



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:37 PM UTC

PDB ID : 6U4P / pdb_00006u4p
Title : Structure-based discovery of a novel small-molecule inhibitor of methicillin-resistant *S. aureus*
Authors : Liu, J.; Kozhaya, L.; Torres, V.J.; Unutmaz, D.; Lu, M.
Deposited on : 2019-08-26
Resolution : 2.49 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

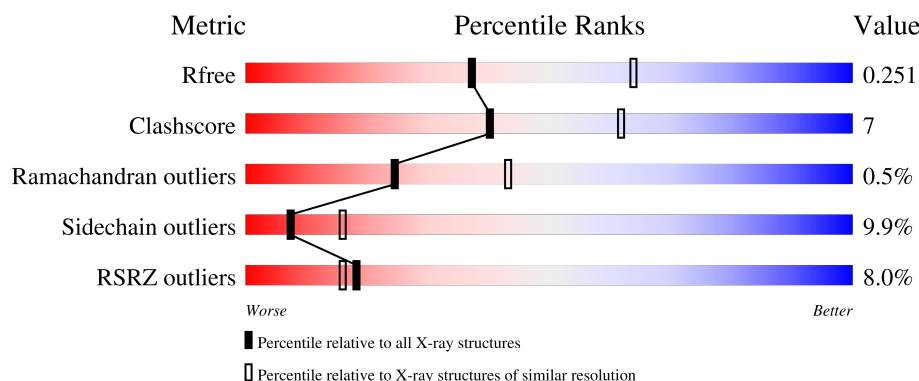
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	293	9% 76% 20% .
1	B	293	9% 77% 21% .
1	C	293	9% 73% 24% .
1	D	293	7% 73% 24% .
1	E	293	9% 72% 24% .

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Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	E	403	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16814 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.

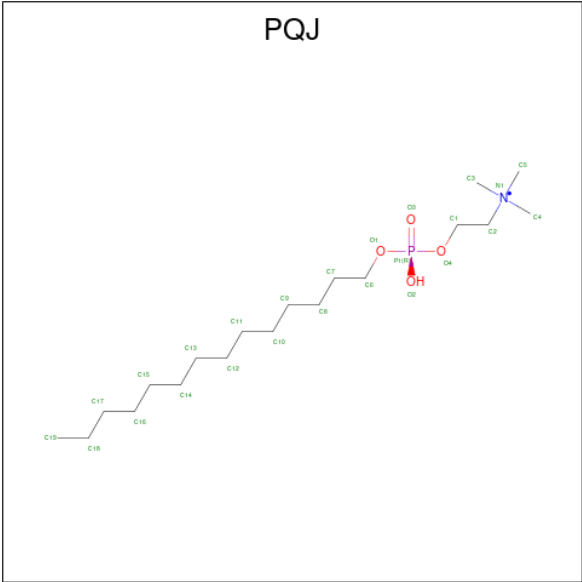
- Molecule 1 is a protein called Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2340	1469	399	465	7			
1	B	293	Total	C	N	O	S	0	0	0
			2340	1469	399	465	7			
1	C	293	Total	C	N	O	S	0	0	0
			2340	1469	399	465	7			
1	D	293	Total	C	N	O	S	0	0	0
			2340	1469	399	465	7			
1	E	293	Total	C	N	O	S	0	0	0
			2340	1469	399	465	7			
1	F	293	Total	C	N	O	S	0	0	0
			2340	1469	399	465	7			
1	G	293	Total	C	N	O	S	0	0	0
			2340	1469	399	465	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	ALA	HIS	engineered mutation	UNP P09616
B	35	ALA	HIS	engineered mutation	UNP P09616
C	35	ALA	HIS	engineered mutation	UNP P09616
D	35	ALA	HIS	engineered mutation	UNP P09616
E	35	ALA	HIS	engineered mutation	UNP P09616
F	35	ALA	HIS	engineered mutation	UNP P09616
G	35	ALA	HIS	engineered mutation	UNP P09616

- Molecule 2 is fos-choline-14 (CCD ID: PQJ) (formula: $C_{19}H_{43}NO_4P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	G	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	G	1	Total	C	N	O	P	0	0
			12	6	1	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

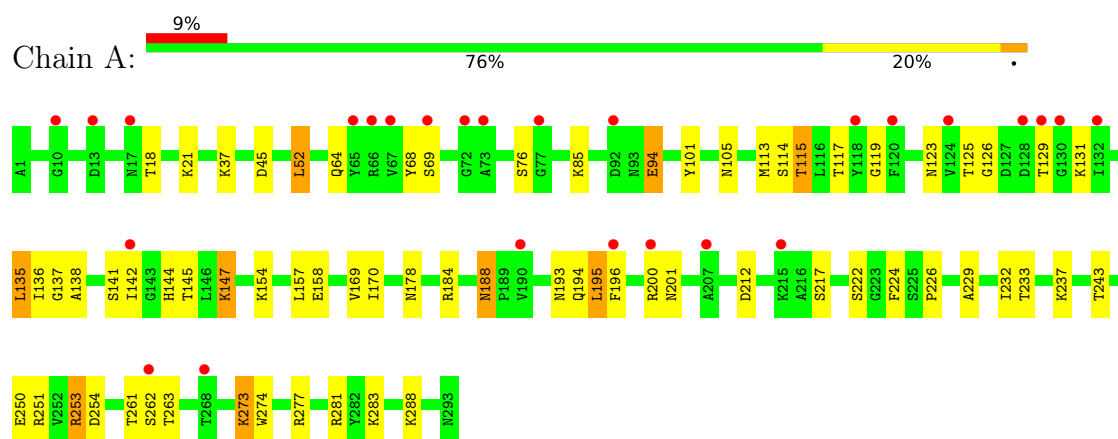
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	13	Total 13	O 13	0	0
4	C	15	Total 15	O 15	0	0
4	D	22	Total 22	O 22	0	0
4	E	15	Total 15	O 15	0	0
4	F	25	Total 25	O 25	0	0
4	G	11	Total 11	O 11	0	0

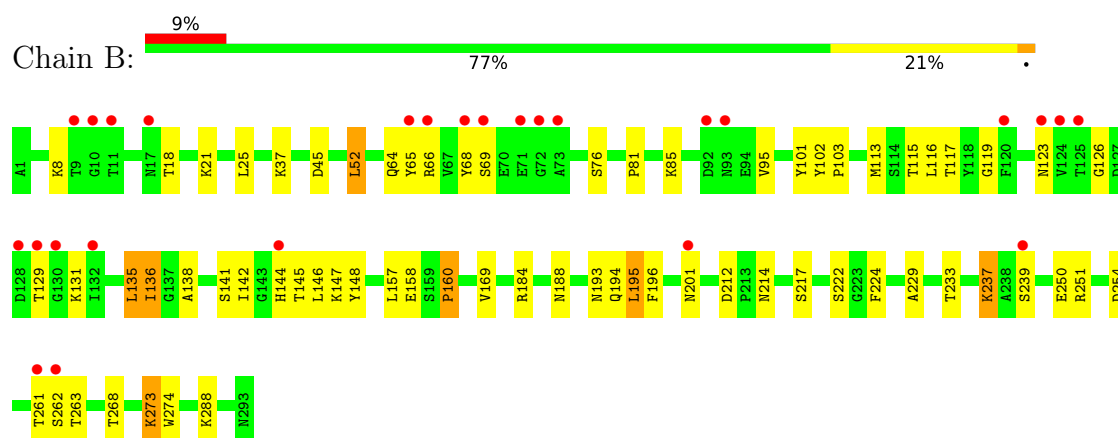
3 Residue-property plots [i](#)

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

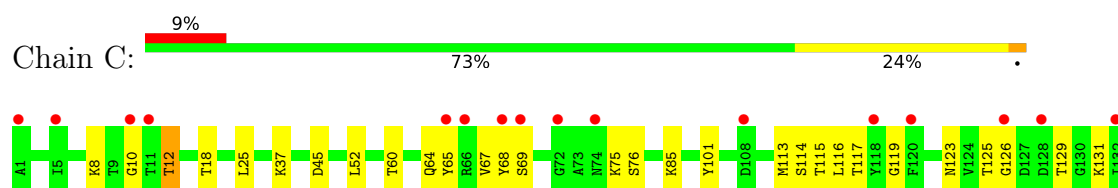
• Molecule 1: Alpha-hemolysin

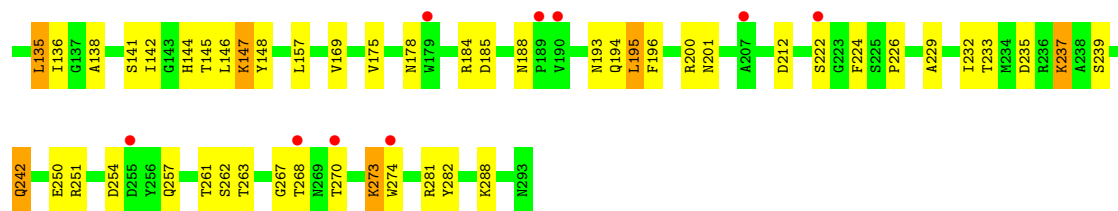


• Molecule 1: Alpha-hemolysin

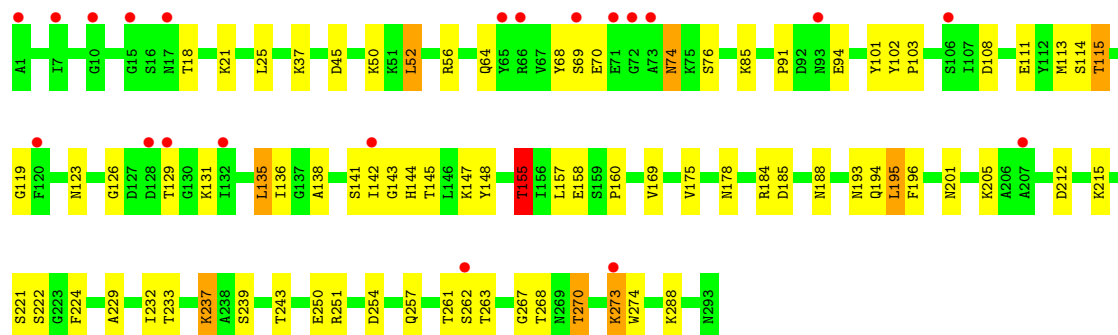
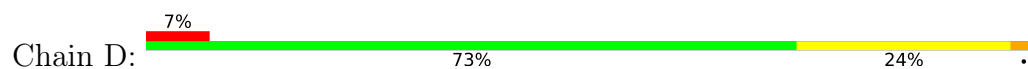


• Molecule 1: Alpha-hemolysin

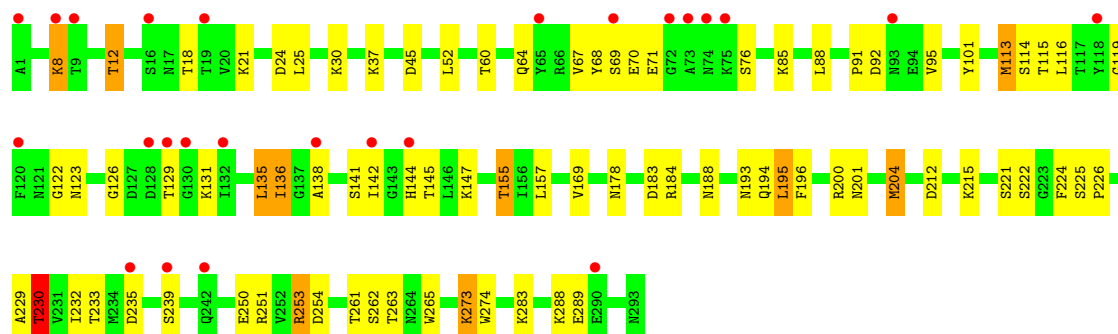




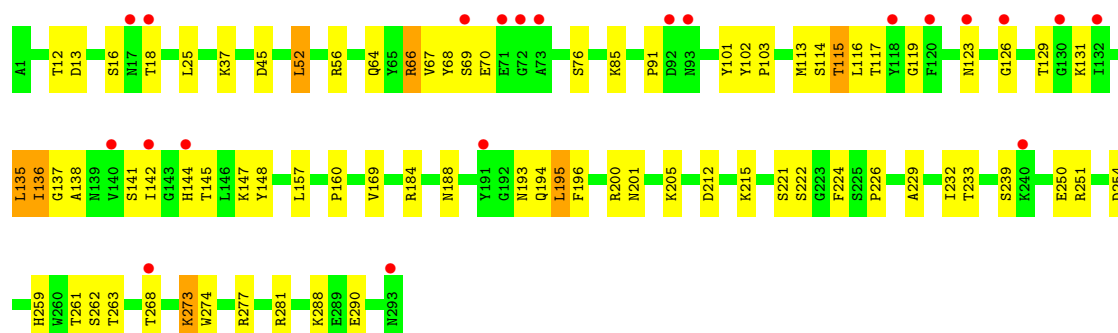
• Molecule 1: Alpha-hemolysin



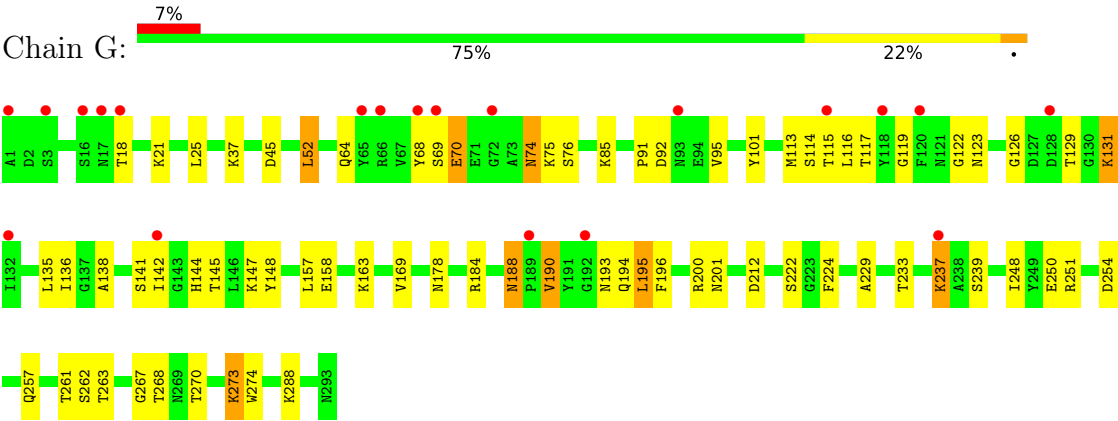
• Molecule 1: Alpha-hemolysin



• Molecule 1: Alpha-hemolysin



● Molecule 1: Alpha-hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.17Å 134.62Å 130.70Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	37.80 – 2.49 37.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (37.80-2.49) 96.2 (37.80-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.212 , 0.249 0.213 , 0.251	Depositor DCC
R_{free} test set	4257 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16814	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: SO4, PQJ

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	0.72	0/2391	1.30	16/3235 (0.5%)
1	B	0.72	0/2391	1.31	13/3235 (0.4%)
1	C	0.70	0/2391	1.29	13/3235 (0.4%)
1	D	0.76	1/2391 (0.0%)	1.33	13/3235 (0.4%)
1	E	0.74	1/2391 (0.0%)	1.34	13/3235 (0.4%)
1	F	0.75	1/2391 (0.0%)	1.32	17/3235 (0.5%)
1	G	0.71	0/2391	1.31	12/3235 (0.4%)
All	All	0.73	3/16737 (0.0%)	1.31	97/22645 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	144	HIS	CE1-NE2	5.84	1.38	1.32
1	D	108	ASP	CG-OD2	5.20	1.35	1.25
1	F	259	HIS	CE1-NE2	5.00	1.37	1.32

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	CB-CG-CD	10.99	136.57	111.30
1	D	155	THR	CA-CB-OG1	-7.25	98.73	109.60
1	D	212	ASP	CA-CB-CG	7.24	119.84	112.60
1	E	230	THR	CB-CA-C	7.03	122.80	109.37
1	A	253	ARG	CB-CG-CD	-6.90	95.42	111.30
1	B	212	ASP	CA-CB-CG	6.76	119.36	112.60
1	G	212	ASP	CA-CB-CG	6.66	119.26	112.60
1	E	212	ASP	CA-CB-CG	6.65	119.25	112.60
1	F	212	ASP	CA-CB-CG	6.63	119.23	112.60
1	C	226	PRO	CB-CA-C	-6.58	102.80	111.23
1	G	18	THR	CA-CB-OG1	6.48	119.32	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	253	ARG	CB-CG-CD	-6.41	96.57	111.30
1	D	144	HIS	CB-CA-C	6.40	122.37	109.38
1	C	268	THR	CA-CB-OG1	-6.34	100.09	109.60
1	F	144	HIS	CB-CA-C	6.32	122.21	109.38
1	A	144	HIS	CB-CA-C	6.31	122.17	109.68
1	A	226	PRO	CB-CA-C	-6.24	103.24	111.23
1	D	188	ASN	CB-CA-C	6.24	116.98	109.31
1	G	251	ARG	CG-CD-NE	-6.24	98.28	112.00
1	B	251	ARG	CG-CD-NE	-6.23	98.29	112.00
1	D	18	THR	CA-CB-OG1	6.23	118.94	109.60
1	A	18	THR	CA-CB-OG1	6.17	118.85	109.60
1	B	144	HIS	CB-CA-C	6.15	121.87	109.38
1	B	18	THR	CA-CB-OG1	6.15	118.82	109.60
1	F	18	THR	CA-CB-OG1	6.15	118.82	109.60
1	E	144	HIS	CB-CA-C	6.14	121.83	109.68
1	A	212	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	144	HIS	CB-CA-C	6.11	121.77	109.68
1	E	188	ASN	CB-CA-C	6.11	116.82	109.31
1	B	268	THR	CA-CB-OG1	-6.09	100.46	109.60
1	E	251	ARG	CG-CD-NE	-6.06	98.66	112.00
1	C	212	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	251	ARG	CG-CD-NE	-6.00	98.79	112.00
1	E	18	THR	CA-CB-OG1	6.00	118.61	109.60
1	A	45	ASP	CA-CB-CG	5.99	118.59	112.60
1	B	188	ASN	CB-CA-C	5.99	116.68	109.31
1	F	226	PRO	CB-CA-C	-5.96	103.60	111.23
1	G	144	HIS	CB-CA-C	5.95	121.45	109.38
1	G	268	THR	CA-CB-OG1	-5.95	100.68	109.60
1	E	45	ASP	CA-CB-CG	5.93	118.53	112.60
1	G	188	ASN	CB-CA-C	5.93	116.60	109.31
1	F	115	THR	CA-CB-OG1	-5.90	100.75	109.60
1	F	160	PRO	CB-CA-C	-5.83	103.31	110.95
1	A	158	GLU	CB-CG-CD	5.82	122.49	112.60
1	A	64	GLN	CA-C-N	5.78	131.74	122.32
1	A	64	GLN	C-N-CA	5.78	131.74	122.32
1	F	188	ASN	CB-CA-C	5.75	116.39	109.31
1	A	188	ASN	CB-CA-C	5.71	116.34	109.31
1	C	188	ASN	CB-CA-C	5.71	116.33	109.31
1	D	64	GLN	CA-C-N	5.71	131.62	122.32
1	D	64	GLN	C-N-CA	5.71	131.62	122.32
1	G	115	THR	CA-CB-OG1	-5.69	101.06	109.60
1	D	158	GLU	CB-CG-CD	5.68	122.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	THR	CA-CB-OG1	-5.67	101.09	109.60
1	E	64	GLN	CA-C-N	5.65	131.53	122.32
1	E	64	GLN	C-N-CA	5.65	131.53	122.32
1	F	64	GLN	CA-C-N	5.65	131.53	122.32
1	F	64	GLN	C-N-CA	5.65	131.53	122.32
1	B	81	PRO	N-CA-CB	-5.61	99.78	102.92
1	G	158	GLU	CB-CG-CD	5.60	122.12	112.60
1	G	70	GLU	CB-CG-CD	5.58	122.09	112.60
1	F	290	GLU	CB-CG-CD	5.57	122.07	112.60
1	F	117	THR	OG1-CB-CG2	-5.56	98.18	109.30
1	C	251	ARG	CG-CD-NE	-5.55	99.80	112.00
1	D	155	THR	CB-CA-C	5.49	119.73	110.79
1	F	268	THR	CA-CB-OG1	-5.47	101.39	109.60
1	D	45	ASP	CA-CB-CG	5.46	118.06	112.60
1	F	45	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	64	GLN	CA-C-N	5.44	131.93	121.54
1	C	64	GLN	C-N-CA	5.44	131.93	121.54
1	D	251	ARG	CG-CD-NE	-5.43	100.05	112.00
1	C	147	LYS	N-CA-CB	-5.42	101.69	110.81
1	C	18	THR	CA-CB-OG1	5.42	117.73	109.60
1	B	64	GLN	CA-C-N	5.41	131.88	121.54
1	B	64	GLN	C-N-CA	5.41	131.88	121.54
1	D	270	THR	CB-CA-C	5.41	119.08	109.72
1	B	45	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	268	THR	CA-CB-CG2	5.32	119.54	110.50
1	G	64	GLN	CA-C-N	5.26	130.89	122.32
1	G	64	GLN	C-N-CA	5.26	130.89	122.32
1	G	45	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	45	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	268	THR	CA-CB-OG1	-5.24	101.74	109.60
1	E	226	PRO	CB-CA-C	-5.21	104.57	111.23
1	A	147	LYS	N-CA-CB	-5.18	102.11	110.81
1	F	277	ARG	CG-CD-NE	-5.12	100.73	112.00
1	B	158	GLU	CB-CG-CD	5.11	121.29	112.60
1	E	289	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	200	ARG	CB-CG-CD	5.08	122.98	111.30
1	A	115	THR	CA-CB-OG1	-5.07	101.99	109.60
1	B	160	PRO	CB-CA-C	-5.06	104.33	110.95
1	F	251	ARG	CG-CD-NE	-5.05	100.90	112.00
1	A	105	ASN	CA-C-N	-5.04	113.56	122.74
1	A	105	ASN	C-N-CA	-5.04	113.56	122.74
1	E	115	THR	CA-CB-OG1	-5.03	102.05	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	ASP	CA-C-N	5.03	130.54	122.50
1	F	13	ASP	C-N-CA	5.03	130.54	122.50

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	2340	0	2268	33	0
1	B	2340	0	2268	36	0
1	C	2340	0	2268	41	0
1	D	2340	0	2268	47	0
1	E	2340	0	2268	40	0
1	F	2340	0	2268	33	0
1	G	2340	0	2268	35	0
2	A	22	0	0	0	0
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
2	E	22	0	0	2	0
2	F	22	0	0	0	0
2	G	23	0	0	2	0
3	A	35	0	0	2	0
3	B	15	0	0	0	0
3	C	25	0	0	0	0
3	D	15	0	0	0	0
3	E	25	0	0	2	0
3	F	20	0	0	0	0
3	G	30	0	0	0	0
4	A	13	0	0	1	0
4	B	13	0	0	0	0
4	C	15	0	0	0	0
4	D	22	0	0	0	1
4	E	15	0	0	0	0
4	F	25	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	11	0	0	0	0
All	All	16814	0	15876	214	1

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 (214) 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:E:113:MET:HG3	1:F:147:LYS:HG3	1.53	0.88
1:G:237:LYS:HE2	1:G:237:LYS:HA	1.59	0.83
1:E:123:ASN:HB2	1:E:135:LEU:HB3	1.61	0.81
1:C:123:ASN:HB2	1:C:135:LEU:HB3	1.63	0.80
1:A:123:ASN:HB2	1:A:135:LEU:HB3	1.63	0.79
1:G:92:ASP:O	1:G:163:LYS:NZ	2.14	0.79
1:F:123:ASN:HB2	1:F:135:LEU:HB3	1.65	0.79
1:C:12:THR:HG21	1:D:56:ARG:HH12	1.49	0.77
1:G:123:ASN:HB2	1:G:135:LEU:HB3	1.66	0.77
1:D:123:ASN:HB2	1:D:135:LEU:HB3	1.66	0.75
1:B:123:ASN:HB2	1:B:135:LEU:HB3	1.67	0.74
1:D:237:LYS:HA	1:D:237:LYS:HE2	1.67	0.74
1:D:52:LEU:CD2	1:D:233:THR:HG22	2.18	0.73
1:B:52:LEU:CD2	1:B:233:THR:HG22	2.20	0.72
1:C:12:THR:HG21	1:D:56:ARG:NH1	2.04	0.72
1:A:52:LEU:CD2	1:A:233:THR:HG22	2.21	0.71
1:C:52:LEU:CD2	1:C:233:THR:HG22	2.20	0.70
1:F:52:LEU:CD2	1:F:233:THR:HG22	2.22	0.70
1:G:52:LEU:CD2	1:G:233:THR:HG22	2.22	0.70
1:E:52:LEU:CD2	1:E:233:THR:HG22	2.22	0.69
1:C:237:LYS:HE2	1:C:237:LYS:HA	1.74	0.69
1:B:115:THR:HG22	1:C:145:THR:OG1	1.92	0.69
1:E:88:LEU:HD13	1:E:230:THR:HG21	1.77	0.65
1:D:115:THR:OG1	1:E:145:THR:HG22	1.97	0.65
1:B:237:LYS:HE2	1:B:237:LYS:HA	1.79	0.65
1:D:113:MET:HG3	1:E:147:LYS:HG3	1.80	0.64
1:E:204:MET:HE1	1:E:265:TRP:HE1	1.63	0.64
1:E:184:ARG:HD2	1:E:254:ASP:OD2	1.99	0.63
1:A:237:LYS:HA	1:A:237:LYS:HE2	1.81	0.62
1:B:184:ARG:HD2	1:B:254:ASP:OD2	2.00	0.61
1:F:184:ARG:HD2	1:F:254:ASP:OD2	2.00	0.61
1:A:178:ASN:ND2	1:G:148:TYR:OH	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HD2	1:D:254:ASP:OD2	2.00	0.61
1:D:148:TYR:OH	1:E:178:ASN:ND2	2.33	0.60
1:A:184:ARG:HD2	1:A:254:ASP:OD2	2.01	0.60
1:B:85:LYS:HB2	1:B:250:GLU:HB3	1.83	0.60
1:G:184:ARG:HD2	1:G:254:ASP:OD2	2.01	0.60
1:G:194:GLN:OE1	2:G:402:PQJ:O2	2.18	0.60
1:C:195:LEU:HD13	1:C:196:PHE:CE2	2.36	0.59
1:D:195:LEU:HD13	1:D:196:PHE:CE2	2.38	0.59
1:G:85:LYS:HB2	1:G:250:GLU:HB3	1.84	0.59
1:A:195:LEU:HD13	1:A:196:PHE:CE2	2.38	0.59
1:E:85:LYS:HB2	1:E:250:GLU:HB3	1.85	0.59
1:A:113:MET:HG3	1:B:147:LYS:HG3	1.85	0.58
1:B:52:LEU:HD22	1:B:233:THR:HG22	1.85	0.58
1:C:184:ARG:HD2	1:C:254:ASP:OD2	2.02	0.58
1:E:157:LEU:O	1:F:222:SER:HB3	2.04	0.58
1:E:195:LEU:HD13	1:E:196:PHE:CE2	2.39	0.58
1:A:169:VAL:HG21	1:A:224:PHE:CZ	2.39	0.58
1:E:12:THR:HG21	1:F:56:ARG:NH1	2.19	0.57
1:G:195:LEU:HD13	1:G:196:PHE:CE2	2.39	0.57
1:A:52:LEU:HD22	1:A:233:THR:HG22	1.85	0.57
1:A:157:LEU:O	1:B:222:SER:HB3	2.04	0.57
1:E:204:MET:N	1:E:204:MET:HE2	2.19	0.57
1:C:85:LYS:HB2	1:C:250:GLU:HB3	1.85	0.57
1:E:12:THR:HG21	1:F:56:ARG:HH12	1.70	0.57
1:C:157:LEU:O	1:D:222:SER:HB3	2.05	0.57
1:F:195:LEU:HD13	1:F:196:PHE:CE2	2.40	0.56
1:B:195:LEU:HD13	1:B:196:PHE:CE2	2.40	0.56
1:C:169:VAL:HG21	1:C:224:PHE:CZ	2.41	0.56
1:D:85:LYS:HB2	1:D:250:GLU:HB3	1.88	0.56
1:F:114:SER:O	1:G:145:THR:HA	2.06	0.56
1:C:126:GLY:HA2	1:C:131:LYS:O	2.06	0.56
1:F:126:GLY:HA2	1:F:131:LYS:O	2.06	0.56
1:C:193:ASN:OD1	1:C:195:LEU:HB2	2.07	0.55
1:F:194:GLN:NE2	1:F:200:ARG:HE	2.04	0.55
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.42	0.55
1:D:52:LEU:HD22	1:D:233:THR:HG22	1.89	0.55
1:G:52:LEU:HD22	1:G:233:THR:HG22	1.88	0.55
1:E:8:LYS:NZ	1:F:16:SER:HB3	2.21	0.55
1:G:194:GLN:NE2	1:G:200:ARG:HE	2.05	0.55
1:E:193:ASN:OD1	1:E:195:LEU:HB2	2.07	0.55
1:C:194:GLN:NE2	1:C:200:ARG:HE	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:402:PQJ:C3	3:E:403:SO4:O2	2.54	0.54
1:G:126:GLY:HA2	1:G:131:LYS:O	2.07	0.54
2:G:402:PQJ:C1	2:G:402:PQJ:C6	2.85	0.54
1:E:194:GLN:NE2	1:E:200:ARG:HE	2.05	0.54
1:A:126:GLY:HA2	1:A:131:LYS:O	2.06	0.54
2:E:402:PQJ:C5	3:E:403:SO4:O2	2.56	0.54
1:D:115:THR:HG22	1:D:143:GLY:HA3	1.90	0.54
1:C:52:LEU:HD22	1:C:233:THR:HG22	1.90	0.54
1:F:193:ASN:OD1	1:F:195:LEU:HB2	2.08	0.54
1:D:94:GLU:HG2	1:D:243:THR:HG23	1.88	0.54
1:D:126:GLY:HA2	1:D:131:LYS:O	2.07	0.54
1:E:126:GLY:HA2	1:E:131:LYS:O	2.07	0.54
1:A:193:ASN:OD1	1:A:195:LEU:HB2	2.08	0.54
1:D:155:THR:HB	1:D:169:VAL:HG22	1.88	0.54
1:F:169:VAL:HG21	1:F:224:PHE:CZ	2.43	0.54
1:A:85:LYS:HB2	1:A:250:GLU:HB3	1.90	0.53
1:B:193:ASN:OD1	1:B:195:LEU:HB2	2.08	0.53
1:G:169:VAL:HG21	1:G:224:PHE:CZ	2.43	0.53
1:B:126:GLY:HA2	1:B:131:LYS:O	2.08	0.53
1:D:193:ASN:OD1	1:D:195:LEU:HB2	2.08	0.53
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.43	0.53
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.44	0.53
1:G:193:ASN:OD1	1:G:195:LEU:HB2	2.08	0.53
1:B:157:LEU:O	1:C:222:SER:HB3	2.09	0.52
1:E:68:TYR:CG	1:E:69:SER:N	2.78	0.52
1:A:68:TYR:CG	1:A:69:SER:N	2.78	0.52
1:C:68:TYR:CG	1:C:69:SER:N	2.78	0.51
1:B:68:TYR:CG	1:B:69:SER:N	2.78	0.51
1:F:68:TYR:CG	1:F:69:SER:N	2.78	0.51
1:A:94:GLU:HG2	1:A:243:THR:HG23	1.91	0.51
1:F:66:ARG:HB3	1:F:66:ARG:NH1	2.25	0.51
1:A:222:SER:HB3	1:G:157:LEU:O	2.10	0.51
1:D:68:TYR:CG	1:D:69:SER:N	2.79	0.51
1:F:52:LEU:HD22	1:F:233:THR:HG22	1.93	0.51
1:F:85:LYS:HB2	1:F:250:GLU:HB3	1.93	0.51
1:A:145:THR:HA	1:G:114:SER:O	2.12	0.50
1:E:155:THR:HB	1:E:169:VAL:HG22	1.94	0.50
1:C:125:THR:HG22	1:D:135:LEU:CD2	2.41	0.50
1:G:237:LYS:HE2	1:G:237:LYS:CA	2.36	0.50
1:E:52:LEU:HD22	1:E:233:THR:HG22	1.94	0.50
3:A:408:SO4:O2	1:B:217:SER:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD13	1:B:136:ILE:N	2.27	0.49
1:G:68:TYR:CG	1:G:69:SER:N	2.78	0.49
1:D:135:LEU:HD13	1:D:136:ILE:N	2.26	0.49
1:C:146:LEU:HD21	1:D:175:VAL:HG22	1.95	0.49
1:D:50:LYS:HE2	1:E:24:ASP:O	2.12	0.49
1:D:123:ASN:OD1	1:E:135:LEU:HD11	2.13	0.49
1:A:217:SER:HA	3:A:409:SO4:O1	2.12	0.49
1:C:125:THR:CG2	1:D:135:LEU:HD22	2.42	0.49
1:B:148:TYR:OH	1:C:178:ASN:ND2	2.45	0.48
1:A:135:LEU:HD13	1:A:136:ILE:N	2.27	0.48
1:C:114:SER:O	1:D:145:THR:HA	2.14	0.47
1:C:135:LEU:HD13	1:C:136:ILE:N	2.29	0.47
1:D:74:ASN:H	1:D:74:ASN:ND2	2.11	0.47
1:F:135:LEU:HD13	1:F:136:ILE:N	2.29	0.47
1:B:8:LYS:HE3	1:C:10:GLY:HA3	1.96	0.47
1:C:237:LYS:HE2	1:C:237:LYS:CA	2.44	0.47
1:C:273:LYS:HD3	1:C:274:TRP:CZ2	2.50	0.47
1:E:183:ASP:OD2	1:F:215:LYS:HE2	2.15	0.46
1:F:157:LEU:O	1:G:222:SER:HB3	2.15	0.46
1:B:273:LYS:HD3	1:B:274:TRP:CZ2	2.49	0.46
1:C:113:MET:HE2	1:D:147:LYS:HD2	1.97	0.46
1:C:125:THR:CG2	1:D:135:LEU:CD2	2.94	0.46
1:G:85:LYS:HD2	1:G:250:GLU:OE1	2.15	0.46
1:F:148:TYR:OH	1:G:178:ASN:ND2	2.41	0.46
1:G:74:ASN:ND2	1:G:74:ASN:H	2.14	0.46
1:E:135:LEU:HD13	1:E:136:ILE:N	2.31	0.46
1:A:115:THR:HG22	1:B:145:THR:HB	1.98	0.45
1:E:204:MET:HE1	1:E:265:TRP:NE1	2.27	0.45
1:A:114:SER:O	1:B:145:THR:HA	2.16	0.45
1:C:125:THR:HG22	1:D:135:LEU:HD22	1.98	0.45
1:D:123:ASN:HD22	1:D:135:LEU:HB3	1.82	0.45
1:C:148:TYR:OH	1:D:178:ASN:ND2	2.49	0.44
1:B:113:MET:HG3	1:C:147:LYS:HG3	1.99	0.44
1:F:273:LYS:HD3	1:F:274:TRP:CZ2	2.53	0.44
1:F:194:GLN:HE22	1:F:200:ARG:HE	1.66	0.44
1:C:119:GLY:O	1:C:138:ALA:HA	2.18	0.44
1:G:194:GLN:HE22	1:G:200:ARG:HE	1.66	0.44
1:D:237:LYS:HE2	1:D:237:LYS:CA	2.42	0.43
1:E:101:TYR:HA	1:E:229:ALA:O	2.18	0.43
1:G:119:GLY:O	1:G:138:ALA:HA	2.19	0.43
1:A:170:ILE:CD1	1:B:214:ASN:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:LYS:HD3	1:G:274:TRP:CZ2	2.54	0.43
1:A:125:THR:CG2	1:B:135:LEU:HD22	2.48	0.43
1:D:101:TYR:HA	1:D:229:ALA:O	2.19	0.43
1:E:60:THR:OG1	1:E:225:SER:OG	2.31	0.43
1:D:185:ASP:OD2	1:E:215:LYS:NZ	2.51	0.43
1:D:194:GLN:O	1:D:195:LEU:C	2.62	0.43
1:B:123:ASN:HD22	1:B:135:LEU:HB3	1.82	0.43
1:F:101:TYR:HA	1:F:229:ALA:O	2.18	0.43
1:A:154:LYS:HE3	1:B:214:ASN:O	2.18	0.42
1:C:101:TYR:HA	1:C:229:ALA:O	2.19	0.42
1:C:194:GLN:HE22	1:C:200:ARG:HE	1.67	0.42
1:D:111:GLU:OE1	1:D:113:MET:CE	2.67	0.42
1:F:119:GLY:O	1:F:138:ALA:HA	2.19	0.42
1:E:194:GLN:HE22	1:E:200:ARG:HE	1.67	0.42
1:F:115:THR:HG22	1:G:145:THR:OG1	2.19	0.42
1:C:194:GLN:O	1:C:195:LEU:C	2.62	0.42
1:A:125:THR:HG22	1:B:135:LEU:CD2	2.48	0.42
1:D:111:GLU:OE1	1:D:113:MET:HE2	2.20	0.42
1:E:122:GLY:O	1:F:137:GLY:HA2	2.20	0.42
1:E:273:LYS:HD3	1:E:274:TRP:CZ2	2.54	0.42
1:D:114:SER:O	1:E:145:THR:HA	2.20	0.42
1:A:137:GLY:HA2	1:G:122:GLY:O	2.20	0.42
1:A:273:LYS:HD3	1:A:274:TRP:CZ2	2.54	0.42
1:C:185:ASP:OD2	1:D:215:LYS:NZ	2.52	0.42
1:B:119:GLY:O	1:B:138:ALA:HA	2.20	0.42
1:A:277:ARG:HD2	4:A:512:HOH:O	2.20	0.42
1:E:119:GLY:O	1:E:138:ALA:HA	2.20	0.42
1:A:125:THR:CG2	1:B:135:LEU:CD2	2.98	0.41
1:A:194:GLN:O	1:A:195:LEU:C	2.63	0.41
1:B:101:TYR:HA	1:B:229:ALA:O	2.19	0.41
1:E:114:SER:O	1:F:145:THR:HA	2.19	0.41
1:F:102:TYR:CG	1:F:103:PRO:HA	2.56	0.41
1:F:113:MET:HG3	1:G:147:LYS:HG3	2.03	0.41
1:B:160:PRO:HD2	1:C:60:THR:HG21	2.02	0.41
1:D:157:LEU:O	1:E:222:SER:HB3	2.20	0.41
1:C:242:GLN:HE21	1:C:242:GLN:HB2	1.74	0.41
1:D:273:LYS:HD3	1:D:274:TRP:CZ2	2.55	0.41
1:C:281:ARG:HG3	1:C:282:TYR:N	2.35	0.41
1:D:119:GLY:O	1:D:138:ALA:HA	2.21	0.41
1:E:204:MET:HE2	1:E:204:MET:H	1.85	0.41
1:G:101:TYR:HA	1:G:229:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ASN:OD1	1:G:190:VAL:HG13	2.21	0.41
1:A:101:TYR:HA	1:A:229:ALA:O	2.20	0.41
1:B:102:TYR:CD1	1:B:103:PRO:HA	2.56	0.41
1:E:194:GLN:O	1:E:195:LEU:C	2.63	0.41
1:A:119:GLY:O	1:A:138:ALA:HA	2.21	0.41
1:B:146:LEU:HD21	1:C:175:VAL:HG22	2.03	0.40
1:C:257:GLN:O	1:C:267:GLY:HA2	2.21	0.40
1:D:102:TYR:CD1	1:D:103:PRO:HA	2.56	0.40
1:A:147:LYS:HG3	1:G:113:MET:HG3	2.03	0.40
1:B:102:TYR:CG	1:B:103:PRO:HA	2.56	0.40
1:B:194:GLN:O	1:B:195:LEU:C	2.64	0.40
1:D:257:GLN:O	1:D:267:GLY:HA2	2.21	0.40
1:G:194:GLN:O	1:G:195:LEU:C	2.64	0.40
1:F:102:TYR:CD1	1:F:103:PRO:HA	2.56	0.40
1:G:248:ILE:N	1:G:248:ILE:HD12	2.36	0.40
1:D:101:TYR:CZ	1:D:160:PRO:HG2	2.56	0.40
1:F:194:GLN:O	1:F:195:LEU:C	2.64	0.40
1:G:257:GLN:O	1:G:267:GLY:HA2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:521:HOH:O	4:F:517:HOH:O[4_446]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	291/293 (99%)	272 (94%)	18 (6%)	1 (0%)	36 55
1	B	291/293 (99%)	272 (94%)	17 (6%)	2 (1%)	18 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	291/293 (99%)	271 (93%)	18 (6%)	2 (1%)	18	34
1	D	291/293 (99%)	272 (94%)	17 (6%)	2 (1%)	18	34
1	E	291/293 (99%)	270 (93%)	19 (6%)	2 (1%)	18	34
1	F	291/293 (99%)	271 (93%)	19 (6%)	1 (0%)	36	55
1	G	291/293 (99%)	270 (93%)	20 (7%)	1 (0%)	36	55
All	All	2037/2051 (99%)	1898 (93%)	128 (6%)	11 (0%)	24	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
1	B	261	THR
1	C	261	THR
1	D	261	THR
1	E	261	THR
1	F	261	THR
1	G	261	THR
1	B	65	TYR
1	C	65	TYR
1	E	91	PRO
1	D	91	PRO

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	258/258 (100%)	237 (92%)	21 (8%)	11	23
1	B	258/258 (100%)	237 (92%)	21 (8%)	11	23
1	C	258/258 (100%)	233 (90%)	25 (10%)	8	17
1	D	258/258 (100%)	233 (90%)	25 (10%)	8	17
1	E	258/258 (100%)	224 (87%)	34 (13%)	4	8
1	F	258/258 (100%)	232 (90%)	26 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	258/258 (100%)	231 (90%)	27 (10%)	6	14
All	All	1806/1806 (100%)	1627 (90%)	179 (10%)	7	16

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	37	LYS
1	A	52	LEU
1	A	76	SER
1	A	94	GLU
1	A	117	THR
1	A	129	THR
1	A	135	LEU
1	A	141	SER
1	A	142	ILE
1	A	188	ASN
1	A	195	LEU
1	A	201	ASN
1	A	232	ILE
1	A	253	ARG
1	A	262	SER
1	A	263	THR
1	A	273	LYS
1	A	281	ARG
1	A	283	LYS
1	A	288	LYS
1	B	21	LYS
1	B	25	LEU
1	B	37	LYS
1	B	52	LEU
1	B	76	SER
1	B	95	VAL
1	B	116	LEU
1	B	117	THR
1	B	129	THR
1	B	135	LEU
1	B	136	ILE
1	B	141	SER
1	B	142	ILE
1	B	195	LEU
1	B	201	ASN

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Mol	Chain	Res	Type
1	B	237	LYS
1	B	239	SER
1	B	262	SER
1	B	263	THR
1	B	273	LYS
1	B	288	LYS
1	C	8	LYS
1	C	12	THR
1	C	25	LEU
1	C	37	LYS
1	C	67	VAL
1	C	75	LYS
1	C	76	SER
1	C	116	LEU
1	C	117	THR
1	C	129	THR
1	C	135	LEU
1	C	141	SER
1	C	142	ILE
1	C	195	LEU
1	C	201	ASN
1	C	232	ILE
1	C	235	ASP
1	C	237	LYS
1	C	239	SER
1	C	242	GLN
1	C	262	SER
1	C	263	THR
1	C	270	THR
1	C	273	LYS
1	C	288	LYS
1	D	21	LYS
1	D	25	LEU
1	D	37	LYS
1	D	52	LEU
1	D	70	GLU
1	D	74	ASN
1	D	76	SER
1	D	115	THR
1	D	129	THR
1	D	135	LEU
1	D	141	SER

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Mol	Chain	Res	Type
1	D	142	ILE
1	D	155	THR
1	D	195	LEU
1	D	201	ASN
1	D	205	LYS
1	D	221	SER
1	D	232	ILE
1	D	237	LYS
1	D	239	SER
1	D	262	SER
1	D	263	THR
1	D	270	THR
1	D	273	LYS
1	D	288	LYS
1	E	8	LYS
1	E	12	THR
1	E	21	LYS
1	E	25	LEU
1	E	30	LYS
1	E	37	LYS
1	E	67	VAL
1	E	70	GLU
1	E	71	GLU
1	E	76	SER
1	E	92	ASP
1	E	95	VAL
1	E	113	MET
1	E	116	LEU
1	E	129	THR
1	E	135	LEU
1	E	136	ILE
1	E	141	SER
1	E	142	ILE
1	E	155	THR
1	E	195	LEU
1	E	201	ASN
1	E	204	MET
1	E	221	SER
1	E	230	THR
1	E	232	ILE
1	E	235	ASP
1	E	239	SER

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Mol	Chain	Res	Type
1	E	253	ARG
1	E	262	SER
1	E	263	THR
1	E	273	LYS
1	E	283	LYS
1	E	288	LYS
1	F	12	THR
1	F	25	LEU
1	F	37	LYS
1	F	52	LEU
1	F	66	ARG
1	F	67	VAL
1	F	70	GLU
1	F	76	SER
1	F	91	PRO
1	F	116	LEU
1	F	129	THR
1	F	135	LEU
1	F	136	ILE
1	F	141	SER
1	F	142	ILE
1	F	195	LEU
1	F	201	ASN
1	F	205	LYS
1	F	221	SER
1	F	232	ILE
1	F	239	SER
1	F	262	SER
1	F	263	THR
1	F	273	LYS
1	F	281	ARG
1	F	288	LYS
1	G	21	LYS
1	G	25	LEU
1	G	37	LYS
1	G	52	LEU
1	G	70	GLU
1	G	74	ASN
1	G	75	LYS
1	G	76	SER
1	G	91	PRO
1	G	95	VAL

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Mol	Chain	Res	Type
1	G	116	LEU
1	G	117	THR
1	G	129	THR
1	G	131	LYS
1	G	136	ILE
1	G	141	SER
1	G	142	ILE
1	G	190	VAL
1	G	195	LEU
1	G	201	ASN
1	G	237	LYS
1	G	239	SER
1	G	262	SER
1	G	263	THR
1	G	270	THR
1	G	273	LYS
1	G	288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	74	ASN
1	A	89	GLN
1	A	121	ASN
1	A	178	ASN
1	A	194	GLN
1	B	64	GLN
1	B	89	GLN
1	B	178	ASN
1	B	201	ASN
1	B	259	HIS
1	C	6	ASN
1	C	64	GLN
1	C	121	ASN
1	C	178	ASN
1	C	194	GLN
1	C	242	GLN
1	D	6	ASN
1	D	64	GLN
1	D	74	ASN
1	D	87	GLN

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Mol	Chain	Res	Type
1	D	121	ASN
1	D	178	ASN
1	E	64	GLN
1	E	74	ASN
1	E	121	ASN
1	E	178	ASN
1	E	194	GLN
1	F	64	GLN
1	F	121	ASN
1	F	178	ASN
1	F	194	GLN
1	G	64	GLN
1	G	74	ASN
1	G	178	ASN
1	G	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

47 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	PQJ	A	402	-	10,10,24	0.94	0	15,15,29	1.29	2 (13%)
3	SO4	B	405	-	4,4,4	0.30	0	6,6,6	0.04	0
3	SO4	D	405	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	B	404	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	A	406	-	4,4,4	0.31	0	6,6,6	0.07	0
3	SO4	C	404	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	G	408	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	A	405	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	G	405	-	4,4,4	0.28	0	6,6,6	0.12	0
2	PQJ	A	401	-	10,10,24	1.08	1 (10%)	15,15,29	2.10	3 (20%)
3	SO4	D	404	-	4,4,4	0.29	0	6,6,6	0.13	0
2	PQJ	B	401	-	10,10,24	0.95	0	15,15,29	1.80	3 (20%)
3	SO4	E	403	-	4,4,4	0.27	0	6,6,6	0.12	0
2	PQJ	E	401	-	10,10,24	1.52	1 (10%)	15,15,29	1.17	1 (6%)
2	PQJ	D	402	-	10,10,24	0.93	0	15,15,29	1.38	3 (20%)
3	SO4	C	406	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	C	405	-	4,4,4	0.30	0	6,6,6	0.11	0
3	SO4	G	403	-	4,4,4	0.27	0	6,6,6	0.13	0
2	PQJ	G	401	-	10,10,24	1.57	1 (10%)	15,15,29	1.44	3 (20%)
3	SO4	E	406	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	A	403	-	4,4,4	0.32	0	6,6,6	0.07	0
2	PQJ	G	402	-	11,11,24	0.84	0	15,16,29	0.83	1 (6%)
3	SO4	E	405	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	G	404	-	4,4,4	0.33	0	6,6,6	0.09	0
2	PQJ	F	402	-	10,10,24	1.01	1 (10%)	15,15,29	1.18	2 (13%)
3	SO4	A	409	-	4,4,4	0.29	0	6,6,6	0.19	0
3	SO4	C	403	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	F	406	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SO4	E	407	-	4,4,4	0.27	0	6,6,6	0.10	0
2	PQJ	F	401	-	10,10,24	1.47	1 (10%)	15,15,29	1.75	4 (26%)
3	SO4	C	407	-	4,4,4	0.31	0	6,6,6	0.08	0
3	SO4	B	403	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	F	404	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	A	407	-	4,4,4	0.31	0	6,6,6	0.14	0
2	PQJ	D	401	-	10,10,24	1.41	1 (10%)	15,15,29	1.42	3 (20%)
2	PQJ	C	402	-	10,10,24	1.01	1 (10%)	15,15,29	0.85	0
3	SO4	A	408	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	E	404	-	4,4,4	0.30	0	6,6,6	0.10	0
3	SO4	F	405	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	G	406	-	4,4,4	0.31	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	G	407	-	4,4,4	0.31	0	6,6,6	0.05	0
3	SO4	A	404	-	4,4,4	0.33	0	6,6,6	0.13	0
2	PQJ	C	401	-	10,10,24	1.34	1 (10%)	15,15,29	1.26	2 (13%)
2	PQJ	B	402	-	10,10,24	1.47	1 (10%)	15,15,29	1.28	3 (20%)
3	SO4	D	403	-	4,4,4	0.30	0	6,6,6	0.10	0
2	PQJ	E	402	-	10,10,24	1.39	1 (10%)	15,15,29	1.19	2 (13%)
3	SO4	F	403	-	4,4,4	0.28	0	6,6,6	0.15	0

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	PQJ	A	402	-	-	2/8/8/24	-
2	PQJ	B	401	-	-	0/8/8/24	-
2	PQJ	D	401	-	-	3/8/8/24	-
2	PQJ	C	402	-	-	4/8/8/24	-
2	PQJ	G	402	-	-	4/11/11/24	-
2	PQJ	E	401	-	-	0/8/8/24	-
2	PQJ	D	402	-	-	3/8/8/24	-
2	PQJ	F	401	-	-	2/8/8/24	-
2	PQJ	C	401	-	-	4/8/8/24	-
2	PQJ	B	402	-	-	2/8/8/24	-
2	PQJ	F	402	-	-	6/8/8/24	-
2	PQJ	G	401	-	-	4/8/8/24	-
2	PQJ	E	402	-	-	7/8/8/24	-
2	PQJ	A	401	-	-	4/8/8/24	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	PQJ	P1-O3	4.14	1.63	1.50
2	B	402	PQJ	P1-O3	3.97	1.62	1.50
2	G	401	PQJ	P1-O3	3.93	1.62	1.50
2	F	401	PQJ	P1-O3	3.79	1.62	1.50
2	D	401	PQJ	P1-O3	3.76	1.62	1.50
2	C	401	PQJ	P1-O3	3.55	1.61	1.50
2	E	402	PQJ	P1-O3	3.27	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PQJ	P1-O1	2.26	1.63	1.54
2	F	402	PQJ	P1-O1	2.12	1.62	1.54
2	C	402	PQJ	P1-O1	2.09	1.62	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PQJ	O1-P1-O4	-5.91	91.25	106.67
2	B	401	PQJ	O1-P1-O4	-4.59	94.70	106.67
2	F	401	PQJ	O4-P1-O3	-4.48	94.32	106.44
2	A	401	PQJ	O2-P1-O4	4.21	117.65	106.67
2	B	401	PQJ	O2-P1-O4	3.87	116.77	106.67
2	C	401	PQJ	O1-P1-O2	3.08	119.36	107.80
2	E	402	PQJ	O1-P1-O2	3.03	119.17	107.80
2	G	401	PQJ	P1-O4-C1	3.01	126.39	118.21
2	F	401	PQJ	O1-P1-O2	2.78	118.24	107.80
2	B	402	PQJ	P1-O4-C1	2.77	125.75	118.21
2	D	401	PQJ	O4-P1-O3	-2.72	99.08	106.44
2	D	401	PQJ	O1-P1-O2	2.72	117.99	107.80
2	F	402	PQJ	O2-P1-O4	2.70	113.71	106.67
2	D	402	PQJ	O1-P1-O4	-2.69	99.65	106.67
2	A	402	PQJ	O2-P1-O4	2.62	113.50	106.67
2	B	401	PQJ	P1-O4-C1	2.61	125.32	118.21
2	E	402	PQJ	O4-P1-O3	-2.53	99.61	106.44
2	A	401	PQJ	O4-P1-O3	2.52	113.26	106.44
2	E	401	PQJ	P1-O4-C1	2.52	125.06	118.21
2	G	401	PQJ	O4-P1-O3	-2.49	99.70	106.44
2	G	402	PQJ	C1-C2-N1	-2.49	107.82	115.82
2	G	401	PQJ	C3-N1-C5	-2.48	102.47	108.98
2	F	401	PQJ	O2-P1-O4	2.45	113.05	106.67
2	A	402	PQJ	O2-P1-O3	2.43	120.31	110.83
2	D	402	PQJ	O4-P1-O3	2.41	112.97	106.44
2	B	402	PQJ	O1-P1-O2	2.36	116.64	107.80
2	F	402	PQJ	O1-P1-O4	-2.36	100.53	106.67
2	D	401	PQJ	P1-O4-C1	2.32	124.50	118.21
2	B	402	PQJ	O1-P1-O4	2.27	112.58	106.67
2	F	401	PQJ	P1-O4-C1	2.26	124.34	118.21
2	C	401	PQJ	O4-P1-O3	-2.18	100.54	106.44
2	D	402	PQJ	O2-P1-O3	2.01	118.65	110.83

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PQJ	O4-C1-C2-N1
2	B	402	PQJ	C1-O4-P1-O1
2	C	401	PQJ	C1-O4-P1-O2
2	C	401	PQJ	C1-O4-P1-O3
2	C	401	PQJ	C1-O4-P1-O1
2	E	402	PQJ	C1-O4-P1-O2
2	E	402	PQJ	C1-O4-P1-O1
2	F	401	PQJ	C1-O4-P1-O2
2	F	401	PQJ	O4-C1-C2-N1
2	F	402	PQJ	C1-O4-P1-O2
2	F	402	PQJ	O4-C1-C2-N1
2	G	401	PQJ	C1-O4-P1-O2
2	G	401	PQJ	C1-O4-P1-O3
2	G	401	PQJ	C1-O4-P1-O1
2	G	401	PQJ	O4-C1-C2-N1
2	G	402	PQJ	C1-O4-P1-O2
2	G	402	PQJ	C1-O4-P1-O3
2	G	402	PQJ	C1-O4-P1-O1
2	G	402	PQJ	O4-C1-C2-N1
2	F	402	PQJ	C1-C2-N1-C3
2	F	402	PQJ	C1-C2-N1-C4
2	A	401	PQJ	C1-C2-N1-C5
2	A	401	PQJ	C1-C2-N1-C4
2	A	401	PQJ	C1-C2-N1-C3
2	F	402	PQJ	C1-C2-N1-C5
2	E	402	PQJ	C1-O4-P1-O3
2	F	402	PQJ	C1-O4-P1-O3
2	D	402	PQJ	C1-C2-N1-C3
2	A	402	PQJ	C1-O4-P1-O2
2	B	402	PQJ	C2-C1-O4-P1
2	A	402	PQJ	O4-C1-C2-N1
2	C	402	PQJ	O4-C1-C2-N1
2	E	402	PQJ	O4-C1-C2-N1
2	D	402	PQJ	C1-C2-N1-C4
2	D	401	PQJ	C1-C2-N1-C4
2	D	402	PQJ	C1-C2-N1-C5
2	D	401	PQJ	C1-C2-N1-C5
2	C	401	PQJ	C1-C2-N1-C4
2	C	402	PQJ	C1-C2-N1-C3
2	E	402	PQJ	C1-C2-N1-C3
2	C	402	PQJ	C1-C2-N1-C5
2	C	402	PQJ	C1-C2-N1-C4
2	D	401	PQJ	C1-C2-N1-C3

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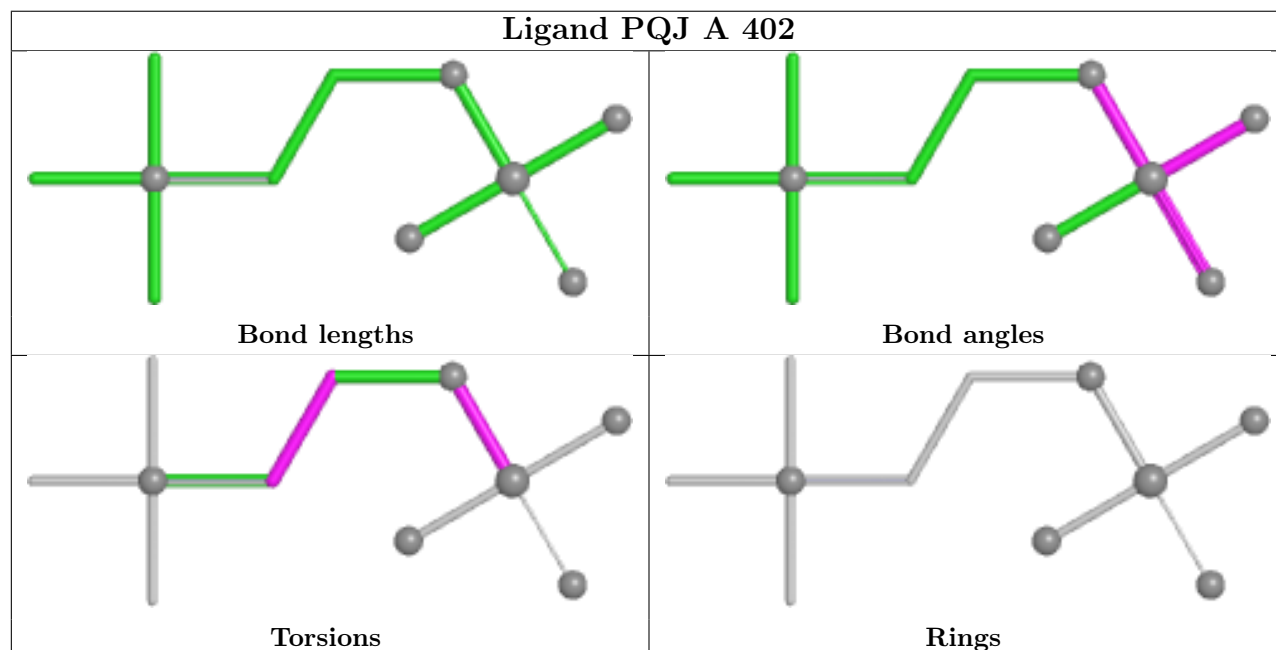
Mol	Chain	Res	Type	Atoms
2	E	402	PQJ	C1-C2-N1-C5
2	E	402	PQJ	C1-C2-N1-C4

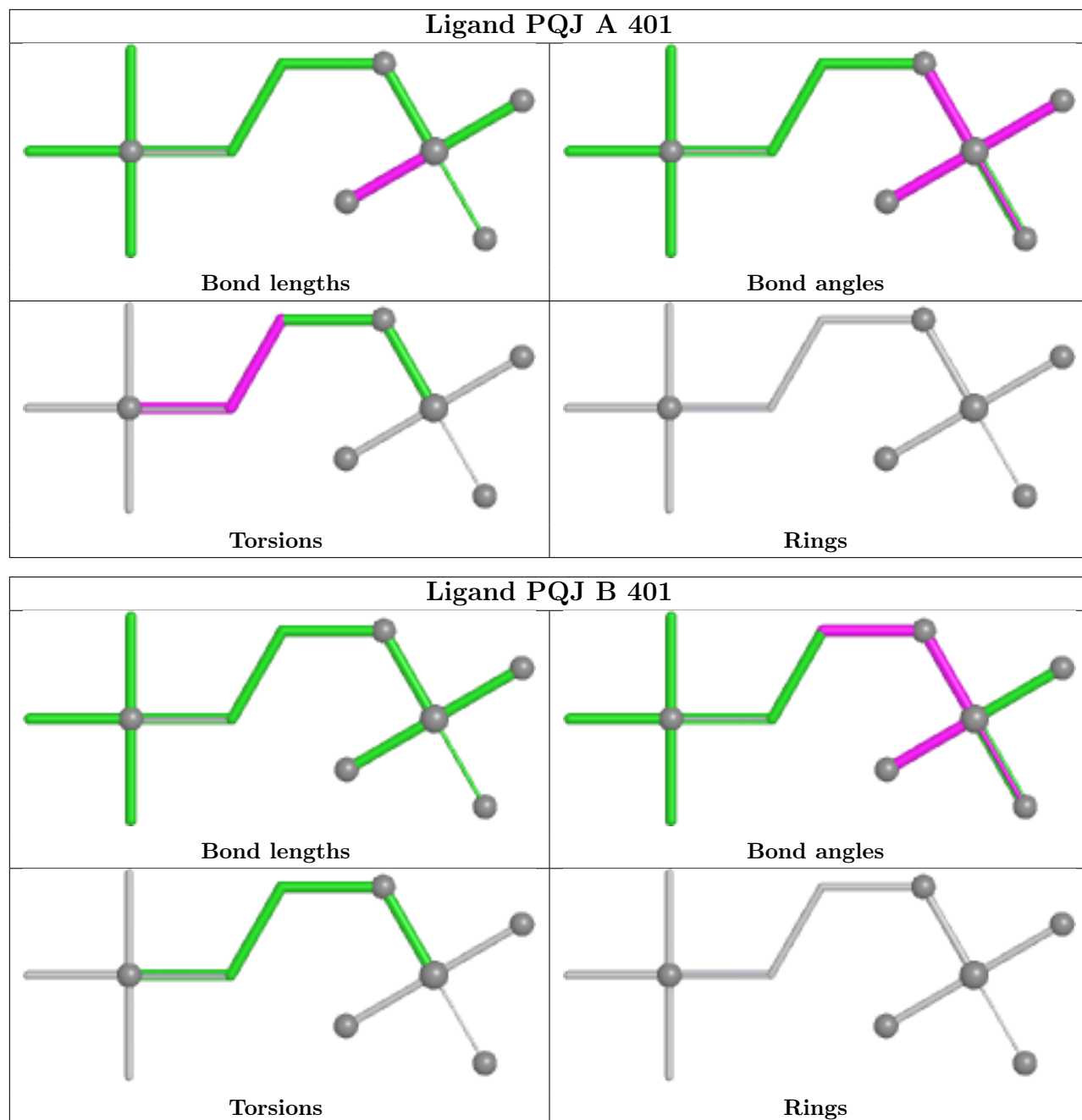
There are no ring outliers.

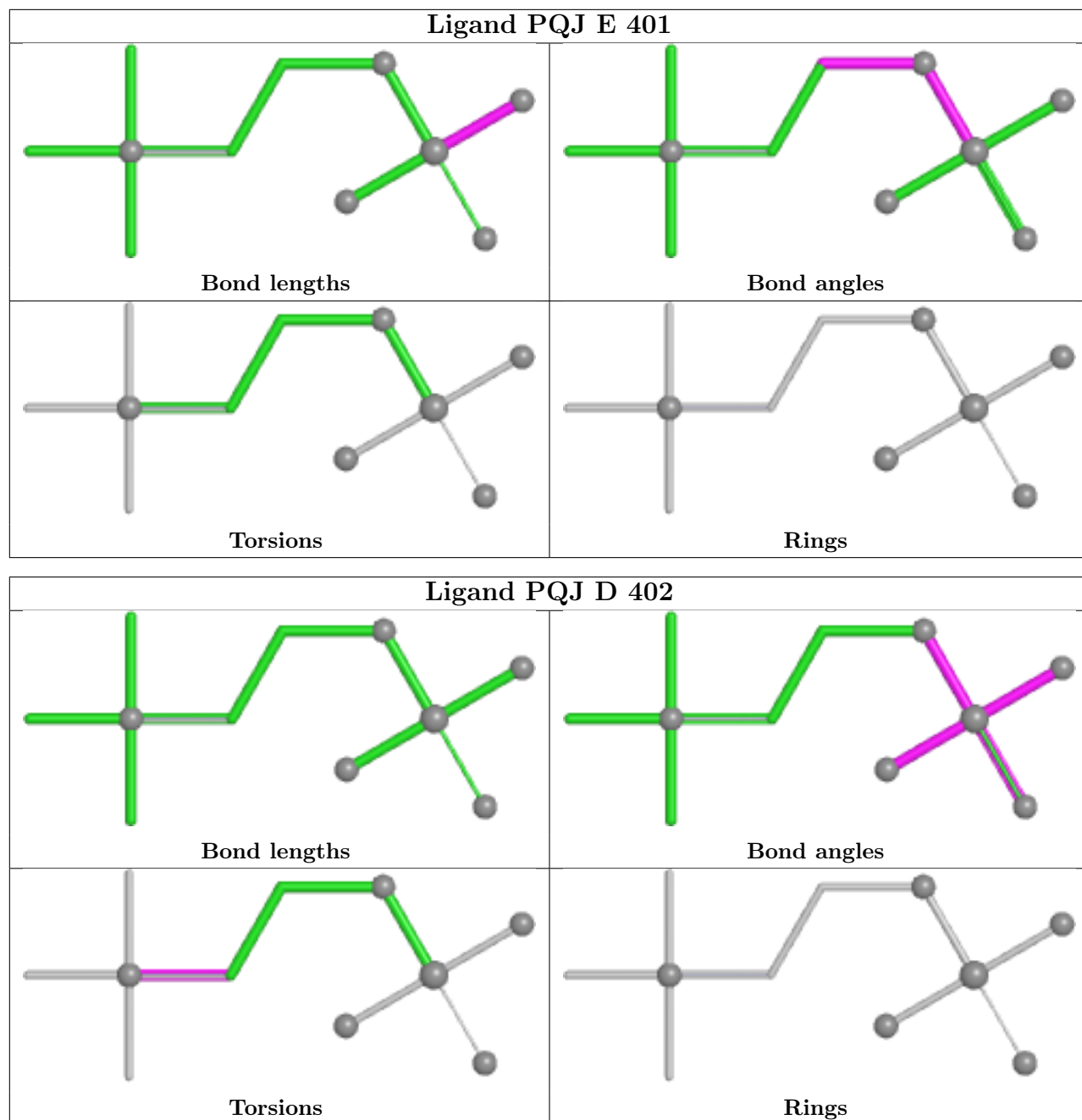
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	403	SO4	2	0
2	G	402	PQJ	2	0
3	A	409	SO4	1	0
3	A	408	SO4	1	0
2	E	402	PQJ	2	0

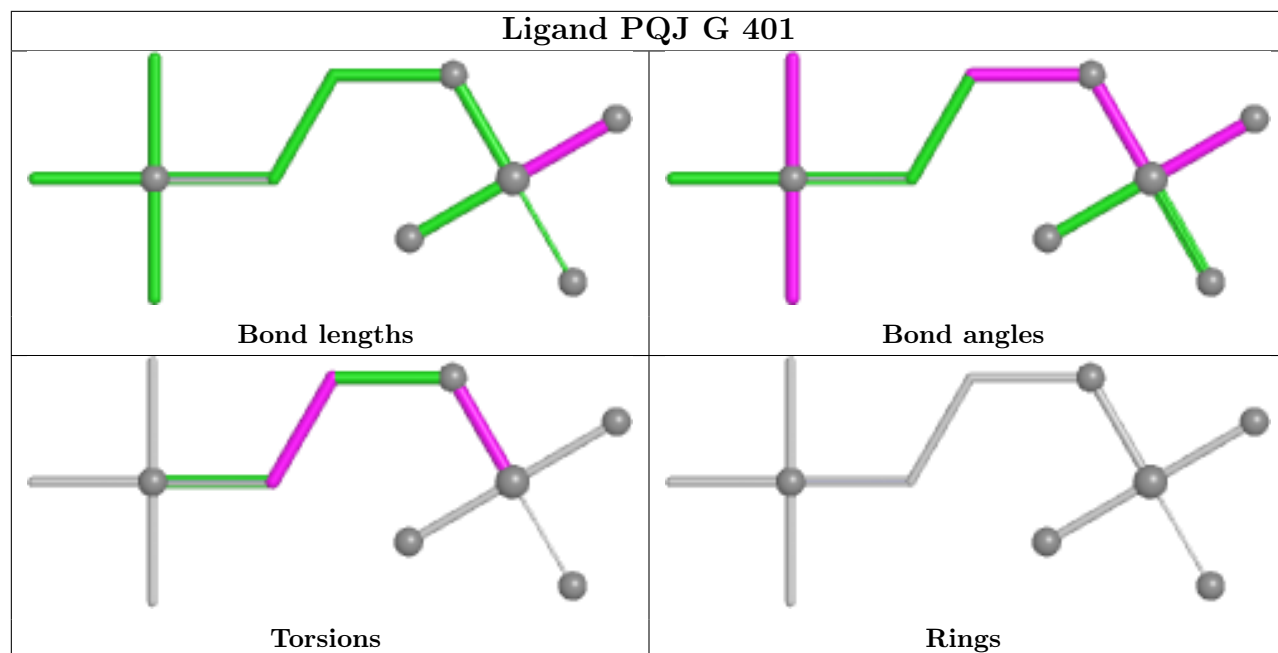
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



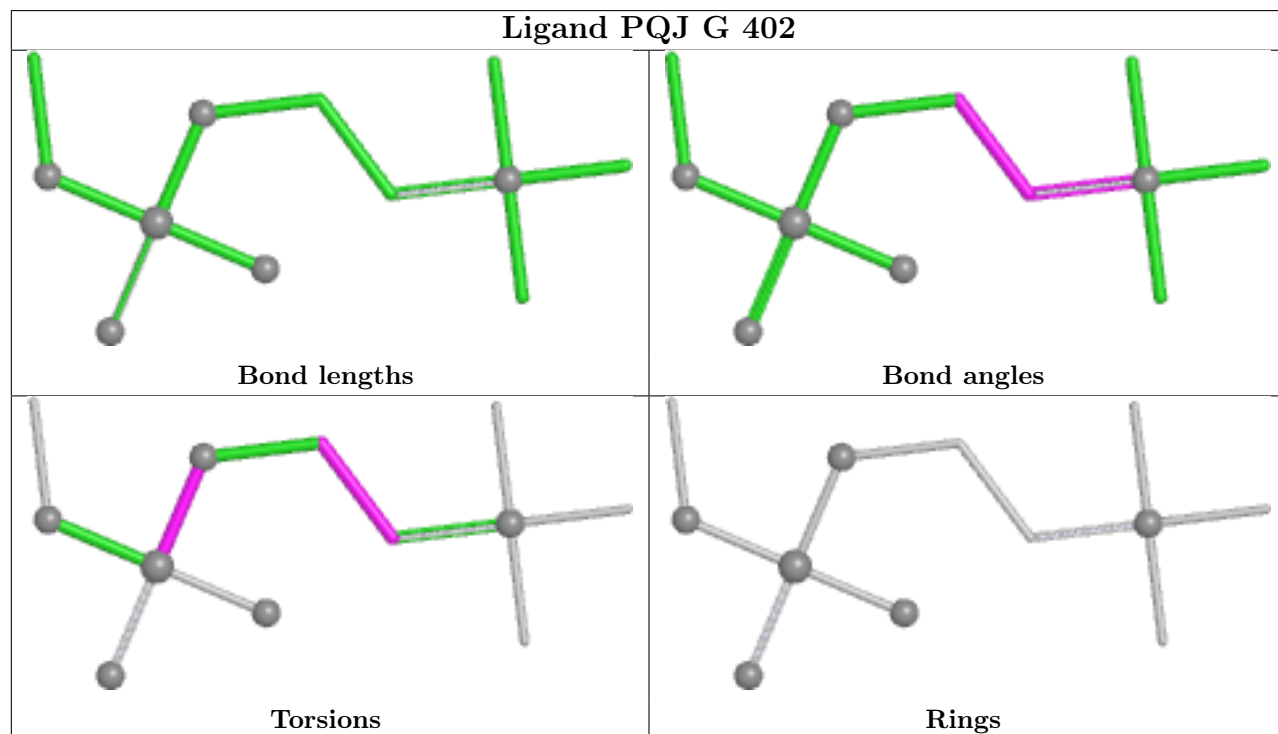


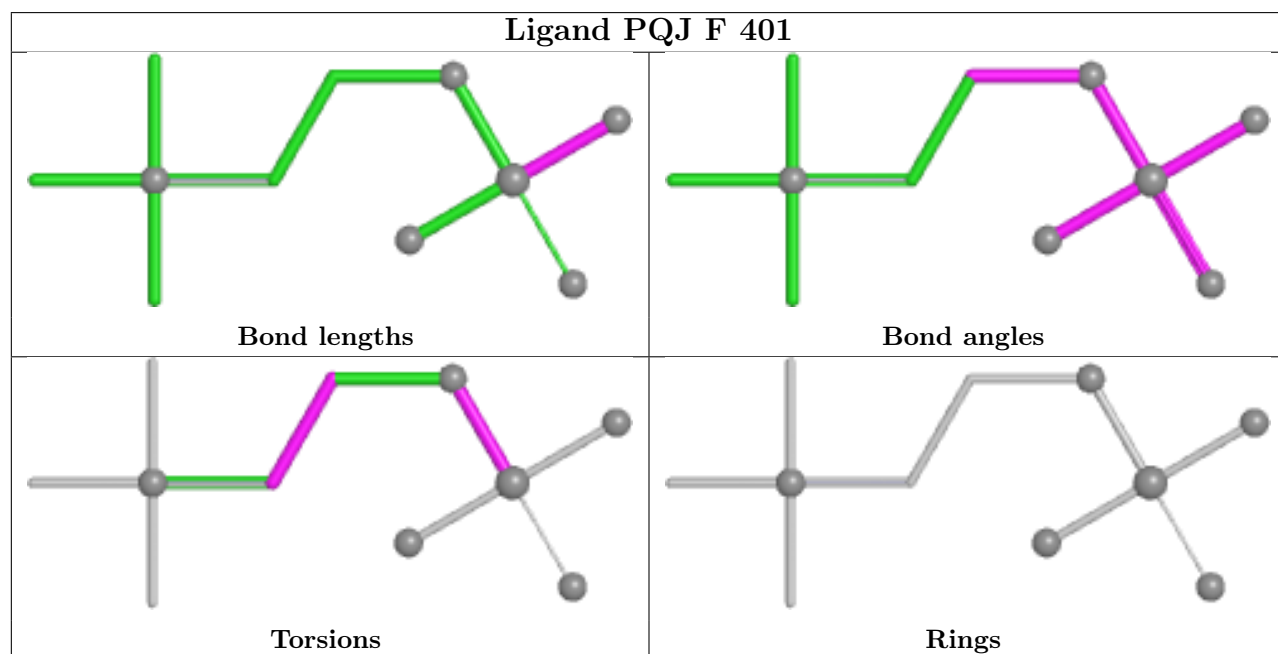
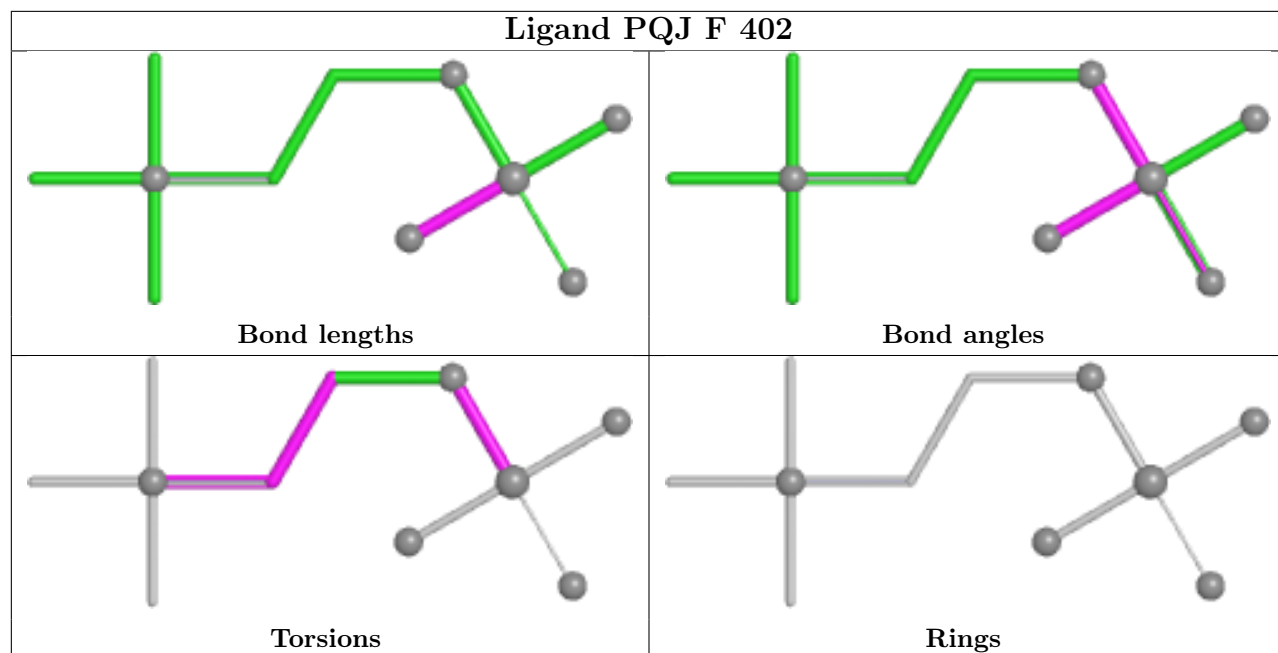


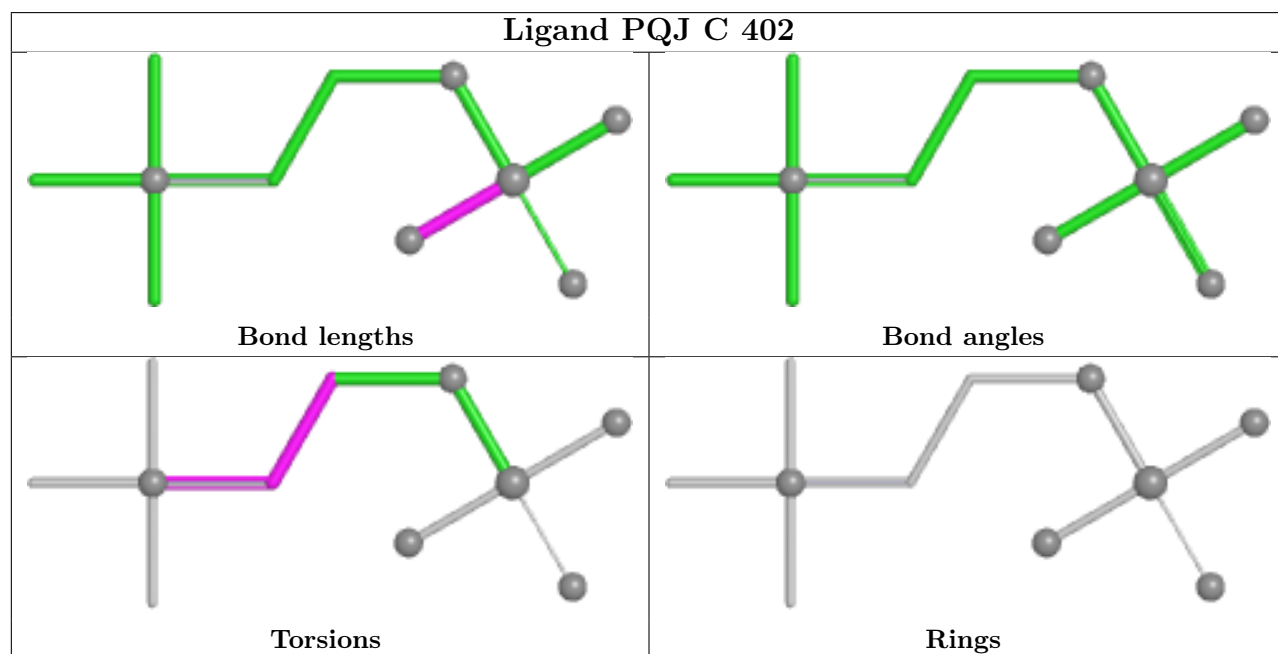
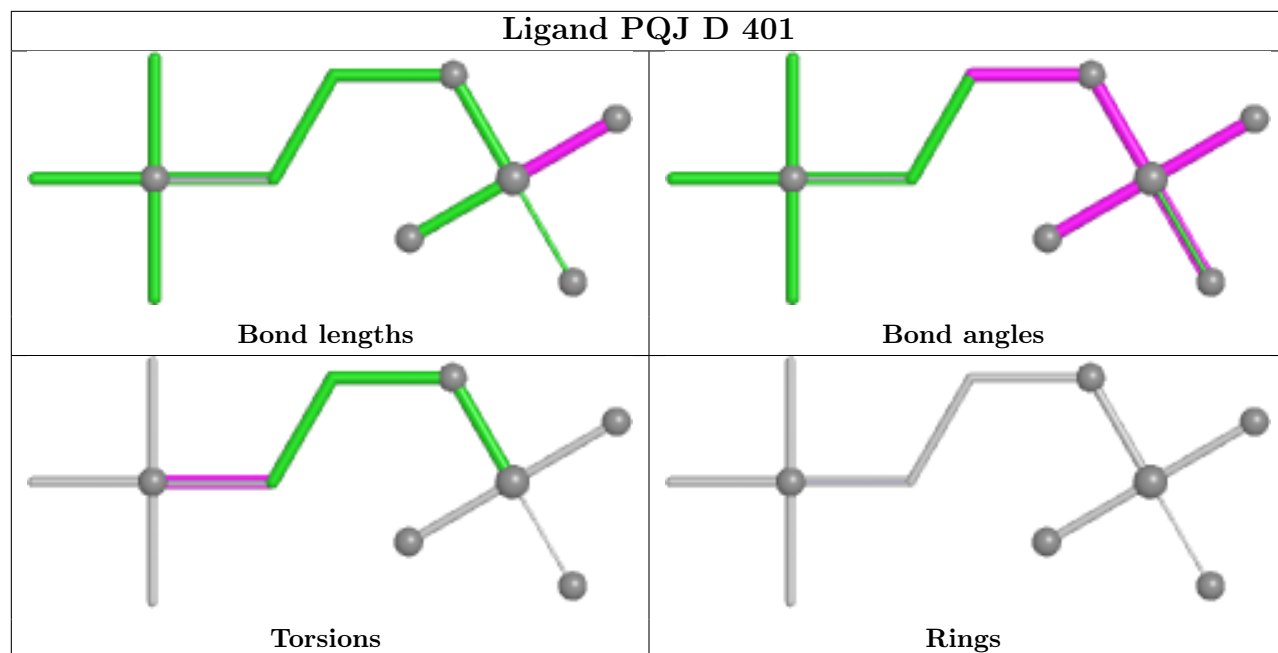
Ligand PQJ G 401

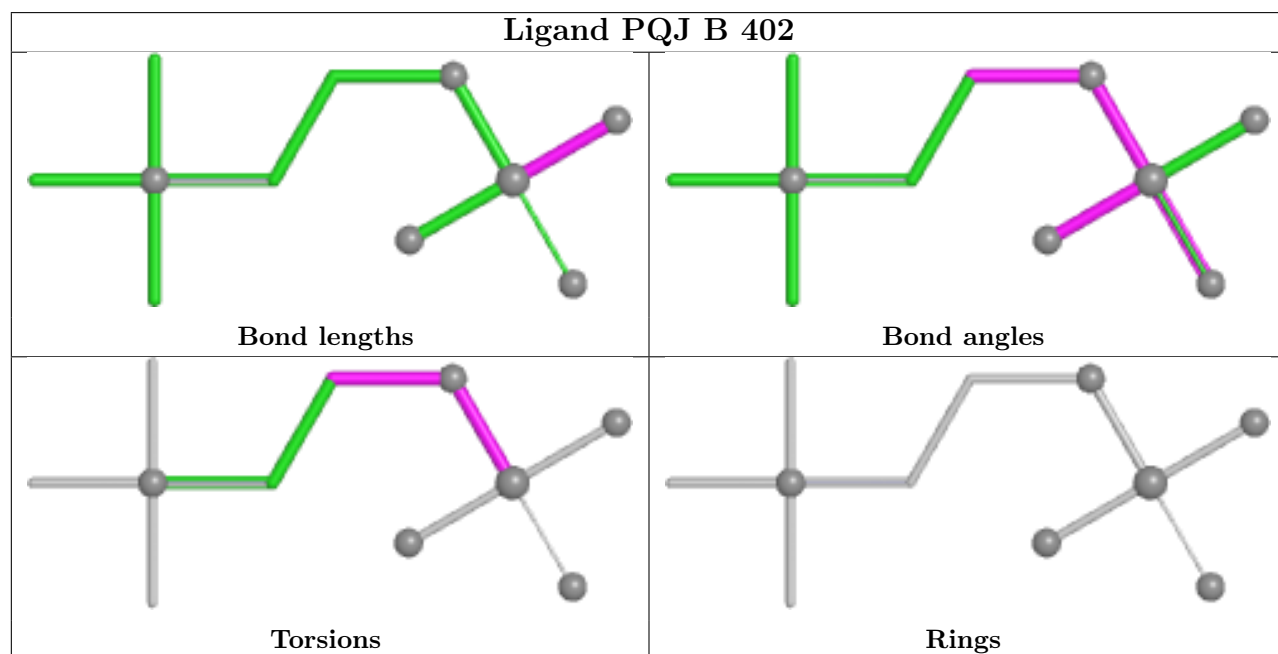
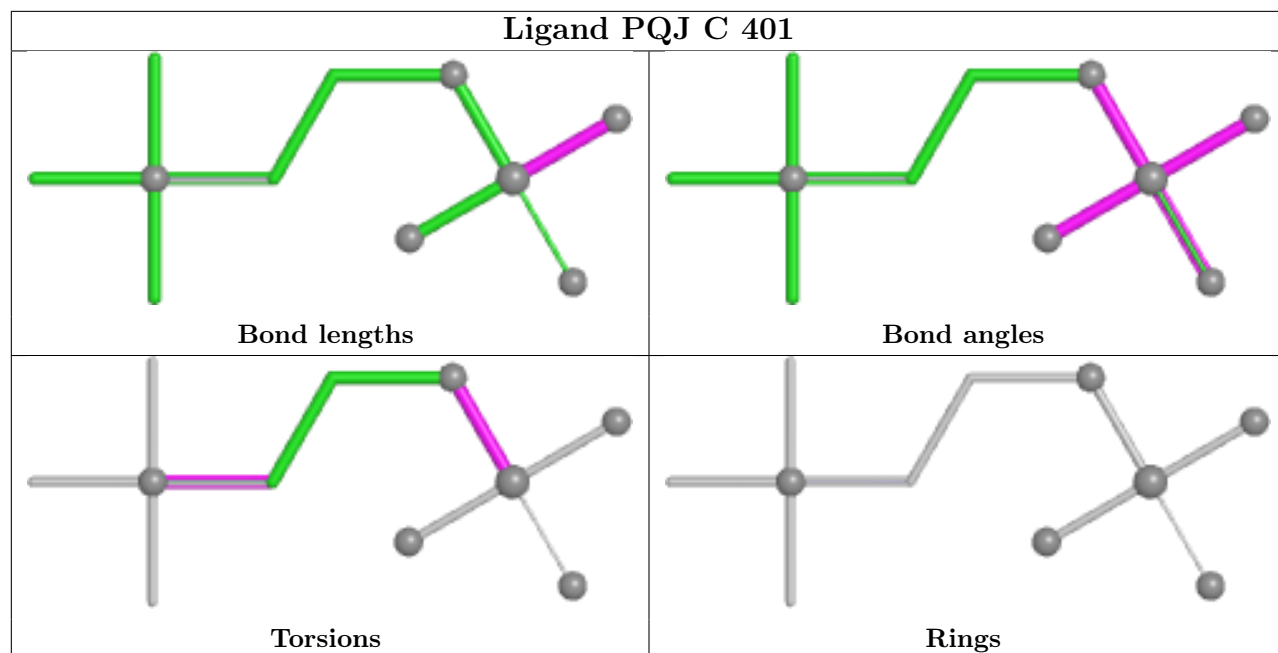


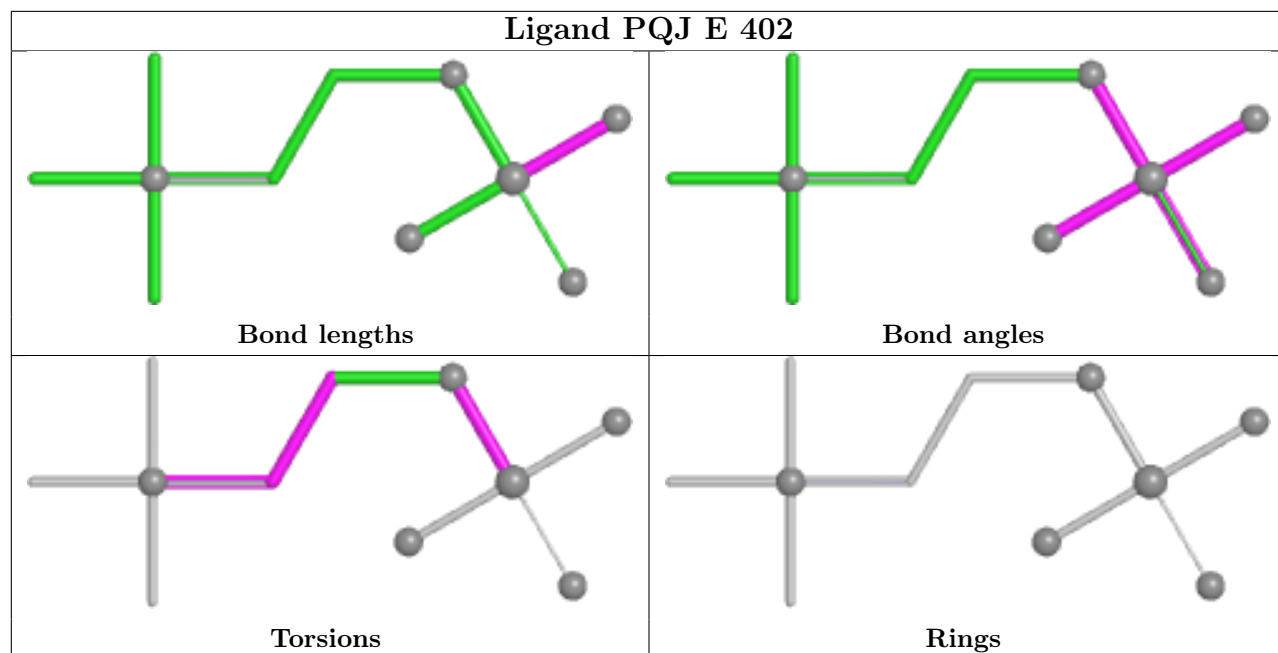
Ligand PQJ G 402











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	293/293 (100%)	0.84	26 (8%)	15 13	52, 73, 119, 186	0
1	B	293/293 (100%)	0.79	26 (8%)	15 13	48, 72, 122, 212	0
1	C	293/293 (100%)	0.81	25 (8%)	16 14	51, 72, 127, 173	0
1	D	293/293 (100%)	0.70	21 (7%)	21 19	47, 67, 123, 176	0
1	E	293/293 (100%)	0.64	25 (8%)	16 14	47, 65, 115, 167	0
1	F	293/293 (100%)	0.66	21 (7%)	21 19	47, 66, 122, 171	0
1	G	293/293 (100%)	0.70	20 (6%)	23 20	47, 68, 115, 148	0
All	All	2051/2051 (100%)	0.73	164 (7%)	18 16	47, 69, 121, 212	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	65	TYR	5.7
1	B	65	TYR	5.4
1	E	120	PHE	5.3
1	F	120	PHE	4.8
1	F	69	SER	4.8
1	D	69	SER	4.4
1	E	69	SER	4.0
1	A	65	TYR	3.9
1	B	10	GLY	3.7
1	B	69	SER	3.7
1	G	65	TYR	3.7
1	D	1	ALA	3.7
1	D	132	ILE	3.6
1	B	72	GLY	3.5
1	C	207	ALA	3.5
1	A	132	ILE	3.5
1	E	138	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	73	ALA	3.4
1	D	66	ARG	3.3
1	D	71	GLU	3.3
1	D	7	ILE	3.3
1	D	120	PHE	3.2
1	C	69	SER	3.2
1	A	17	ASN	3.2
1	F	118	TYR	3.2
1	A	118	TYR	3.2
1	E	65	TYR	3.2
1	C	66	ARG	3.1
1	B	132	ILE	3.1
1	E	1	ALA	3.1
1	B	128	ASP	3.1
1	D	65	TYR	3.1
1	G	132	ILE	3.1
1	B	129	THR	3.1
1	G	68	TYR	3.1
1	B	71	GLU	3.1
1	C	120	PHE	3.1
1	G	72	GLY	3.0
1	A	77	GLY	3.0
1	E	118	TYR	2.9
1	F	71	GLU	2.9
1	A	120	PHE	2.9
1	A	72	GLY	2.9
1	B	124	VAL	2.9
1	E	72	GLY	2.9
1	D	10	GLY	2.8
1	E	93	ASN	2.8
1	G	3	SER	2.8
1	A	73	ALA	2.8
1	B	125	THR	2.8
1	B	66	ARG	2.8
1	A	10	GLY	2.7
1	F	132	ILE	2.7
1	B	239	SER	2.7
1	D	207	ALA	2.7
1	G	69	SER	2.7
1	E	128	ASP	2.7
1	G	142	ILE	2.7
1	B	93	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	68	TYR	2.7
1	A	128	ASP	2.7
1	D	128	ASP	2.7
1	C	72	GLY	2.7
1	A	67	VAL	2.7
1	B	73	ALA	2.7
1	E	290	GLU	2.7
1	B	130	GLY	2.6
1	D	142	ILE	2.6
1	G	120	PHE	2.6
1	A	69	SER	2.6
1	E	73	ALA	2.6
1	G	128	ASP	2.6
1	B	68	TYR	2.6
1	F	93	ASN	2.6
1	C	1	ALA	2.6
1	F	142	ILE	2.6
1	F	268	THR	2.6
1	G	18	THR	2.6
1	F	240	LYS	2.6
1	G	93	ASN	2.5
1	B	9	THR	2.5
1	D	129	THR	2.5
1	E	235	ASP	2.5
1	B	144	HIS	2.5
1	F	123	ASN	2.5
1	F	73	ALA	2.5
1	F	126	GLY	2.5
1	F	130	GLY	2.5
1	A	92	ASP	2.5
1	E	142	ILE	2.5
1	G	237	LYS	2.5
1	B	123	ASN	2.5
1	B	120	PHE	2.5
1	E	132	ILE	2.4
1	G	1	ALA	2.4
1	E	129	THR	2.4
1	A	190	VAL	2.4
1	A	129	THR	2.4
1	A	262	SER	2.4
1	C	128	ASP	2.4
1	E	144	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	17	ASN	2.4
1	D	273	LYS	2.4
1	E	130	GLY	2.3
1	A	66	ARG	2.3
1	G	118	TYR	2.3
1	G	189	PRO	2.3
1	E	9	THR	2.3
1	D	15	GLY	2.3
1	C	255	ASP	2.3
1	A	142	ILE	2.3
1	B	262	SER	2.3
1	E	75	LYS	2.3
1	G	66	ARG	2.3
1	A	207	ALA	2.2
1	B	261	THR	2.2
1	D	72	GLY	2.2
1	D	93	ASN	2.2
1	C	270	THR	2.2
1	E	19	THR	2.2
1	E	239	SER	2.2
1	C	189	PRO	2.2
1	C	190	VAL	2.2
1	E	242	GLN	2.2
1	C	5	ILE	2.2
1	C	108	ASP	2.2
1	A	215	LYS	2.2
1	G	17	ASN	2.2
1	B	11	THR	2.2
1	C	11	THR	2.2
1	G	115	THR	2.2
1	C	222	SER	2.2
1	D	106	SER	2.2
1	A	196	PHE	2.2
1	F	144	HIS	2.1
1	G	16	SER	2.1
1	F	140	VAL	2.1
1	D	17	ASN	2.1
1	F	18	THR	2.1
1	A	200	ARG	2.1
1	A	124	VAL	2.1
1	C	179	TRP	2.1
1	E	74	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	268	THR	2.1
1	C	10	GLY	2.1
1	F	92	ASP	2.1
1	B	201	ASN	2.1
1	C	74	ASN	2.1
1	F	293	ASN	2.1
1	C	126	GLY	2.1
1	C	268	THR	2.1
1	B	92	ASP	2.1
1	F	191	TYR	2.1
1	A	130	GLY	2.0
1	F	72	GLY	2.0
1	C	132	ILE	2.0
1	E	8	LYS	2.0
1	A	13	ASP	2.0
1	C	118	TYR	2.0
1	D	262	SER	2.0
1	E	16	SER	2.0
1	B	17	ASN	2.0
1	G	192	GLY	2.0
1	C	274	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	403	5/5	0.53	0.14	123,129,142,154	0
3	SO4	A	406	5/5	0.58	0.16	119,131,140,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	G	403	5/5	0.63	0.15	98,101,118,121	0
3	SO4	F	403	5/5	0.67	0.13	114,117,124,136	0
3	SO4	B	404	5/5	0.67	0.14	107,112,122,134	0
3	SO4	G	405	5/5	0.68	0.12	129,131,144,159	0
3	SO4	G	406	5/5	0.69	0.16	101,107,130,143	0
3	SO4	G	404	5/5	0.70	0.13	106,106,131,132	0
3	SO4	G	408	5/5	0.70	0.15	100,117,135,141	0
3	SO4	E	403	5/5	0.71	0.12	89,102,111,117	0
3	SO4	F	406	5/5	0.72	0.17	95,106,112,136	0
3	SO4	C	407	5/5	0.72	0.20	135,139,149,164	0
3	SO4	A	405	5/5	0.74	0.09	104,110,118,122	0
3	SO4	B	405	5/5	0.74	0.13	94,116,126,145	0
2	PQJ	B	402	11/25	0.74	0.23	84,124,144,147	0
3	SO4	D	403	5/5	0.74	0.12	116,118,128,135	0
3	SO4	B	403	5/5	0.75	0.13	109,117,134,143	0
3	SO4	E	404	5/5	0.75	0.10	108,122,130,131	0
3	SO4	C	403	5/5	0.75	0.14	120,123,125,135	0
3	SO4	A	409	5/5	0.76	0.17	113,115,119,121	0
3	SO4	A	404	5/5	0.76	0.11	113,113,120,124	0
3	SO4	F	404	5/5	0.76	0.11	103,108,128,132	0
2	PQJ	G	402	12/25	0.77	0.23	89,114,126,128	0
3	SO4	C	404	5/5	0.77	0.11	96,110,124,133	0
3	SO4	E	405	5/5	0.79	0.14	99,106,117,118	0
3	SO4	E	407	5/5	0.79	0.18	105,113,128,143	0
3	SO4	D	405	5/5	0.79	0.12	91,117,124,129	0
2	PQJ	D	402	11/25	0.79	0.21	77,109,127,128	0
3	SO4	C	405	5/5	0.79	0.09	92,106,116,127	0
3	SO4	F	405	5/5	0.80	0.12	90,111,118,125	0
2	PQJ	E	402	11/25	0.81	0.24	76,108,151,154	0
2	PQJ	F	402	11/25	0.81	0.19	79,101,118,127	0
3	SO4	E	406	5/5	0.83	0.12	101,112,124,126	0
3	SO4	D	404	5/5	0.84	0.10	93,124,129,134	0
2	PQJ	C	402	11/25	0.84	0.20	94,113,128,130	0
3	SO4	G	407	5/5	0.85	0.10	106,108,113,141	0
3	SO4	A	408	5/5	0.86	0.13	95,95,115,127	0
2	PQJ	A	402	11/25	0.87	0.16	73,108,116,121	0
3	SO4	C	406	5/5	0.87	0.09	97,111,121,123	0
2	PQJ	G	401	11/25	0.87	0.13	68,92,117,127	0
2	PQJ	A	401	11/25	0.88	0.15	68,91,108,110	0
2	PQJ	D	401	11/25	0.89	0.14	70,83,102,103	0
2	PQJ	E	401	11/25	0.90	0.12	69,79,91,94	0
3	SO4	A	407	5/5	0.90	0.10	102,116,123,123	0

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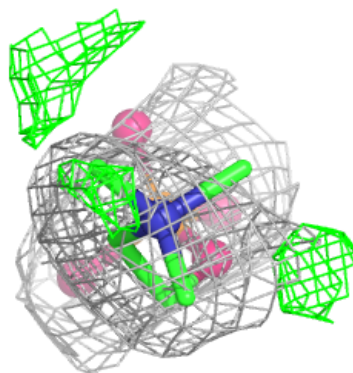
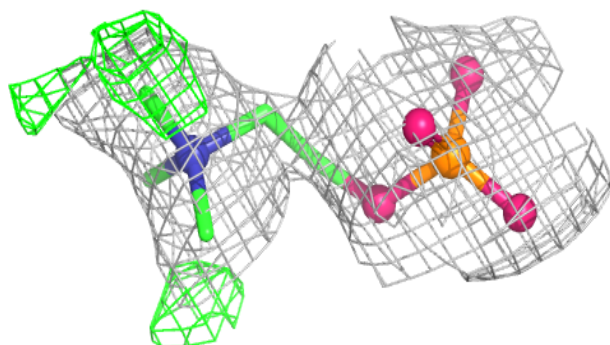
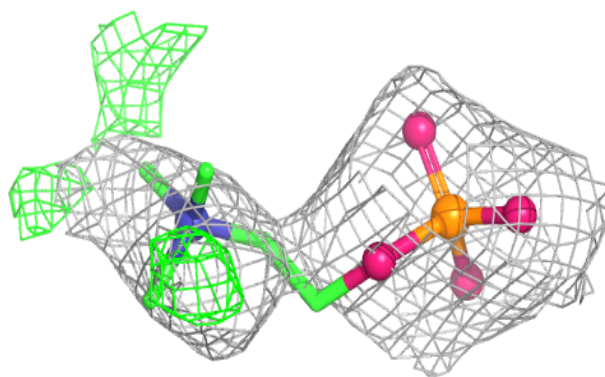
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PQJ	B	401	11/25	0.90	0.12	70,89,105,107	0
2	PQJ	C	401	11/25	0.91	0.12	76,93,110,126	0
2	PQJ	F	401	11/25	0.91	0.11	62,75,98,101	0

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.

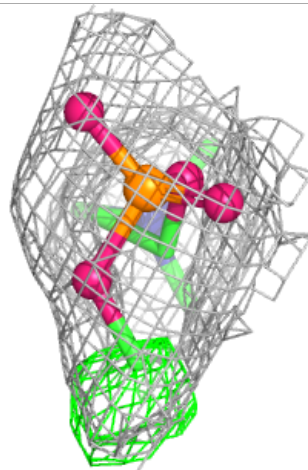
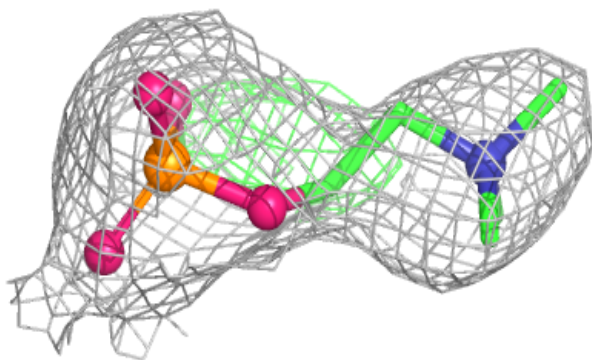
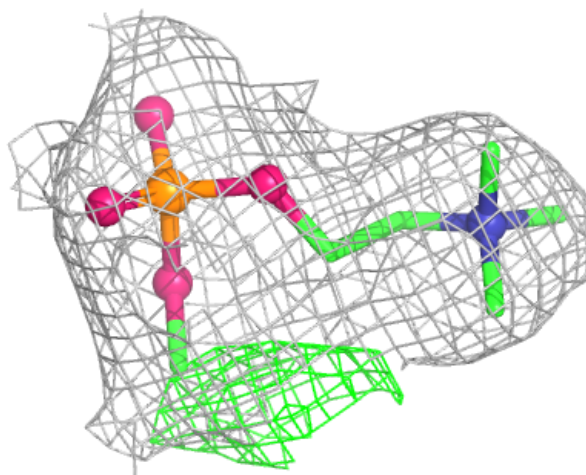
Electron density around PQJ B 402:

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



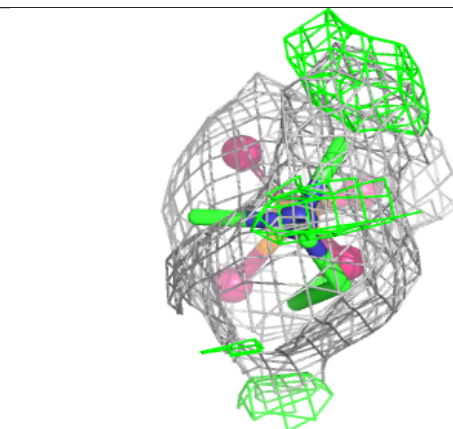
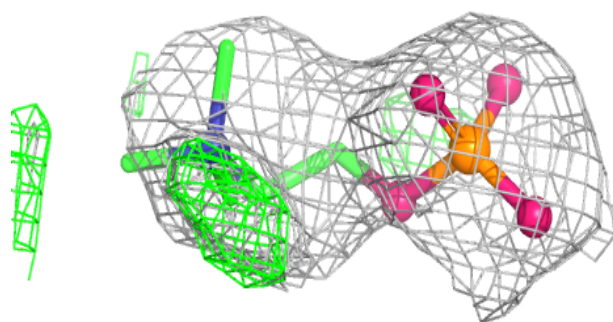
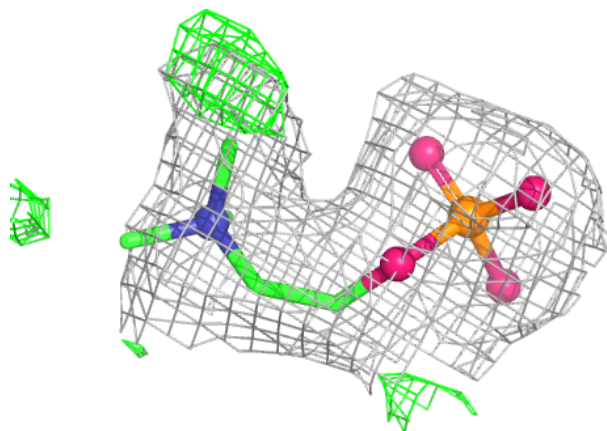
Electron density around PQJ G 402:

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

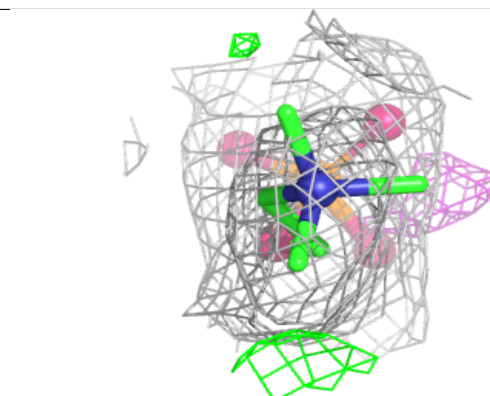
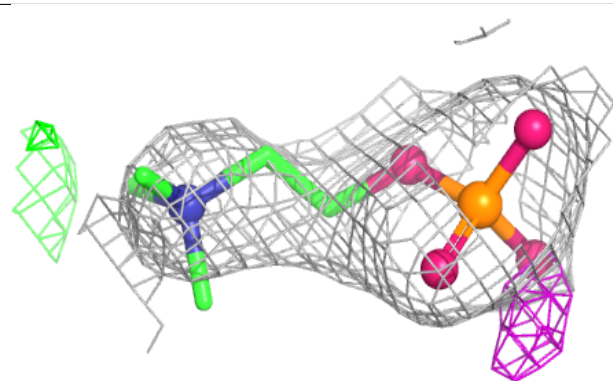
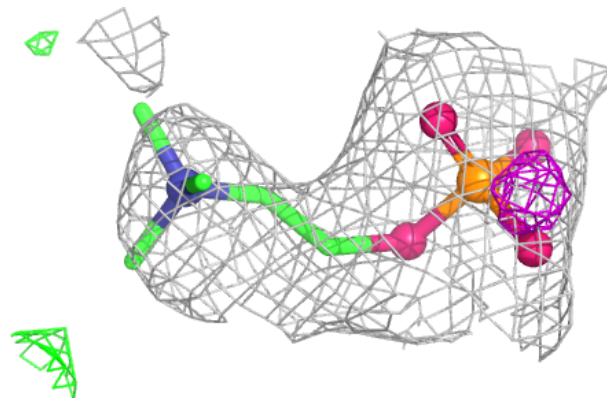


Electron density around PQJ D 402:

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

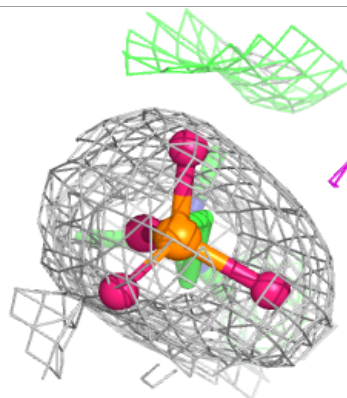
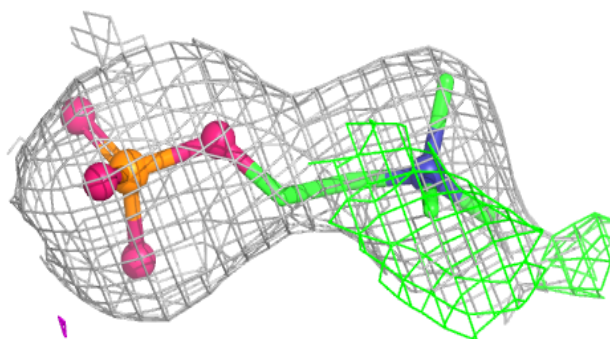
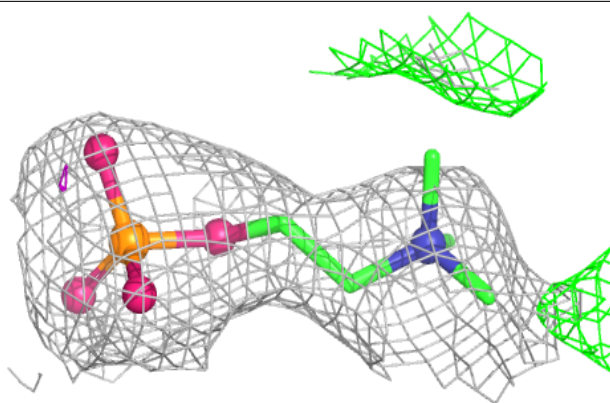
**Electron density around PQJ E 402:**

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

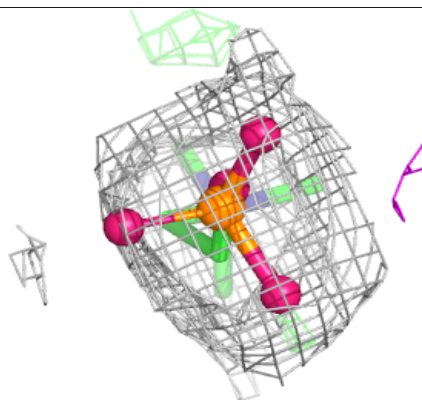
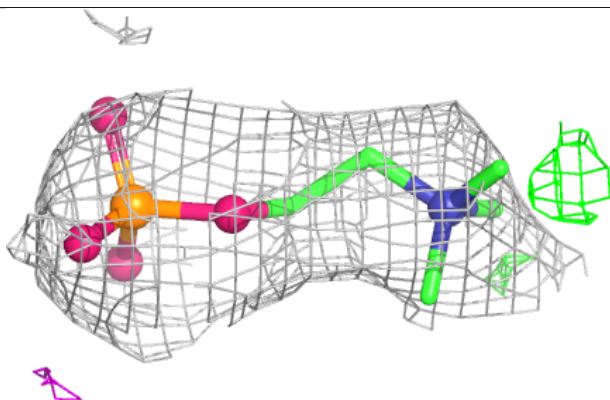
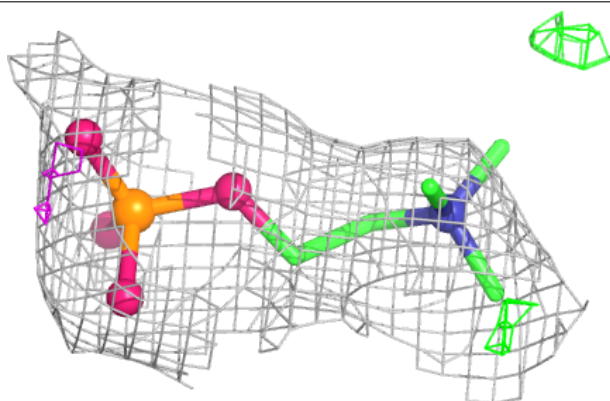


Electron density around PQJ F 402:

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

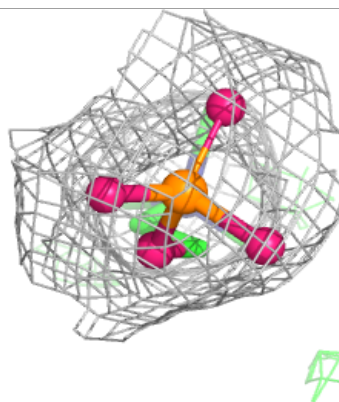
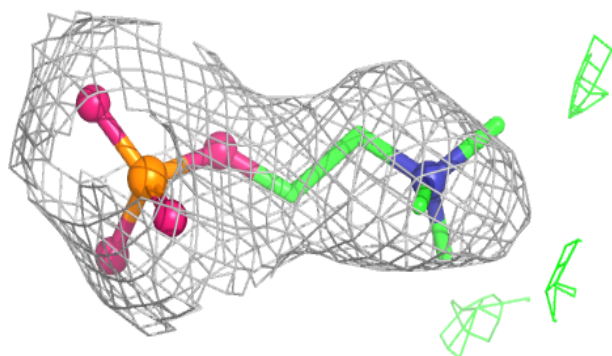
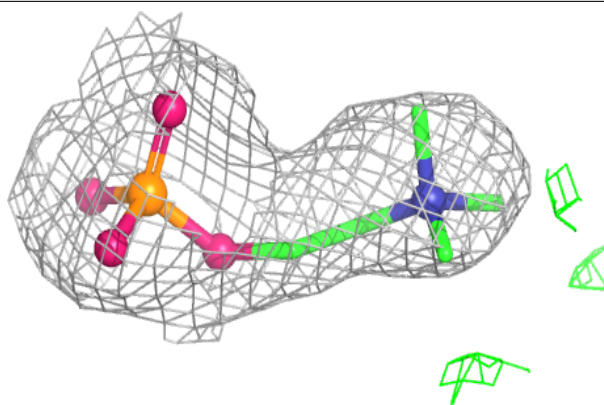
**Electron density around PQJ C 402:**

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

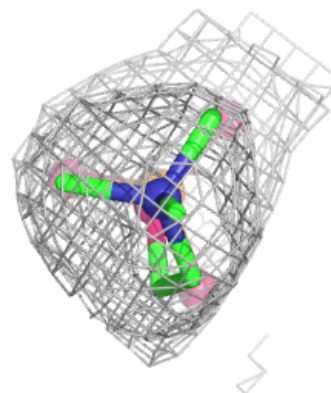
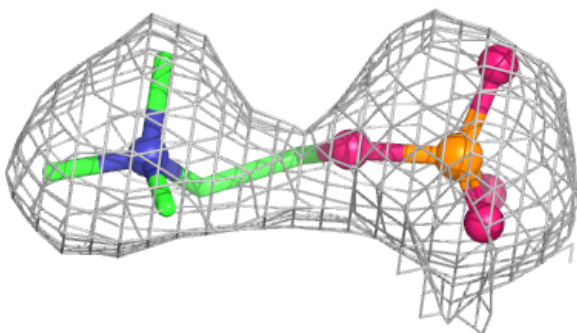
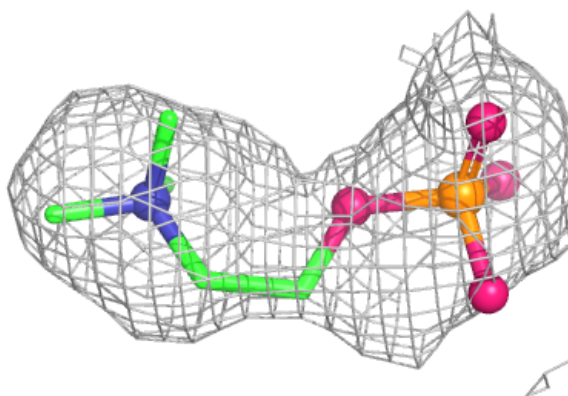


Electron density around PQJ A 402:

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

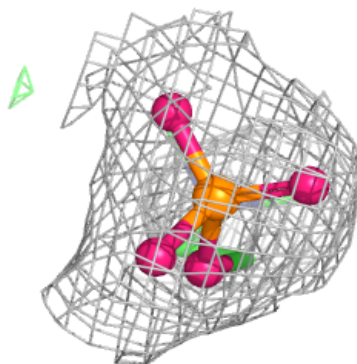
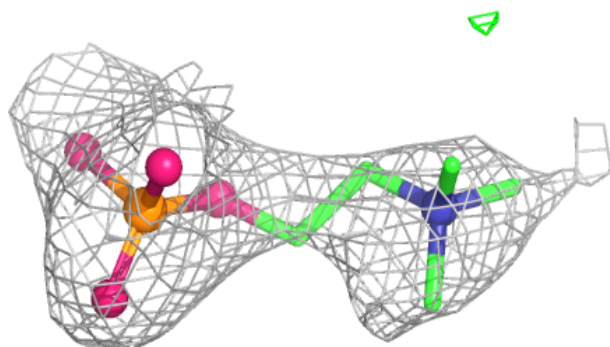
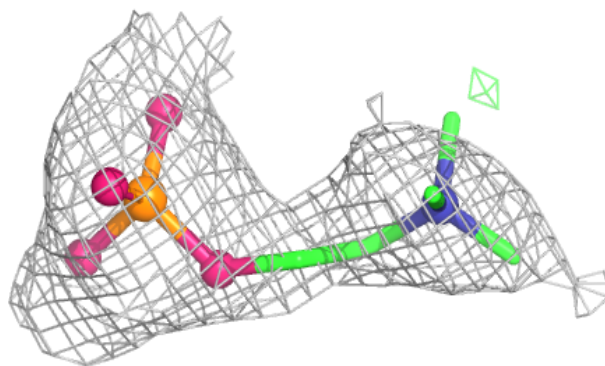
**Electron density around PQJ G 401:**

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

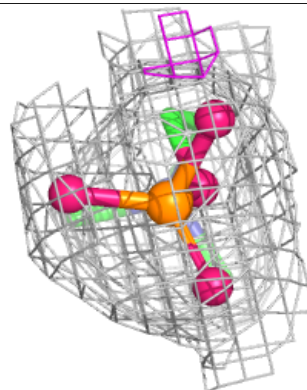
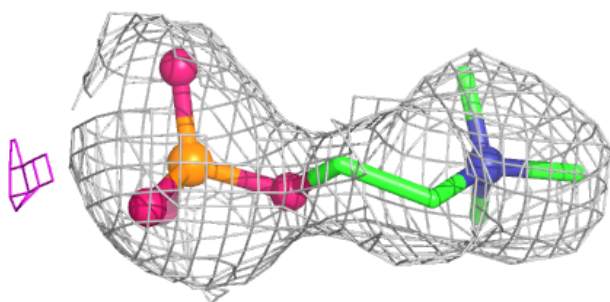
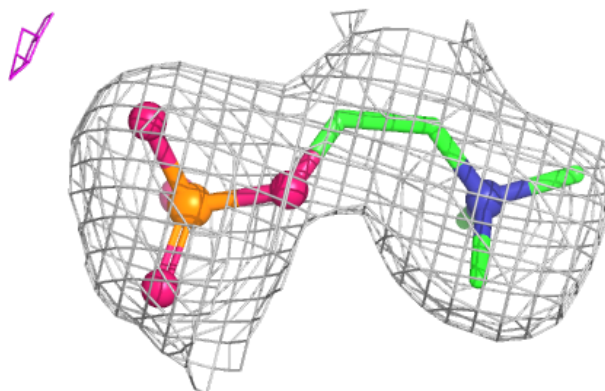


Electron density around PQJ A 401:

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

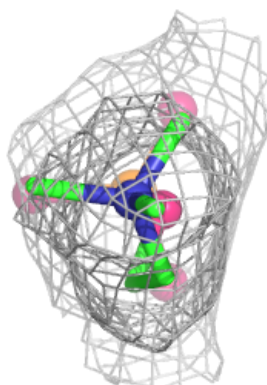
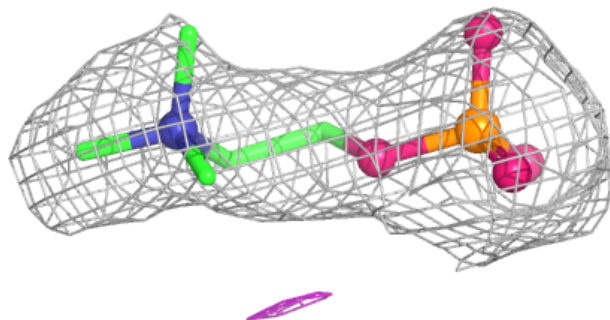
**Electron density around PQJ D 401:**

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

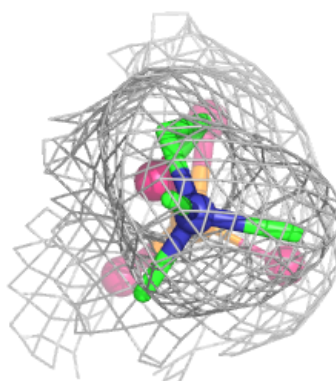
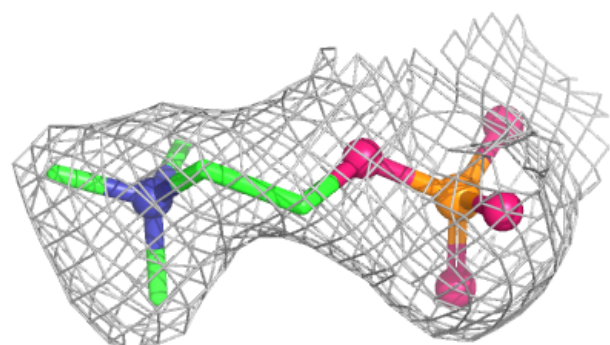
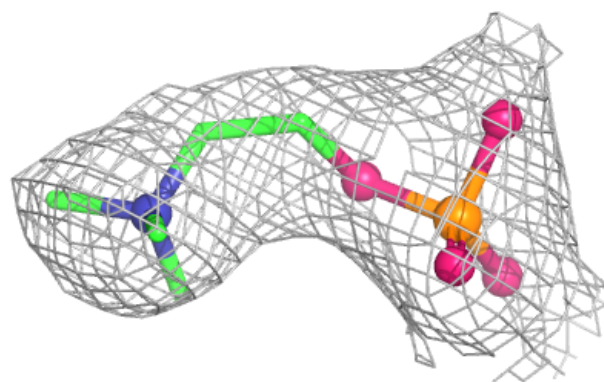


Electron density around PQJ E 401:

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

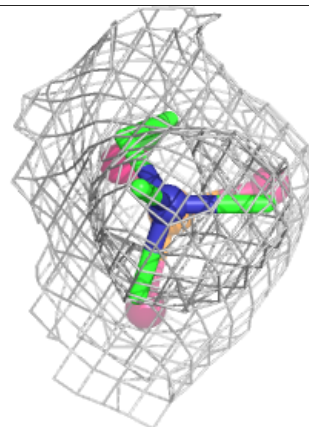
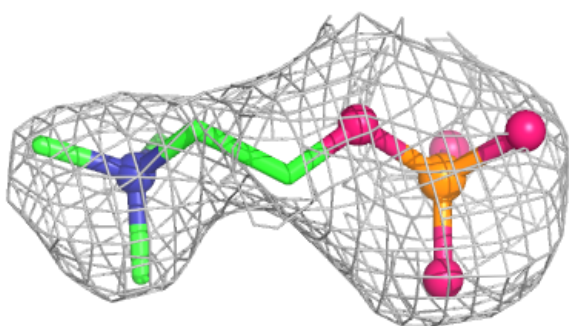
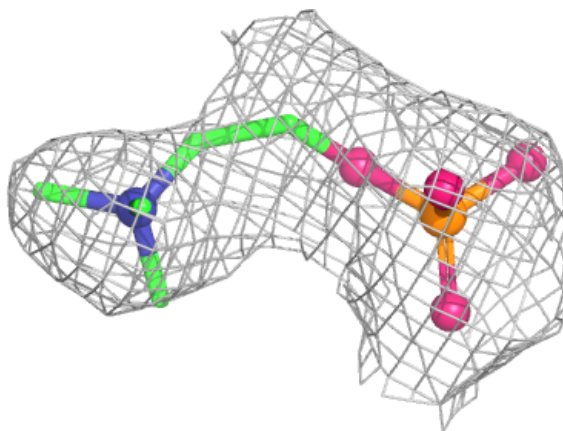
**Electron density around PQJ B 401:**

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

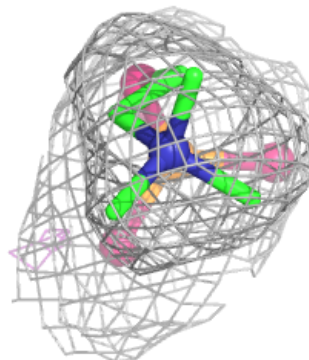
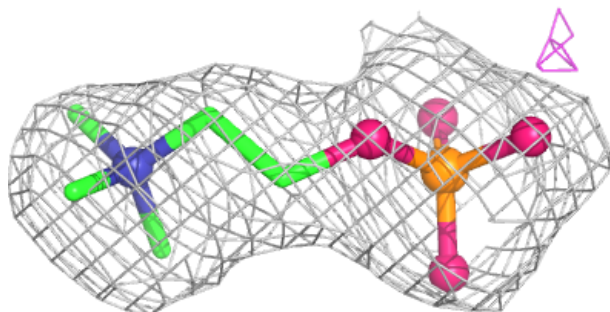
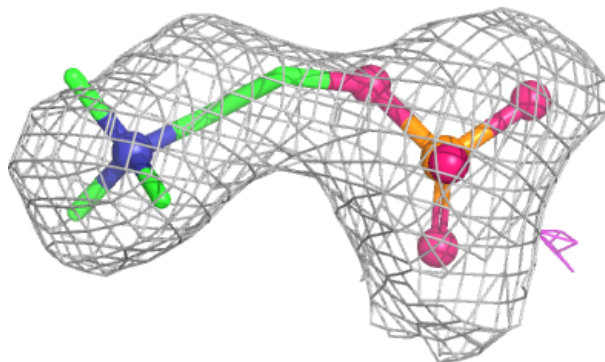


Electron density around PQJ C 401:

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

**Electron density around PQJ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.