW2	C8A-C4A-C4	-2.37	115.61	118.73
3	A	901	XMP	C8-N9-C4	2.35	108.65	106.67
4	B	702	AMZ	C3-C2-C1	2.32	105.86	101.46
4	D	704	AMZ	OP1-P-O3	2.32	112.71	106.67
3	C	903	XMP	C8-N9-C4	2.30	108.61	106.67
4	D	704	AMZ	C2-C3-C	-2.29	98.19	102.61
4	D	704	AMZ	N-C5-N1	-2.27	109.19	113.40
5	B	802	BW2	O17-C17-C11	2.27	122.37	119.60
4	B	702	AMZ	N-C5-N1	-2.25	109.22	113.40
3	A	901	XMP	C4'-O4'-C1'	-2.09	104.85	109.47
5	D	804	BW2	C8A-C4A-C4	-2.07	116.00	118.73
3	C	903	XMP	C8-N7-C5	2.06	107.93	104.26
3	C	903	XMP	OP2-P-O5'	2.05	112.02	106.67
3	A	901	XMP	C3'-C2'-C1'	2.02	105.29	101.46
3	A	901	XMP	OP2-P-O5'	2.00	111.89	106.67
5	B	802	BW2	O2-S10-N9	-2.00	101.86	106.74

There are no chirality outliers.

All (10) torsion outliers are listed below:

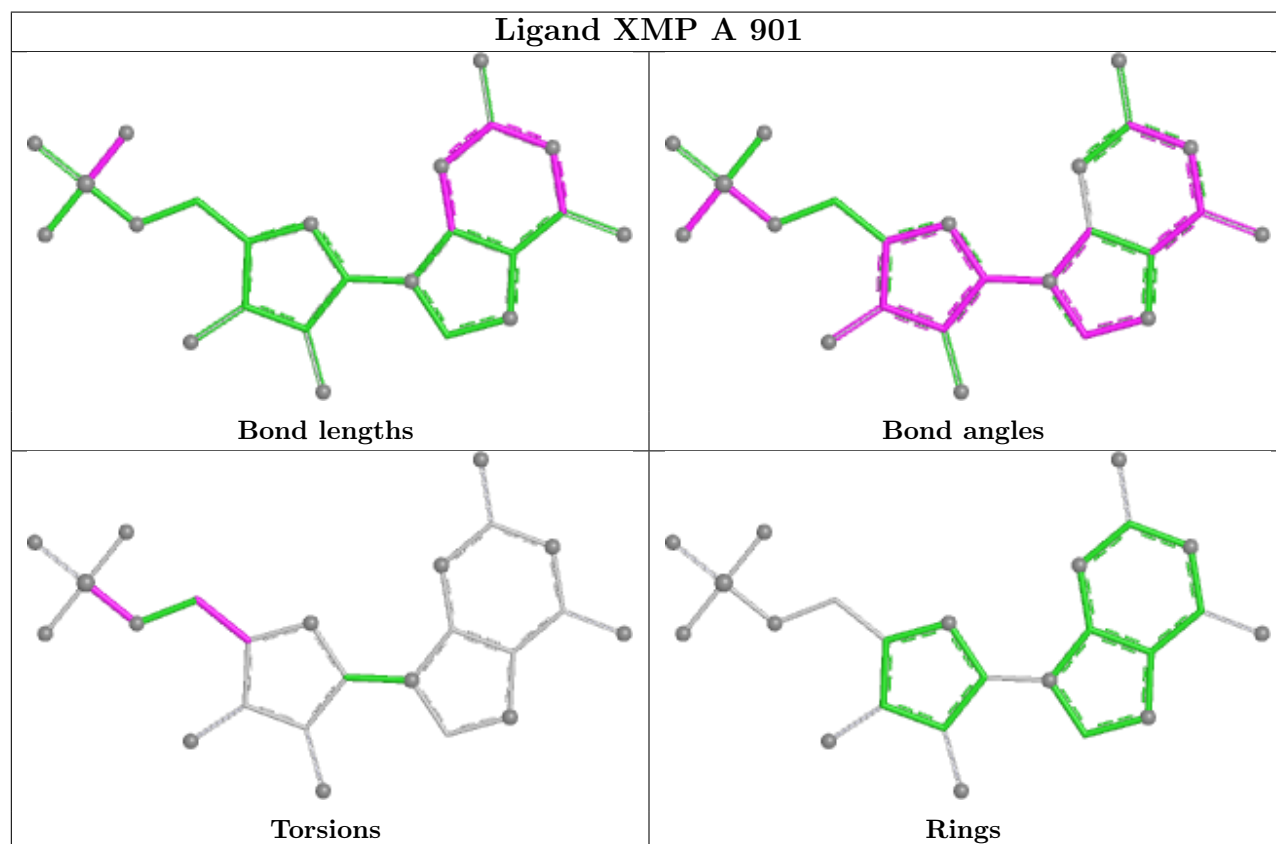
Mol	Chain	Res	Type	Atoms
3	A	901	XMP	C5'-O5'-P-OP3
3	A	901	XMP	C5'-O5'-P-OP2
3	A	901	XMP	C5'-O5'-P-OP1
3	A	901	XMP	O4'-C4'-C5'-O5'
3	C	903	XMP	C5'-O5'-P-OP3
3	C	903	XMP	C5'-O5'-P-OP2
3	C	903	XMP	C5'-O5'-P-OP1
3	C	903	XMP	O4'-C4'-C5'-O5'
3	C	903	XMP	C3'-C4'-C5'-O5'
3	A	901	XMP	C3'-C4'-C5'-O5'

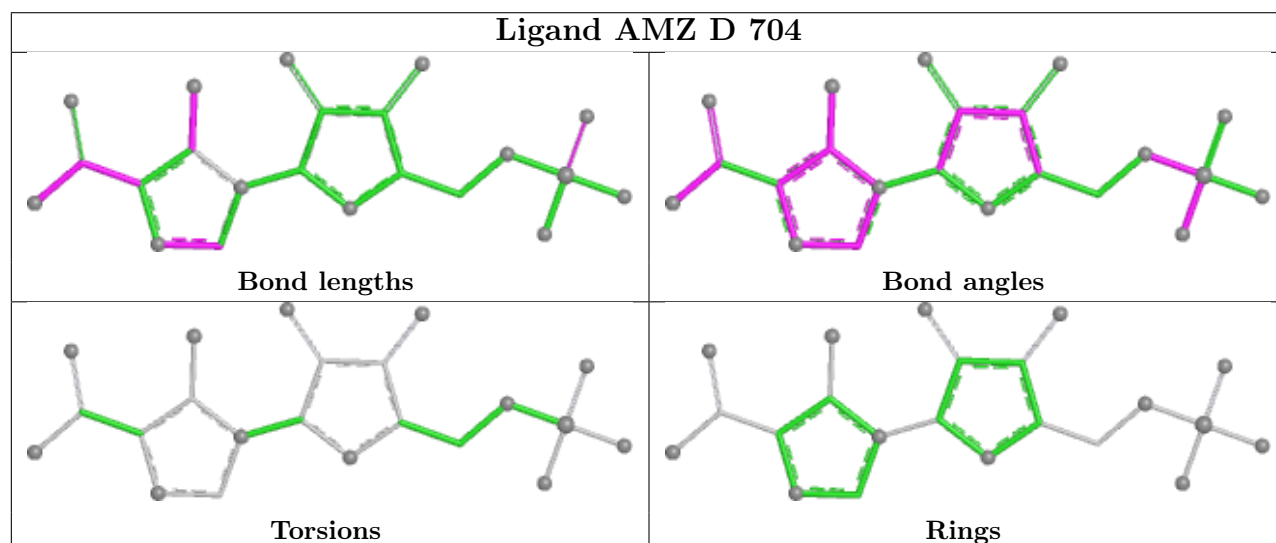
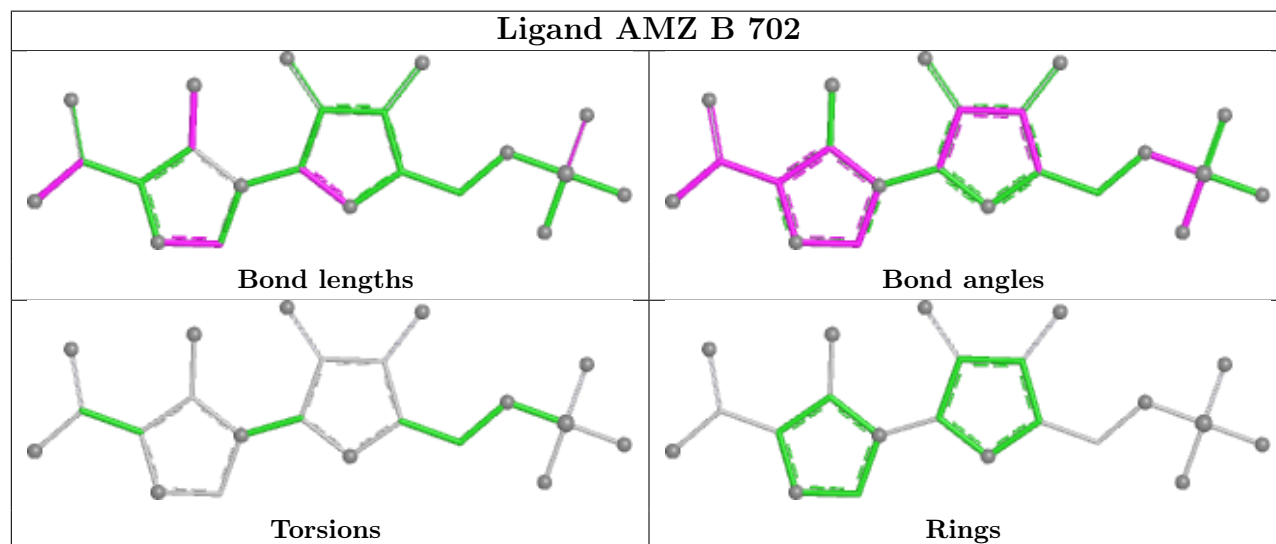
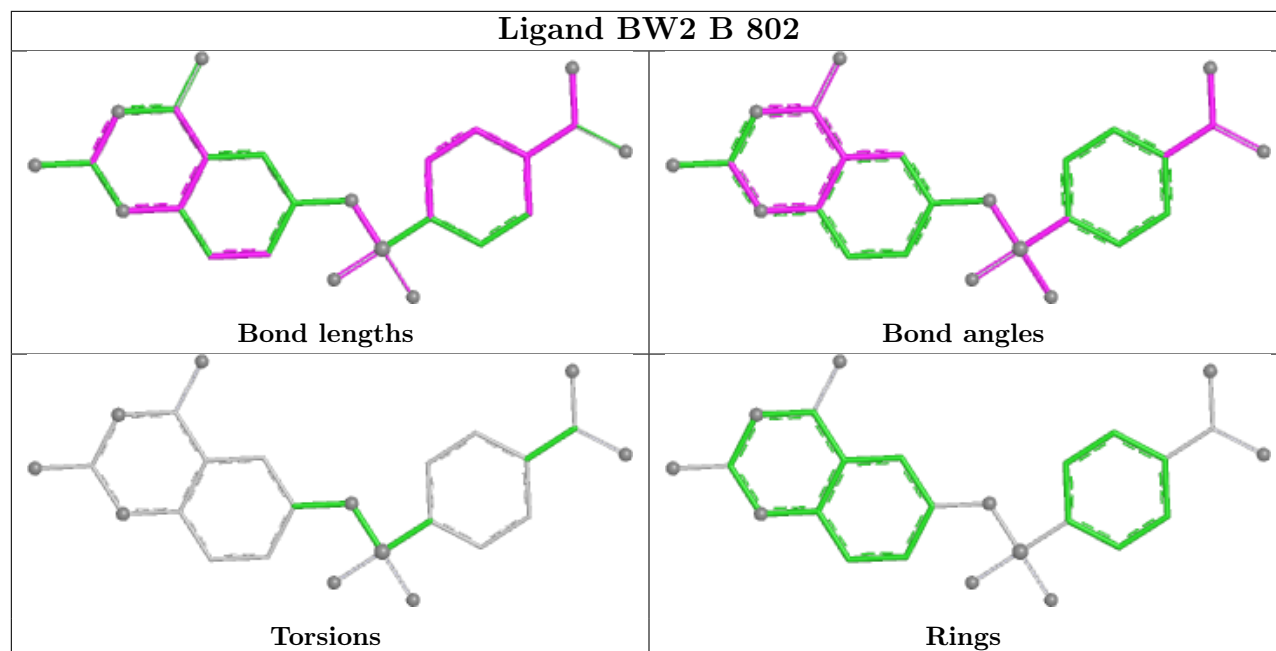
There are no ring outliers.

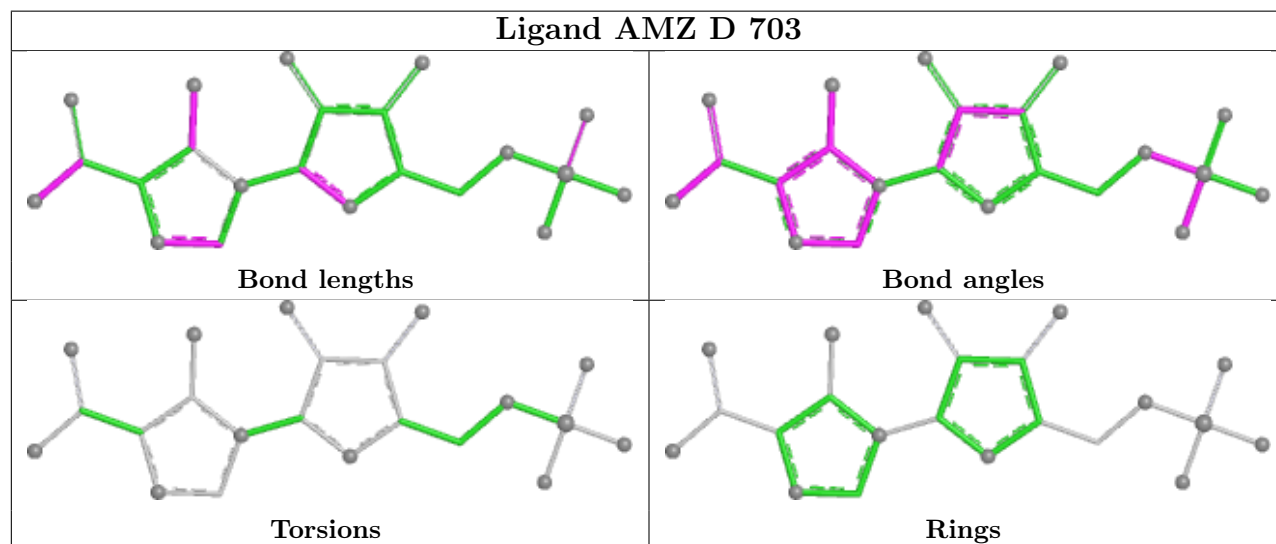
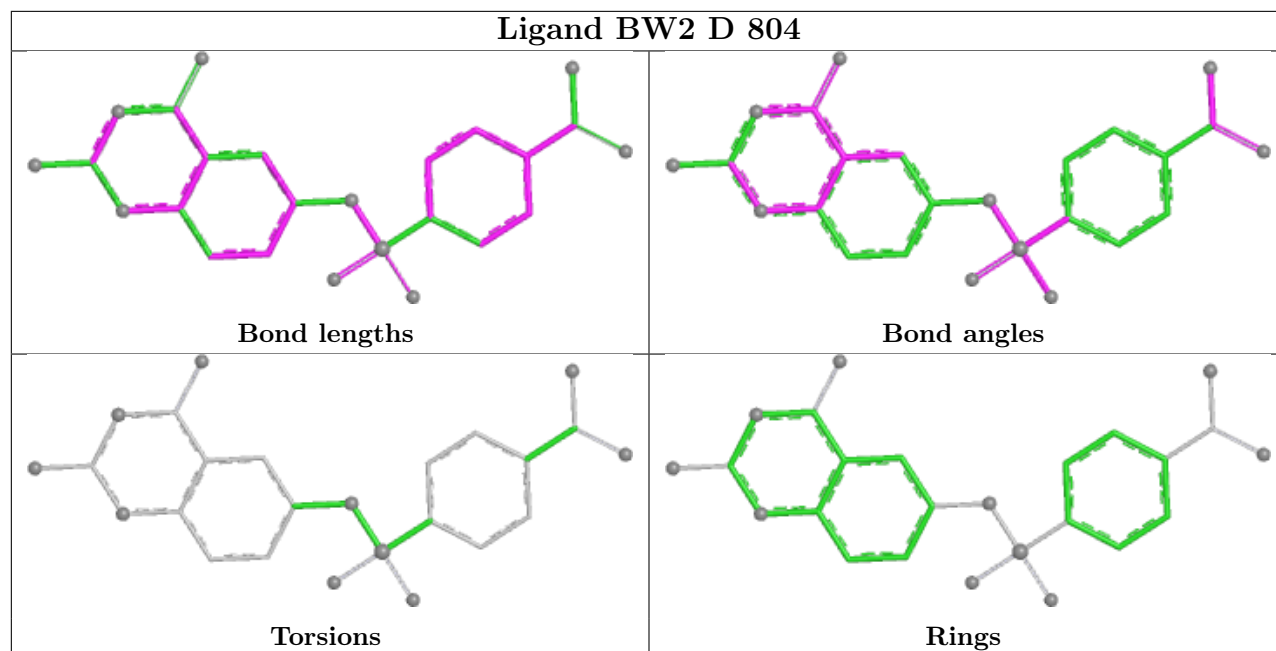
5 monomers are involved in 13 short contacts:

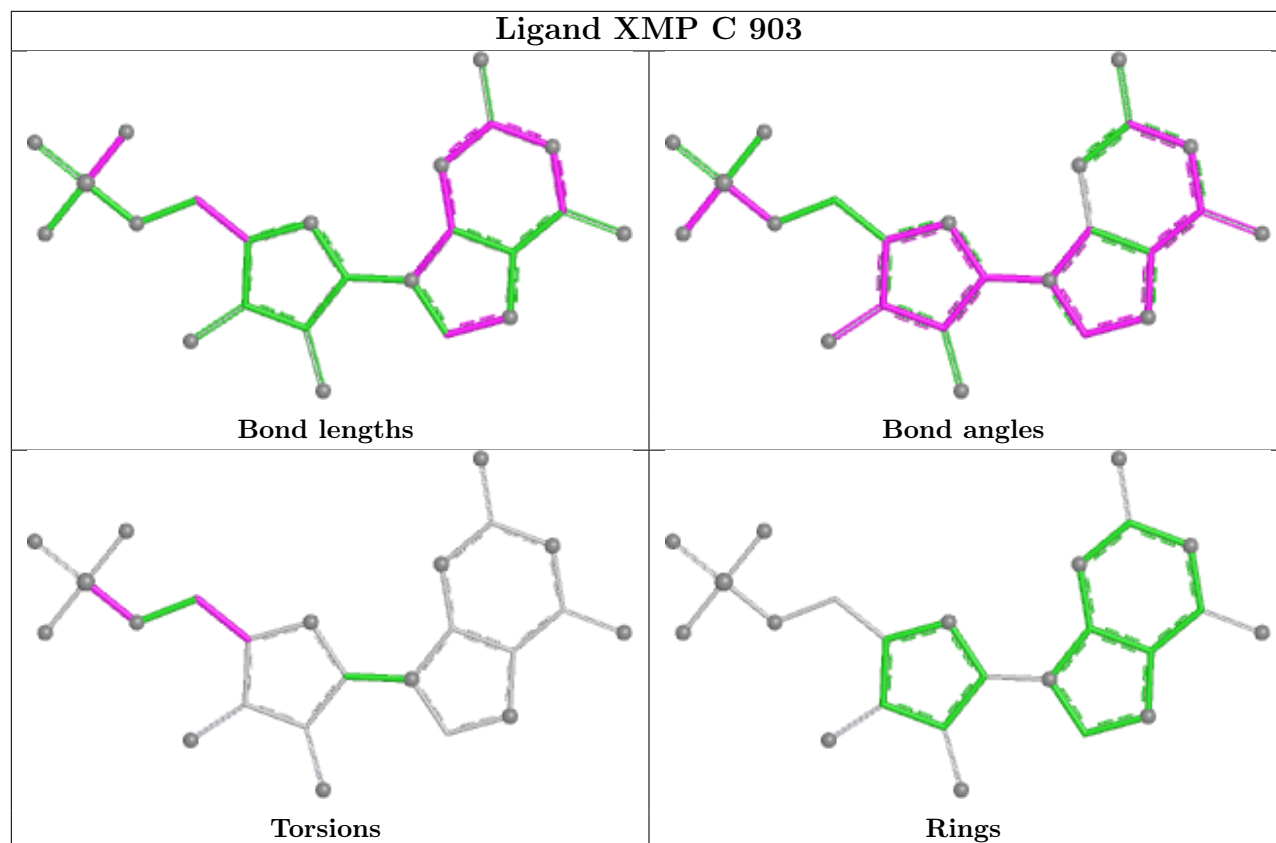
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	XMP	3	0
5	B	802	BW2	2	0
4	B	702	AMZ	1	0
5	D	804	BW2	6	0
4	D	703	AMZ	1	0

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%)	-1.78	0 100 100	6, 26, 51, 64	0
1	B	587/592 (99%)	-1.79	0 100 100	3, 22, 51, 74	0
1	C	585/592 (98%)	-1.75	0 100 100	8, 29, 54, 66	0
1	D	579/592 (97%)	-1.76	0 100 100	4, 25, 54, 75	0
All	All	2340/2368 (98%)	-1.77	0 100 100	3, 25, 53, 75	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AMZ	D	703	22/22	0.99	0.03	34,39,40,41	0
2	K	B	1002	1/1	1.00	0.01	12,12,12,12	0
2	K	C	1003	1/1	1.00	0.01	17,17,17,17	0
2	K	D	1004	1/1	1.00	0.01	17,17,17,17	0

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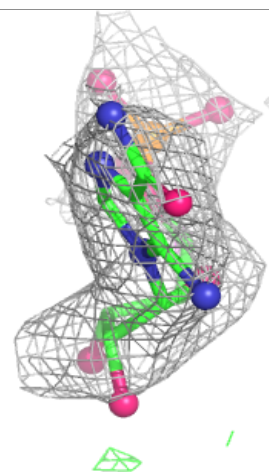
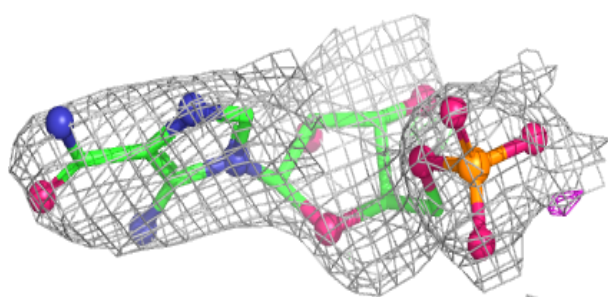
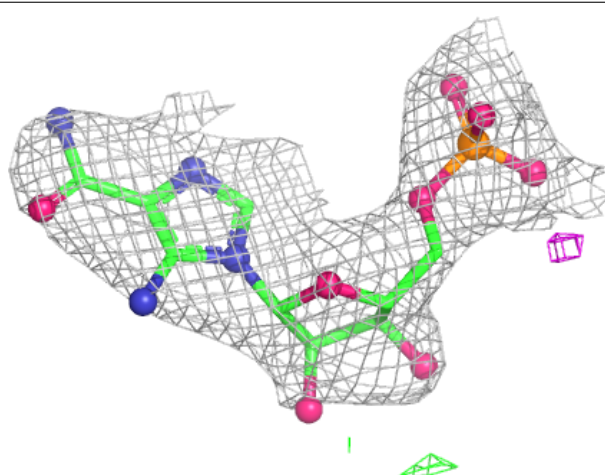
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XMP	A	901	24/24	1.00	0.02	19,21,26,31	0
3	XMP	C	903	24/24	1.00	0.02	17,21,28,30	0
4	AMZ	B	702	22/22	1.00	0.03	27,30,32,33	0
2	K	A	1001	1/1	1.00	0.02	16,16,16,16	0
4	AMZ	D	704	22/22	1.00	0.02	20,22,25,27	0
5	BW2	B	802	25/34	1.00	0.02	21,25,32,33	0
5	BW2	D	804	25/34	1.00	0.02	27,31,33,34	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.

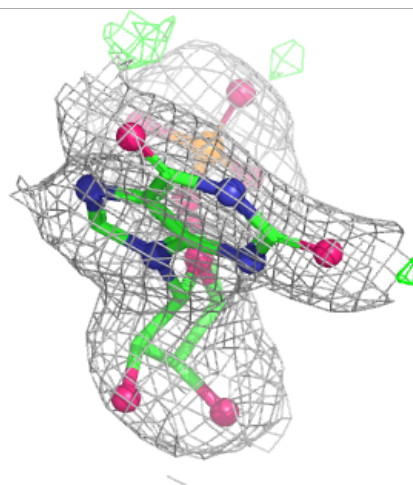
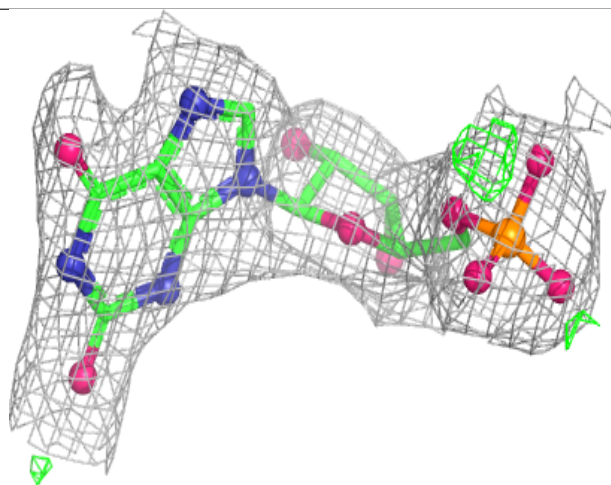
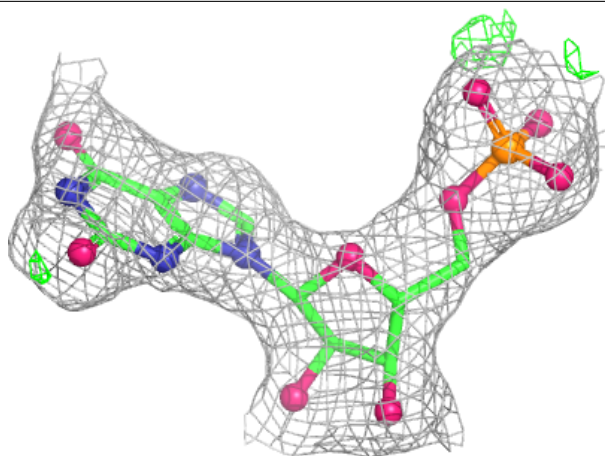
Electron density around AMZ D 703:

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



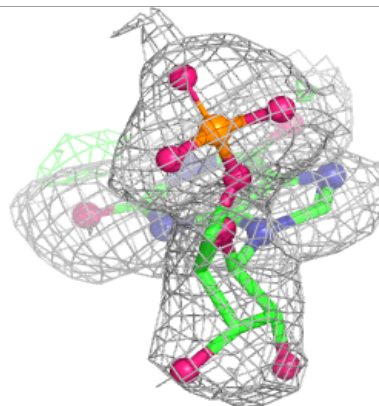
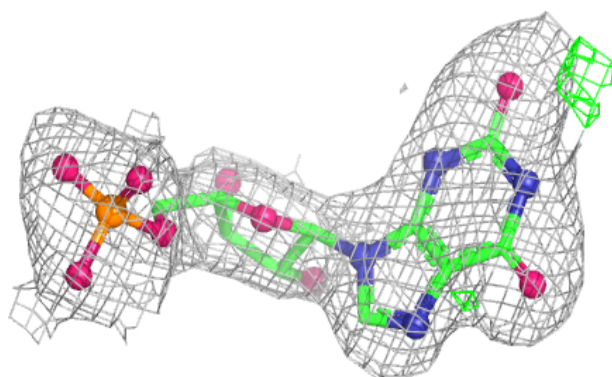
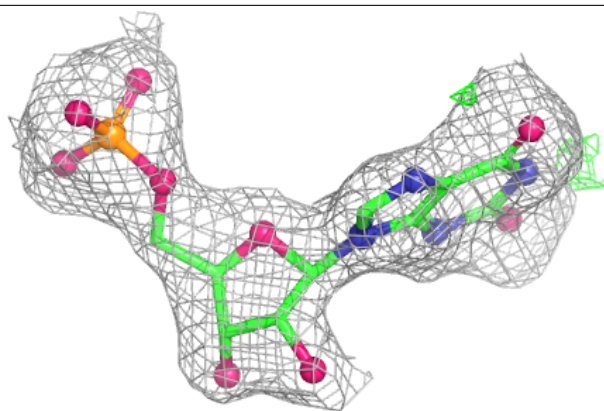
Electron density around XMP A 901:

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



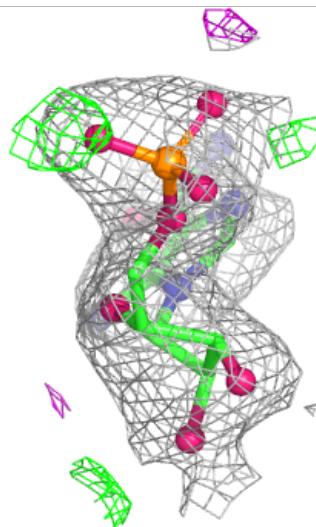
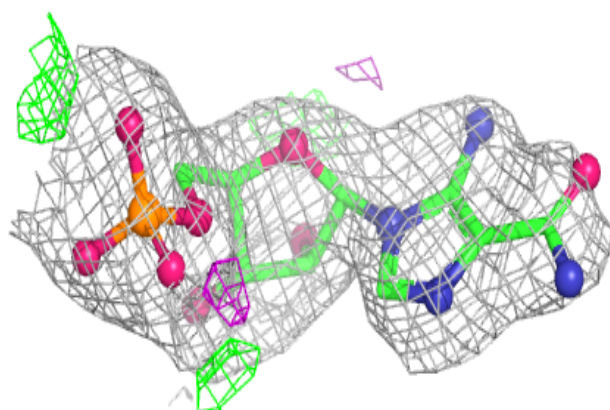
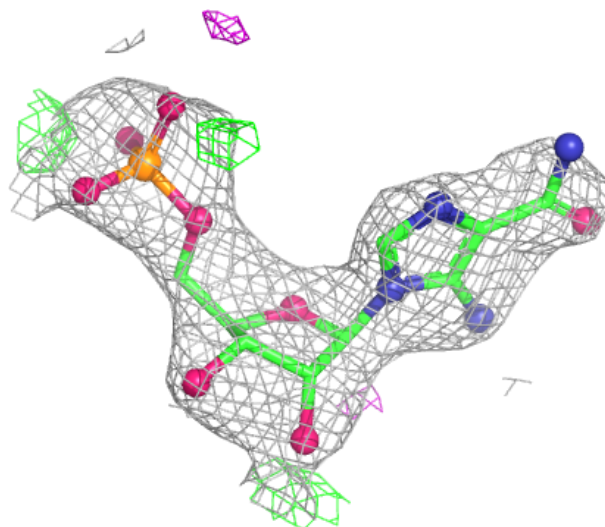
Electron density around XMP C 903:

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



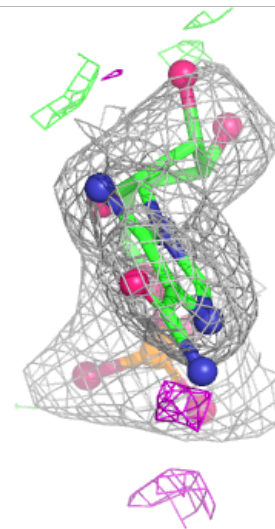
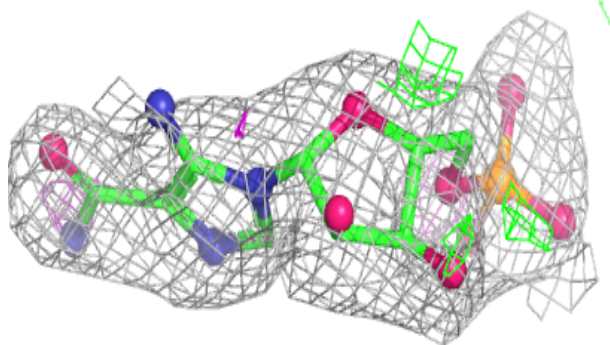
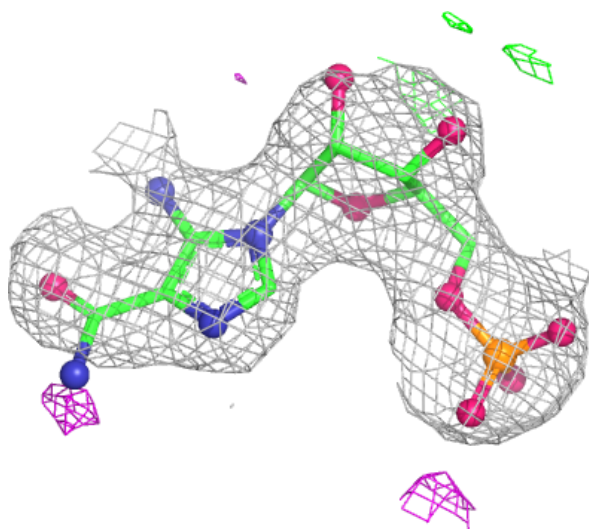
Electron density around AMZ B 702:

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



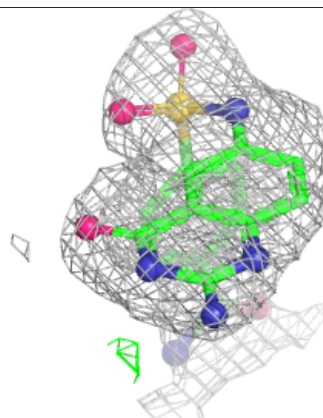
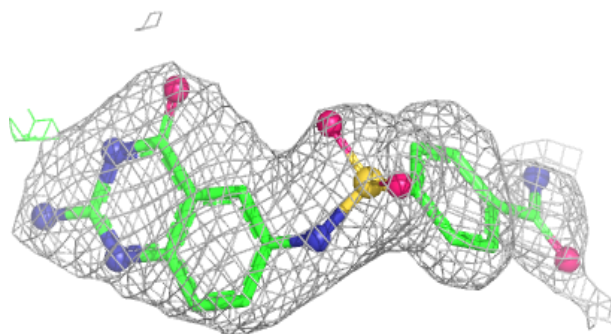
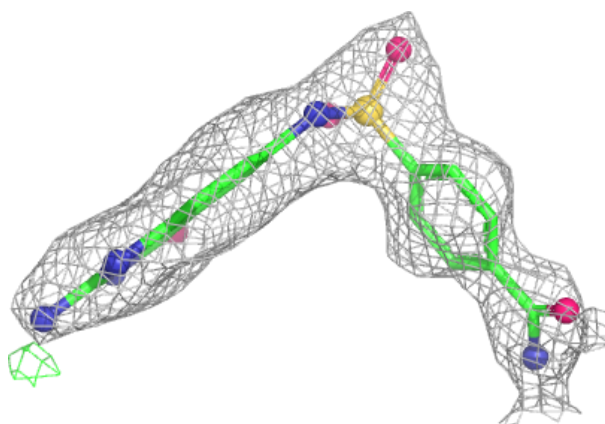
Electron density around AMZ D 704:

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



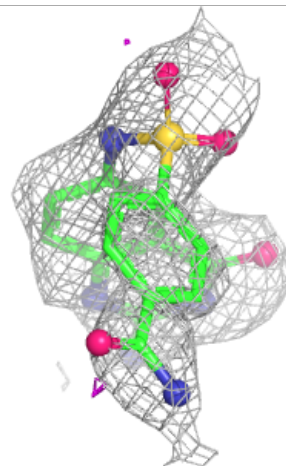
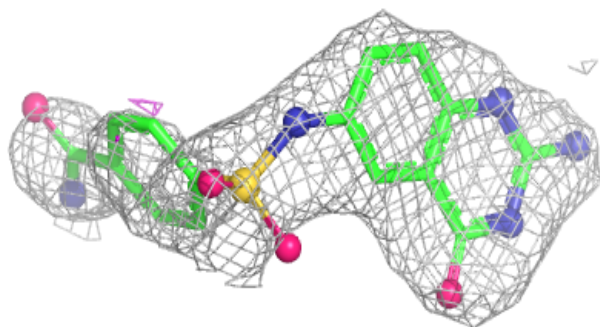
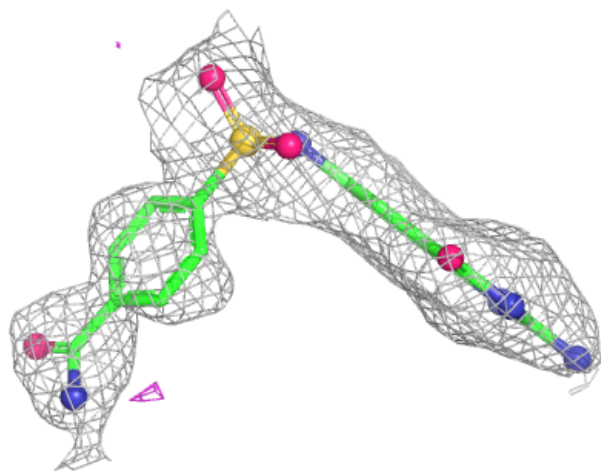
Electron density around BW2 B 802:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.