



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:31 PM UTC

PDB ID : 5W5O / pdb_00005w5o
Title : Identification of potent and selective RIPK2 inhibitors for the treatment of inflammatory diseases.
Authors : Kreusch, A.; Spraggon, G.
Deposited on : 2017-06-15
Resolution : 2.89 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

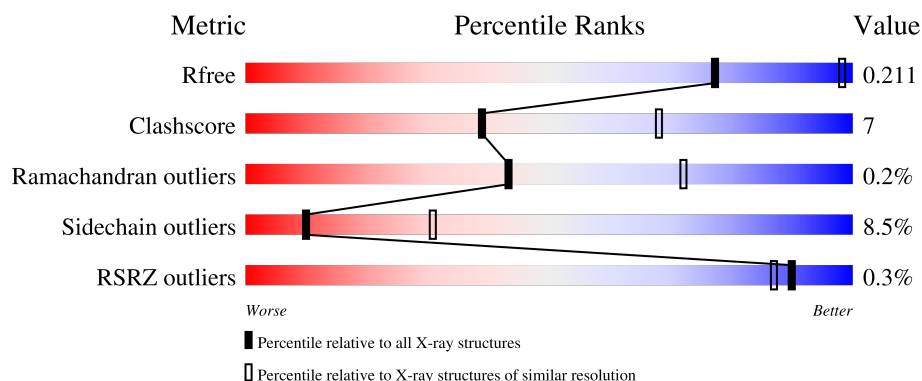
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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.



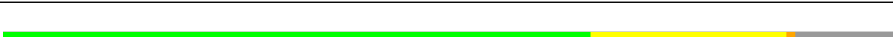
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	310	67% 20% • 11%
1	B	310	65% 21% • 11%
1	C	310	61% 23% • • 11%
1	D	310	68% 19% • 11%
1	E	310	68% 17% • • 11%

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Mol	Chain	Length	Quality of chain
1	F	310	 68%20% • 11%
1	G	310	 69%18% • 11%
1	H	310	 69%18% • 11%
1	I	310	 71%16% • 11%
1	J	310	 69%16% • 11%
1	K	310	 %66%20% • 11%
1	L	310	 69%19% • 11%
1	M	310	 70%18% • 11%
1	N	310	 65%19% • • 12%
1	O	310	 69%17% • 11%
1	P	310	 66%22% • 11%

2 Entry composition

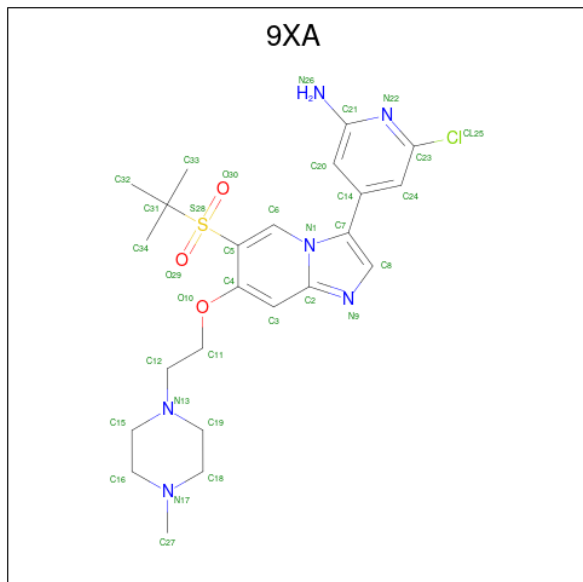
There are 3 unique types of molecules in this entry. The entry contains 35681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Receptor-interacting serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2165	1401	365	391	8			
1	B	275	Total	C	N	O	S	0	0	0
			2177	1408	370	391	8			
1	C	275	Total	C	N	O	S	0	0	0
			2170	1406	368	388	8			
1	D	275	Total	C	N	O	S	0	0	0
			2174	1408	372	386	8			
1	E	275	Total	C	N	O	S	0	0	0
			2197	1422	373	394	8			
1	F	275	Total	C	N	O	S	0	0	0
			2184	1413	373	390	8			
1	G	275	Total	C	N	O	S	0	0	0
			2198	1420	374	396	8			
1	H	275	Total	C	N	O	S	0	0	0
			2188	1416	372	392	8			
1	I	275	Total	C	N	O	S	0	0	0
			2176	1410	372	386	8			
1	J	275	Total	C	N	O	S	0	0	0
			2199	1421	377	393	8			
1	K	275	Total	C	N	O	S	0	0	0
			2198	1418	373	399	8			
1	L	275	Total	C	N	O	S	0	0	0
			2182	1412	369	393	8			
1	M	276	Total	C	N	O	S	0	0	0
			2159	1398	365	388	8			
1	N	272	Total	C	N	O	S	0	0	0
			2118	1376	357	377	8			
1	O	276	Total	C	N	O	S	0	0	0
			2185	1414	369	394	8			
1	P	275	Total	C	N	O	S	0	0	0
			2163	1401	362	392	8			

- Molecule 2 is 4-{6-(tert-butylsulfonyl)-7-[2-(4-methylpiperazin-1-yl)ethoxy]imidazo[1,2-a]pyridin-3-yl}-6-chloropyridin-2-amine (CCD ID: 9XA) (formula: C₂₃H₃₁ClN₆O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	E	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	F	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	G	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	H	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	I	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	J	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	K	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		
2	L	1	Total	C	Cl	N	O	S	0	0
			34	23	1	6	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	Cl	N	O	S	
			34	23	1	6	3	1	
2	N	1	Total	C	Cl	N	O	S	
			34	23	1	6	3	1	
2	O	1	Total	C	Cl	N	O	S	
			34	23	1	6	3	1	
2	P	1	Total	C	Cl	N	O	S	
			34	23	1	6	3	1	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O		
			13	13	0	0
3	B	20	Total	O		
			20	20	0	0
3	C	15	Total	O		
			15	15	0	0
3	D	25	Total	O		
			25	25	0	0
3	E	16	Total	O		
			16	16	0	0
3	F	20	Total	O		
			20	20	0	0
3	G	16	Total	O		
			16	16	0	0
3	H	24	Total	O		
			24	24	0	0
3	I	23	Total	O		
			23	23	0	0
3	J	19	Total	O		
			19	19	0	0
3	K	19	Total	O		
			19	19	0	0
3	L	12	Total	O		
			12	12	0	0
3	M	15	Total	O		
			15	15	0	0
3	N	25	Total	O		
			25	25	0	0
3	O	16	Total	O		
			16	16	0	0

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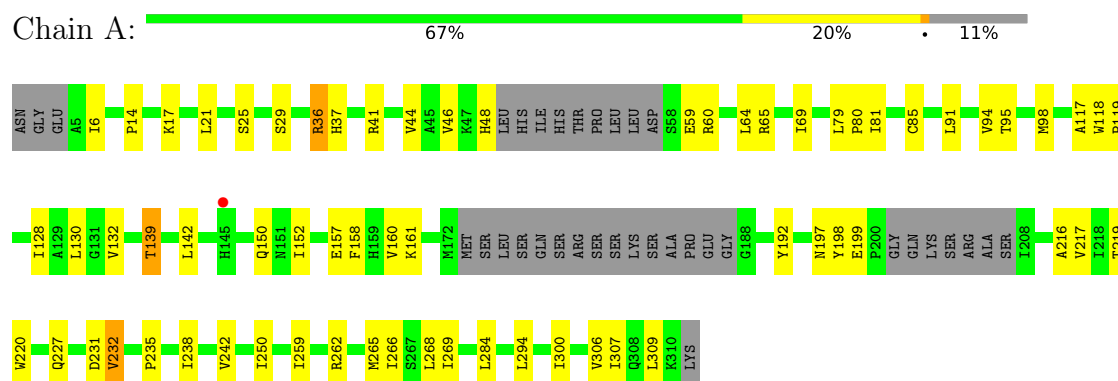
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	26	Total	O	0	0
			26	26		

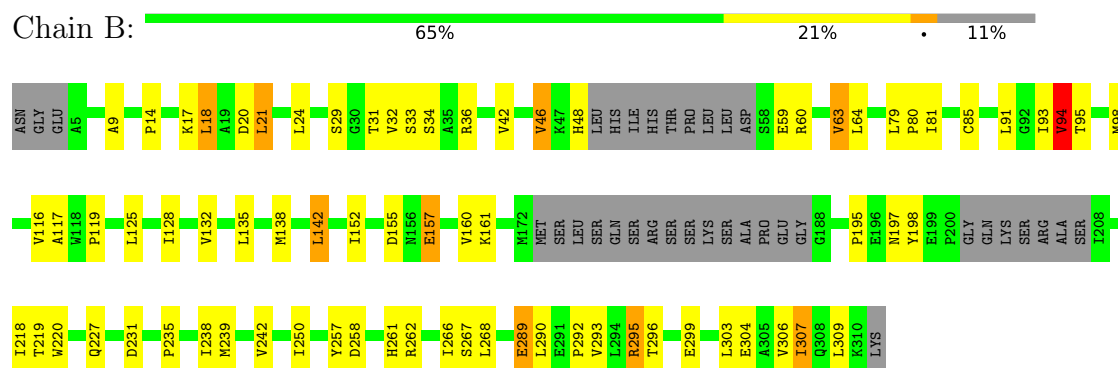
3 Residue-property plots

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.

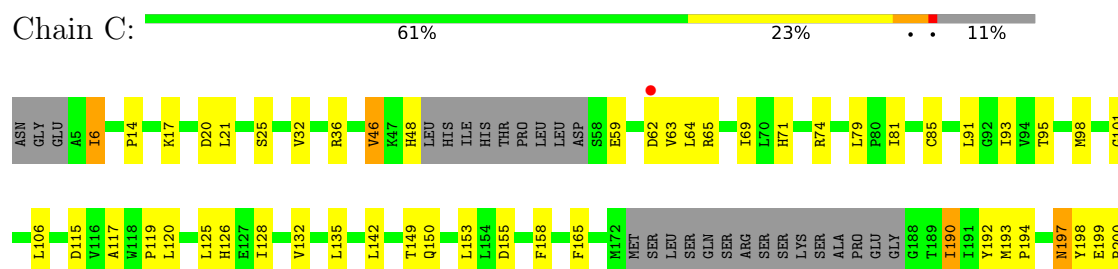
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

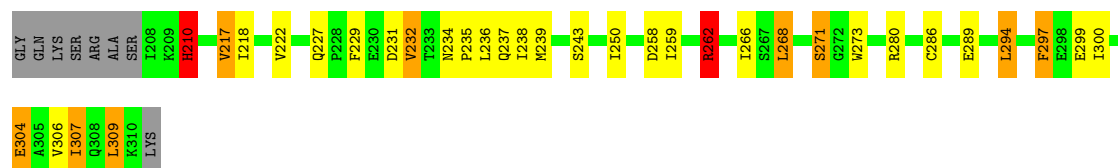


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

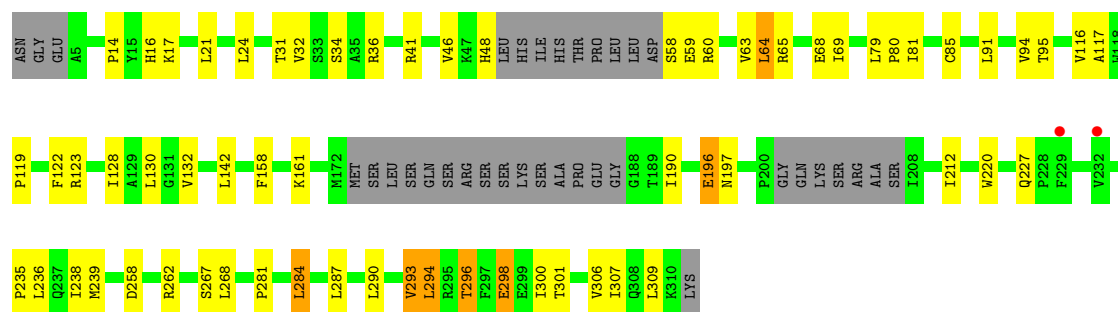


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

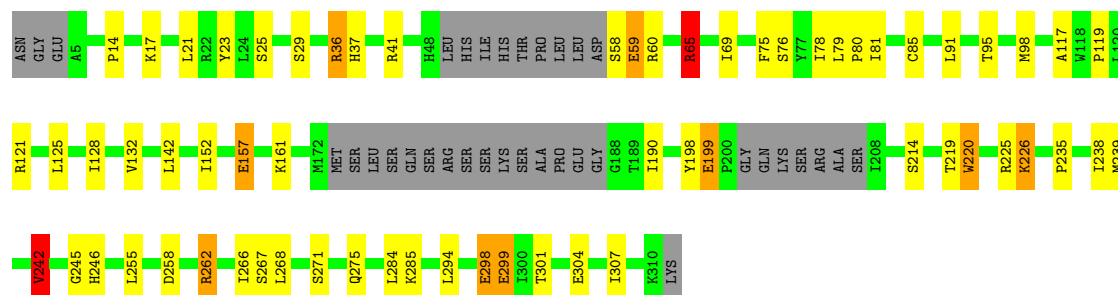




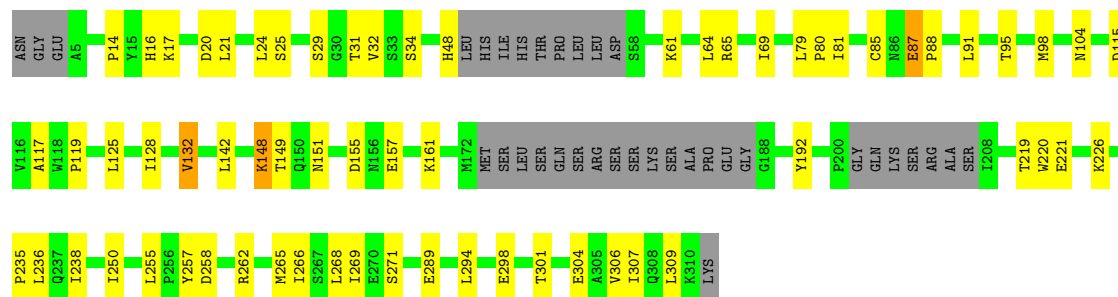
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

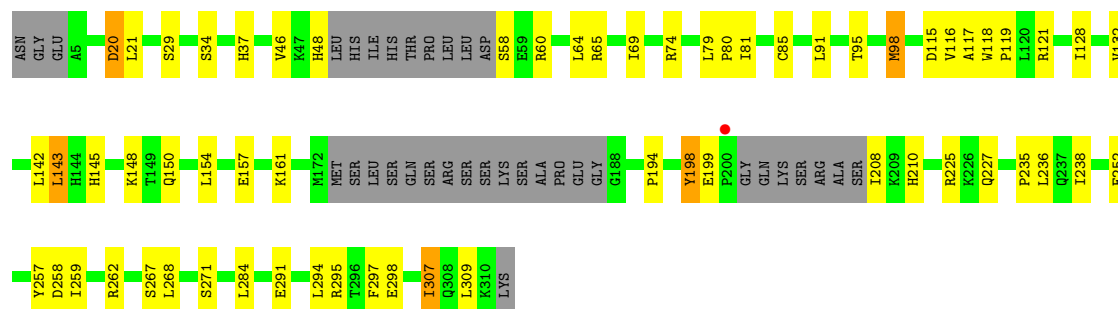


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2



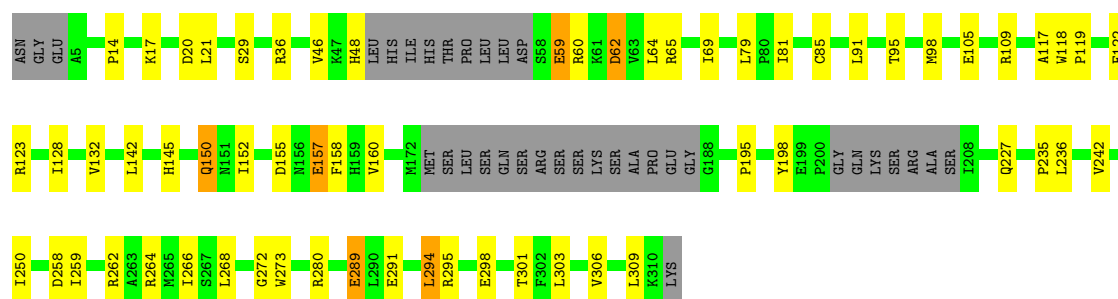
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2





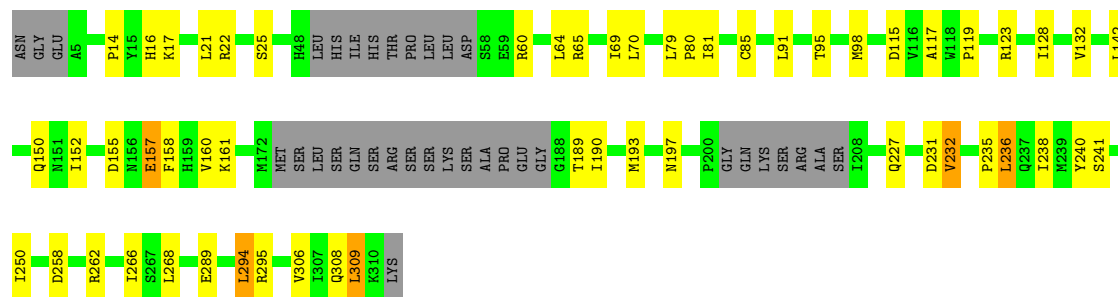
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain H: 69% 18% 11%



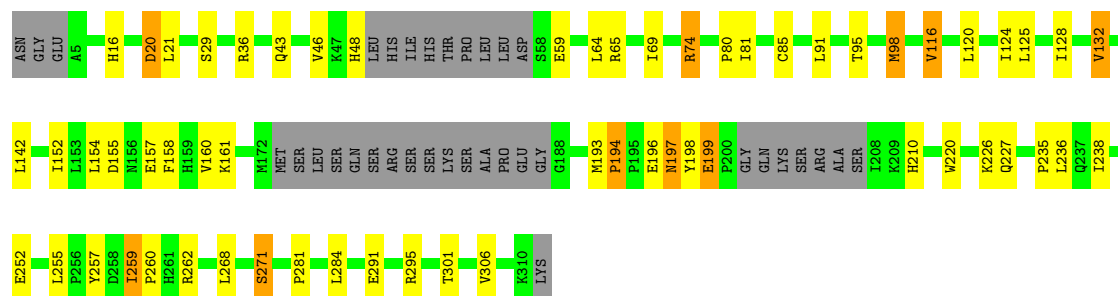
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

Chain I: 71% 16% 11%

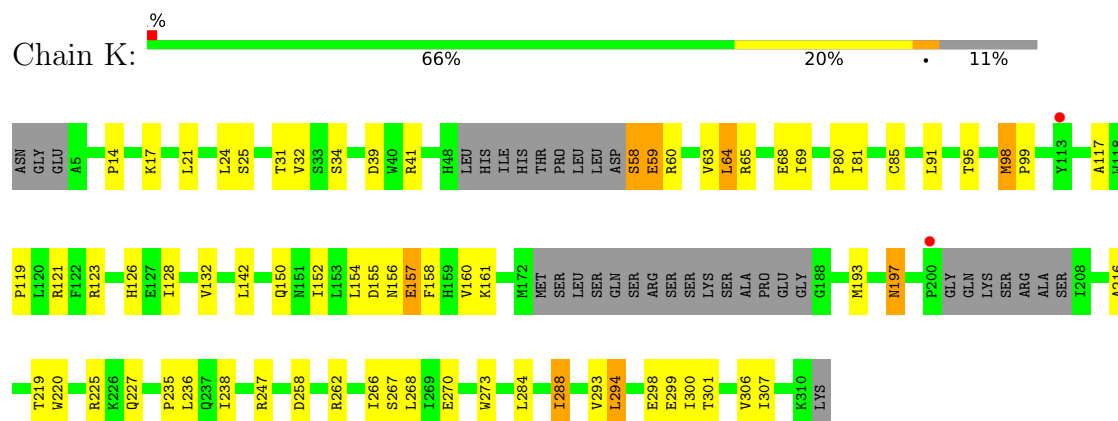


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2

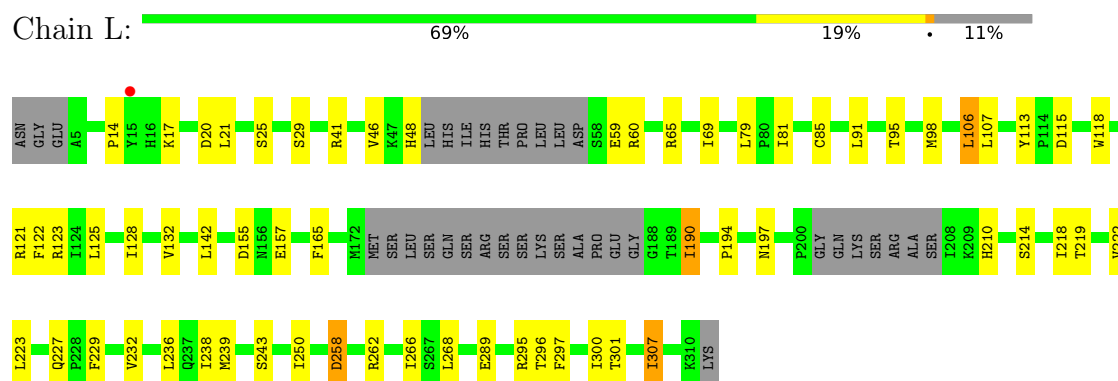
Chain J: 69% 16% 11%



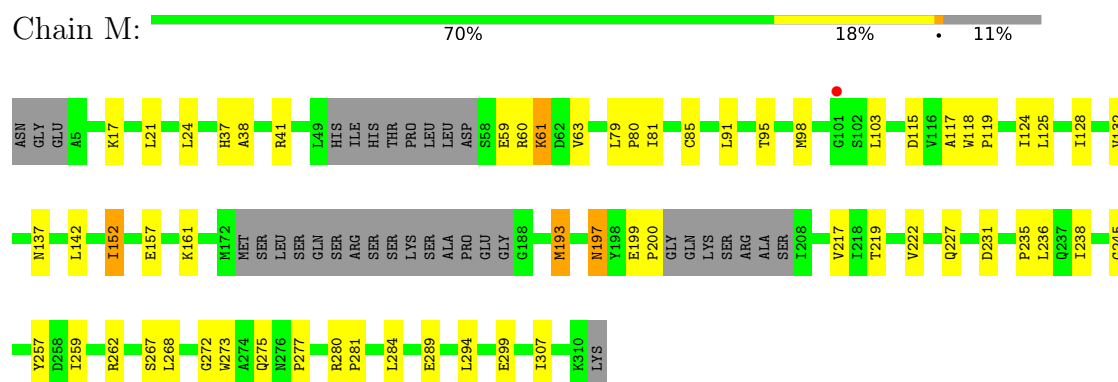
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2



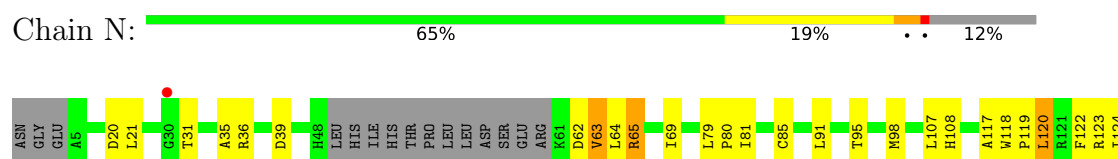
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.31Å 107.47Å 210.19Å 90.15° 89.77° 89.96°	Depositor
Resolution (Å)	47.90 – 2.89 47.90 – 2.89	Depositor EDS
% Data completeness (in resolution range)	88.4 (47.90-2.89) 87.8 (47.90-2.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.217 , 0.252 0.182 , 0.211	Depositor DCC
R_{free} test set	6905 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.366 for h,-k,-l 0.370 for -h,k,-l 0.417 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35681	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: 9XA

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	0.90	0/2224	1.41	12/3040 (0.4%)
1	B	0.89	0/2237	1.39	11/3056 (0.4%)
1	C	0.90	0/2230	1.43	17/3048 (0.6%)
1	D	0.92	0/2234	1.36	2/3052 (0.1%)
1	E	0.93	0/2257	1.40	14/3079 (0.5%)
1	F	0.91	0/2244	1.38	6/3063 (0.2%)
1	G	0.88	1/2258 (0.0%)	1.40	7/3082 (0.2%)
1	H	0.88	0/2248	1.36	8/3069 (0.3%)
1	I	0.90	1/2236 (0.0%)	1.37	9/3054 (0.3%)
1	J	0.89	2/2259 (0.1%)	1.39	6/3081 (0.2%)
1	K	0.90	1/2258 (0.0%)	1.37	10/3081 (0.3%)
1	L	0.87	0/2242	1.39	14/3063 (0.5%)
1	M	0.90	1/2218 (0.0%)	1.38	9/3033 (0.3%)
1	N	0.89	0/2177	1.39	17/2981 (0.6%)
1	O	0.90	1/2244 (0.0%)	1.38	11/3064 (0.4%)
1	P	0.90	1/2223 (0.0%)	1.41	14/3040 (0.5%)
All	All	0.90	8/35789 (0.0%)	1.39	167/48886 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	193	MET	SD-CE	-6.54	1.63	1.79
1	J	98	MET	SD-CE	-6.33	1.63	1.79
1	M	193	MET	SD-CE	-6.13	1.64	1.79
1	G	98	MET	SD-CE	-5.59	1.65	1.79
1	I	193	MET	SD-CE	-5.38	1.66	1.79
1	J	194	PRO	CA-C	5.30	1.55	1.52
1	K	98	MET	SD-CE	-5.16	1.66	1.79
1	P	98	MET	SD-CE	-5.15	1.66	1.79

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	199	GLU	N-CA-C	9.26	116.55	108.22
1	C	59	GLU	CA-C-N	8.13	131.18	120.28
1	C	59	GLU	C-N-CA	8.13	131.18	120.28
1	H	157	GLU	CA-C-N	7.81	133.72	122.40
1	H	157	GLU	C-N-CA	7.81	133.72	122.40
1	M	63	VAL	CA-C-N	7.27	130.99	120.38
1	M	63	VAL	C-N-CA	7.27	130.99	120.38
1	C	210	HIS	CA-C-N	7.21	130.26	120.38
1	C	210	HIS	C-N-CA	7.21	130.26	120.38
1	I	60	ARG	N-CA-C	-7.07	103.62	111.82
1	A	231	ASP	CA-CB-CG	7.02	119.62	112.60
1	N	209	LYS	CA-C-N	6.94	129.46	120.44
1	N	209	LYS	C-N-CA	6.94	129.46	120.44
1	I	309	LEU	N-CA-C	-6.80	105.12	113.41
1	I	157	GLU	CA-C-N	6.78	132.22	122.40
1	I	157	GLU	C-N-CA	6.78	132.22	122.40
1	A	232	VAL	CA-C-N	6.77	132.01	120.71
1	A	232	VAL	C-N-CA	6.77	132.01	120.71
1	G	20	ASP	CA-CB-CG	6.66	119.26	112.60
1	N	232	VAL	N-CA-CB	6.58	117.89	110.72
1	P	298	GLU	CA-C-N	6.57	134.09	121.54
1	P	298	GLU	C-N-CA	6.57	134.09	121.54
1	I	232	VAL	CA-C-N	6.51	129.83	120.79
1	I	232	VAL	C-N-CA	6.51	129.83	120.79
1	L	296	THR	N-CA-C	-6.47	104.08	112.23
1	F	20	ASP	CA-CB-CG	6.45	119.05	112.60
1	O	48	HIS	N-CA-C	6.42	116.55	108.45
1	O	66	GLU	CB-CG-CD	6.34	123.38	112.60
1	L	59	GLU	CA-C-N	6.28	130.64	120.60
1	L	59	GLU	C-N-CA	6.28	130.64	120.60
1	E	242	VAL	N-CA-CB	6.18	118.94	110.54
1	P	86	ASN	CA-CB-CG	6.14	118.74	112.60
1	N	196	GLU	CB-CG-CD	6.07	122.92	112.60
1	H	59	GLU	CA-C-N	5.98	128.22	120.44
1	H	59	GLU	C-N-CA	5.98	128.22	120.44
1	P	21	LEU	CA-C-N	5.95	130.58	122.19
1	P	21	LEU	C-N-CA	5.95	130.58	122.19
1	B	289	GLU	CB-CG-CD	5.95	122.71	112.60
1	N	268	LEU	CA-C-N	5.89	127.99	120.56
1	N	268	LEU	C-N-CA	5.89	127.99	120.56
1	M	37	HIS	CA-C-N	5.77	128.01	120.28
1	M	37	HIS	C-N-CA	5.77	128.01	120.28
1	P	295	ARG	CA-C-N	5.76	128.32	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	295	ARG	C-N-CA	5.76	128.32	120.54
1	E	59	GLU	CA-C-N	5.76	129.06	120.31
1	E	59	GLU	C-N-CA	5.76	129.06	120.31
1	J	20	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	155	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	20	ASP	CA-CB-CG	5.67	118.27	112.60
1	E	271	SER	CA-C-N	5.67	126.23	119.94
1	E	271	SER	C-N-CA	5.67	126.23	119.94
1	M	61	LYS	CA-C-N	5.64	127.83	120.28
1	M	61	LYS	C-N-CA	5.64	127.83	120.28
1	N	122	PHE	CA-C-N	5.63	127.83	120.28
1	N	122	PHE	C-N-CA	5.63	127.83	120.28
1	L	165	PHE	CA-C-N	5.63	126.19	120.00
1	L	165	PHE	C-N-CA	5.63	126.19	120.00
1	M	60	ARG	CA-C-N	5.58	132.19	121.54
1	M	60	ARG	C-N-CA	5.58	132.19	121.54
1	F	155	ASP	CA-CB-CG	5.57	118.17	112.60
1	G	58	SER	CA-C-N	5.57	128.06	120.54
1	G	58	SER	C-N-CA	5.57	128.06	120.54
1	B	59	GLU	CA-C-N	5.54	127.65	120.44
1	B	59	GLU	C-N-CA	5.54	127.65	120.44
1	E	65	ARG	N-CA-C	-5.52	105.33	112.68
1	A	60	ARG	CA-C-N	5.51	127.93	120.38
1	A	60	ARG	C-N-CA	5.51	127.93	120.38
1	C	165	PHE	CA-C-N	5.51	126.06	120.00
1	C	165	PHE	C-N-CA	5.51	126.06	120.00
1	A	37	HIS	CA-C-N	5.47	127.88	120.38
1	A	37	HIS	C-N-CA	5.47	127.88	120.38
1	C	271	SER	CA-C-N	5.47	125.90	119.94
1	C	271	SER	C-N-CA	5.47	125.90	119.94
1	B	20	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	94	VAL	N-CA-CB	5.46	118.94	111.41
1	L	214	SER	CA-C-N	5.41	127.97	120.29
1	L	214	SER	C-N-CA	5.41	127.97	120.29
1	A	139	THR	CB-CA-C	5.40	118.97	110.71
1	C	236	LEU	CA-C-N	5.39	127.50	120.28
1	C	236	LEU	C-N-CA	5.39	127.50	120.28
1	A	59	GLU	CA-C-N	5.38	127.43	120.44
1	A	59	GLU	C-N-CA	5.38	127.43	120.44
1	J	155	ASP	CA-CB-CG	5.37	117.97	112.60
1	H	20	ASP	CA-CB-CG	5.34	117.94	112.60
1	J	271	SER	CA-C-N	5.33	125.86	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	271	SER	C-N-CA	5.33	125.86	119.94
1	B	295	ARG	CA-C-N	5.31	127.39	120.28
1	B	295	ARG	C-N-CA	5.31	127.39	120.28
1	F	220	TRP	CA-C-N	5.30	127.64	120.38
1	F	220	TRP	C-N-CA	5.30	127.64	120.38
1	C	262	ARG	CA-C-N	5.30	127.33	120.44
1	C	262	ARG	C-N-CA	5.30	127.33	120.44
1	B	220	TRP	CA-C-N	5.29	127.63	120.38
1	B	220	TRP	C-N-CA	5.29	127.63	120.38
1	J	124	ILE	CA-C-N	5.27	127.65	120.54
1	J	124	ILE	C-N-CA	5.27	127.65	120.54
1	E	37	HIS	CA-C-N	5.26	127.59	120.38
1	E	37	HIS	C-N-CA	5.26	127.59	120.38
1	B	157	GLU	CB-CG-CD	5.25	121.52	112.60
1	O	275	GLN	N-CA-C	-5.24	105.48	111.14
1	K	157	GLU	CB-CG-CD	5.23	121.50	112.60
1	K	220	TRP	CA-C-N	5.23	127.55	120.38
1	K	220	TRP	C-N-CA	5.23	127.55	120.38
1	K	155	ASP	CA-CB-CG	5.22	117.82	112.60
1	K	58	SER	CA-C-N	5.20	131.10	121.52
1	K	58	SER	C-N-CA	5.20	131.10	121.52
1	N	120	LEU	CA-C-N	5.19	127.49	120.38
1	N	120	LEU	C-N-CA	5.19	127.49	120.38
1	N	220	TRP	CA-C-N	5.19	127.49	120.38
1	N	220	TRP	C-N-CA	5.19	127.49	120.38
1	E	220	TRP	CA-C-N	5.18	127.48	120.38
1	E	220	TRP	C-N-CA	5.18	127.48	120.38
1	L	60	ARG	CA-C-N	5.18	127.94	120.38
1	L	60	ARG	C-N-CA	5.18	127.94	120.38
1	O	155	ASP	CA-CB-CG	5.17	117.77	112.60
1	L	155	ASP	CA-CB-CG	5.17	117.77	112.60
1	N	238	ILE	CB-CG1-CD1	5.17	124.66	113.80
1	C	243	SER	N-CA-C	-5.16	106.49	112.89
1	C	304	GLU	CB-CG-CD	5.16	121.38	112.60
1	D	220	TRP	CA-C-N	5.16	127.45	120.38
1	D	220	TRP	C-N-CA	5.16	127.45	120.38
1	P	268	LEU	CA-C-N	5.16	127.07	120.56
1	P	268	LEU	C-N-CA	5.16	127.07	120.56
1	L	197	ASN	CA-C-N	5.16	127.14	120.44
1	L	197	ASN	C-N-CA	5.16	127.14	120.44
1	O	60	ARG	CA-C-N	5.13	127.41	120.38
1	O	60	ARG	C-N-CA	5.13	127.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	220	TRP	CA-C-N	5.13	127.41	120.38
1	P	220	TRP	C-N-CA	5.13	127.41	120.38
1	E	157	GLU	CB-CG-CD	5.13	121.32	112.60
1	F	271	SER	CA-C-N	5.13	125.63	119.94
1	F	271	SER	C-N-CA	5.13	125.63	119.94
1	O	252	GLU	CB-CG-CD	5.12	121.31	112.60
1	A	220	TRP	CA-C-N	5.12	127.40	120.38
1	A	220	TRP	C-N-CA	5.12	127.40	120.38
1	C	59	GLU	N-CA-C	-5.12	105.78	111.36
1	G	37	HIS	CA-C-N	5.12	127.39	120.38
1	G	37	HIS	C-N-CA	5.12	127.39	120.38
1	O	61	LYS	CA-C-N	5.11	127.12	120.28
1	O	61	LYS	C-N-CA	5.11	127.12	120.28
1	K	59	GLU	CA-C-N	5.10	127.53	120.29
1	K	59	GLU	C-N-CA	5.10	127.53	120.29
1	E	304	GLU	CA-C-N	5.08	127.09	120.28
1	E	304	GLU	C-N-CA	5.08	127.09	120.28
1	H	62	ASP	CA-C-N	5.08	127.06	120.56
1	H	62	ASP	C-N-CA	5.08	127.06	120.56
1	I	155	ASP	CA-CB-CG	5.08	117.68	112.60
1	L	20	ASP	CA-CB-CG	5.08	117.67	112.60
1	O	220	TRP	CA-C-N	5.07	127.33	120.38
1	O	220	TRP	C-N-CA	5.07	127.33	120.38
1	P	155	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	155	ASP	CA-CB-CG	5.06	117.66	112.60
1	P	58	SER	CA-C-N	5.06	129.17	120.72
1	P	58	SER	C-N-CA	5.06	129.17	120.72
1	H	155	ASP	CA-CB-CG	5.05	117.65	112.60
1	K	68	GLU	CA-C-N	5.04	127.00	120.70
1	K	68	GLU	C-N-CA	5.04	127.00	120.70
1	N	299	GLU	CA-C-N	5.04	128.91	120.64
1	N	299	GLU	C-N-CA	5.04	128.91	120.64
1	N	151	ASN	CA-C-N	5.04	128.02	122.22
1	N	151	ASN	C-N-CA	5.04	128.02	122.22
1	I	60	ARG	CA-C-N	5.04	127.73	120.38
1	I	60	ARG	C-N-CA	5.04	127.73	120.38
1	M	152	ILE	CB-CA-C	5.03	118.37	111.88
1	L	258	ASP	CA-CB-CG	5.02	117.62	112.60
1	G	271	SER	CA-C-N	5.00	125.49	119.94
1	G	271	SER	C-N-CA	5.00	125.49	119.94

There are no chirality outliers.

There are no planarity outliers.

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	2165	0	2091	35	0
1	B	2177	0	2105	41	0
1	C	2170	0	2101	42	0
1	D	2174	0	2111	32	0
1	E	2197	0	2148	27	0
1	F	2184	0	2123	28	0
1	G	2198	0	2139	31	0
1	H	2188	0	2131	31	0
1	I	2176	0	2119	19	0
1	J	2199	0	2150	33	0
1	K	2198	0	2131	35	0
1	L	2182	0	2115	21	0
1	M	2159	0	2073	29	0
1	N	2118	0	2035	35	0
1	O	2185	0	2122	29	0
1	P	2163	0	2078	28	0
2	A	34	0	0	0	0
2	B	34	0	0	2	0
2	C	34	0	0	5	0
2	D	34	0	0	2	0
2	E	34	0	0	0	0
2	F	34	0	0	1	0
2	G	34	0	0	0	0
2	H	34	0	0	0	0
2	I	34	0	0	0	0
2	J	34	0	0	0	0
2	K	34	0	0	1	0
2	L	34	0	0	0	0
2	M	34	0	0	1	0
2	N	34	0	0	0	0
2	O	34	0	0	0	0
2	P	34	0	0	0	0
3	A	13	0	0	0	0
3	B	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	15	0	0	0	0
3	D	25	0	0	0	0
3	E	16	0	0	0	0
3	F	20	0	0	0	0
3	G	16	0	0	0	0
3	H	24	0	0	3	0
3	I	23	0	0	0	0
3	J	19	0	0	0	0
3	K	19	0	0	0	0
3	L	12	0	0	0	0
3	M	15	0	0	1	0
3	N	25	0	0	1	0
3	O	16	0	0	3	0
3	P	26	0	0	0	0
All	All	35681	0	33772	468	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 7.

All (468) 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:M:125:LEU:HD22	1:M:219:THR:HG22	1.47	0.95
1:J:236:LEU:HD21	1:M:235:PRO:HB2	1.50	0.93
1:N:290:LEU:O	1:N:293:VAL:HG12	1.77	0.85
1:A:157:GLU:HG2	1:B:157:GLU:HG2	1.56	0.85
1:M:157:GLU:HG2	1:N:157:GLU:HG2	1.61	0.83
1:I:157:GLU:HG2	1:J:157:GLU:HG2	1.61	0.82
1:A:219:THR:HG23	1:A:269:ILE:HG12	1.64	0.80
1:O:157:GLU:HG2	1:P:157:GLU:HG2	1.64	0.79
1:B:60:ARG:HG2	1:B:91:LEU:HD22	1.65	0.79
1:D:32:VAL:HG11	2:D:401:9XA:O29	1.82	0.78
1:G:157:GLU:HG2	1:H:157:GLU:HG2	1.67	0.76
1:H:60:ARG:HG3	1:H:91:LEU:HD22	1.70	0.74
1:K:288:ILE:HG22	1:L:41:ARG:NH1	2.03	0.73
1:K:17:LYS:HE3	1:K:39:ASP:OD2	1.91	0.70
1:E:284:LEU:HD23	1:J:284:LEU:HD23	1.73	0.69
1:K:157:GLU:HG2	1:L:157:GLU:HG2	1.74	0.69
1:M:103:LEU:HD22	1:M:152:ILE:HD11	1.75	0.69
1:K:284:LEU:HD23	1:M:284:LEU:HD23	1.75	0.69
1:A:192:TYR:HD1	1:A:217:VAL:HG23	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:MET:HE2	1:J:161:LYS:HB2	1.75	0.67
1:N:81:ILE:HA	1:N:95:THR:HG22	1.77	0.67
1:P:78:ILE:HD12	1:P:165:PHE:HZ	1.60	0.66
1:D:81:ILE:HA	1:D:95:THR:HG22	1.78	0.66
1:F:87:GLU:HB2	1:F:88:PRO:HD2	1.76	0.66
1:I:81:ILE:HA	1:I:95:THR:HG22	1.77	0.66
1:K:98:MET:HE2	1:K:161:LYS:HB2	1.77	0.66
1:C:235:PRO:HA	1:C:238:ILE:HD12	1.77	0.65
1:G:98:MET:HE2	1:G:161:LYS:HB2	1.77	0.65
1:C:81:ILE:HA	1:C:95:THR:HG22	1.79	0.65
1:G:81:ILE:HA	1:G:95:THR:HG22	1.79	0.65
1:H:81:ILE:HA	1:H:95:THR:HG22	1.79	0.65
1:A:284:LEU:HD23	1:G:284:LEU:HD23	1.78	0.64
1:O:262:ARG:O	1:O:266:ILE:HG23	1.97	0.64
1:C:234:ASN:HB3	1:C:237:GLN:HB2	1.78	0.64
1:C:125:LEU:HD21	1:C:222:VAL:HG21	1.78	0.64
1:E:81:ILE:HA	1:E:95:THR:HG22	1.80	0.64
1:L:81:ILE:HA	1:L:95:THR:HG22	1.79	0.64
1:J:128:ILE:O	1:J:132:VAL:HG12	1.96	0.63
1:J:81:ILE:HA	1:J:95:THR:HG22	1.81	0.63
1:A:81:ILE:HA	1:A:95:THR:HG22	1.81	0.62
1:A:128:ILE:HG12	1:A:152:ILE:HD12	1.81	0.62
1:P:81:ILE:HA	1:P:95:THR:HG22	1.81	0.62
1:O:81:ILE:HA	1:O:95:THR:HG22	1.81	0.62
1:F:81:ILE:HA	1:F:95:THR:HG22	1.82	0.62
1:C:306:VAL:HA	1:C:309:LEU:HD22	1.82	0.62
1:B:81:ILE:HA	1:B:95:THR:HG22	1.81	0.62
1:C:229:PHE:O	1:C:232:VAL:HG12	2.00	0.62
1:J:194:PRO:HB2	1:J:196:GLU:OE1	2.00	0.61
1:C:194:PRO:HD2	1:C:210:HIS:CD2	2.34	0.61
1:A:192:TYR:HA	1:A:217:VAL:HG21	1.81	0.61
1:M:128:ILE:HD11	1:M:152:ILE:HD12	1.83	0.61
1:F:128:ILE:O	1:F:132:VAL:HG12	2.00	0.61
1:C:101:GLY:HA2	2:C:401:9XA:C11	2.31	0.60
1:M:81:ILE:HA	1:M:95:THR:HG22	1.83	0.60
1:M:128:ILE:CD1	1:M:152:ILE:HD12	2.31	0.60
1:D:293:VAL:O	1:D:296:THR:HB	2.01	0.60
1:P:128:ILE:HG12	1:P:152:ILE:HD12	1.82	0.60
1:J:220:TRP:HH2	1:J:226:LYS:HE3	1.67	0.60
1:N:192:TYR:HA	1:N:217:VAL:HG11	1.84	0.60
1:K:81:ILE:HA	1:K:95:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:158:PHE:CD1	1:K:306:VAL:HG23	2.37	0.59
1:A:158:PHE:HD2	1:A:306:VAL:HG13	1.66	0.59
1:H:123:ARG:HA	1:H:294:LEU:HD21	1.83	0.59
1:O:17:LYS:HD3	1:O:38:ALA:HB3	1.83	0.59
1:F:235:PRO:HA	1:F:238:ILE:HD12	1.85	0.59
1:E:235:PRO:HA	1:E:238:ILE:HD12	1.85	0.59
1:O:125:LEU:HD22	1:O:219:THR:CG2	2.32	0.58
1:E:128:ILE:O	1:E:132:VAL:HG23	2.04	0.58
1:B:290:LEU:O	1:B:293:VAL:HG12	2.02	0.58
1:D:158:PHE:CD1	1:D:306:VAL:HG23	2.38	0.58
1:M:199:GLU:OE2	1:M:200:PRO:HD2	2.03	0.58
1:J:158:PHE:CD1	1:J:306:VAL:HG23	2.39	0.58
1:J:193:MET:HE3	1:J:197:ASN:HB3	1.86	0.58
1:O:125:LEU:HD22	1:O:219:THR:HG22	1.86	0.58
1:O:307:ILE:HG13	1:P:300:ILE:HD11	1.85	0.58
1:O:48:HIS:HB2	3:O:505:HOH:O	2.03	0.57
1:O:273:TRP:O	1:O:273:TRP:CD1	2.57	0.57
1:A:235:PRO:HA	1:A:238:ILE:HD12	1.86	0.57
1:C:232:VAL:HG11	1:C:238:ILE:HG12	1.87	0.57
1:F:25:SER:HB3	2:F:401:9XA:C32	2.34	0.57
1:I:115:ASP:HB2	1:I:308:GLN:OE1	2.05	0.56
1:M:235:PRO:HA	1:M:238:ILE:HD12	1.87	0.56
1:O:235:PRO:HA	1:O:238:ILE:HD12	1.85	0.56
1:B:235:PRO:HA	1:B:238:ILE:HD12	1.87	0.56
1:D:59:GLU:O	1:D:63:VAL:HG23	2.04	0.56
1:H:145:HIS:CE1	3:H:502:HOH:O	2.58	0.56
1:I:128:ILE:O	1:I:132:VAL:HG23	2.05	0.56
1:G:128:ILE:O	1:G:132:VAL:HG23	2.06	0.56
1:K:32:VAL:HG11	2:K:401:9XA:O29	2.05	0.56
1:L:125:LEU:HD22	1:L:219:THR:HG22	1.87	0.56
1:F:31:THR:HG23	1:F:48:HIS:CD2	2.41	0.56
2:C:401:9XA:C34	2:C:401:9XA:C4	2.84	0.55
1:F:104:ASN:HB2	1:F:149:THR:HG23	1.88	0.55
1:H:128:ILE:O	1:H:132:VAL:HG23	2.06	0.55
1:B:128:ILE:O	1:B:132:VAL:HG23	2.07	0.55
1:D:60:ARG:O	1:D:64:LEU:HD12	2.07	0.55
1:A:36:ARG:HH11	1:A:41:ARG:HG2	1.70	0.55
1:C:304:GLU:HA	1:C:307:ILE:HG22	1.88	0.55
1:H:158:PHE:CD2	1:H:306:VAL:HG23	2.42	0.55
1:N:152:ILE:HG23	1:N:160:VAL:CG2	2.36	0.55
1:P:78:ILE:HD13	1:P:162:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:199:GLU:CD	1:M:200:PRO:HD2	2.31	0.55
1:B:267:SER:HA	1:J:16:HIS:HB2	1.89	0.55
1:P:235:PRO:HA	1:P:238:ILE:HD12	1.89	0.55
1:I:123:ARG:HA	1:I:294:LEU:HD21	1.89	0.54
1:K:60:ARG:NH2	1:K:91:LEU:HB2	2.22	0.54
1:L:128:ILE:O	1:L:132:VAL:HG23	2.06	0.54
1:G:98:MET:CE	1:G:161:LYS:HG3	2.38	0.54
1:C:125:LEU:HD11	1:C:222:VAL:HG21	1.90	0.54
1:H:150:GLN:H	1:H:150:GLN:HE21	1.55	0.54
1:P:98:MET:HE2	1:P:161:LYS:HB2	1.88	0.54
1:P:192:TYR:HA	1:P:217:VAL:HG11	1.89	0.54
1:N:63:VAL:HG22	1:N:91:LEU:HD21	1.89	0.54
1:E:65:ARG:O	1:E:69:ILE:HG12	2.08	0.54
1:J:98:MET:CE	1:J:161:LYS:HG3	2.38	0.54
1:P:128:ILE:O	1:P:132:VAL:HG23	2.07	0.54
1:C:128:ILE:O	1:C:132:VAL:HG23	2.08	0.54
1:E:117:ALA:HB1	1:E:119:PRO:HD2	1.90	0.54
1:A:128:ILE:O	1:A:132:VAL:HG23	2.06	0.53
1:C:193:MET:HE2	1:C:197:ASN:HB3	1.91	0.53
1:D:14:PRO:HD2	1:D:17:LYS:HE2	1.91	0.53
1:O:245:GLY:HA2	1:O:275:GLN:OE1	2.08	0.53
1:P:117:ALA:HB1	1:P:119:PRO:HD2	1.90	0.53
1:E:58:SER:HB3	1:E:60:ARG:HG2	1.90	0.53
1:C:117:ALA:HB1	1:C:119:PRO:HD2	1.89	0.53
1:J:36:ARG:HG2	1:J:43:GLN:HA	1.90	0.53
1:E:190:ILE:HG12	1:E:239:MET:HE2	1.89	0.53
1:K:17:LYS:HE3	1:K:39:ASP:CG	2.32	0.53
1:H:105:GLU:O	1:H:109:ARG:HB2	2.08	0.53
1:K:216:ALA:HA	1:K:219:THR:HG22	1.91	0.53
1:D:122:PHE:O	1:D:294:LEU:HD11	2.09	0.53
1:B:24:LEU:HD22	2:B:401:9XA:C11	2.38	0.53
1:E:128:ILE:HG12	1:E:152:ILE:HD12	1.91	0.53
1:N:98:MET:HE2	1:N:161:LYS:HB2	1.90	0.52
1:J:271:SER:OG	1:J:281:PRO:HD3	2.10	0.52
1:N:125:LEU:HD11	1:N:222:VAL:CG1	2.40	0.52
1:D:130:LEU:HD23	1:D:287:LEU:HD21	1.89	0.52
1:F:24:LEU:HD11	1:F:34:SER:HB3	1.91	0.52
1:F:298:GLU:HG3	1:F:301:THR:HG23	1.91	0.52
1:N:80:PRO:HD3	1:N:161:LYS:HD2	1.92	0.52
1:K:21:LEU:HA	1:K:34:SER:O	2.10	0.52
1:P:78:ILE:HD12	1:P:165:PHE:CZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:PRO:HA	1:G:238:ILE:HD12	1.92	0.52
1:M:24:LEU:HG	2:M:401:9XA:O30	2.10	0.52
1:N:125:LEU:HD11	1:N:222:VAL:HG11	1.91	0.52
1:A:192:TYR:CD1	1:A:217:VAL:HG23	2.41	0.52
1:C:259:ILE:HB	1:C:262:ARG:HG3	1.90	0.52
1:D:60:ARG:HG3	1:D:91:LEU:HD22	1.91	0.52
1:N:128:ILE:O	1:N:132:VAL:HG23	2.10	0.52
1:C:192:TYR:HA	1:C:217:VAL:HG11	1.91	0.52
1:K:98:MET:HE3	1:K:154:LEU:C	2.34	0.52
1:L:190:ILE:HG12	1:L:239:MET:HE3	1.91	0.51
1:K:98:MET:CE	1:K:161:LYS:HG3	2.40	0.51
1:B:33:SER:HB2	1:B:48:HIS:HE1	1.75	0.51
1:C:6:ILE:HD13	1:D:68:GLU:HG3	1.91	0.51
1:N:20:ASP:HB2	1:N:36:ARG:HD3	1.92	0.51
1:H:118:TRP:CH2	1:H:259:ILE:HG12	2.45	0.51
1:E:121:ARG:HH12	1:E:225:ARG:NE	2.09	0.51
1:H:298:GLU:HG3	1:H:301:THR:HG23	1.92	0.51
1:M:245:GLY:HA2	1:M:275:GLN:OE1	2.08	0.51
1:B:46:VAL:HA	1:B:93:ILE:O	2.10	0.51
1:G:121:ARG:HH22	1:G:225:ARG:HG3	1.76	0.51
1:O:93:ILE:HD12	1:O:95:THR:HG23	1.92	0.51
1:G:121:ARG:NH2	1:G:225:ARG:HG3	2.26	0.51
1:D:290:LEU:O	1:D:293:VAL:HG13	2.10	0.51
1:K:128:ILE:O	1:K:132:VAL:HG23	2.10	0.51
1:H:117:ALA:HB1	1:H:119:PRO:HD2	1.92	0.51
1:G:143:LEU:HD22	1:G:145:HIS:NE2	2.26	0.50
1:M:128:ILE:O	1:M:132:VAL:HG23	2.12	0.50
1:P:194:PRO:HG3	1:P:210:HIS:HA	1.93	0.50
1:C:271:SER:O	1:C:280:ARG:HA	2.12	0.50
1:B:32:VAL:HG11	2:B:401:9XA:C6	2.41	0.50
1:F:117:ALA:HB1	1:F:119:PRO:HD2	1.93	0.50
1:O:273:TRP:O	1:O:273:TRP:HD1	1.95	0.50
1:E:307:ILE:CD1	1:F:307:ILE:HG21	2.42	0.50
1:D:46:VAL:HG12	1:D:48:HIS:HD2	1.76	0.50
1:M:117:ALA:HB1	1:M:119:PRO:HD2	1.93	0.50
1:N:209:LYS:O	1:N:212:ILE:HG22	2.12	0.50
1:O:65:ARG:O	1:O:69:ILE:HG12	2.10	0.50
1:L:107:LEU:HD11	1:L:222:VAL:HG22	1.94	0.50
1:F:148:LYS:HG2	1:F:151:ASN:ND2	2.27	0.49
1:L:229:PHE:HB3	1:L:232:VAL:HG22	1.92	0.49
1:G:65:ARG:O	1:G:69:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:TRP:NE1	1:J:255:LEU:HD11	2.27	0.49
1:N:65:ARG:O	1:N:69:ILE:HG12	2.13	0.49
1:N:214:SER:O	1:N:217:VAL:HG13	2.13	0.49
1:A:192:TYR:HD1	1:A:217:VAL:CG2	2.24	0.49
1:J:291:GLU:HB3	1:J:295:ARG:HH21	1.76	0.49
1:K:117:ALA:HB1	1:K:119:PRO:HD2	1.95	0.49
1:N:299:GLU:HA	1:N:302:PHE:CD2	2.47	0.49
1:O:117:ALA:HB1	1:O:119:PRO:HD2	1.95	0.49
1:I:117:ALA:HB1	1:I:119:PRO:HD2	1.93	0.49
1:K:284:LEU:O	1:K:288:ILE:HG23	2.13	0.49
1:K:298:GLU:HG2	1:K:301:THR:HG23	1.95	0.49
1:M:80:PRO:HD3	1:M:161:LYS:HD2	1.95	0.49
1:B:117:ALA:HB1	1:B:119:PRO:HD2	1.94	0.49
1:J:235:PRO:HA	1:J:238:ILE:HD12	1.94	0.49
1:P:214:SER:O	1:P:217:VAL:HG13	2.13	0.49
1:N:229:PHE:HB3	1:N:232:VAL:HG22	1.94	0.49
1:C:14:PRO:HD2	1:C:17:LYS:HG3	1.95	0.49
1:G:291:GLU:O	1:G:295:ARG:HG2	2.12	0.49
1:A:80:PRO:HD3	1:A:161:LYS:HD2	1.95	0.49
1:D:298:GLU:HG2	1:D:301:THR:HG23	1.94	0.49
1:H:59:GLU:HA	1:H:62:ASP:OD2	2.13	0.49
1:M:137:ASN:ND2	1:N:39:ASP:HB3	2.28	0.49
1:M:193:MET:HE3	1:M:197:ASN:HB3	1.94	0.49
1:E:80:PRO:HD3	1:E:161:LYS:HD2	1.95	0.48
1:J:98:MET:HE3	1:J:154:LEU:C	2.38	0.48
1:J:198:TYR:HB2	1:J:199:GLU:OE2	2.13	0.48
1:N:277:PRO:HB2	3:N:505:HOH:O	2.12	0.48
1:C:65:ARG:O	1:C:69:ILE:HG12	2.13	0.48
1:D:116:VAL:HG12	1:D:309:LEU:HD21	1.95	0.48
1:D:117:ALA:HB1	1:D:119:PRO:HD2	1.95	0.48
1:G:148:LYS:HG3	1:G:150:GLN:HB2	1.94	0.48
1:A:117:ALA:HB1	1:A:119:PRO:HD2	1.96	0.48
1:D:235:PRO:HA	1:D:238:ILE:HD12	1.95	0.48
1:E:75:PHE:HB3	1:E:78:ILE:HG12	1.95	0.48
1:G:117:ALA:HB1	1:G:119:PRO:HD2	1.95	0.48
1:K:216:ALA:O	1:K:219:THR:HG22	2.13	0.48
1:L:46:VAL:HG12	1:L:48:HIS:HD2	1.79	0.48
1:O:15:TYR:HA	1:O:18:LEU:HD12	1.95	0.48
1:B:14:PRO:HD2	1:B:17:LYS:HG3	1.96	0.48
1:G:98:MET:HE3	1:G:154:LEU:C	2.39	0.48
1:C:46:VAL:HG22	1:C:48:HIS:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ILE:O	1:D:132:VAL:HG23	2.13	0.48
1:H:79:LEU:HD12	1:H:98:MET:HE3	1.96	0.47
1:C:190:ILE:HD12	1:C:239:MET:SD	2.54	0.47
1:A:79:LEU:HD12	1:A:98:MET:HE3	1.96	0.47
1:G:116:VAL:HG12	1:G:309:LEU:HD21	1.95	0.47
1:I:79:LEU:HD12	1:I:98:MET:HE3	1.96	0.47
1:H:273:TRP:CD1	1:H:273:TRP:C	2.91	0.47
1:B:257:TYR:HA	1:B:262:ARG:HD2	1.96	0.47
1:B:299:GLU:H	1:B:299:GLU:CD	2.23	0.47
1:E:157:GLU:HB3	1:F:157:GLU:HG2	1.96	0.47
1:J:236:LEU:HD21	1:M:235:PRO:CB	2.35	0.47
1:G:198:TYR:O	1:G:199:GLU:HG3	2.14	0.47
1:H:46:VAL:HG12	1:H:48:HIS:HD2	1.79	0.47
1:H:122:PHE:O	1:H:294:LEU:HD11	2.15	0.47
1:A:157:GLU:HG2	1:B:157:GLU:CG	2.38	0.47
1:A:192:TYR:CD1	1:A:217:VAL:CG2	2.98	0.47
1:F:85:CYS:O	1:F:91:LEU:HA	2.15	0.47
1:H:235:PRO:HB2	1:P:236:LEU:HD22	1.96	0.47
1:A:157:GLU:CG	1:B:157:GLU:HG2	2.37	0.46
1:H:264:ARG:HH11	1:H:289:GLU:HG3	1.79	0.46
1:K:235:PRO:HA	1:K:238:ILE:HD12	1.96	0.46
1:B:24:LEU:HD11	1:B:34:SER:HB3	1.97	0.46
1:F:65:ARG:O	1:F:69:ILE:HG12	2.15	0.46
1:N:299:GLU:HA	1:N:302:PHE:HD2	1.80	0.46
1:K:247:ARG:HG3	1:K:273:TRP:CD1	2.50	0.46
1:O:257:TYR:HA	1:O:262:ARG:HD2	1.98	0.46
1:L:121:ARG:O	1:L:125:LEU:HG	2.15	0.46
1:L:218:ILE:O	1:L:222:VAL:HG23	2.16	0.46
1:N:85:CYS:O	1:N:91:LEU:HA	2.16	0.46
1:F:14:PRO:HD2	1:F:17:LYS:HG3	1.97	0.46
1:O:246:HIS:HA	3:O:507:HOH:O	2.15	0.46
1:B:138:MET:CE	1:B:142:LEU:HB3	2.46	0.46
1:C:158:PHE:CD2	1:C:306:VAL:HG13	2.51	0.46
1:I:14:PRO:HD2	1:I:17:LYS:HG3	1.98	0.46
1:O:192:TYR:HB3	1:O:214:SER:HB3	1.98	0.46
1:B:18:LEU:HB3	1:B:21:LEU:HD12	1.98	0.46
1:K:193:MET:HE3	1:K:197:ASN:HB3	1.98	0.46
1:N:127:GLU:HB3	1:N:160:VAL:CG1	2.46	0.46
1:H:14:PRO:HD2	1:H:17:LYS:HG3	1.98	0.46
1:L:14:PRO:HD2	1:L:17:LYS:HG3	1.98	0.46
1:N:119:PRO:HG2	1:N:301:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:127:GLU:HB3	1:N:160:VAL:HG12	1.97	0.46
1:E:79:LEU:HD12	1:E:98:MET:HE3	1.97	0.46
1:P:65:ARG:O	1:P:69:ILE:HG12	2.16	0.46
1:E:14:PRO:HD2	1:E:17:LYS:HG3	1.98	0.45
1:K:121:ARG:HH11	1:K:225:ARG:HD2	1.81	0.45
1:K:123:ARG:HA	1:K:294:LEU:HD21	1.98	0.45
1:P:152:ILE:HD13	1:P:162:ILE:HG12	1.98	0.45
1:E:36:ARG:NH2	1:E:41:ARG:HG2	2.31	0.45
1:H:85:CYS:O	1:H:91:LEU:HA	2.16	0.45
1:I:235:PRO:HA	1:I:238:ILE:HD12	1.97	0.45
1:M:79:LEU:HD12	1:M:98:MET:HE3	1.97	0.45
1:O:85:CYS:O	1:O:91:LEU:HA	2.16	0.45
1:C:32:VAL:HG11	2:C:401:9XA:C6	2.47	0.45
1:E:245:GLY:HA2	1:E:275:GLN:OE1	2.17	0.45
1:G:194:PRO:HG3	1:G:210:HIS:HA	1.98	0.45
1:O:132:VAL:HG21	1:O:147:LEU:HD21	1.97	0.45
1:O:144:HIS:ND1	1:O:147:LEU:HD13	2.31	0.45
1:C:158:PHE:HD2	1:C:306:VAL:HG13	1.80	0.45
1:C:268:LEU:HD21	1:C:286:CYS:HA	1.98	0.45
1:I:158:PHE:CD2	1:I:306:VAL:HG23	2.52	0.45
1:N:232:VAL:HG21	1:N:238:ILE:HB	1.98	0.45
1:A:265:MET:O	1:A:269:ILE:HG13	2.16	0.45
1:E:85:CYS:O	1:E:91:LEU:HA	2.16	0.45
1:J:259:ILE:HA	1:J:260:PRO:HD3	1.83	0.45
1:K:60:ARG:O	1:K:64:LEU:HD12	2.17	0.45
1:P:250:ILE:HD13	1:P:266:ILE:HG23	1.98	0.45
1:D:65:ARG:O	1:D:69:ILE:HG12	2.17	0.45
1:D:80:PRO:HD3	1:D:161:LYS:HD2	1.99	0.45
1:E:198:TYR:CZ	1:E:239:MET:HG2	2.52	0.45
1:K:14:PRO:HD2	1:K:17:LYS:HG3	1.98	0.45
1:K:266:ILE:O	1:K:270:GLU:HG2	2.16	0.45
1:A:14:PRO:HD2	1:A:17:LYS:HG3	1.98	0.45
1:M:257:TYR:HA	1:M:262:ARG:HD2	1.99	0.45
1:G:294:LEU:HA	1:G:297:PHE:CD2	2.52	0.45
1:L:232:VAL:HG21	1:L:238:ILE:HG12	1.99	0.45
1:O:80:PRO:HD3	1:O:161:LYS:HD2	1.98	0.45
1:O:276:ASN:HB3	1:O:279:GLU:HB2	1.99	0.45
1:G:80:PRO:HD3	1:G:161:LYS:HD2	1.99	0.45
1:I:306:VAL:HA	1:I:309:LEU:HD12	1.99	0.45
1:J:252:GLU:HB3	1:J:257:TYR:CE1	2.52	0.45
1:P:33:SER:HB2	1:P:48:HIS:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HA	1:B:138:MET:HE2	1.99	0.45
1:C:294:LEU:HA	1:C:297:PHE:CE2	2.52	0.45
1:O:79:LEU:HD12	1:O:98:MET:HE3	1.99	0.45
1:K:65:ARG:O	1:K:69:ILE:HG12	2.17	0.44
1:A:6:ILE:O	1:B:9:ALA:HA	2.17	0.44
1:E:23:TYR:CD1	1:E:23:TYR:N	2.84	0.44
1:G:118:TRP:CH2	1:G:259:ILE:HG12	2.52	0.44
1:E:36:ARG:HH21	1:E:41:ARG:HG2	1.81	0.44
1:F:16:HIS:HE1	1:F:17:LYS:HE3	1.82	0.44
1:F:16:HIS:CE1	1:F:17:LYS:HE3	2.53	0.44
1:I:80:PRO:HD3	1:I:161:LYS:HD2	1.99	0.44
1:J:152:ILE:HG23	1:J:160:VAL:HG13	2.00	0.44
1:B:250:ILE:HD13	1:B:266:ILE:HG23	2.00	0.44
1:F:306:VAL:HA	1:F:309:LEU:HD12	2.00	0.44
1:B:261:HIS:ND1	1:B:293:VAL:HG23	2.33	0.44
1:O:193:MET:HE3	1:O:197:ASN:HB3	2.00	0.44
1:B:29:SER:HB3	3:B:507:HOH:O	2.17	0.44
1:C:79:LEU:HD12	1:C:98:MET:HE3	2.00	0.44
1:F:80:PRO:HD3	1:F:161:LYS:HD2	1.99	0.44
1:F:148:LYS:HB3	1:F:192:TYR:CD2	2.52	0.44
1:G:143:LEU:HD21	1:G:208:ILE:HA	2.00	0.44
1:G:294:LEU:HA	1:G:297:PHE:HD2	1.83	0.44
1:M:85:CYS:O	1:M:91:LEU:HA	2.17	0.44
1:I:16:HIS:CE1	1:I:17:LYS:HE2	2.53	0.44
1:K:300:ILE:HD11	1:L:307:ILE:HG13	1.99	0.44
1:P:152:ILE:HG23	1:P:160:VAL:HG13	2.00	0.44
1:A:130:LEU:HD22	1:B:42:VAL:HG13	1.99	0.43
1:B:85:CYS:O	1:B:91:LEU:HA	2.17	0.43
1:C:273:TRP:O	1:C:273:TRP:CD1	2.71	0.43
1:D:85:CYS:O	1:D:91:LEU:HA	2.18	0.43
1:D:196:GLU:H	1:D:196:GLU:HG3	1.60	0.43
1:G:98:MET:HE1	1:G:161:LYS:HG3	2.00	0.43
1:M:17:LYS:HD3	1:M:38:ALA:HB3	2.00	0.43
1:G:46:VAL:HG12	1:G:48:HIS:HD2	1.82	0.43
1:J:98:MET:HE1	1:J:161:LYS:HG3	1.99	0.43
1:P:85:CYS:O	1:P:91:LEU:HA	2.18	0.43
1:B:46:VAL:HB	1:B:94:VAL:HB	2.01	0.43
1:D:32:VAL:CG1	2:D:401:9XA:O29	2.62	0.43
1:H:250:ILE:HD13	1:H:266:ILE:HG23	2.00	0.43
1:J:65:ARG:O	1:J:69:ILE:HG12	2.17	0.43
1:K:85:CYS:O	1:K:91:LEU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:276:ASN:HB3	1:P:279:GLU:HB2	1.99	0.43
1:H:306:VAL:HA	1:H:309:LEU:HD12	2.00	0.43
1:K:80:PRO:HD3	1:K:161:LYS:HD2	1.99	0.43
1:L:85:CYS:O	1:L:91:LEU:HA	2.17	0.43
1:N:79:LEU:HA	1:N:80:PRO:HD3	1.94	0.43
1:B:306:VAL:HA	1:B:309:LEU:HD12	2.01	0.43
1:C:135:LEU:HD22	1:C:142:LEU:HD12	1.99	0.43
1:D:16:HIS:HB2	1:N:285:LYS:HD3	2.01	0.43
1:D:212:ILE:HG12	1:D:281:PRO:O	2.19	0.43
1:I:85:CYS:O	1:I:91:LEU:HA	2.18	0.43
1:I:236:LEU:HD22	1:I:240:TYR:CE2	2.53	0.43
1:L:250:ILE:HD13	1:L:266:ILE:HG23	2.01	0.43
1:P:14:PRO:HD2	1:P:17:LYS:HG3	2.01	0.43
1:B:80:PRO:HD3	1:B:161:LYS:HD2	2.00	0.43
1:M:231:ASP:HA	3:M:509:HOH:O	2.18	0.43
1:N:117:ALA:HB1	1:N:119:PRO:HD2	1.99	0.43
1:P:80:PRO:HD3	1:P:161:LYS:HD2	2.00	0.43
1:B:292:PRO:HA	1:B:295:ARG:HB2	2.01	0.43
1:F:304:GLU:O	1:F:307:ILE:HG13	2.18	0.43
1:G:257:TYR:HA	1:G:262:ARG:HD2	2.01	0.43
1:A:85:CYS:O	1:A:91:LEU:HA	2.18	0.43
1:B:79:LEU:HD12	1:B:98:MET:HE3	2.01	0.43
1:C:85:CYS:O	1:C:91:LEU:HA	2.18	0.43
1:D:190:ILE:HG12	1:D:239:MET:HE2	2.00	0.43
1:A:250:ILE:HD13	1:A:266:ILE:HG23	2.00	0.43
1:B:116:VAL:HG12	1:B:309:LEU:HD21	2.01	0.43
1:C:125:LEU:HD11	1:C:222:VAL:CG2	2.49	0.43
1:F:250:ILE:HD13	1:F:266:ILE:HG23	2.01	0.43
1:I:16:HIS:HE1	1:I:17:LYS:HE2	1.83	0.43
1:L:118:TRP:O	1:L:122:PHE:HD2	2.01	0.43
1:N:35:ALA:C	1:N:36:ARG:HD2	2.44	0.43
1:B:195:PRO:HA	1:B:198:TYR:CE2	2.54	0.42
1:E:298:GLU:HG3	1:E:301:THR:HG23	2.01	0.42
1:G:252:GLU:HB3	1:G:257:TYR:CE1	2.54	0.42
1:A:79:LEU:HA	1:A:80:PRO:HD3	1.91	0.42
1:J:193:MET:CE	1:J:197:ASN:HB3	2.48	0.42
1:N:118:TRP:CH2	1:N:259:ILE:HG12	2.54	0.42
1:D:212:ILE:HD12	1:D:212:ILE:HA	1.94	0.42
1:A:216:ALA:HA	1:A:219:THR:HG22	2.00	0.42
1:B:60:ARG:O	1:B:63:VAL:HG13	2.19	0.42
1:B:304:GLU:O	1:B:307:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG12	1:A:48:HIS:HD2	1.84	0.42
1:C:273:TRP:O	1:C:273:TRP:HD1	2.02	0.42
1:J:194:PRO:HG3	1:J:210:HIS:HA	2.00	0.42
1:E:125:LEU:HD13	1:E:219:THR:HG23	2.02	0.42
1:A:158:PHE:CD2	1:A:306:VAL:HG13	2.49	0.42
1:D:14:PRO:HD2	1:D:17:LYS:CE	2.48	0.42
1:F:149:THR:HG21	1:F:221:GLU:OE2	2.20	0.42
1:G:79:LEU:HA	1:G:80:PRO:HD3	1.90	0.42
1:B:125:LEU:HD13	1:B:219:THR:HG23	2.01	0.42
1:H:65:ARG:O	1:H:69:ILE:HG12	2.20	0.42
1:I:65:ARG:O	1:I:69:ILE:HG12	2.19	0.42
1:I:250:ILE:HD13	1:I:266:ILE:HG23	2.02	0.42
1:J:74:ARG:HE	1:J:74:ARG:HB3	1.47	0.42
1:M:277:PRO:HA	1:M:280:ARG:HE	1.84	0.42
1:K:158:PHE:HD1	1:K:306:VAL:HG23	1.84	0.42
1:M:272:GLY:HA2	1:M:281:PRO:HD2	2.02	0.42
1:A:65:ARG:O	1:A:69:ILE:HG12	2.19	0.42
1:B:198:TYR:CD1	1:B:239:MET:HE3	2.55	0.42
1:N:250:ILE:HD13	1:N:266:ILE:HG23	2.00	0.42
1:A:158:PHE:CZ	1:A:309:LEU:HD23	2.55	0.41
1:A:198:TYR:OH	1:A:242:VAL:HG21	2.20	0.41
1:C:101:GLY:HA2	2:C:401:9XA:C34	2.50	0.41
1:D:24:LEU:HD11	1:D:34:SER:HB3	2.02	0.41
1:H:272:GLY:O	1:H:280:ARG:HG2	2.20	0.41
1:C:149:THR:HG22	1:C:218:ILE:HG23	2.01	0.41
1:L:194:PRO:HG3	1:L:210:HIS:HA	2.01	0.41
1:M:118:TRP:CH2	1:M:259:ILE:HG12	2.56	0.41
1:M:273:TRP:CD1	1:M:273:TRP:C	2.97	0.41
1:O:125:LEU:HD22	1:O:219:THR:HG23	2.01	0.41
1:C:250:ILE:HD13	1:C:266:ILE:HG23	2.01	0.41
1:F:257:TYR:HA	1:F:262:ARG:HD2	2.02	0.41
1:J:194:PRO:HB2	1:J:196:GLU:CD	2.45	0.41
1:C:153:LEU:HD11	2:C:401:9XA:C20	2.50	0.41
1:E:262:ARG:O	1:E:266:ILE:HG12	2.20	0.41
1:F:265:MET:O	1:F:269:ILE:HG13	2.20	0.41
1:G:85:CYS:O	1:G:91:LEU:HA	2.20	0.41
1:J:46:VAL:HG12	1:J:48:HIS:HD2	1.85	0.41
1:L:106:LEU:HA	1:L:113:TYR:CD2	2.55	0.41
1:B:152:ILE:HG23	1:B:160:VAL:HG13	2.03	0.41
1:E:220:TRP:CH2	1:E:226:LYS:HG3	2.55	0.41
1:G:307:ILE:HD12	1:H:303:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:PRO:HB3	1:H:242:VAL:HG12	2.02	0.41
1:B:198:TYR:HE2	1:B:242:VAL:CG2	2.34	0.41
1:H:291:GLU:HB3	3:H:520:HOH:O	2.20	0.41
1:C:199:GLU:HB2	1:C:200:PRO:HD2	2.03	0.41
1:J:80:PRO:HD3	1:J:161:LYS:HD2	2.02	0.41
1:A:152:ILE:HG23	1:A:160:VAL:HG13	2.02	0.41
1:H:152:ILE:HG23	1:H:160:VAL:HG13	2.02	0.41
1:C:71:HIS:ND1	1:C:74:ARG:NH2	2.69	0.41
1:C:190:ILE:H	1:C:190:ILE:HG12	1.65	0.41
1:D:123:ARG:HA	1:D:294:LEU:HD21	2.02	0.41
1:E:242:VAL:HA	1:E:246:HIS:O	2.21	0.41
1:J:85:CYS:O	1:J:91:LEU:HA	2.20	0.41
1:N:107:LEU:HD21	1:N:222:VAL:HG23	2.01	0.41
1:N:123:ARG:HA	1:N:294:LEU:HD21	2.03	0.41
1:N:306:VAL:HA	1:N:309:LEU:HD12	2.03	0.41
1:O:192:TYR:HB2	3:O:512:HOH:O	2.20	0.41
1:I:152:ILE:HG23	1:I:160:VAL:HG13	2.03	0.41
1:K:152:ILE:HG23	1:K:160:VAL:HG13	2.03	0.41
1:L:65:ARG:O	1:L:69:ILE:HG12	2.20	0.41
1:N:108:HIS:CE1	1:N:227:GLN:HE21	2.39	0.41
1:P:158:PHE:CD1	1:P:306:VAL:HG13	2.56	0.41
1:C:46:VAL:HA	1:C:93:ILE:O	2.21	0.40
1:P:286:CYS:O	1:P:290:LEU:HD12	2.20	0.40
1:A:118:TRP:CH2	1:A:259:ILE:HG12	2.56	0.40
1:D:284:LEU:HD21	1:O:288:ILE:HD13	2.04	0.40
1:G:21:LEU:HA	1:G:34:SER:O	2.22	0.40
1:H:198:TYR:HB3	1:P:240:TYR:CD2	2.56	0.40
1:A:307:ILE:HG22	1:B:303:LEU:HB3	2.03	0.40
1:F:79:LEU:HD12	1:F:98:MET:HE3	2.02	0.40
1:F:125:LEU:HD13	1:F:219:THR:HG23	2.03	0.40
1:J:116:VAL:HG12	1:J:120:LEU:HD23	2.03	0.40
1:K:99:PRO:HG2	1:K:156:ASN:HB2	2.04	0.40
1:K:126:HIS:HB2	1:K:294:LEU:HD11	2.02	0.40
1:D:79:LEU:HA	1:D:80:PRO:HD3	1.92	0.40
1:M:103:LEU:HD21	1:M:222:VAL:HG22	2.03	0.40
1:C:126:HIS:HB2	1:C:294:LEU:HD11	2.01	0.40
1:H:145:HIS:HE1	3:H:502:HOH:O	1.97	0.40
1:L:79:LEU:HD12	1:L:98:MET:HE3	2.04	0.40
1:P:98:MET:HE3	1:P:154:LEU:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/310 (86%)	255 (96%)	12 (4%)	0	100	100
1	B	267/310 (86%)	255 (96%)	12 (4%)	0	100	100
1	C	267/310 (86%)	256 (96%)	9 (3%)	2 (1%)	18	48
1	D	267/310 (86%)	260 (97%)	7 (3%)	0	100	100
1	E	267/310 (86%)	255 (96%)	11 (4%)	1 (0%)	30	59
1	F	267/310 (86%)	254 (95%)	12 (4%)	1 (0%)	30	59
1	G	267/310 (86%)	258 (97%)	9 (3%)	0	100	100
1	H	267/310 (86%)	257 (96%)	10 (4%)	0	100	100
1	I	267/310 (86%)	255 (96%)	12 (4%)	0	100	100
1	J	267/310 (86%)	258 (97%)	9 (3%)	0	100	100
1	K	267/310 (86%)	256 (96%)	11 (4%)	0	100	100
1	L	267/310 (86%)	259 (97%)	8 (3%)	0	100	100
1	M	268/310 (86%)	257 (96%)	10 (4%)	1 (0%)	30	59
1	N	264/310 (85%)	252 (96%)	10 (4%)	2 (1%)	16	44
1	O	268/310 (86%)	259 (97%)	9 (3%)	0	100	100
1	P	267/310 (86%)	255 (96%)	10 (4%)	2 (1%)	18	48
All	All	4271/4960 (86%)	4101 (96%)	161 (4%)	9 (0%)	43	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	61	LYS
1	P	299	GLU
1	N	209	LYS
1	C	198	TYR
1	C	299	GLU
1	E	299	GLU

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Mol	Chain	Res	Type
1	N	299	GLU
1	F	61	LYS
1	P	274	ALA

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	231/279 (83%)	213 (92%)	18 (8%)	11	35
1	B	232/279 (83%)	214 (92%)	18 (8%)	11	35
1	C	231/279 (83%)	203 (88%)	28 (12%)	5	16
1	D	231/279 (83%)	208 (90%)	23 (10%)	7	24
1	E	237/279 (85%)	216 (91%)	21 (9%)	9	28
1	F	233/279 (84%)	217 (93%)	16 (7%)	14	41
1	G	237/279 (85%)	221 (93%)	16 (7%)	14	42
1	H	235/279 (84%)	221 (94%)	14 (6%)	17	47
1	I	232/279 (83%)	211 (91%)	21 (9%)	9	28
1	J	237/279 (85%)	220 (93%)	17 (7%)	13	39
1	K	237/279 (85%)	215 (91%)	22 (9%)	8	27
1	L	234/279 (84%)	213 (91%)	21 (9%)	9	28
1	M	227/279 (81%)	211 (93%)	16 (7%)	14	40
1	N	222/279 (80%)	200 (90%)	22 (10%)	7	24
1	O	234/279 (84%)	211 (90%)	23 (10%)	7	25
1	P	230/279 (82%)	208 (90%)	22 (10%)	8	26
All	All	3720/4464 (83%)	3402 (92%)	318 (8%)	10	31

All (318) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU

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Mol	Chain	Res	Type
1	A	25	SER
1	A	29	SER
1	A	36	ARG
1	A	44	VAL
1	A	64	LEU
1	A	94	VAL
1	A	139	THR
1	A	142	LEU
1	A	150	GLN
1	A	197	ASN
1	A	199	GLU
1	A	227	GLN
1	A	232	VAL
1	A	262	ARG
1	A	268	LEU
1	A	294	LEU
1	A	300	ILE
1	B	18	LEU
1	B	21	LEU
1	B	31	THR
1	B	36	ARG
1	B	46	VAL
1	B	63	VAL
1	B	64	LEU
1	B	94	VAL
1	B	142	LEU
1	B	197	ASN
1	B	218	ILE
1	B	227	GLN
1	B	231	ASP
1	B	258	ASP
1	B	268	LEU
1	B	289	GLU
1	B	296	THR
1	B	307	ILE
1	C	6	ILE
1	C	21	LEU
1	C	25	SER
1	C	36	ARG
1	C	46	VAL
1	C	62	ASP
1	C	63	VAL

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Mol	Chain	Res	Type
1	C	64	LEU
1	C	106	LEU
1	C	115	ASP
1	C	120	LEU
1	C	150	GLN
1	C	190	ILE
1	C	197	ASN
1	C	210	HIS
1	C	217	VAL
1	C	227	GLN
1	C	231	ASP
1	C	232	VAL
1	C	258	ASP
1	C	262	ARG
1	C	268	LEU
1	C	289	GLU
1	C	294	LEU
1	C	297	PHE
1	C	300	ILE
1	C	307	ILE
1	C	309	LEU
1	D	21	LEU
1	D	31	THR
1	D	36	ARG
1	D	41	ARG
1	D	58	SER
1	D	64	LEU
1	D	94	VAL
1	D	142	LEU
1	D	196	GLU
1	D	197	ASN
1	D	227	GLN
1	D	236	LEU
1	D	258	ASP
1	D	262	ARG
1	D	267	SER
1	D	268	LEU
1	D	284	LEU
1	D	293	VAL
1	D	294	LEU
1	D	296	THR
1	D	298	GLU

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Mol	Chain	Res	Type
1	D	300	ILE
1	D	307	ILE
1	E	21	LEU
1	E	25	SER
1	E	29	SER
1	E	36	ARG
1	E	59	GLU
1	E	65	ARG
1	E	76	SER
1	E	142	LEU
1	E	199	GLU
1	E	214	SER
1	E	226	LYS
1	E	242	VAL
1	E	255	LEU
1	E	258	ASP
1	E	262	ARG
1	E	267	SER
1	E	268	LEU
1	E	285	LYS
1	E	294	LEU
1	E	298	GLU
1	E	299	GLU
1	F	21	LEU
1	F	29	SER
1	F	32	VAL
1	F	64	LEU
1	F	87	GLU
1	F	115	ASP
1	F	132	VAL
1	F	142	LEU
1	F	148	LYS
1	F	226	LYS
1	F	236	LEU
1	F	255	LEU
1	F	258	ASP
1	F	268	LEU
1	F	289	GLU
1	F	294	LEU
1	G	20	ASP
1	G	29	SER
1	G	60	ARG

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Mol	Chain	Res	Type
1	G	64	LEU
1	G	74	ARG
1	G	115	ASP
1	G	142	LEU
1	G	143	LEU
1	G	198	TYR
1	G	227	GLN
1	G	236	LEU
1	G	258	ASP
1	G	267	SER
1	G	268	LEU
1	G	298	GLU
1	G	307	ILE
1	H	21	LEU
1	H	29	SER
1	H	36	ARG
1	H	64	LEU
1	H	142	LEU
1	H	150	GLN
1	H	227	GLN
1	H	236	LEU
1	H	258	ASP
1	H	262	ARG
1	H	268	LEU
1	H	289	GLU
1	H	294	LEU
1	H	295	ARG
1	I	21	LEU
1	I	22	ARG
1	I	25	SER
1	I	64	LEU
1	I	70	LEU
1	I	142	LEU
1	I	150	GLN
1	I	189	THR
1	I	190	ILE
1	I	197	ASN
1	I	227	GLN
1	I	231	ASP
1	I	232	VAL
1	I	236	LEU
1	I	241	SER

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Mol	Chain	Res	Type
1	I	258	ASP
1	I	262	ARG
1	I	268	LEU
1	I	289	GLU
1	I	294	LEU
1	I	295	ARG
1	J	20	ASP
1	J	21	LEU
1	J	29	SER
1	J	59	GLU
1	J	64	LEU
1	J	74	ARG
1	J	116	VAL
1	J	125	LEU
1	J	132	VAL
1	J	142	LEU
1	J	197	ASN
1	J	199	GLU
1	J	227	GLN
1	J	259	ILE
1	J	262	ARG
1	J	268	LEU
1	J	301	THR
1	K	24	LEU
1	K	25	SER
1	K	31	THR
1	K	41	ARG
1	K	58	SER
1	K	59	GLU
1	K	63	VAL
1	K	64	LEU
1	K	142	LEU
1	K	150	GLN
1	K	197	ASN
1	K	227	GLN
1	K	236	LEU
1	K	258	ASP
1	K	262	ARG
1	K	267	SER
1	K	268	LEU
1	K	288	ILE
1	K	293	VAL

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Mol	Chain	Res	Type
1	K	294	LEU
1	K	299	GLU
1	K	307	ILE
1	L	21	LEU
1	L	25	SER
1	L	29	SER
1	L	106	LEU
1	L	115	ASP
1	L	123	ARG
1	L	142	LEU
1	L	190	ILE
1	L	223	LEU
1	L	227	GLN
1	L	236	LEU
1	L	243	SER
1	L	258	ASP
1	L	262	ARG
1	L	268	LEU
1	L	289	GLU
1	L	295	ARG
1	L	297	PHE
1	L	300	ILE
1	L	301	THR
1	L	307	ILE
1	M	21	LEU
1	M	41	ARG
1	M	59	GLU
1	M	115	ASP
1	M	124	ILE
1	M	142	LEU
1	M	197	ASN
1	M	217	VAL
1	M	227	GLN
1	M	236	LEU
1	M	267	SER
1	M	268	LEU
1	M	289	GLU
1	M	294	LEU
1	M	299	GLU
1	M	307	ILE
1	N	21	LEU
1	N	31	THR

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Mol	Chain	Res	Type
1	N	62	ASP
1	N	63	VAL
1	N	64	LEU
1	N	65	ARG
1	N	120	LEU
1	N	124	ILE
1	N	142	LEU
1	N	150	GLN
1	N	153	LEU
1	N	160	VAL
1	N	197	ASN
1	N	209	LYS
1	N	217	VAL
1	N	227	GLN
1	N	238	ILE
1	N	284	LEU
1	N	289	GLU
1	N	294	LEU
1	N	296	THR
1	N	307	ILE
1	O	17	LYS
1	O	21	LEU
1	O	25	SER
1	O	64	LEU
1	O	93	ILE
1	O	105	GLU
1	O	142	LEU
1	O	147	LEU
1	O	150	GLN
1	O	197	ASN
1	O	214	SER
1	O	219	THR
1	O	226	LYS
1	O	227	GLN
1	O	236	LEU
1	O	258	ASP
1	O	266	ILE
1	O	267	SER
1	O	268	LEU
1	O	285	LYS
1	O	289	GLU
1	O	294	LEU

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Mol	Chain	Res	Type
1	O	299	GLU
1	P	21	LEU
1	P	25	SER
1	P	29	SER
1	P	31	THR
1	P	60	ARG
1	P	62	ASP
1	P	64	LEU
1	P	76	SER
1	P	94	VAL
1	P	120	LEU
1	P	142	LEU
1	P	196	GLU
1	P	197	ASN
1	P	217	VAL
1	P	225	ARG
1	P	227	GLN
1	P	257	TYR
1	P	268	LEU
1	P	282	SER
1	P	284	LEU
1	P	294	LEU
1	P	304	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	150	GLN
1	A	156	ASN
1	B	48	HIS
1	C	210	HIS
1	C	237	GLN
1	C	244	GLN
1	D	108	HIS
1	D	126	HIS
1	D	151	ASN
1	D	156	ASN
1	D	227	GLN
1	D	261	HIS
1	E	104	ASN
1	F	48	HIS

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Mol	Chain	Res	Type
1	F	151	ASN
1	F	156	ASN
1	F	197	ASN
1	G	108	HIS
1	G	156	ASN
1	G	210	HIS
1	G	227	GLN
1	G	244	GLN
1	H	16	HIS
1	H	104	ASN
1	H	150	GLN
1	I	104	ASN
1	I	150	GLN
1	I	156	ASN
1	I	244	GLN
1	J	100	ASN
1	J	156	ASN
1	J	244	GLN
1	J	308	GLN
1	K	104	ASN
1	K	126	HIS
1	K	145	HIS
1	K	150	GLN
1	K	156	ASN
1	L	43	GLN
1	L	133	ASN
1	L	145	HIS
1	M	43	GLN
1	M	108	HIS
1	M	137	ASN
1	M	227	GLN
1	N	108	HIS
1	N	150	GLN
1	N	227	GLN
1	N	237	GLN
1	O	151	ASN
1	O	156	ASN
1	P	16	HIS
1	P	197	ASN
1	P	261	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	9XA	B	401	-	34,37,37	2.49	12 (35%)	47,56,56	3.09	21 (44%)
2	9XA	C	401	-	34,37,37	3.06	10 (29%)	47,56,56	3.30	22 (46%)
2	9XA	J	401	-	34,37,37	2.60	12 (35%)	47,56,56	3.14	21 (44%)
2	9XA	I	401	-	34,37,37	2.67	11 (32%)	47,56,56	3.05	23 (48%)
2	9XA	O	401	-	34,37,37	2.47	11 (32%)	47,56,56	2.96	20 (42%)
2	9XA	P	401	-	34,37,37	2.51	11 (32%)	47,56,56	2.90	19 (40%)
2	9XA	K	401	-	34,37,37	2.50	10 (29%)	47,56,56	2.86	18 (38%)
2	9XA	F	401	-	34,37,37	2.56	10 (29%)	47,56,56	3.27	21 (44%)
2	9XA	A	401	-	34,37,37	2.55	10 (29%)	47,56,56	3.21	22 (46%)
2	9XA	L	401	-	34,37,37	2.52	9 (26%)	47,56,56	2.87	19 (40%)
2	9XA	N	401	-	34,37,37	2.54	9 (26%)	47,56,56	2.94	20 (42%)
2	9XA	E	401	-	34,37,37	2.62	12 (35%)	47,56,56	2.95	22 (46%)
2	9XA	G	401	-	34,37,37	2.52	11 (32%)	47,56,56	3.03	19 (40%)
2	9XA	D	401	-	34,37,37	2.51	12 (35%)	47,56,56	2.87	20 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9XA	M	401	-	34,37,37	2.53	10 (29%)	47,56,56	2.98	22 (46%)
2	9XA	H	401	-	34,37,37	2.69	13 (38%)	47,56,56	2.92	18 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9XA	B	401	-	-	4/23/35/35	0/4/4/4
2	9XA	C	401	-	-	13/23/35/35	0/4/4/4
2	9XA	J	401	-	-	2/23/35/35	0/4/4/4
2	9XA	I	401	-	-	2/23/35/35	0/4/4/4
2	9XA	O	401	-	-	3/23/35/35	0/4/4/4
2	9XA	P	401	-	-	1/23/35/35	0/4/4/4
2	9XA	K	401	-	-	2/23/35/35	0/4/4/4
2	9XA	F	401	-	-	6/23/35/35	0/4/4/4
2	9XA	A	401	-	-	1/23/35/35	0/4/4/4
2	9XA	L	401	-	-	2/23/35/35	0/4/4/4
2	9XA	N	401	-	-	2/23/35/35	0/4/4/4
2	9XA	E	401	-	-	2/23/35/35	0/4/4/4
2	9XA	G	401	-	-	2/23/35/35	0/4/4/4
2	9XA	D	401	-	-	2/23/35/35	0/4/4/4
2	9XA	M	401	-	-	2/23/35/35	0/4/4/4
2	9XA	H	401	-	-	2/23/35/35	0/4/4/4

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	9XA	C2-N1	-8.52	1.27	1.39
2	C	401	9XA	C7-N1	-8.16	1.30	1.39
2	C	401	9XA	C2-N9	-7.45	1.23	1.33
2	H	401	9XA	C2-N1	-7.19	1.29	1.39
2	I	401	9XA	C2-N1	-7.19	1.29	1.39
2	K	401	9XA	C2-N1	-6.99	1.29	1.39
2	D	401	9XA	C2-N1	-6.93	1.29	1.39
2	H	401	9XA	C7-N1	-6.79	1.32	1.39
2	L	401	9XA	C2-N1	-6.73	1.29	1.39
2	L	401	9XA	C7-N1	-6.71	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	9XA	C2-N9	-6.67	1.24	1.33
2	I	401	9XA	C7-N1	-6.61	1.32	1.39
2	P	401	9XA	C2-N9	-6.55	1.24	1.33
2	B	401	9XA	C2-N1	-6.49	1.30	1.39
2	F	401	9XA	C2-N1	-6.45	1.30	1.39
2	I	401	9XA	C2-N9	-6.41	1.24	1.33
2	J	401	9XA	C2-N9	-6.36	1.25	1.33
2	E	401	9XA	C2-N1	-6.31	1.30	1.39
2	K	401	9XA	C7-N1	-6.30	1.32	1.39
2	J	401	9XA	C2-N1	-6.30	1.30	1.39
2	N	401	9XA	C2-N1	-6.29	1.30	1.39
2	F	401	9XA	C2-N9	-6.28	1.25	1.33
2	G	401	9XA	C7-N1	-6.27	1.32	1.39
2	M	401	9XA	C2-N1	-6.27	1.30	1.39
2	G	401	9XA	C2-N9	-6.27	1.25	1.33
2	M	401	9XA	C7-N1	-6.25	1.32	1.39
2	N	401	9XA	C2-N9	-6.25	1.25	1.33
2	B	401	9XA	C2-N9	-6.21	1.25	1.33
2	L	401	9XA	C2-N9	-6.20	1.25	1.33
2	K	401	9XA	C2-N9	-6.20	1.25	1.33
2	D	401	9XA	C7-N1	-6.17	1.32	1.39
2	N	401	9XA	C7-N1	-6.14	1.32	1.39
2	A	401	9XA	C2-N1	-6.12	1.30	1.39
2	J	401	9XA	C7-N1	-6.12	1.32	1.39
2	O	401	9XA	C7-N1	-6.08	1.32	1.39
2	A	401	9XA	C2-N9	-6.08	1.25	1.33
2	O	401	9XA	C2-N1	-6.07	1.30	1.39
2	E	401	9XA	C2-N9	-6.07	1.25	1.33
2	P	401	9XA	C2-N1	-6.04	1.30	1.39
2	G	401	9XA	C2-N1	-6.01	1.30	1.39
2	M	401	9XA	C2-N9	-5.99	1.25	1.33
2	D	401	9XA	C2-N9	-5.98	1.25	1.33
2	O	401	9XA	C2-N9	-5.91	1.25	1.33
2	E	401	9XA	C7-N1	-5.77	1.33	1.39
2	C	401	9XA	C6-N1	-5.70	1.29	1.38
2	A	401	9XA	C7-N1	-5.69	1.33	1.39
2	C	401	9XA	C31-S28	-5.33	1.77	1.82
2	F	401	9XA	C7-N1	-5.33	1.33	1.39
2	P	401	9XA	C7-N1	-5.25	1.33	1.39
2	F	401	9XA	O30-S28	5.01	1.48	1.43
2	B	401	9XA	C7-N1	-4.81	1.34	1.39
2	E	401	9XA	O30-S28	4.38	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	9XA	C6-N1	-4.33	1.31	1.38
2	A	401	9XA	O30-S28	4.25	1.47	1.43
2	E	401	9XA	C6-N1	-4.23	1.31	1.38
2	A	401	9XA	C6-N1	-4.23	1.31	1.38
2	E	401	9XA	O29-S28	4.21	1.47	1.43
2	M	401	9XA	C6-N1	-4.21	1.31	1.38
2	G	401	9XA	C6-N1	-4.18	1.31	1.38
2	O	401	9XA	C6-N1	-4.16	1.32	1.38
2	H	401	9XA	C6-N1	-4.15	1.32	1.38
2	L	401	9XA	C6-N1	-4.14	1.32	1.38
2	K	401	9XA	C6-N1	-4.12	1.32	1.38
2	J	401	9XA	O29-S28	4.12	1.47	1.43
2	F	401	9XA	C6-N1	-4.06	1.32	1.38
2	D	401	9XA	C6-N1	-4.05	1.32	1.38
2	C	401	9XA	C8-C7	-4.04	1.33	1.37
2	N	401	9XA	C6-N1	-4.01	1.32	1.38
2	J	401	9XA	C6-N1	-3.95	1.32	1.38
2	P	401	9XA	C6-N1	-3.94	1.32	1.38
2	B	401	9XA	O29-S28	3.87	1.46	1.43
2	N	401	9XA	O30-S28	3.74	1.46	1.43
2	E	401	9XA	C8-N9	3.59	1.44	1.37
2	A	401	9XA	O29-S28	3.54	1.46	1.43
2	M	401	9XA	O29-S28	3.52	1.46	1.43
2	A	401	9XA	C8-N9	3.51	1.44	1.37
2	H	401	9XA	O30-S28	3.48	1.46	1.43
2	G	401	9XA	O29-S28	3.39	1.46	1.43
2	F	401	9XA	O29-S28	3.38	1.46	1.43
2	B	401	9XA	C14-C7	3.29	1.53	1.48
2	J	401	9XA	C8-N9	3.29	1.43	1.37
2	O	401	9XA	C8-N9	3.29	1.43	1.37
2	M	401	9XA	C8-N9	3.29	1.43	1.37
2	N	401	9XA	O29-S28	3.27	1.46	1.43
2	G	401	9XA	C8-N9	3.27	1.43	1.37
2	P	401	9XA	C14-C7	3.25	1.52	1.48
2	P	401	9XA	O29-S28	3.24	1.46	1.43
2	N	401	9XA	C8-N9	3.23	1.43	1.37
2	P	401	9XA	C8-N9	3.22	1.43	1.37
2	I	401	9XA	O29-S28	3.21	1.46	1.43
2	L	401	9XA	C8-N9	3.13	1.43	1.37
2	D	401	9XA	C8-N9	3.10	1.43	1.37
2	I	401	9XA	C8-N9	3.09	1.43	1.37
2	I	401	9XA	O30-S28	3.08	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	9XA	C8-N9	3.08	1.43	1.37
2	K	401	9XA	C8-N9	3.07	1.43	1.37
2	B	401	9XA	O30-S28	3.05	1.46	1.43
2	H	401	9XA	C8-N9	3.04	1.43	1.37
2	E	401	9XA	C14-C7	3.02	1.52	1.48
2	O	401	9XA	O29-S28	3.02	1.46	1.43
2	B	401	9XA	C3-C2	3.01	1.48	1.41
2	P	401	9XA	O30-S28	2.96	1.46	1.43
2	L	401	9XA	O30-S28	2.94	1.46	1.43
2	H	401	9XA	O29-S28	2.94	1.46	1.43
2	H	401	9XA	C14-C7	2.94	1.52	1.48
2	B	401	9XA	C6-N1	-2.90	1.33	1.38
2	B	401	9XA	C31-S28	2.87	1.85	1.82
2	M	401	9XA	C14-C7	2.87	1.52	1.48
2	J	401	9XA	C8-C7	-2.82	1.34	1.37
2	I	401	9XA	C14-C7	2.82	1.52	1.48
2	O	401	9XA	C3-C2	2.80	1.48	1.41
2	F	401	9XA	C8-N9	2.80	1.42	1.37
2	J	401	9XA	O30-S28	2.80	1.45	1.43
2	D	401	9XA	O29-S28	2.79	1.45	1.43
2	L	401	9XA	C14-C7	2.79	1.52	1.48
2	J	401	9XA	C3-C2	2.78	1.48	1.41
2	C	401	9XA	C8-N9	2.78	1.42	1.37
2	F	401	9XA	C14-C7	2.78	1.52	1.48
2	G	401	9XA	C3-C2	2.77	1.48	1.41
2	O	401	9XA	C14-C7	2.76	1.52	1.48
2	D	401	9XA	C14-C7	2.71	1.52	1.48
2	K	401	9XA	C14-C7	2.69	1.52	1.48
2	O	401	9XA	C31-S28	2.67	1.84	1.82
2	G	401	9XA	C14-C7	2.66	1.52	1.48
2	D	401	9XA	O30-S28	2.66	1.45	1.43
2	M	401	9XA	C3-C2	2.65	1.47	1.41
2	F	401	9XA	C3-C2	2.64	1.47	1.41
2	G	401	9XA	O30-S28	2.64	1.45	1.43
2	E	401	9XA	C3-C2	2.64	1.47	1.41
2	A	401	9XA	C3-C2	2.59	1.47	1.41
2	H	401	9XA	C32-C31	2.52	1.57	1.52
2	B	401	9XA	C8-C7	-2.51	1.35	1.37
2	A	401	9XA	C14-C7	2.51	1.51	1.48
2	P	401	9XA	C3-C2	2.51	1.47	1.41
2	K	401	9XA	O30-S28	2.50	1.45	1.43
2	N	401	9XA	C14-C7	2.50	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	9XA	C3-C2	2.50	1.47	1.41
2	D	401	9XA	C3-C2	2.50	1.47	1.41
2	N	401	9XA	C3-C2	2.46	1.47	1.41
2	O	401	9XA	O30-S28	2.46	1.45	1.43
2	C	401	9XA	C14-C7	2.41	1.51	1.48
2	I	401	9XA	C3-C2	2.40	1.47	1.41
2	M	401	9XA	O30-S28	2.38	1.45	1.43
2	K	401	9XA	C8-C7	-2.37	1.35	1.37
2	L	401	9XA	O29-S28	2.36	1.45	1.43
2	J	401	9XA	C14-C7	2.36	1.51	1.48
2	H	401	9XA	C8-C7	-2.35	1.35	1.37
2	G	401	9XA	C8-C7	-2.32	1.35	1.37
2	I	401	9XA	C32-C31	2.31	1.56	1.52
2	L	401	9XA	C3-C2	2.30	1.47	1.41
2	M	401	9XA	C31-S28	2.29	1.84	1.82
2	H	401	9XA	C3-C2	2.29	1.47	1.41
2	A	401	9XA	C23-N22	2.28	1.37	1.33
2	C	401	9XA	O30-S28	-2.21	1.41	1.43
2	C	401	9XA	C21-N22	-2.19	1.30	1.35
2	K	401	9XA	C32-C31	2.16	1.56	1.52
2	D	401	9XA	C8-C7	-2.14	1.35	1.37
2	D	401	9XA	C32-C31	2.14	1.56	1.52
2	H	401	9XA	C16-N17	2.13	1.51	1.46
2	I	401	9XA	C8-C7	-2.13	1.35	1.37
2	G	401	9XA	C18-N17	2.10	1.51	1.46
2	P	401	9XA	C24-C23	2.09	1.41	1.38
2	P	401	9XA	C31-S28	2.07	1.84	1.82
2	F	401	9XA	C8-C7	-2.05	1.35	1.37
2	H	401	9XA	C33-C31	2.05	1.56	1.52
2	E	401	9XA	C8-C7	-2.04	1.35	1.37
2	O	401	9XA	C33-C31	2.04	1.56	1.52
2	E	401	9XA	C23-N22	2.03	1.37	1.33
2	J	401	9XA	C18-N17	2.02	1.51	1.46
2	J	401	9XA	C24-C23	2.02	1.41	1.38
2	D	401	9XA	C34-C31	2.02	1.56	1.52
2	B	401	9XA	C33-C31	2.02	1.56	1.52
2	E	401	9XA	C24-C23	2.01	1.41	1.38

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	9XA	C7-C8-N9	-11.09	100.45	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	9XA	C7-C8-N9	-10.54	101.03	112.37
2	D	401	9XA	C7-C8-N9	-10.44	101.14	112.37
2	K	401	9XA	C7-C8-N9	-10.30	101.30	112.37
2	A	401	9XA	C7-C8-N9	-10.29	101.31	112.37
2	B	401	9XA	C7-C8-N9	-10.23	101.37	112.37
2	E	401	9XA	C7-C8-N9	-10.23	101.37	112.37
2	H	401	9XA	C7-C8-N9	-10.20	101.41	112.37
2	L	401	9XA	C7-C8-N9	-9.95	101.67	112.37
2	O	401	9XA	C7-C8-N9	-9.90	101.73	112.37
2	J	401	9XA	C7-C8-N9	-9.87	101.76	112.37
2	C	401	9XA	C7-C8-N9	-9.78	101.85	112.37
2	N	401	9XA	C7-C8-N9	-9.77	101.86	112.37
2	M	401	9XA	C7-C8-N9	-9.76	101.88	112.37
2	P	401	9XA	C7-C8-N9	-9.56	102.10	112.37
2	G	401	9XA	C7-C8-N9	-9.53	102.12	112.37
2	C	401	9XA	C24-C23-CL25	9.19	130.73	118.92
2	F	401	9XA	C8-N9-C2	8.44	110.75	105.11
2	A	401	9XA	C23-N22-C21	8.32	122.58	116.70
2	B	401	9XA	C8-N9-C2	8.21	110.59	105.11
2	M	401	9XA	C23-N22-C21	8.13	122.45	116.70
2	A	401	9XA	C8-N9-C2	7.70	110.25	105.11
2	I	401	9XA	C23-N22-C21	7.53	122.03	116.70
2	O	401	9XA	C23-N22-C21	7.51	122.01	116.70
2	J	401	9XA	C18-N17-C16	7.46	121.42	109.54
2	F	401	9XA	C23-N22-C21	7.42	121.95	116.70
2	P	401	9XA	C23-N22-C21	7.28	121.85	116.70
2	E	401	9XA	C8-N9-C2	7.26	109.95	105.11
2	N	401	9XA	C23-N22-C21	7.14	121.75	116.70
2	E	401	9XA	C23-N22-C21	7.11	121.72	116.70
2	G	401	9XA	C18-N17-C16	7.07	120.80	109.54
2	I	401	9XA	C8-N9-C2	7.02	109.80	105.11
2	K	401	9XA	C8-N9-C2	6.94	109.75	105.11
2	J	401	9XA	C23-N22-C21	6.82	121.52	116.70
2	H	401	9XA	C8-N9-C2	6.77	109.63	105.11
2	J	401	9XA	C8-N9-C2	6.67	109.56	105.11
2	D	401	9XA	C8-N9-C2	6.67	109.56	105.11
2	L	401	9XA	C23-N22-C21	6.66	121.41	116.70
2	H	401	9XA	C23-N22-C21	6.57	121.34	116.70
2	O	401	9XA	C8-N9-C2	6.56	109.49	105.11
2	D	401	9XA	C23-N22-C21	6.54	121.33	116.70
2	C	401	9XA	C24-C14-C7	6.50	133.32	120.64
2	P	401	9XA	C8-N9-C2	6.47	109.43	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	9XA	C23-N22-C21	6.42	121.24	116.70
2	G	401	9XA	C8-N9-C2	6.26	109.29	105.11
2	B	401	9XA	C23-N22-C21	6.26	121.13	116.70
2	M	401	9XA	C8-N9-C2	6.24	109.28	105.11
2	G	401	9XA	C23-N22-C21	6.06	120.98	116.70
2	N	401	9XA	C8-N9-C2	5.97	109.10	105.11
2	L	401	9XA	C8-N9-C2	5.94	109.07	105.11
2	A	401	9XA	C24-C23-N22	-5.92	118.75	125.47
2	H	401	9XA	C18-N17-C16	5.88	118.90	109.54
2	F	401	9XA	C14-C7-C8	-5.80	118.83	129.36
2	N	401	9XA	C12-N13-C19	5.80	126.69	111.24
2	M	401	9XA	C18-N17-C16	5.60	118.46	109.54
2	C	401	9XA	C14-C20-C21	5.59	123.04	117.35
2	C	401	9XA	C8-N9-C2	5.42	108.73	105.11
2	C	401	9XA	C23-N22-C21	5.40	120.52	116.70
2	O	401	9XA	C18-N17-C16	5.38	118.11	109.54
2	P	401	9XA	C14-C7-C8	-5.34	119.68	129.36
2	C	401	9XA	C20-C14-C7	-5.28	110.35	120.64
2	B	401	9XA	C14-C7-C8	-5.15	120.02	129.36
2	F	401	9XA	O30-S28-C31	-5.14	104.26	108.54
2	C	401	9XA	C7-N1-C2	5.10	109.40	106.91
2	D	401	9XA	C14-C7-C8	-4.99	120.30	129.36
2	C	401	9XA	CL25-C23-N22	-4.94	104.98	115.45
2	N	401	9XA	C14-C7-C8	-4.81	120.64	129.36
2	L	401	9XA	C18-N17-C16	4.80	117.18	109.54
2	K	401	9XA	C14-C7-C8	-4.79	120.67	129.36
2	J	401	9XA	C14-C7-C8	-4.77	120.72	129.36
2	I	401	9XA	C14-C7-C8	-4.76	120.73	129.36
2	M	401	9XA	C24-C23-N22	-4.62	120.23	125.47
2	L	401	9XA	C14-C7-C8	-4.57	121.06	129.36
2	A	401	9XA	C14-C7-C8	-4.57	121.07	129.36
2	P	401	9XA	C14-C7-N1	4.55	130.71	124.45
2	E	401	9XA	C14-C7-C8	-4.54	121.12	129.36
2	H	401	9XA	C14-C7-C8	-4.54	121.13	129.36
2	G	401	9XA	C14-C7-C8	-4.50	121.19	129.36
2	B	401	9XA	C18-N17-C16	4.49	116.69	109.54
2	O	401	9XA	C14-C7-C8	-4.45	121.30	129.36
2	D	401	9XA	C24-C23-N22	-4.44	120.43	125.47
2	N	401	9XA	C24-C23-N22	-4.42	120.45	125.47
2	O	401	9XA	C24-C23-N22	-4.40	120.48	125.47
2	M	401	9XA	C14-C7-C8	-4.39	121.40	129.36
2	K	401	9XA	C24-C23-N22	-4.33	120.56	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	9XA	C7-N1-C2	4.33	109.02	106.91
2	A	401	9XA	C12-N13-C15	4.28	122.63	111.24
2	F	401	9XA	C14-C7-N1	4.23	130.28	124.45
2	N	401	9XA	C19-N13-C15	4.21	117.91	108.84
2	G	401	9XA	C19-C18-N17	4.21	117.62	110.86
2	J	401	9XA	C24-C23-N22	-4.19	120.71	125.47
2	F	401	9XA	C12-N13-C19	4.18	122.38	111.24
2	L	401	9XA	C24-C23-N22	-4.18	120.73	125.47
2	P	401	9XA	C24-C23-N22	-4.17	120.74	125.47
2	E	401	9XA	C24-C23-N22	-4.17	120.74	125.47
2	B	401	9XA	C14-C7-N1	4.15	130.16	124.45
2	B	401	9XA	C19-N13-C15	4.14	117.76	108.84
2	L	401	9XA	O30-S28-O29	-4.13	114.44	120.28
2	F	401	9XA	C8-C7-N1	4.06	110.84	104.53
2	E	401	9XA	C7-N1-C2	4.06	108.89	106.91
2	G	401	9XA	C27-N17-C18	4.05	118.36	110.63
2	K	401	9XA	O29-S28-C31	-4.05	105.17	108.54
2	B	401	9XA	O30-S28-C31	-4.00	105.21	108.54
2	H	401	9XA	C7-N1-C2	3.99	108.86	106.91
2	O	401	9XA	O30-S28-O29	-3.97	114.67	120.28
2	P	401	9XA	C18-N17-C16	3.97	115.85	109.54
2	L	401	9XA	C19-N13-C15	3.95	117.34	108.84
2	F	401	9XA	C14-C20-C21	3.88	121.30	117.35
2	B	401	9XA	C24-C23-N22	-3.86	121.09	125.47
2	F	401	9XA	C19-N13-C15	3.85	117.14	108.84
2	B	401	9XA	C14-C20-C21	3.79	121.22	117.35
2	J	401	9XA	O30-S28-O29	-3.78	114.94	120.28
2	H	401	9XA	C24-C23-N22	-3.75	121.21	125.47
2	I	401	9XA	C16-C15-N13	3.75	118.21	110.65
2	D	401	9XA	C8-C7-N1	3.74	110.34	104.53
2	F	401	9XA	C34-C31-S28	3.73	116.07	107.72
2	I	401	9XA	C24-C23-N22	-3.70	121.27	125.47
2	G	401	9XA	C24-C23-N22	-3.68	121.30	125.47
2	M	401	9XA	C7-N1-C2	3.62	108.67	106.91
2	G	401	9XA	C15-C16-N17	3.60	116.64	110.86
2	J	401	9XA	C19-C18-N17	3.60	116.64	110.86
2	I	401	9XA	C19-N13-C15	3.56	116.52	108.84
2	A	401	9XA	C18-N17-C16	3.56	115.21	109.54
2	G	401	9XA	C7-N1-C2	3.55	108.64	106.91
2	H	401	9XA	C14-C20-C21	3.53	120.95	117.35
2	J	401	9XA	C14-C7-N1	3.53	129.31	124.45
2	N	401	9XA	C14-C7-N1	3.53	129.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	9XA	C27-N17-C18	3.50	117.30	110.63
2	D	401	9XA	C19-N13-C15	3.50	116.38	108.84
2	J	401	9XA	C15-C16-N17	3.48	116.45	110.86
2	K	401	9XA	C14-C7-N1	3.48	129.24	124.45
2	I	401	9XA	C8-C7-N1	3.47	109.92	104.53
2	H	401	9XA	C14-C7-N1	3.45	129.20	124.45
2	K	401	9XA	C8-C7-N1	3.45	109.89	104.53
2	I	401	9XA	C7-N1-C2	3.45	108.59	106.91
2	E	401	9XA	C14-C20-C21	3.43	120.85	117.35
2	A	401	9XA	C14-C7-N1	3.42	129.17	124.45
2	D	401	9XA	C14-C7-N1	3.42	129.16	124.45
2	I	401	9XA	C14-C20-C21	3.41	120.83	117.35
2	O	401	9XA	C14-C20-C21	3.38	120.80	117.35
2	E	401	9XA	O30-S28-O29	-3.38	115.51	120.28
2	G	401	9XA	C14-C7-N1	3.37	129.09	124.45
2	A	401	9XA	O30-S28-O29	-3.37	115.52	120.28
2	J	401	9XA	C8-C7-N1	3.36	109.76	104.53
2	A	401	9XA	CL25-C23-N22	3.35	122.56	115.45
2	I	401	9XA	O30-S28-O29	-3.35	115.55	120.28
2	K	401	9XA	C7-N1-C2	3.34	108.54	106.91
2	A	401	9XA	C3-C2-N1	3.33	122.59	118.83
2	I	401	9XA	C14-C7-N1	3.33	129.04	124.45
2	N	401	9XA	C8-C7-N1	3.33	109.71	104.53
2	B	401	9XA	C7-N1-C2	3.33	108.53	106.91
2	M	401	9XA	C14-C20-C21	3.32	120.74	117.35
2	L	401	9XA	C8-C7-N1	3.32	109.69	104.53
2	O	401	9XA	C8-C7-N1	3.32	109.69	104.53
2	E	401	9XA	C14-C7-N1	3.31	129.01	124.45
2	M	401	9XA	C14-C7-N1	3.30	128.99	124.45
2	H	401	9XA	O30-S28-O29	-3.30	115.62	120.28
2	E	401	9XA	C8-C7-N1	3.29	109.64	104.53
2	P	401	9XA	C3-C2-N1	3.28	122.53	118.83
2	J	401	9XA	C7-N1-C2	3.28	108.51	106.91
2	L	401	9XA	C14-C7-N1	3.27	128.96	124.45
2	C	401	9XA	C19-N13-C15	3.27	115.88	108.84
2	B	401	9XA	C8-C7-N1	3.26	109.60	104.53
2	M	401	9XA	O30-S28-O29	-3.24	115.70	120.28
2	H	401	9XA	C8-C7-N1	3.23	109.55	104.53
2	P	401	9XA	C14-C20-C21	3.23	120.64	117.35
2	E	401	9XA	C18-N17-C16	3.20	114.64	109.54
2	A	401	9XA	C8-C7-N1	3.20	109.50	104.53
2	F	401	9XA	C18-N17-C16	3.20	114.63	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	9XA	O30-S28-O29	-3.19	115.77	120.28
2	J	401	9XA	C14-C20-C21	3.19	120.60	117.35
2	D	401	9XA	C18-N17-C16	3.19	114.61	109.54
2	B	401	9XA	O30-S28-O29	-3.17	115.80	120.28
2	O	401	9XA	C7-N1-C2	3.16	108.45	106.91
2	G	401	9XA	C8-C7-N1	3.14	109.41	104.53
2	M	401	9XA	C8-C7-N1	3.14	109.41	104.53
2	G	401	9XA	C14-C20-C21	3.14	120.55	117.35
2	P	401	9XA	O30-S28-O29	-3.13	115.86	120.28
2	O	401	9XA	C14-C7-N1	3.13	128.76	124.45
2	E	401	9XA	C3-C2-N1	3.12	122.35	118.83
2	I	401	9XA	C18-N17-C16	3.12	114.51	109.54
2	P	401	9XA	C19-N13-C15	3.11	115.55	108.84
2	G	401	9XA	O10-C4-C5	3.09	121.43	114.29
2	G	401	9XA	O30-S28-O29	-3.07	115.95	120.28
2	E	401	9XA	C15-C16-N17	-3.06	105.94	110.86
2	K	401	9XA	C18-N17-C16	3.06	114.41	109.54
2	F	401	9XA	C24-C23-N22	-3.05	122.01	125.47
2	C	401	9XA	C3-C2-N1	3.04	122.26	118.83
2	L	401	9XA	C32-C31-S28	3.04	114.53	107.72
2	J	401	9XA	O10-C4-C5	3.03	121.29	114.29
2	L	401	9XA	C7-N1-C2	3.02	108.38	106.91
2	G	401	9XA	C12-N13-C19	3.02	119.27	111.24
2	F	401	9XA	C3-C2-N1	3.00	122.21	118.83
2	D	401	9XA	O10-C4-C5	2.97	121.14	114.29
2	P	401	9XA	C8-C7-N1	2.96	109.13	104.53
2	C	401	9XA	C8-C7-N1	2.95	109.12	104.53
2	J	401	9XA	C3-C2-N1	2.95	122.16	118.83
2	G	401	9XA	C3-C2-N1	2.94	122.15	118.83
2	O	401	9XA	C19-C18-N17	2.94	115.58	110.86
2	D	401	9XA	CL25-C23-N22	2.94	121.69	115.45
2	M	401	9XA	O10-C4-C5	2.91	121.01	114.29
2	C	401	9XA	C34-C31-S28	2.90	114.22	107.72
2	N	401	9XA	CL25-C23-N22	2.89	121.59	115.45
2	O	401	9XA	O10-C4-C5	2.89	120.97	114.29
2	N	401	9XA	C16-C15-N13	2.88	116.45	110.65
2	C	401	9XA	C24-C14-C20	-2.86	116.30	119.65
2	L	401	9XA	O10-C4-C5	2.85	120.86	114.29
2	J	401	9XA	C12-N13-C19	2.83	118.77	111.24
2	K	401	9XA	O10-C4-C5	2.83	120.81	114.29
2	M	401	9XA	C12-N13-C19	2.81	118.74	111.24
2	D	401	9XA	O30-S28-O29	-2.78	116.34	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	9XA	O10-C4-C5	2.78	120.71	114.29
2	B	401	9XA	C34-C31-C33	-2.78	106.02	111.05
2	P	401	9XA	O29-S28-C5	-2.77	106.05	110.85
2	C	401	9XA	C16-C15-N13	2.76	116.22	110.65
2	M	401	9XA	C3-C2-N1	2.75	121.94	118.83
2	E	401	9XA	O10-C4-C5	2.75	120.64	114.29
2	K	401	9XA	CL25-C23-N22	2.74	121.26	115.45
2	A	401	9XA	O10-C4-C5	2.74	120.61	114.29
2	N	401	9XA	O30-S28-O29	-2.73	116.43	120.28
2	H	401	9XA	C3-C2-N1	2.71	121.88	118.83
2	P	401	9XA	C12-N13-C19	2.70	118.44	111.24
2	K	401	9XA	C19-N13-C15	2.70	114.66	108.84
2	I	401	9XA	CL25-C23-N22	2.69	121.16	115.45
2	F	401	9XA	O30-S28-O29	-2.68	116.49	120.28
2	N	401	9XA	O10-C4-C5	2.68	120.48	114.29
2	I	401	9XA	C3-C2-N1	2.67	121.84	118.83
2	F	401	9XA	N26-C21-N22	2.67	120.88	116.59
2	I	401	9XA	O10-C4-C5	2.66	120.44	114.29
2	B	401	9XA	C3-C2-N1	2.66	121.83	118.83
2	C	401	9XA	C27-N17-C16	2.65	115.69	110.63
2	D	401	9XA	C12-N13-C19	2.65	118.30	111.24
2	O	401	9XA	C3-C2-N1	2.64	121.80	118.83
2	K	401	9XA	C3-C2-N1	2.63	121.79	118.83
2	D	401	9XA	C14-C20-C21	2.62	120.02	117.35
2	N	401	9XA	C3-C2-N1	2.62	121.78	118.83
2	L	401	9XA	C14-C20-C21	2.62	120.02	117.35
2	C	401	9XA	O30-S28-C31	-2.61	106.37	108.54
2	D	401	9XA	C34-C31-S28	2.59	113.53	107.72
2	E	401	9XA	C19-N13-C15	2.59	114.42	108.84
2	C	401	9XA	O30-S28-O29	-2.58	116.64	120.28
2	J	401	9XA	C27-N17-C16	2.56	115.51	110.63
2	A	401	9XA	C27-N17-C18	2.56	115.51	110.63
2	A	401	9XA	C19-N13-C15	2.54	114.32	108.84
2	P	401	9XA	C7-N1-C2	2.54	108.15	106.91
2	F	401	9XA	C27-N17-C18	2.52	115.44	110.63
2	M	401	9XA	C15-C16-N17	2.50	114.88	110.86
2	E	401	9XA	CL25-C23-N22	2.49	120.74	115.45
2	A	401	9XA	C14-C20-C21	2.48	119.88	117.35
2	L	401	9XA	O29-S28-C31	-2.48	106.47	108.54
2	C	401	9XA	O29-S28-C31	-2.48	106.48	108.54
2	D	401	9XA	C27-N17-C18	2.47	115.35	110.63
2	O	401	9XA	C15-C16-N17	2.47	114.82	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	9XA	C14-C7-C8	-2.46	124.90	129.36
2	N	401	9XA	C27-N17-C18	2.44	115.28	110.63
2	A	401	9XA	C15-C16-N17	-2.44	106.94	110.86
2	B	401	9XA	C27-N17-C18	2.44	115.27	110.63
2	I	401	9XA	C27-N17-C16	2.43	115.27	110.63
2	N	401	9XA	C7-N1-C2	2.43	108.10	106.91
2	P	401	9XA	O10-C4-C5	2.43	119.89	114.29
2	A	401	9XA	C11-O10-C4	2.42	124.15	117.58
2	L	401	9XA	C15-C16-N17	2.42	114.74	110.86
2	F	401	9XA	C34-C31-C33	-2.42	106.68	111.05
2	D	401	9XA	C3-C2-N1	2.41	121.55	118.83
2	J	401	9XA	N26-C21-N22	2.40	120.45	116.59
2	I	401	9XA	C32-C31-S28	2.40	113.10	107.72
2	I	401	9XA	C12-N13-C19	2.39	117.62	111.24
2	H	401	9XA	CL25-C23-N22	2.39	120.52	115.45
2	P	401	9XA	C33-C31-C32	-2.38	106.75	111.05
2	A	401	9XA	C32-C31-S28	2.38	113.04	107.72
2	B	401	9XA	C16-C15-N13	2.37	115.44	110.65
2	O	401	9XA	N26-C21-N22	2.37	120.41	116.59
2	O	401	9XA	C32-C31-S28	2.37	113.03	107.72
2	N	401	9XA	C14-C20-C21	2.37	119.77	117.35
2	H	401	9XA	C32-C31-S28	2.36	113.01	107.72
2	M	401	9XA	N26-C21-N22	2.34	120.36	116.59
2	M	401	9XA	CL25-C23-N22	2.34	120.42	115.45
2	A	401	9XA	C27-N17-C16	2.34	115.09	110.63
2	L	401	9XA	C3-C2-N1	2.33	121.46	118.83
2	F	401	9XA	CL25-C23-N22	2.33	120.40	115.45
2	C	401	9XA	O29-S28-C5	2.33	114.87	110.85
2	D	401	9XA	N26-C21-N22	2.33	120.33	116.59
2	E	401	9XA	C27-N17-C18	2.30	115.01	110.63
2	B	401	9XA	C34-C31-S28	2.28	112.83	107.72
2	I	401	9XA	C27-N17-C18	2.27	114.97	110.63
2	M	401	9XA	C11-O10-C4	2.27	123.75	117.58
2	B	401	9XA	O10-C4-C5	2.26	119.52	114.29
2	O	401	9XA	CL25-C23-N22	2.24	120.21	115.45
2	O	401	9XA	C11-O10-C4	2.23	123.65	117.58
2	E	401	9XA	C27-N17-C16	2.23	114.89	110.63
2	E	401	9XA	C34-C31-S28	2.22	112.70	107.72
2	H	401	9XA	C34-C31-C33	-2.22	107.04	111.05
2	E	401	9XA	C11-O10-C4	2.21	123.59	117.58
2	C	401	9XA	C12-N13-C19	2.21	117.13	111.24
2	A	401	9XA	N26-C21-N22	2.21	120.14	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	9XA	C24-C14-C20	-2.20	117.08	119.65
2	D	401	9XA	C7-N1-C2	2.20	107.98	106.91
2	B	401	9XA	C18-C19-N13	2.19	115.07	110.65
2	G	401	9XA	C11-O10-C4	2.19	123.53	117.58
2	P	401	9XA	C11-O10-C4	2.18	123.50	117.58
2	M	401	9XA	C34-C31-S28	2.18	112.59	107.72
2	P	401	9XA	C19-C18-N17	2.17	114.34	110.86
2	K	401	9XA	C11-O10-C4	2.17	123.47	117.58
2	E	401	9XA	C34-C31-C33	-2.15	107.17	111.05
2	I	401	9XA	C18-C19-N13	2.15	114.98	110.65
2	N	401	9XA	O29-S28-C31	-2.14	106.76	108.54
2	M	401	9XA	C19-C18-N17	2.14	114.29	110.86
2	J	401	9XA	C11-O10-C4	2.14	123.39	117.58
2	M	401	9XA	C32-C31-S28	2.13	112.50	107.72
2	N	401	9XA	N26-C21-N22	2.13	120.01	116.59
2	E	401	9XA	C32-C31-S28	2.13	112.48	107.72
2	K	401	9XA	C14-C20-C21	2.10	119.49	117.35
2	I	401	9XA	C11-O10-C4	2.10	123.28	117.58
2	H	401	9XA	C15-C16-N17	2.09	114.22	110.86
2	D	401	9XA	C11-O10-C4	2.08	123.24	117.58
2	N	401	9XA	C32-C31-S28	2.08	112.38	107.72
2	L	401	9XA	O30-S28-C31	2.07	110.27	108.54
2	K	401	9XA	N26-C21-N22	2.07	119.92	116.59
2	H	401	9XA	C27-N17-C16	2.07	114.58	110.63
2	M	401	9XA	C19-N13-C15	2.07	113.29	108.84
2	O	401	9XA	C34-C31-S28	2.06	112.34	107.72
2	F	401	9XA	O10-C4-C5	2.05	119.03	114.29
2	G	401	9XA	O30-S28-C31	-2.03	106.85	108.54
2	L	401	9XA	C18-C19-N13	2.03	114.74	110.65
2	J	401	9XA	C19-N13-C15	2.02	113.19	108.84
2	F	401	9XA	C27-N17-C16	2.01	114.47	110.63
2	I	401	9XA	O29-S28-C31	-2.00	106.87	108.54

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	9XA	C32-C31-S28-C5
2	C	401	9XA	C33-C31-S28-C5
2	C	401	9XA	C34-C31-S28-C5
2	C	401	9XA	C32-C31-S28-O29
2	C	401	9XA	C33-C31-S28-O29

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Mol	Chain	Res	Type	Atoms
2	C	401	9XA	C34-C31-S28-O29
2	C	401	9XA	C32-C31-S28-O30
2	C	401	9XA	C33-C31-S28-O30
2	C	401	9XA	C34-C31-S28-O30
2	F	401	9XA	C11-C12-N13-C19
2	F	401	9XA	C4-C5-S28-O30
2	F	401	9XA	C6-C5-S28-O30
2	N	401	9XA	C11-C12-N13-C19
2	O	401	9XA	O10-C11-C12-N13
2	C	401	9XA	C12-C11-O10-C4
2	C	401	9XA	O10-C11-C12-N13
2	G	401	9XA	C11-C12-N13-C19
2	J	401	9XA	C11-C12-N13-C19
2	K	401	9XA	C11-C12-N13-C19
2	L	401	9XA	C11-C12-N13-C15
2	F	401	9XA	C11-C12-N13-C15
2	I	401	9XA	C11-C12-N13-C19
2	M	401	9XA	C11-C12-N13-C19
2	F	401	9XA	C3-C4-O10-C11
2	D	401	9XA	C11-C12-N13-C19
2	F	401	9XA	C5-C4-O10-C11
2	O	401	9XA	C11-C12-N13-C15
2	B	401	9XA	C3-C4-O10-C11
2	P	401	9XA	O10-C11-C12-N13
2	B	401	9XA	C5-C4-O10-C11
2	E	401	9XA	C11-C12-N13-C19
2	H	401	9XA	C11-C12-N13-C19
2	O	401	9XA	C11-C12-N13-C19
2	C	401	9XA	C3-C4-O10-C11
2	B	401	9XA	C11-C12-N13-C15
2	D	401	9XA	C11-C12-N13-C15
2	L	401	9XA	C11-C12-N13-C19
2	B	401	9XA	C12-C11-O10-C4
2	H	401	9XA	C11-C12-N13-C15
2	K	401	9XA	C11-C12-N13-C15
2	C	401	9XA	C5-C4-O10-C11
2	E	401	9XA	C11-C12-N13-C15
2	M	401	9XA	C11-C12-N13-C15
2	G	401	9XA	C11-C12-N13-C15
2	J	401	9XA	C11-C12-N13-C15
2	A	401	9XA	C11-C12-N13-C19
2	I	401	9XA	C11-C12-N13-C15

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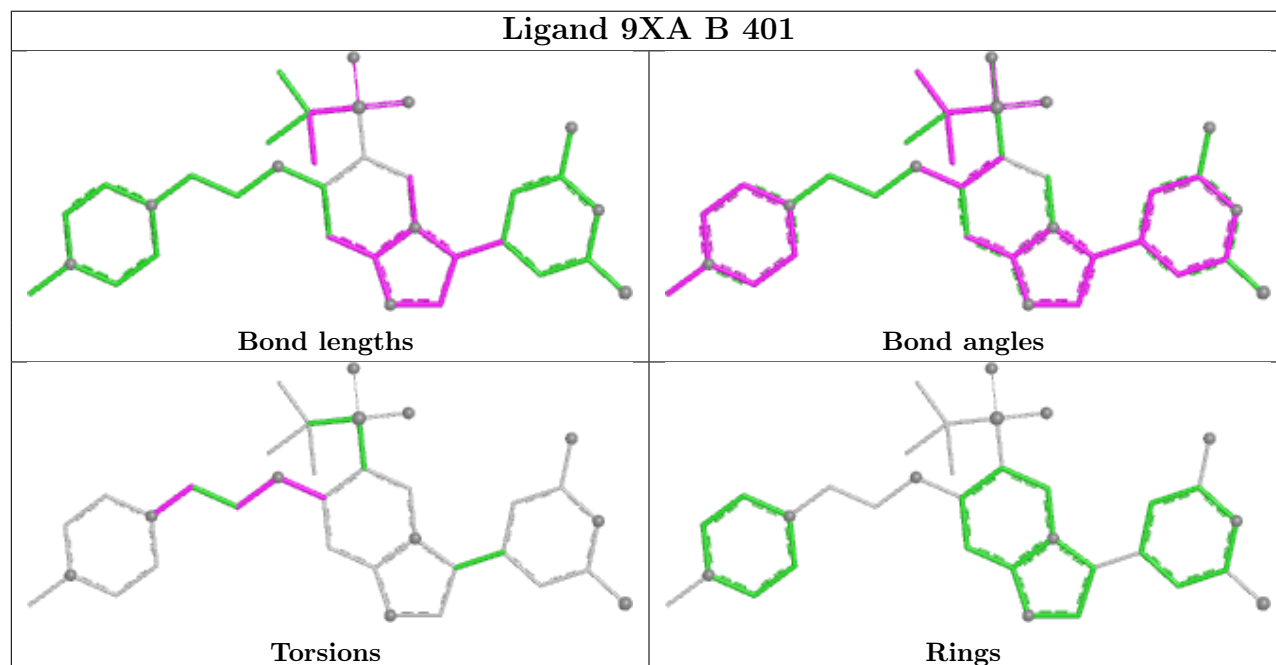
Mol	Chain	Res	Type	Atoms
2	N	401	9XA	C11-C12-N13-C15

There are no ring outliers.

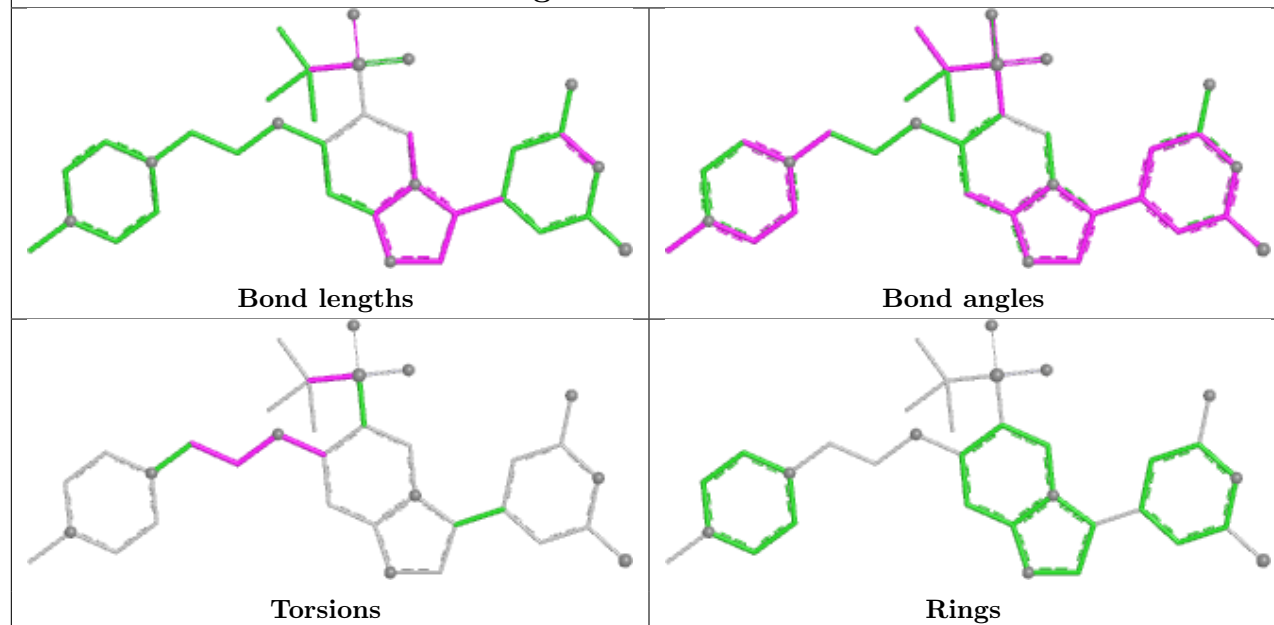
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	9XA	2	0
2	C	401	9XA	5	0
2	K	401	9XA	1	0
2	F	401	9XA	1	0
2	D	401	9XA	2	0
2	M	401	9XA	1	0

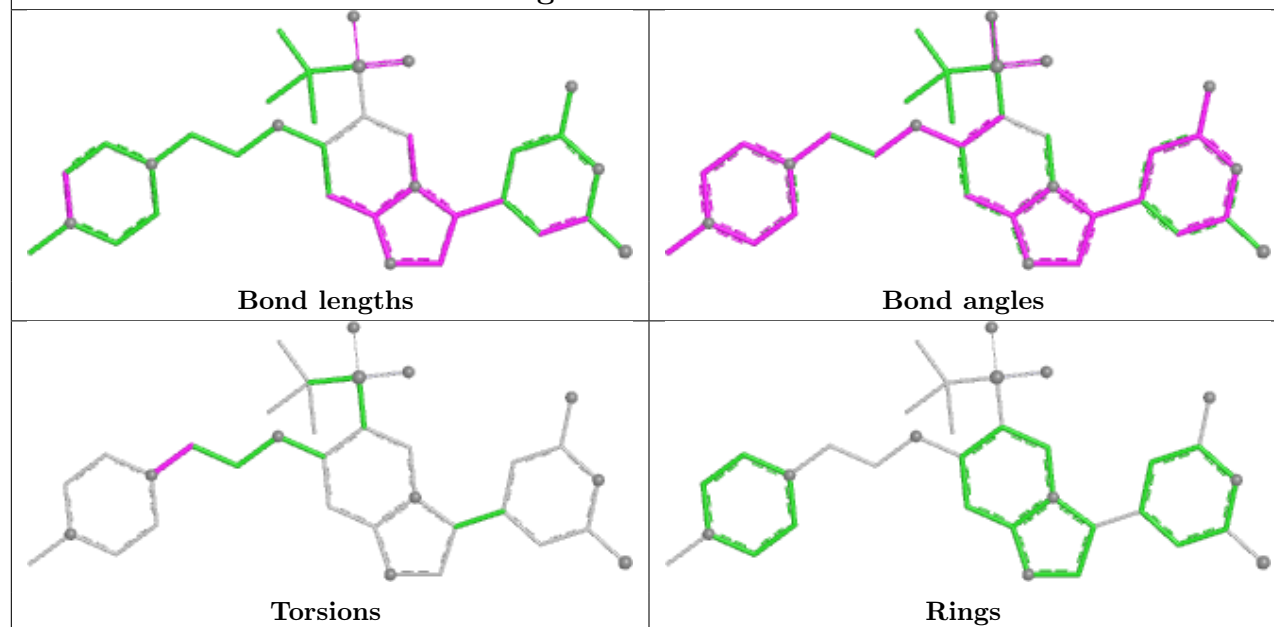
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



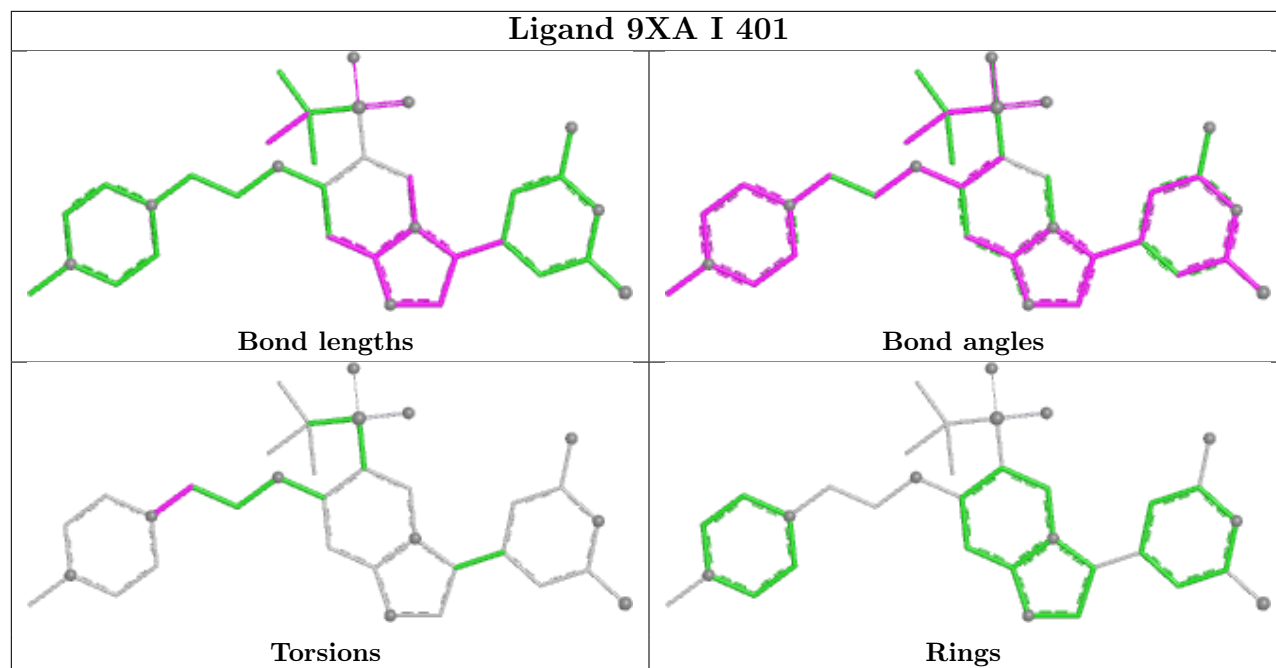
Ligand 9XA C 401



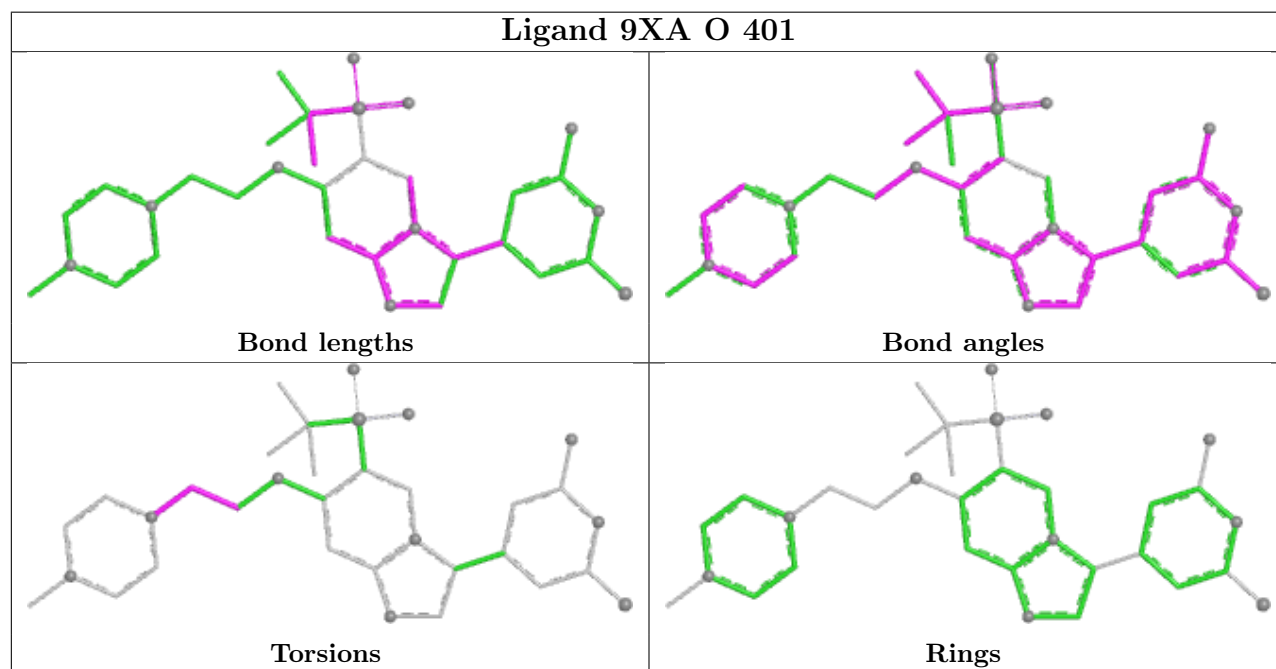
Ligand 9XA J 401



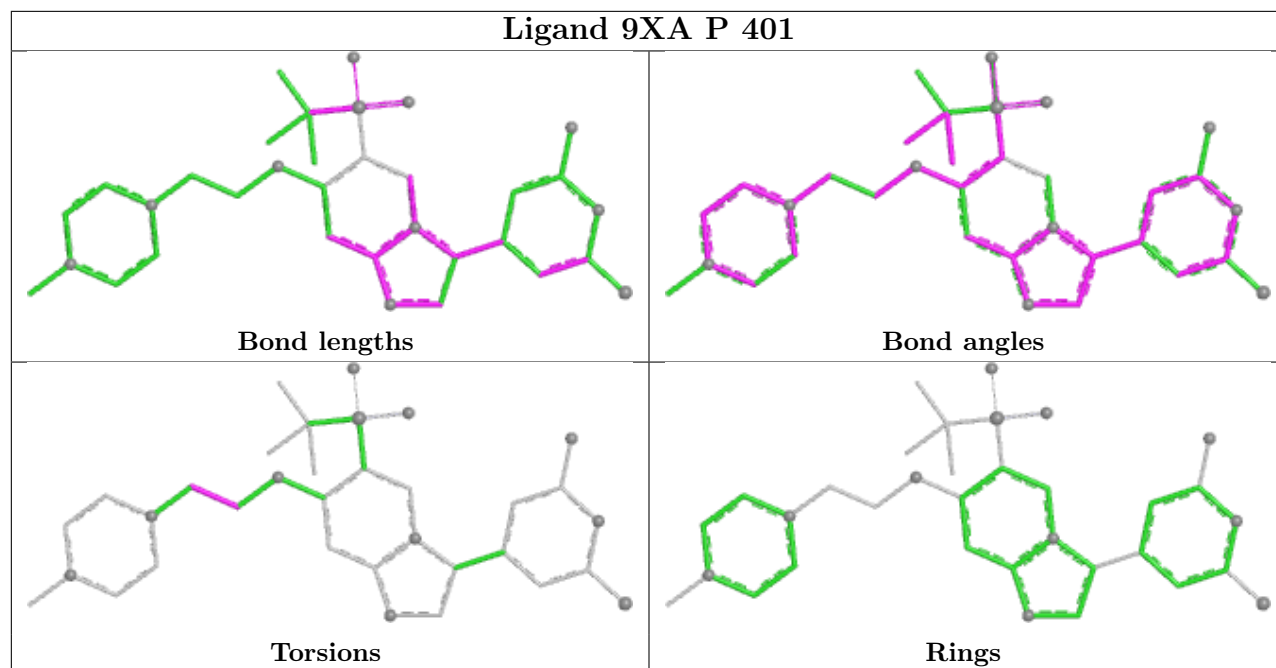
Ligand 9XA I 401



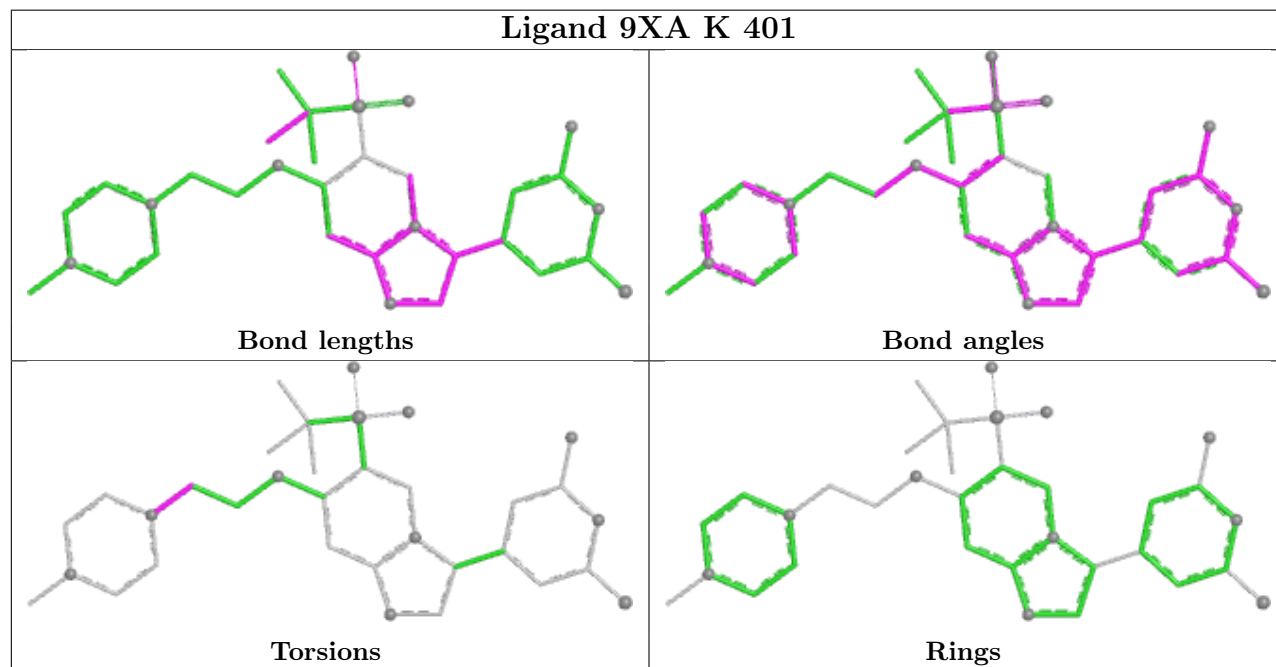
Ligand 9XA O 401



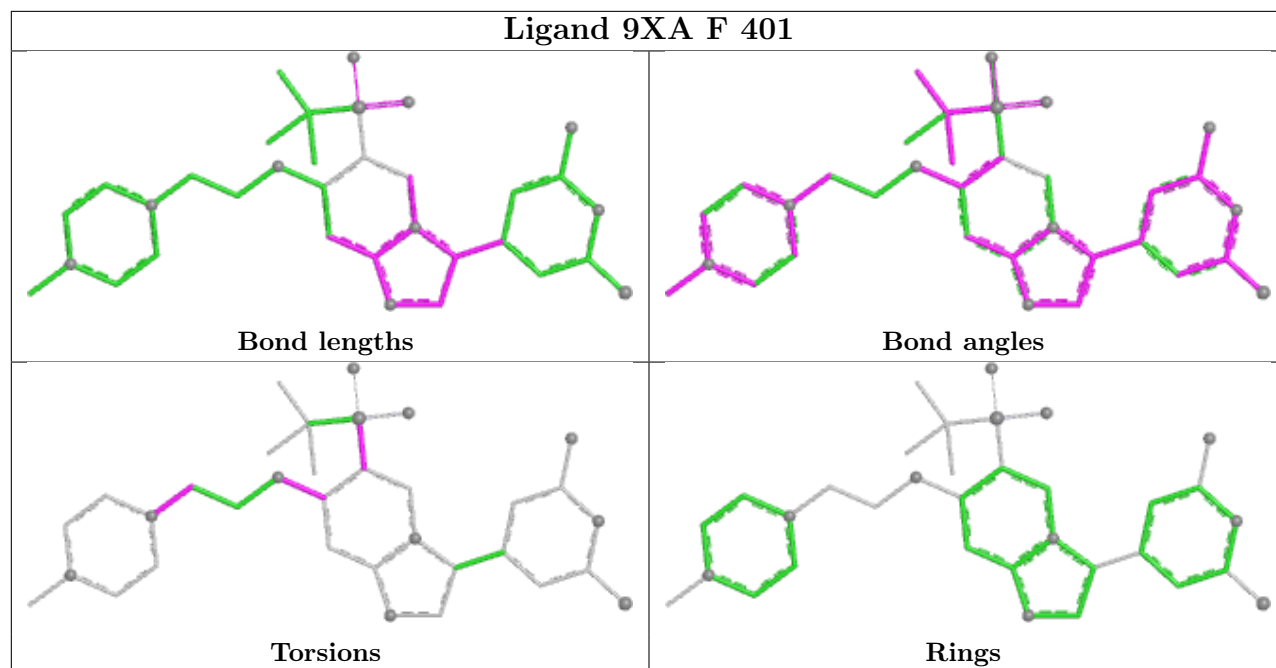
Ligand 9XA P 401



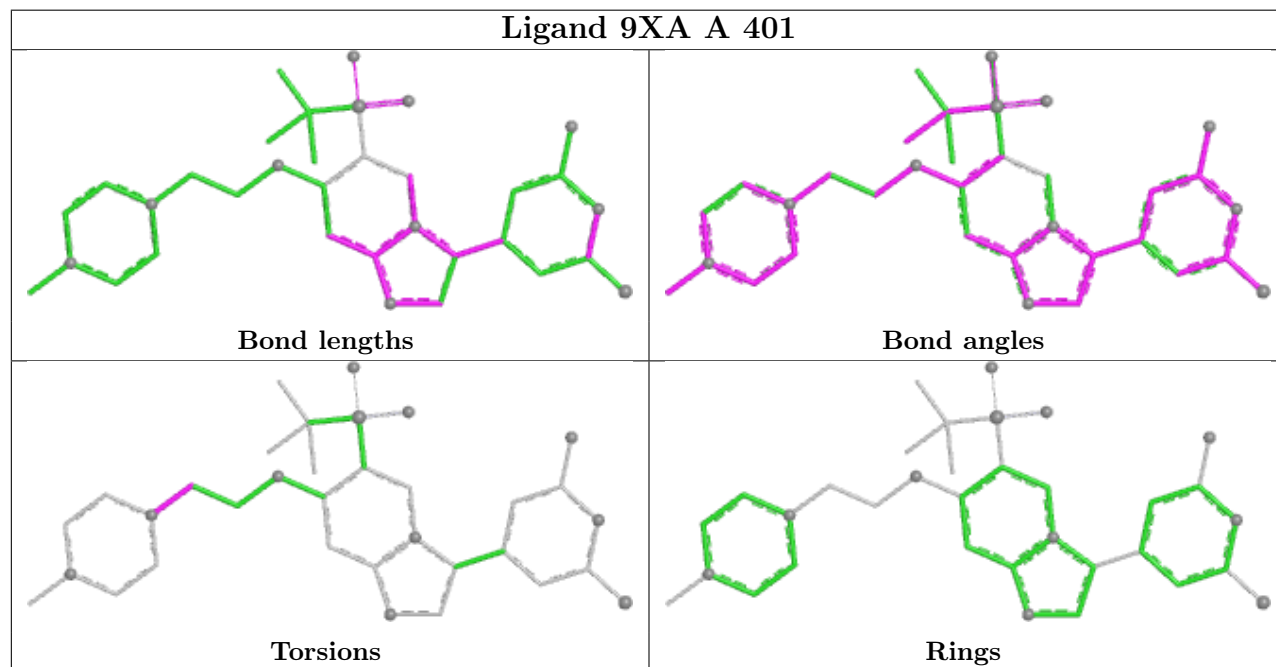
Ligand 9XA K 401



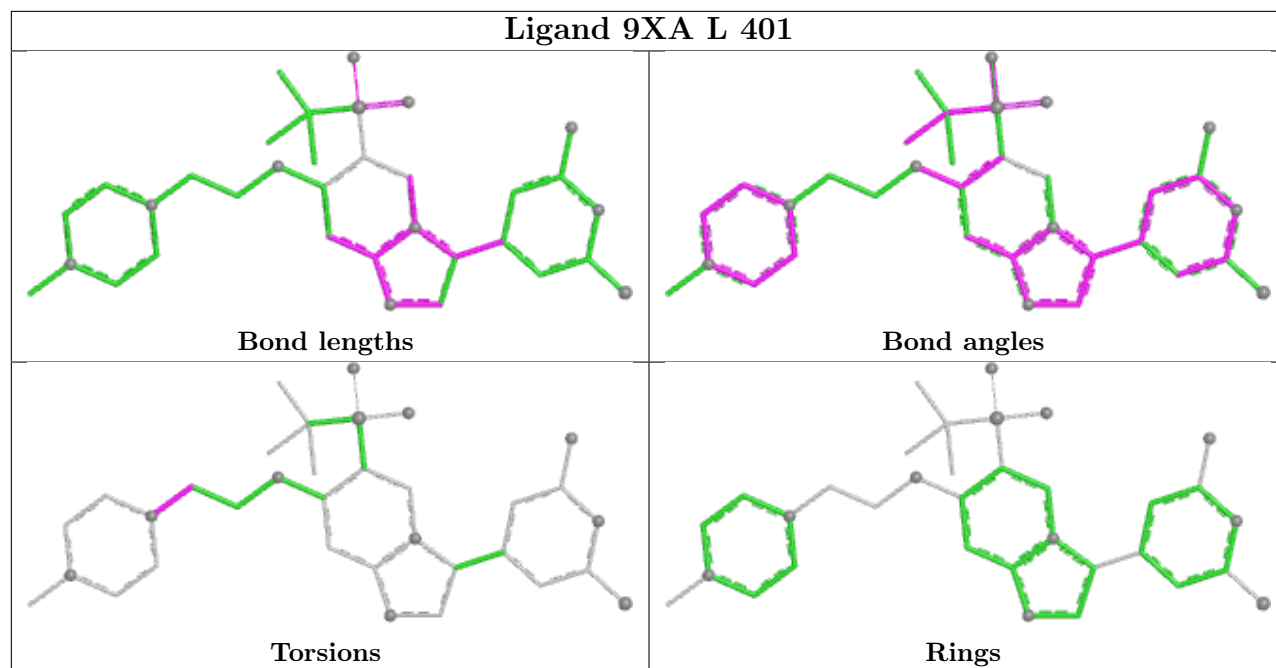
Ligand 9XA F 401



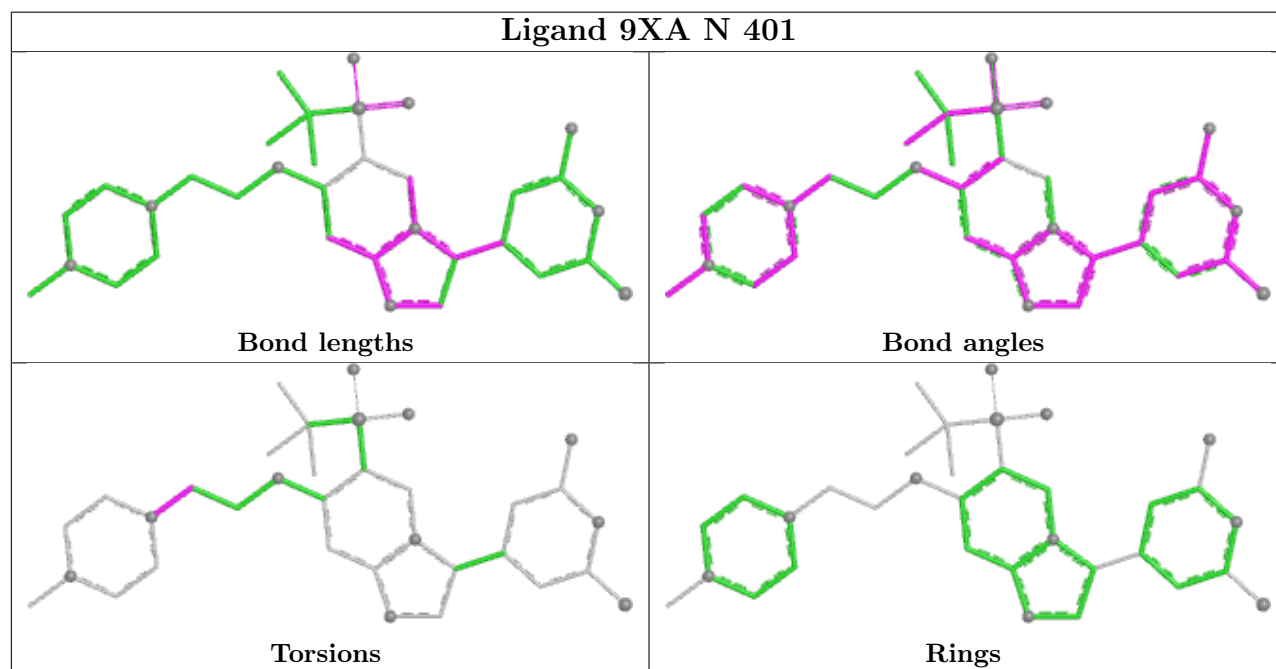
Ligand 9XA A 401



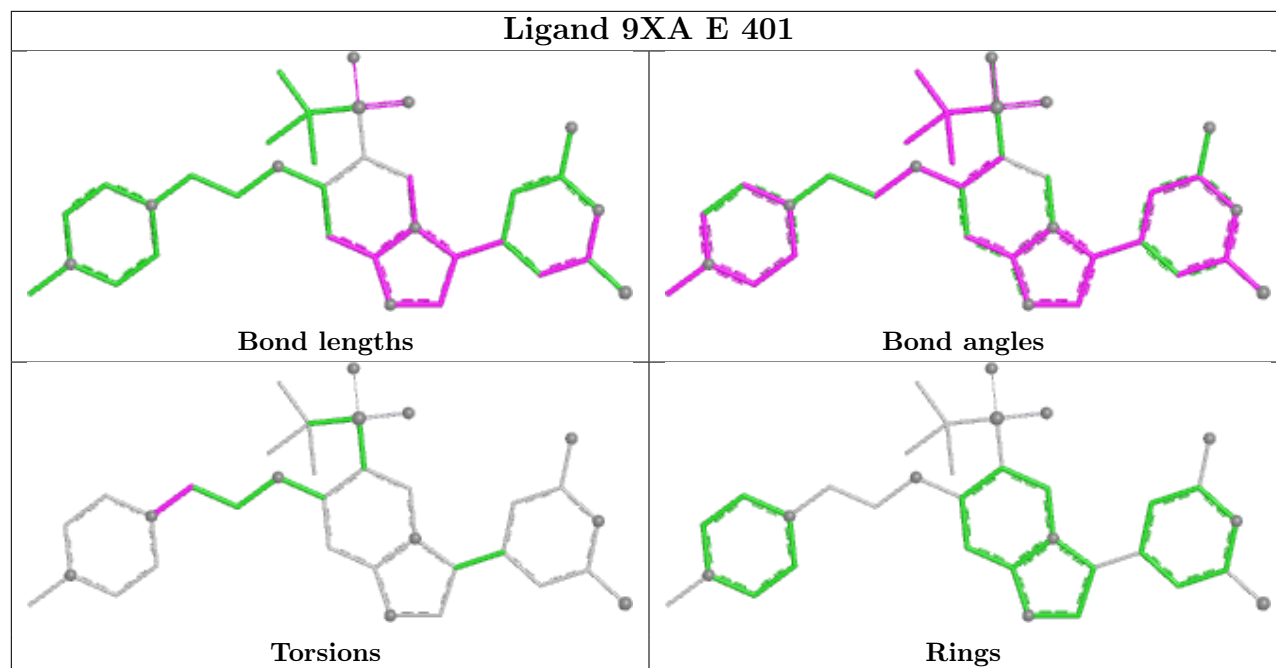
Ligand 9XA L 401



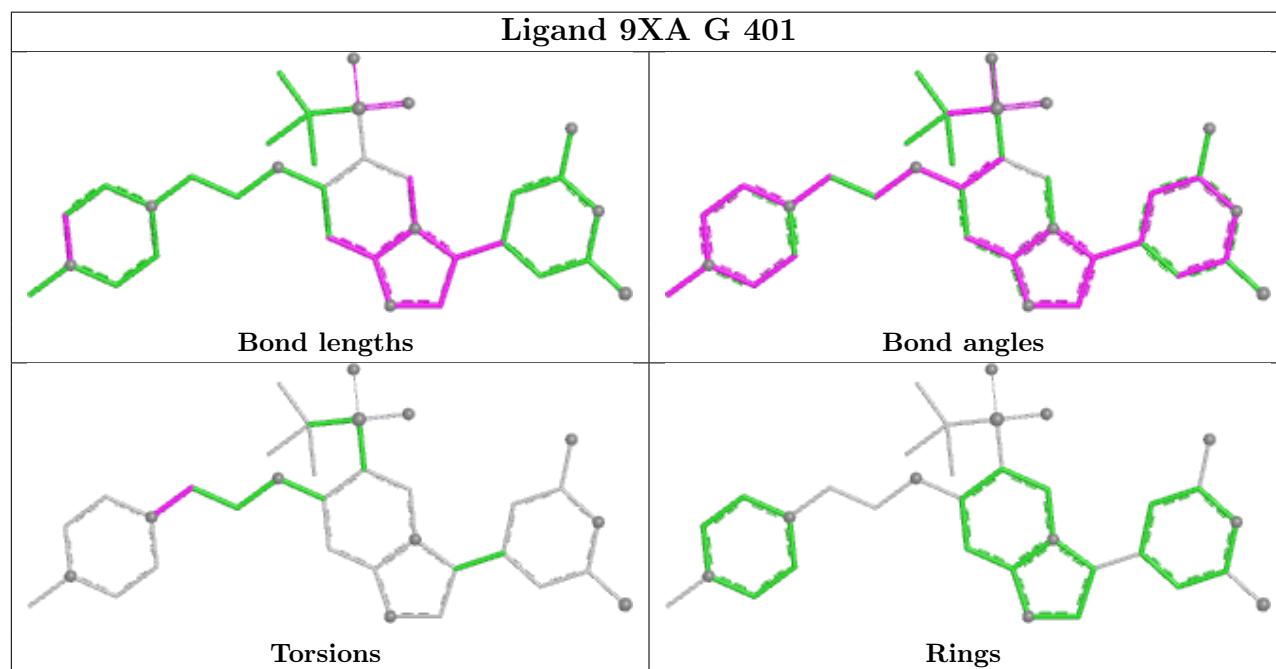
Ligand 9XA N 401



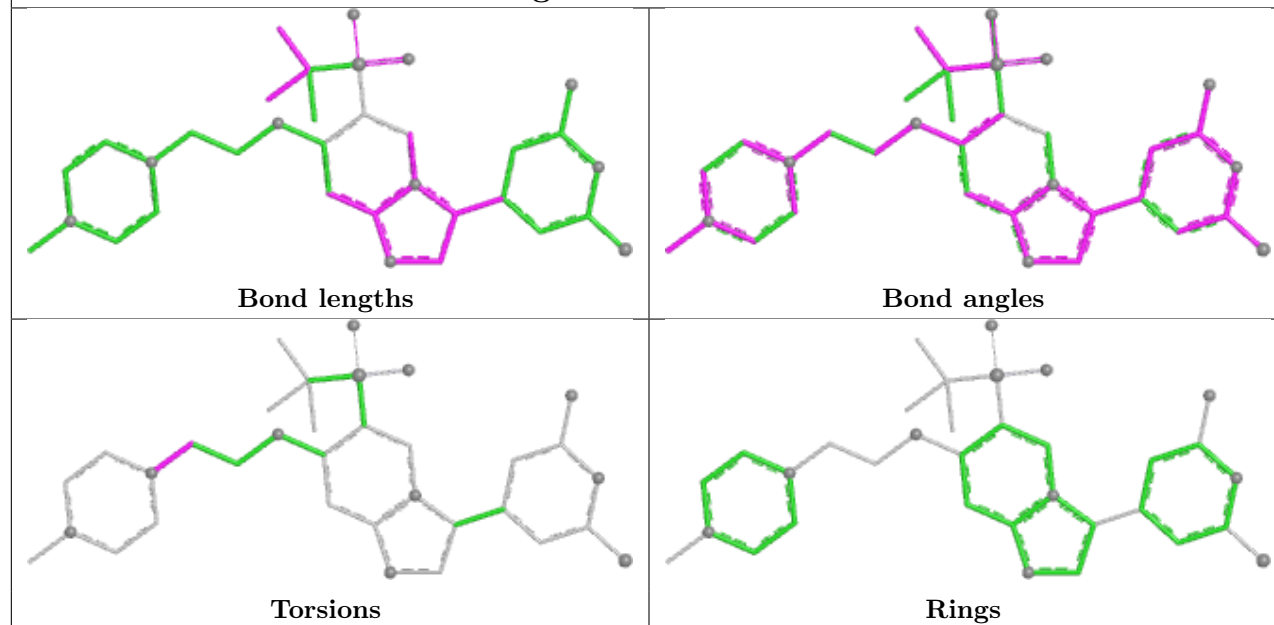
Ligand 9XA E 401



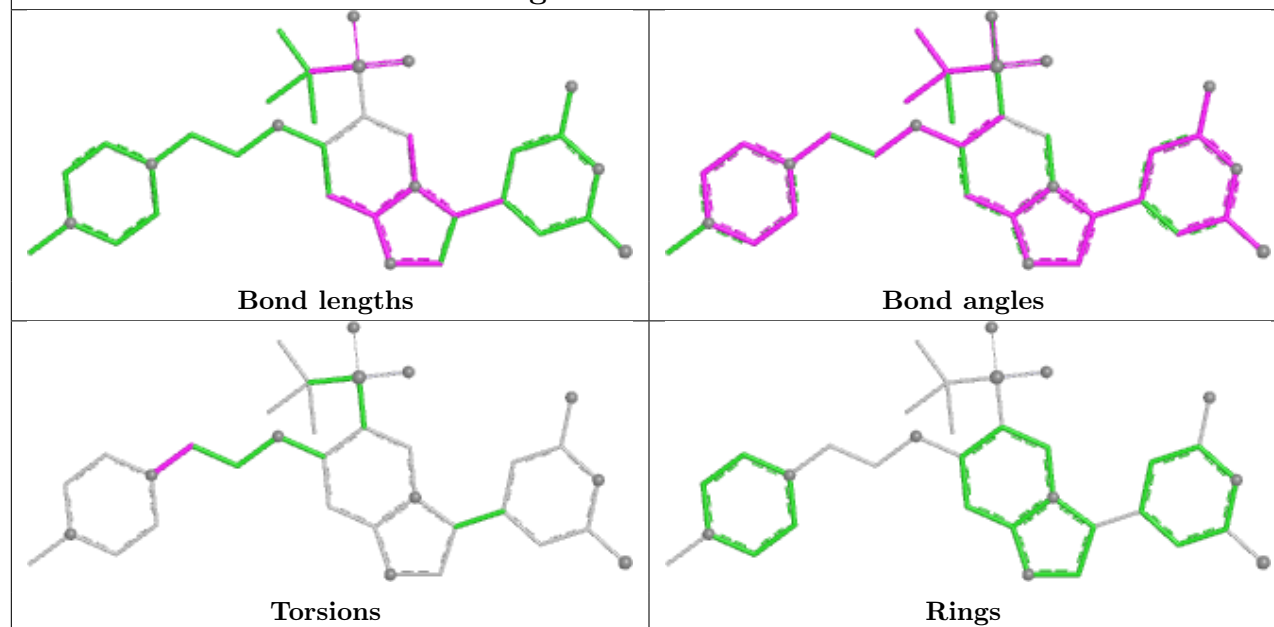
Ligand 9XA G 401

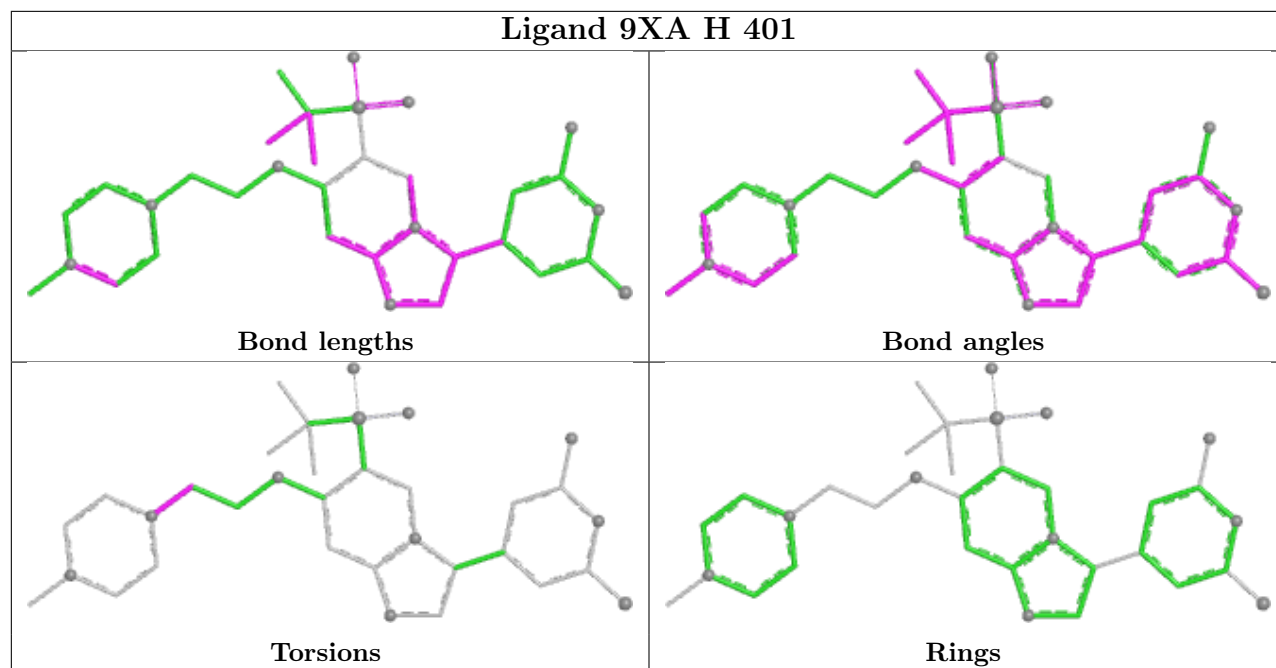


Ligand 9XA D 401



Ligand 9XA M 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	275/310 (88%)	-0.86	1 (0%) 88 85	48, 78, 106, 141	0
1	B	275/310 (88%)	-0.79	0 100 100	51, 82, 109, 128	0
1	C	275/310 (88%)	-0.73	1 (0%) 88 85	59, 91, 121, 133	0
1	D	275/310 (88%)	-0.80	2 (0%) 84 79	47, 83, 110, 126	0
1	E	275/310 (88%)	-0.87	0 100 100	51, 78, 106, 121	0
1	F	275/310 (88%)	-0.85	0 100 100	54, 81, 107, 132	0
1	G	275/310 (88%)	-0.86	1 (0%) 88 85	51, 77, 107, 125	0
1	H	275/310 (88%)	-0.86	0 100 100	50, 82, 114, 139	0
1	I	275/310 (88%)	-0.83	0 100 100	53, 82, 110, 127	0
1	J	275/310 (88%)	-0.81	0 100 100	53, 80, 106, 130	0
1	K	275/310 (88%)	-0.81	2 (0%) 84 79	54, 83, 109, 121	0
1	L	275/310 (88%)	-0.81	1 (0%) 88 85	62, 92, 123, 140	0
1	M	276/310 (89%)	-0.84	1 (0%) 88 85	55, 85, 112, 128	0
1	N	272/310 (87%)	-0.75	1 (0%) 88 85	62, 91, 117, 129	0
1	O	276/310 (89%)	-0.85	1 (0%) 88 85	56, 85, 111, 131	0
1	P	275/310 (88%)	-0.81	1 (0%) 88 85	59, 91, 111, 138	0
All	All	4399/4960 (88%)	-0.82	12 (0%) 90 87	47, 84, 112, 141	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	232	VAL	3.6
1	M	101	GLY	3.3
1	G	200	PRO	3.1
1	K	113	TYR	3.0
1	A	145	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	11	PRO	2.6
1	N	30	GLY	2.2
1	C	62	ASP	2.1
1	K	200	PRO	2.1
1	D	229	PHE	2.1
1	O	171	ARG	2.1
1	L	15	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

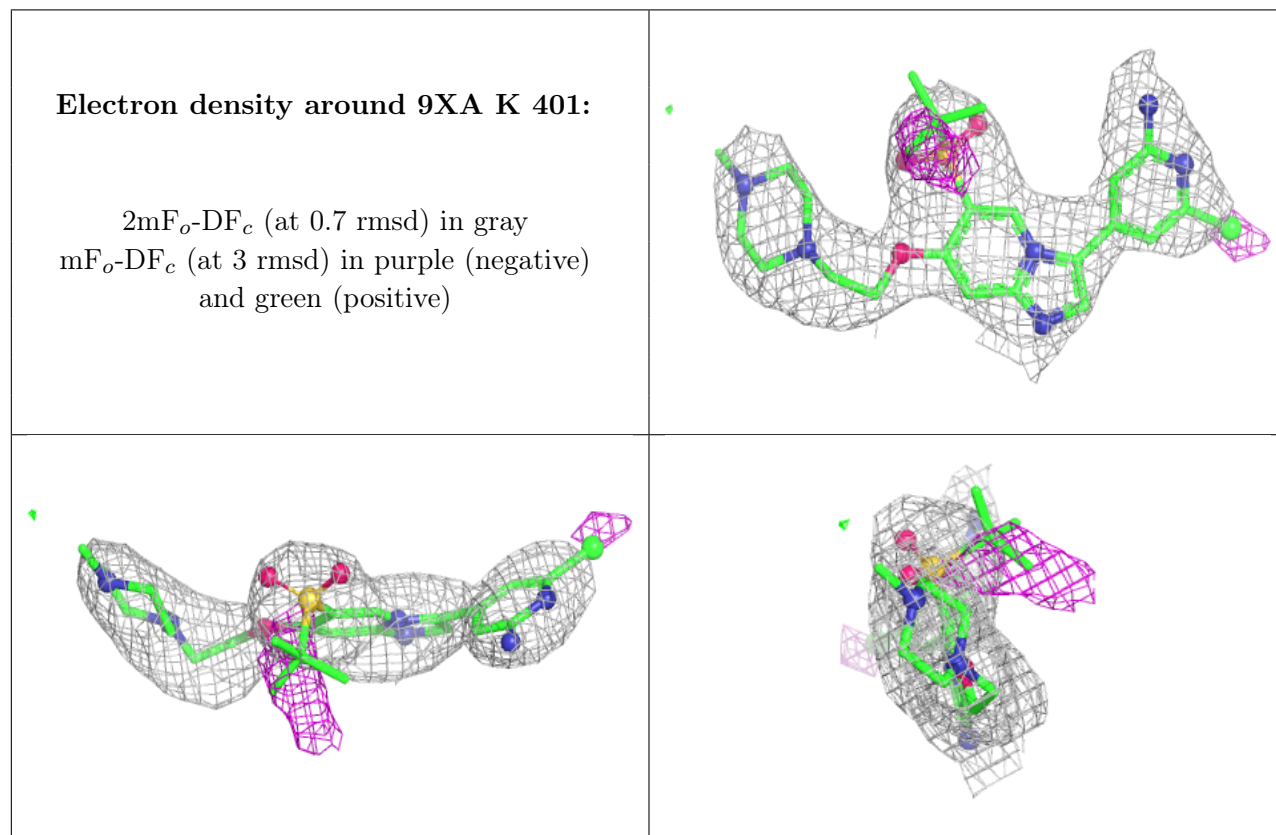
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

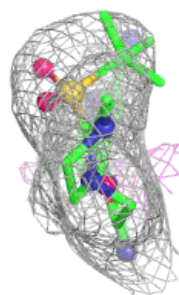
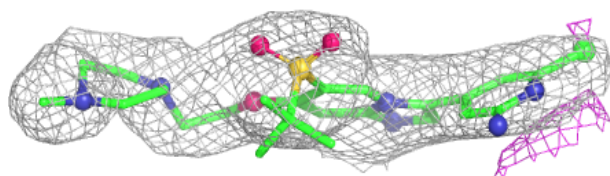
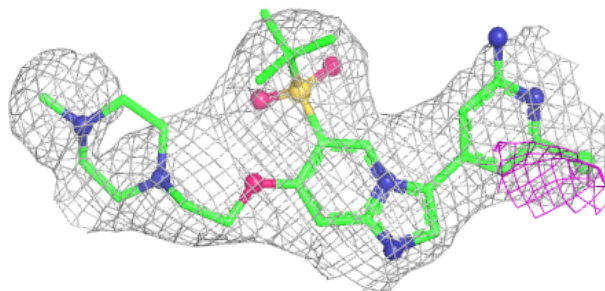
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	9XA	K	401	34/34	0.96	0.10	85,93,109,112	0
2	9XA	I	401	34/34	0.97	0.08	66,81,98,99	0
2	9XA	N	401	34/34	0.97	0.08	107,113,115,115	0
2	9XA	P	401	34/34	0.97	0.09	99,110,123,125	0
2	9XA	E	401	34/34	0.98	0.08	73,88,117,117	0
2	9XA	F	401	34/34	0.98	0.07	71,86,96,98	0
2	9XA	G	401	34/34	0.98	0.07	74,81,89,100	0
2	9XA	H	401	34/34	0.98	0.07	60,75,107,108	0
2	9XA	A	401	34/34	0.98	0.08	78,87,115,117	0
2	9XA	B	401	34/34	0.98	0.07	68,80,89,97	0
2	9XA	L	401	34/34	0.98	0.07	87,97,111,120	0
2	9XA	M	401	34/34	0.98	0.08	80,93,114,115	0
2	9XA	C	401	34/34	0.98	0.07	87,97,112,117	0
2	9XA	D	401	34/34	0.98	0.07	74,88,113,114	0
2	9XA	O	401	34/34	0.99	0.06	83,98,118,119	0
2	9XA	J	401	34/34	0.99	0.07	76,83,98,100	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.

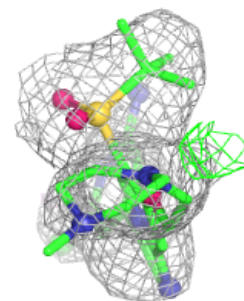
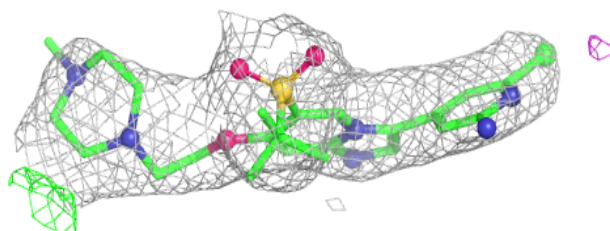
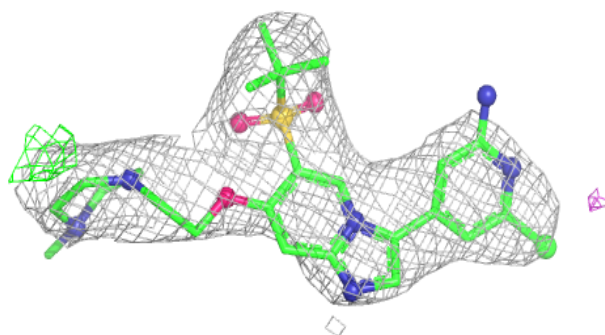


Electron density around 9XA I 401:

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

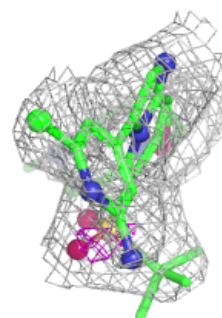
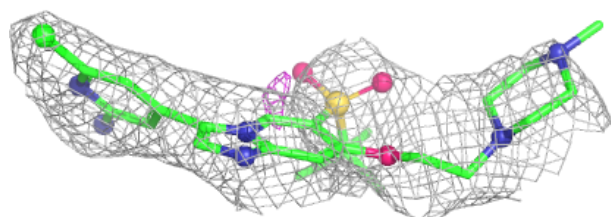
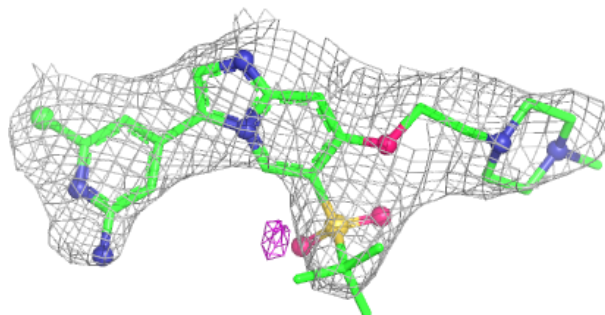
**Electron density around 9XA N 401:**

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

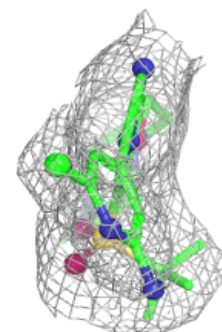
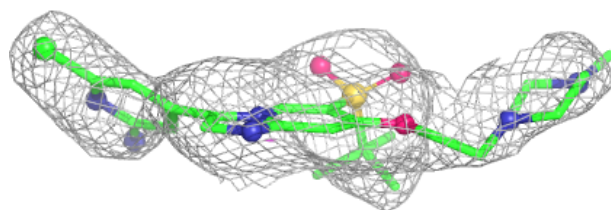
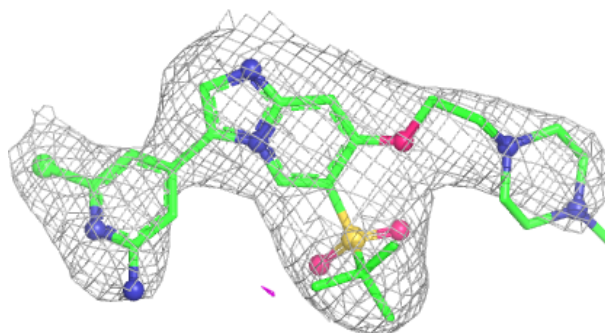


Electron density around 9XA P 401:

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

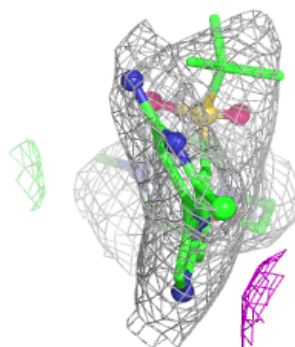
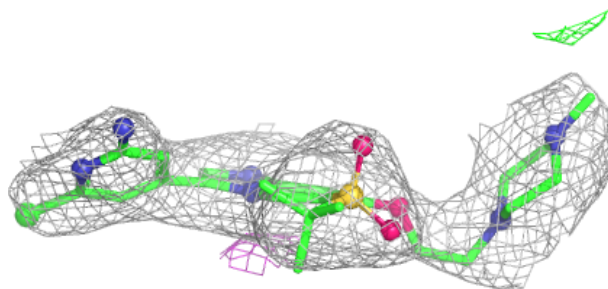
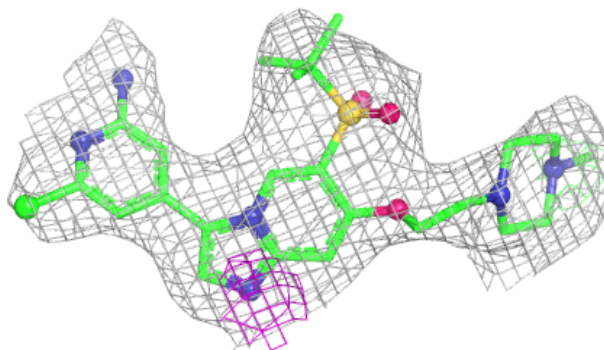
**Electron density around 9XA E 401:**

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

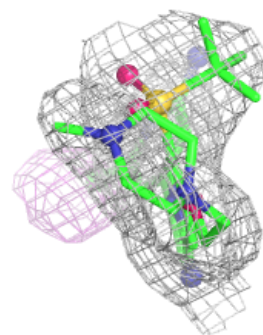
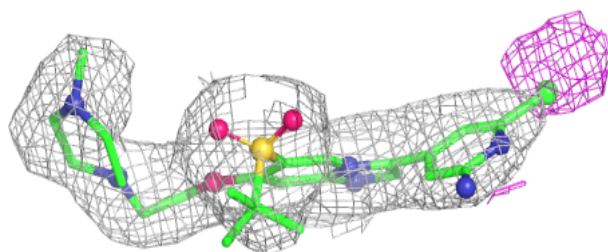
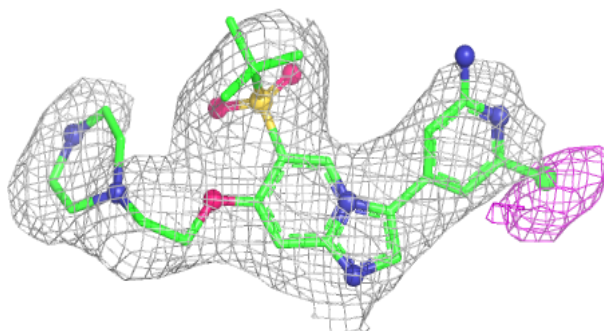


Electron density around 9XA F 401:

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

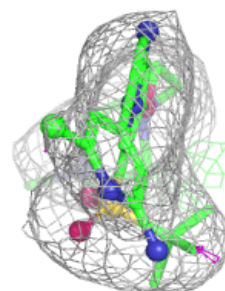
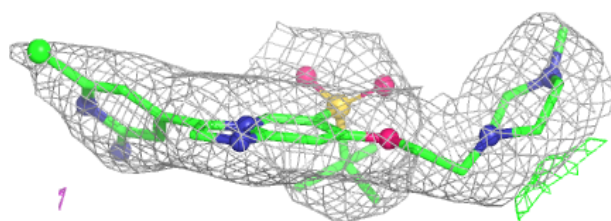
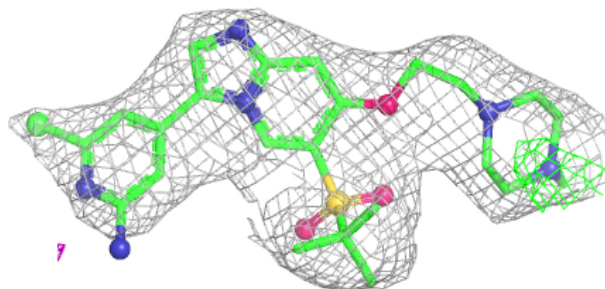
**Electron density around 9XA G 401:**

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

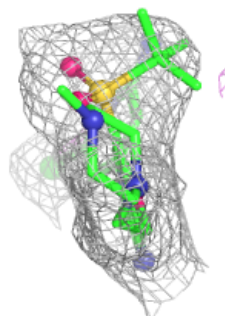
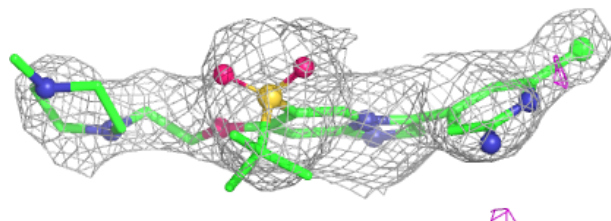
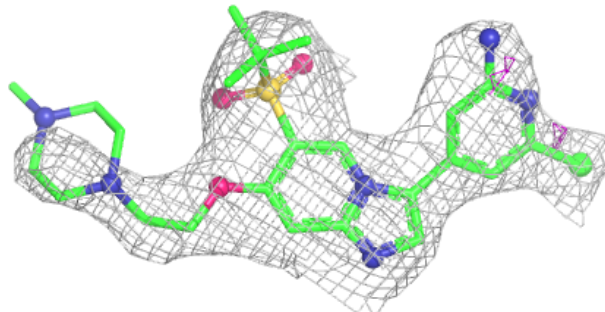


Electron density around 9XA H 401:

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

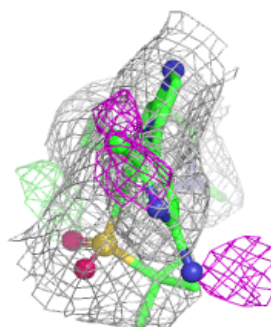
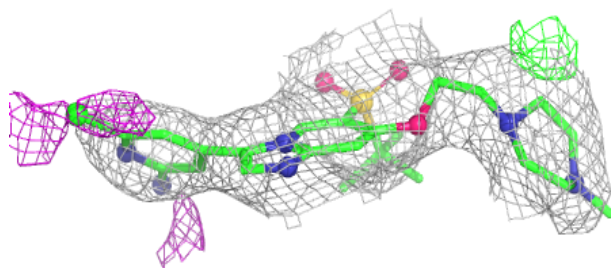
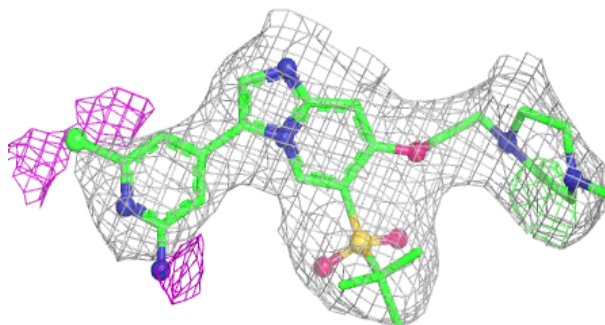
**Electron density around 9XA A 401:**

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

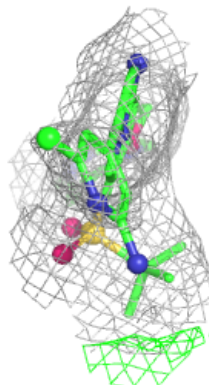
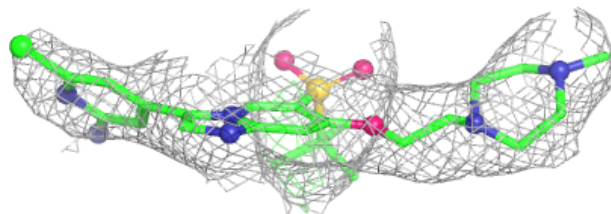
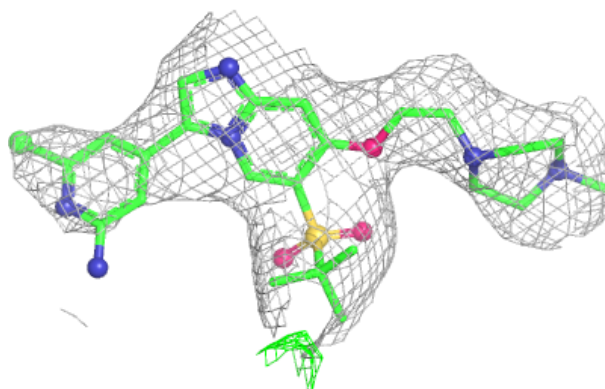


Electron density around 9XA B 401:

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

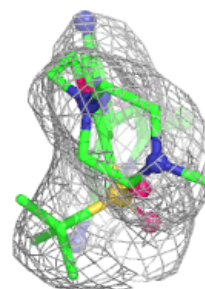
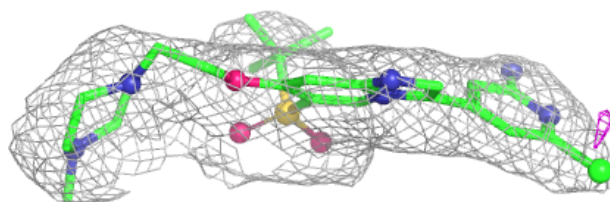
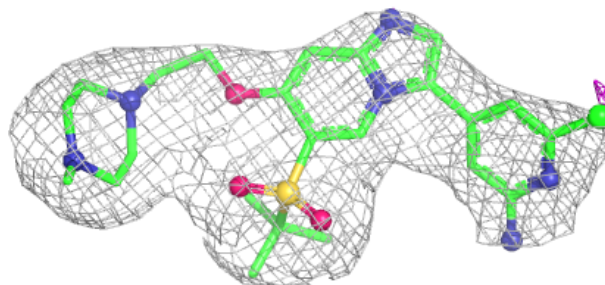
**Electron density around 9XA L 401:**

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

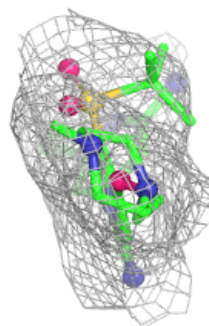
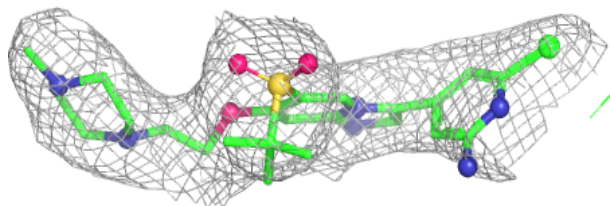
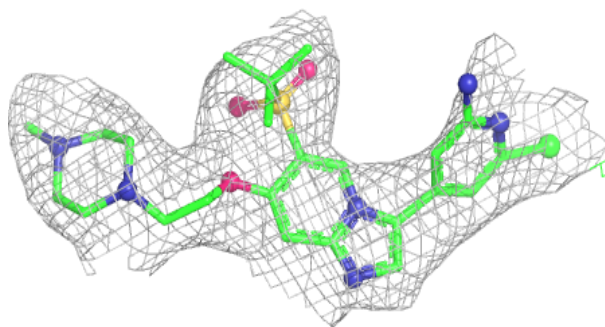


Electron density around 9XA M 401:

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

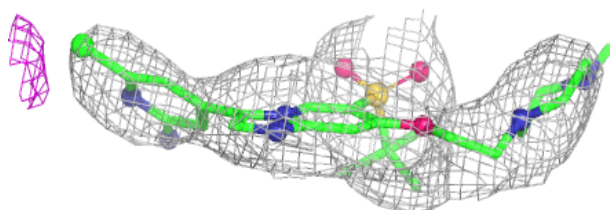
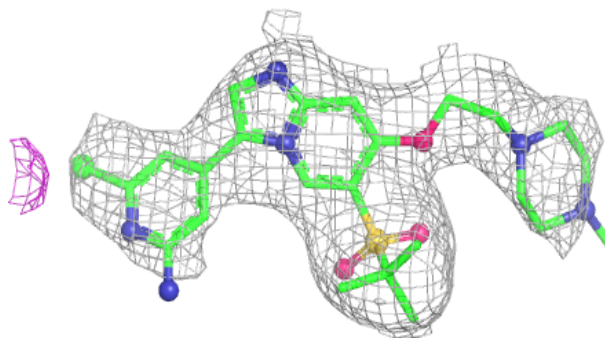
**Electron density around 9XA C 401:**

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

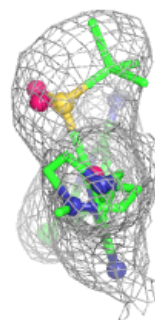
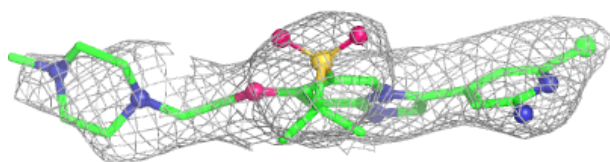
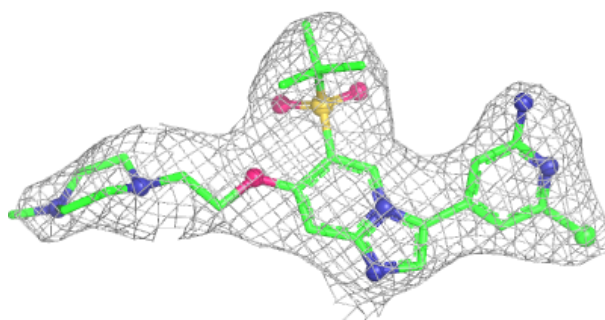


Electron density around 9XA D 401:

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

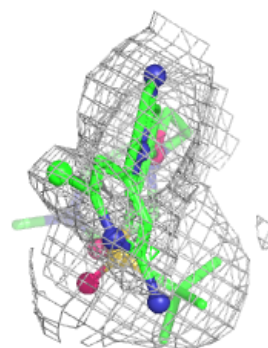
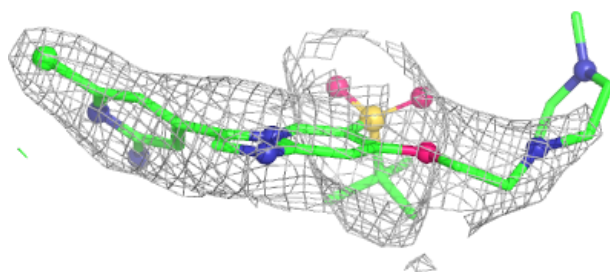
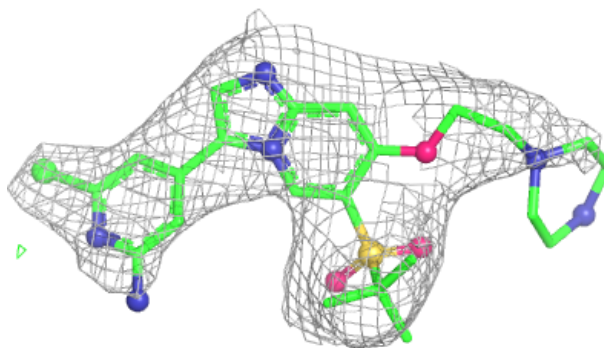
**Electron density around 9XA O 401:**

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



Electron density around 9XA J 401:

$2mF_o-DF_c$ (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.