



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:27 PM UTC

PDB ID : 3GOK / pdb_00003gok
Title : Binding site mapping of protein ligands
Authors : Scheich, C.
Deposited on : 2009-03-19
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

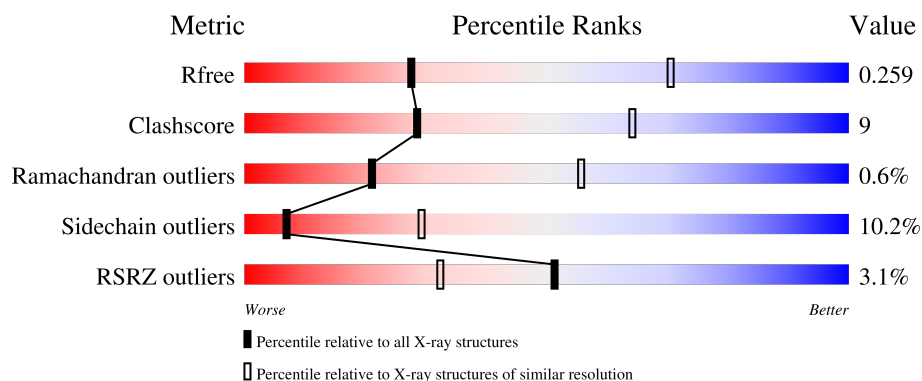
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



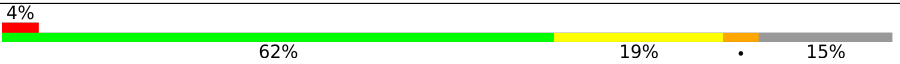
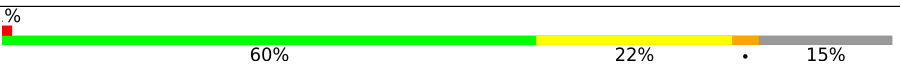
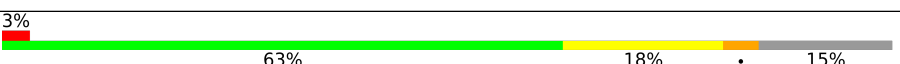
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	334	3% 65% 17% 15%
1	B	334	2% 64% 19% 13%
1	C	334	4% 66% 16% 15%
1	D	334	3% 60% 21% 15%
1	E	334	2% 62% 20% 13%

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Mol	Chain	Length	Quality of chain
1	F	334	
1	G	334	
1	H	334	
1	I	334	
1	J	334	
1	K	334	
1	L	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28332 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2317	1481	401	418	17			
1	B	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	C	285	Total	C	N	O	S	0	0	0
			2322	1488	400	417	17			
1	D	283	Total	C	N	O	S	0	0	0
			2298	1467	399	415	17			
1	E	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	F	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			
1	G	286	Total	C	N	O	S	0	0	0
			2329	1490	402	420	17			
1	H	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	I	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			
1	J	283	Total	C	N	O	S	0	0	0
			2298	1467	399	415	17			
1	K	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	L	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	expression tag	UNP P49137
A	32	ALA	-	expression tag	UNP P49137
A	33	MET	-	expression tag	UNP P49137
A	34	GLY	-	expression tag	UNP P49137
A	35	SER	-	expression tag	UNP P49137

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP P49137
A	37	ALA	-	expression tag	UNP P49137
A	38	MET	-	expression tag	UNP P49137
A	39	GLY	-	expression tag	UNP P49137
A	40	SER	-	expression tag	UNP P49137
B	31	GLY	-	expression tag	UNP P49137
B	32	ALA	-	expression tag	UNP P49137
B	33	MET	-	expression tag	UNP P49137
B	34	GLY	-	expression tag	UNP P49137
B	35	SER	-	expression tag	UNP P49137
B	36	GLY	-	expression tag	UNP P49137
B	37	ALA	-	expression tag	UNP P49137
B	38	MET	-	expression tag	UNP P49137
B	39	GLY	-	expression tag	UNP P49137
B	40	SER	-	expression tag	UNP P49137
C	31	GLY	-	expression tag	UNP P49137
C	32	ALA	-	expression tag	UNP P49137
C	33	MET	-	expression tag	UNP P49137
C	34	GLY	-	expression tag	UNP P49137
C	35	SER	-	expression tag	UNP P49137
C	36	GLY	-	expression tag	UNP P49137
C	37	ALA	-	expression tag	UNP P49137
C	38	MET	-	expression tag	UNP P49137
C	39	GLY	-	expression tag	UNP P49137
C	40	SER	-	expression tag	UNP P49137
D	31	GLY	-	expression tag	UNP P49137
D	32	ALA	-	expression tag	UNP P49137
D	33	MET	-	expression tag	UNP P49137
D	34	GLY	-	expression tag	UNP P49137
D	35	SER	-	expression tag	UNP P49137
D	36	GLY	-	expression tag	UNP P49137
D	37	ALA	-	expression tag	UNP P49137
D	38	MET	-	expression tag	UNP P49137
D	39	GLY	-	expression tag	UNP P49137
D	40	SER	-	expression tag	UNP P49137
E	31	GLY	-	expression tag	UNP P49137
E	32	ALA	-	expression tag	UNP P49137
E	33	MET	-	expression tag	UNP P49137
E	34	GLY	-	expression tag	UNP P49137
E	35	SER	-	expression tag	UNP P49137
E	36	GLY	-	expression tag	UNP P49137
E	37	ALA	-	expression tag	UNP P49137

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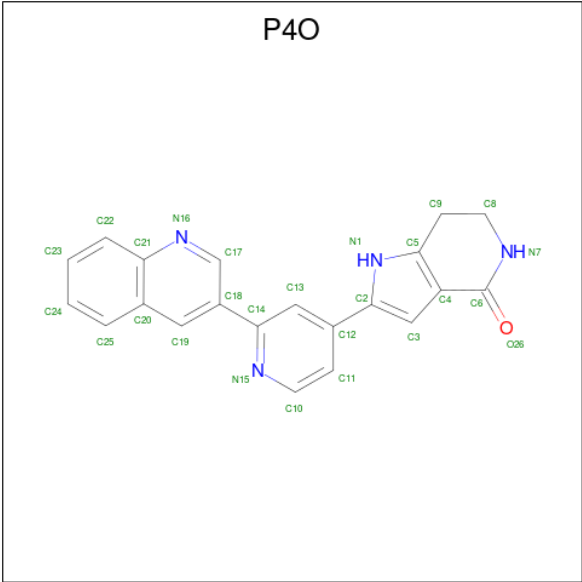
Chain	Residue	Modelled	Actual	Comment	Reference
E	38	MET	-	expression tag	UNP P49137
E	39	GLY	-	expression tag	UNP P49137
E	40	SER	-	expression tag	UNP P49137
F	31	GLY	-	expression tag	UNP P49137
F	32	ALA	-	expression tag	UNP P49137
F	33	MET	-	expression tag	UNP P49137
F	34	GLY	-	expression tag	UNP P49137
F	35	SER	-	expression tag	UNP P49137
F	36	GLY	-	expression tag	UNP P49137
F	37	ALA	-	expression tag	UNP P49137
F	38	MET	-	expression tag	UNP P49137
F	39	GLY	-	expression tag	UNP P49137
F	40	SER	-	expression tag	UNP P49137
G	31	GLY	-	expression tag	UNP P49137
G	32	ALA	-	expression tag	UNP P49137
G	33	MET	-	expression tag	UNP P49137
G	34	GLY	-	expression tag	UNP P49137
G	35	SER	-	expression tag	UNP P49137
G	36	GLY	-	expression tag	UNP P49137
G	37	ALA	-	expression tag	UNP P49137
G	38	MET	-	expression tag	UNP P49137
G	39	GLY	-	expression tag	UNP P49137
G	40	SER	-	expression tag	UNP P49137
H	31	GLY	-	expression tag	UNP P49137
H	32	ALA	-	expression tag	UNP P49137
H	33	MET	-	expression tag	UNP P49137
H	34	GLY	-	expression tag	UNP P49137
H	35	SER	-	expression tag	UNP P49137
H	36	GLY	-	expression tag	UNP P49137
H	37	ALA	-	expression tag	UNP P49137
H	38	MET	-	expression tag	UNP P49137
H	39	GLY	-	expression tag	UNP P49137
H	40	SER	-	expression tag	UNP P49137
I	31	GLY	-	expression tag	UNP P49137
I	32	ALA	-	expression tag	UNP P49137
I	33	MET	-	expression tag	UNP P49137
I	34	GLY	-	expression tag	UNP P49137
I	35	SER	-	expression tag	UNP P49137
I	36	GLY	-	expression tag	UNP P49137
I	37	ALA	-	expression tag	UNP P49137
I	38	MET	-	expression tag	UNP P49137
I	39	GLY	-	expression tag	UNP P49137

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Chain	Residue	Modelled	Actual	Comment	Reference
I	40	SER	-	expression tag	UNP P49137
J	31	GLY	-	expression tag	UNP P49137
J	32	ALA	-	expression tag	UNP P49137
J	33	MET	-	expression tag	UNP P49137
J	34	GLY	-	expression tag	UNP P49137
J	35	SER	-	expression tag	UNP P49137
J	36	GLY	-	expression tag	UNP P49137
J	37	ALA	-	expression tag	UNP P49137
J	38	MET	-	expression tag	UNP P49137
J	39	GLY	-	expression tag	UNP P49137
J	40	SER	-	expression tag	UNP P49137
K	31	GLY	-	expression tag	UNP P49137
K	32	ALA	-	expression tag	UNP P49137
K	33	MET	-	expression tag	UNP P49137
K	34	GLY	-	expression tag	UNP P49137
K	35	SER	-	expression tag	UNP P49137
K	36	GLY	-	expression tag	UNP P49137
K	37	ALA	-	expression tag	UNP P49137
K	38	MET	-	expression tag	UNP P49137
K	39	GLY	-	expression tag	UNP P49137
K	40	SER	-	expression tag	UNP P49137
L	31	GLY	-	expression tag	UNP P49137
L	32	ALA	-	expression tag	UNP P49137
L	33	MET	-	expression tag	UNP P49137
L	34	GLY	-	expression tag	UNP P49137
L	35	SER	-	expression tag	UNP P49137
L	36	GLY	-	expression tag	UNP P49137
L	37	ALA	-	expression tag	UNP P49137
L	38	MET	-	expression tag	UNP P49137
L	39	GLY	-	expression tag	UNP P49137
L	40	SER	-	expression tag	UNP P49137

- Molecule 2 is 2-(2-QUINOLIN-3-YLPYRIDIN-4-YL)-1,5,6,7-TETRAHYDRO-4H-PYRROLO[3,2-C]PYRIDIN-4-ONE (CCD ID: P4O) (formula: C₂₁H₁₆N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	21	4	1		
2	B	1	Total	C	N	O	0	0
			26	21	4	1		
2	C	1	Total	C	N	O	0	0
			26	21	4	1		
2	D	1	Total	C	N	O	0	0
			26	21	4	1		
2	E	1	Total	C	N	O	0	0
			26	21	4	1		
2	F	1	Total	C	N	O	0	0
			26	21	4	1		
2	G	1	Total	C	N	O	0	0
			26	21	4	1		
2	H	1	Total	C	N	O	0	0
			26	21	4	1		
2	I	1	Total	C	N	O	0	0
			26	21	4	1		
2	J	1	Total	C	N	O	0	0
			26	21	4	1		
2	K	1	Total	C	N	O	0	0
			26	21	4	1		
2	L	1	Total	C	N	O	0	0
			26	21	4	1		

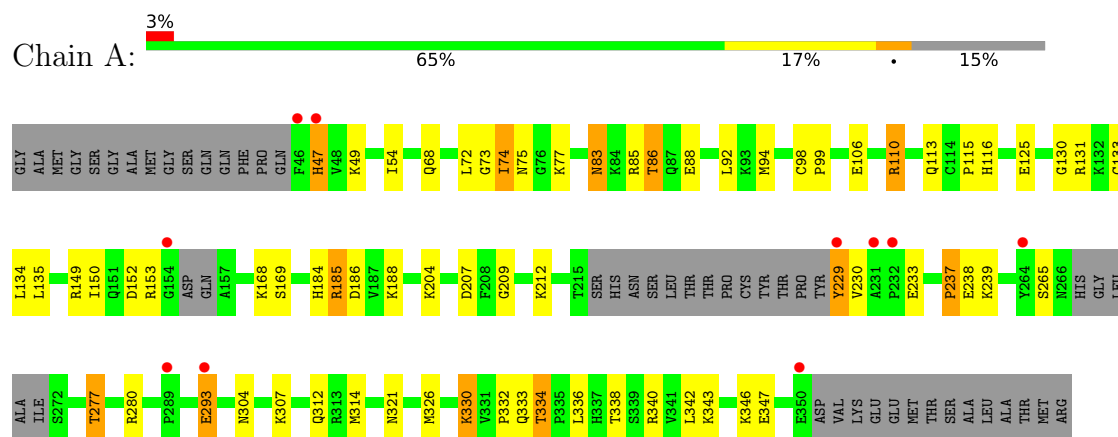
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	8	Total O 8 8	0	0
3	C	6	Total O 6 6	0	0
3	D	8	Total O 8 8	0	0
3	E	5	Total O 5 5	0	0
3	F	2	Total O 2 2	0	0
3	G	6	Total O 6 6	0	0
3	H	7	Total O 7 7	0	0
3	I	2	Total O 2 2	0	0
3	J	6	Total O 6 6	0	0
3	K	4	Total O 4 4	0	0
3	L	7	Total O 7 7	0	0

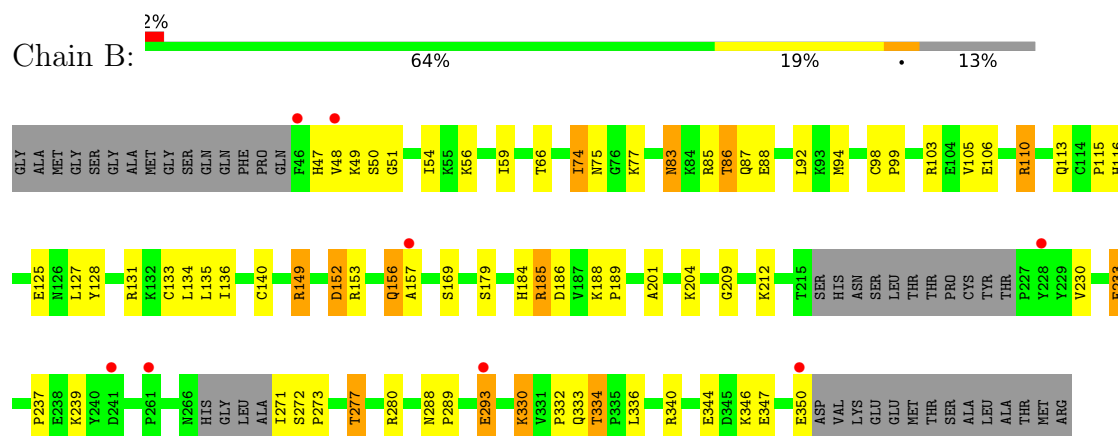
3 Residue-property plots [i](#)

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.

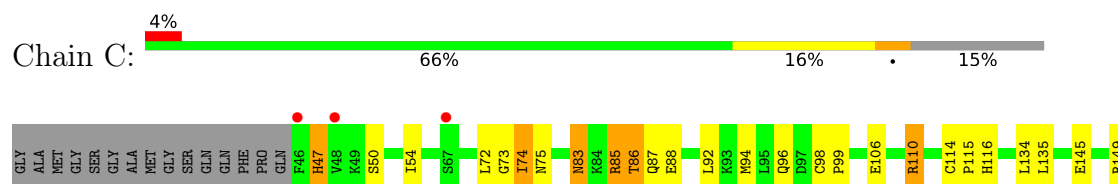
- Molecule 1: MAP kinase-activated protein kinase 2

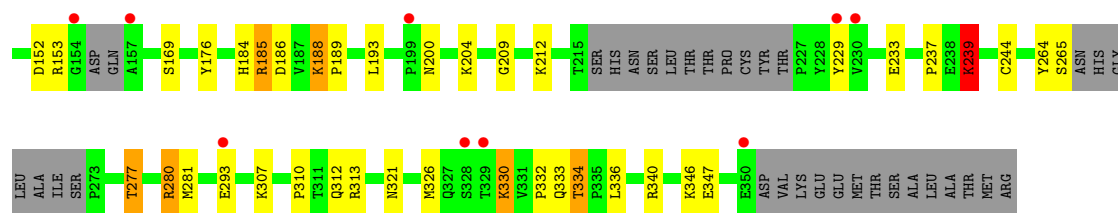


- Molecule 1: MAP kinase-activated protein kinase 2

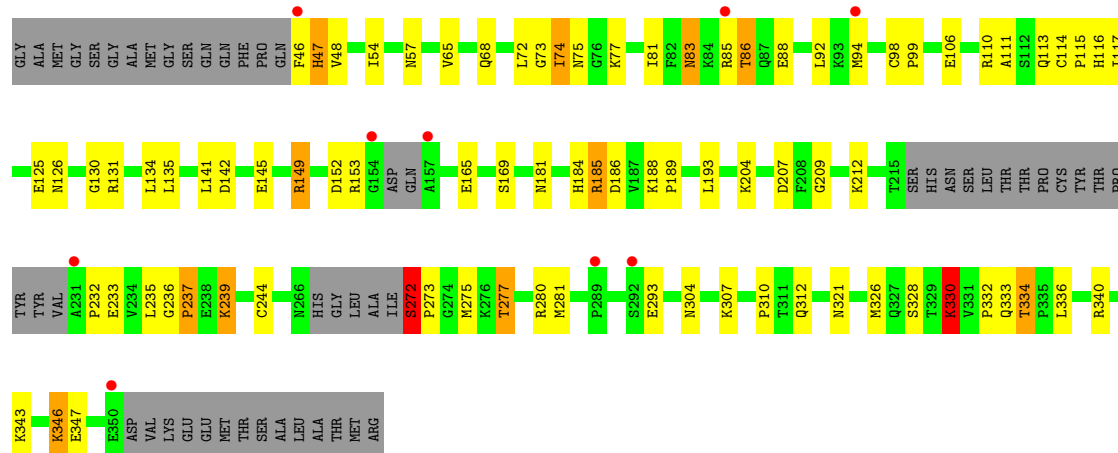


- Molecule 1: MAP kinase-activated protein kinase 2

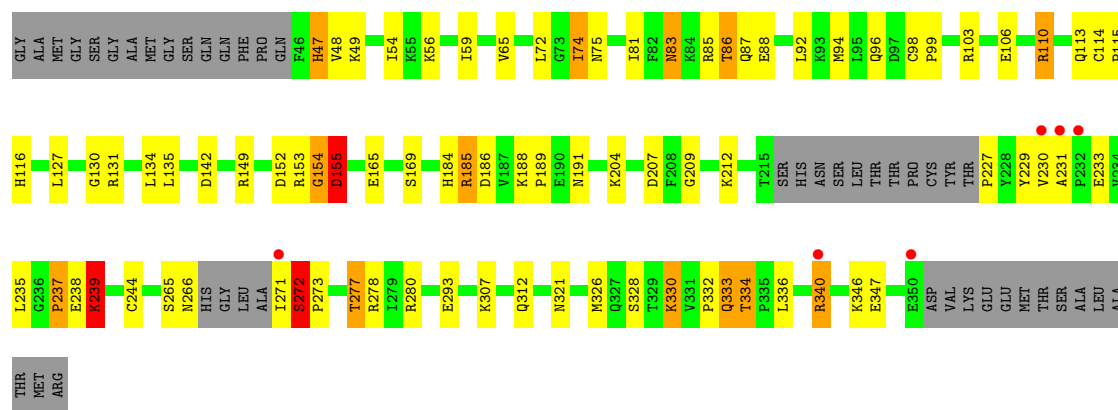




- Molecule 1: MAP kinase-activated protein kinase 2

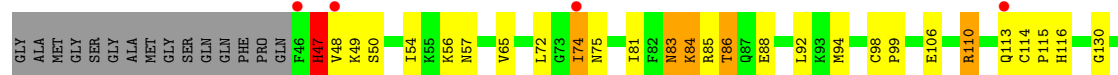


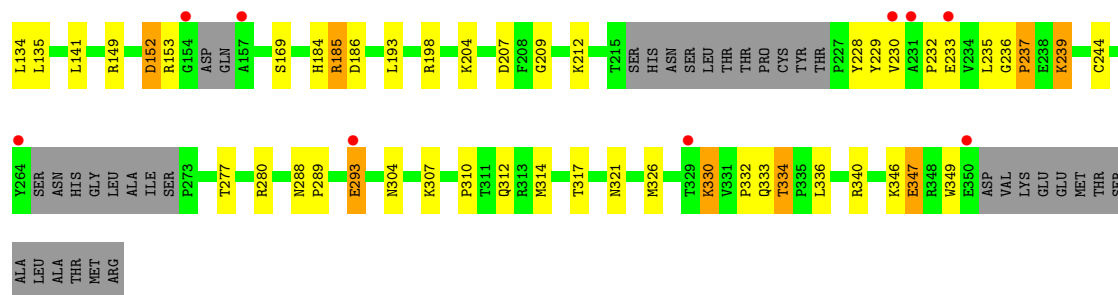
- Molecule 1: MAP kinase-activated protein kinase 2



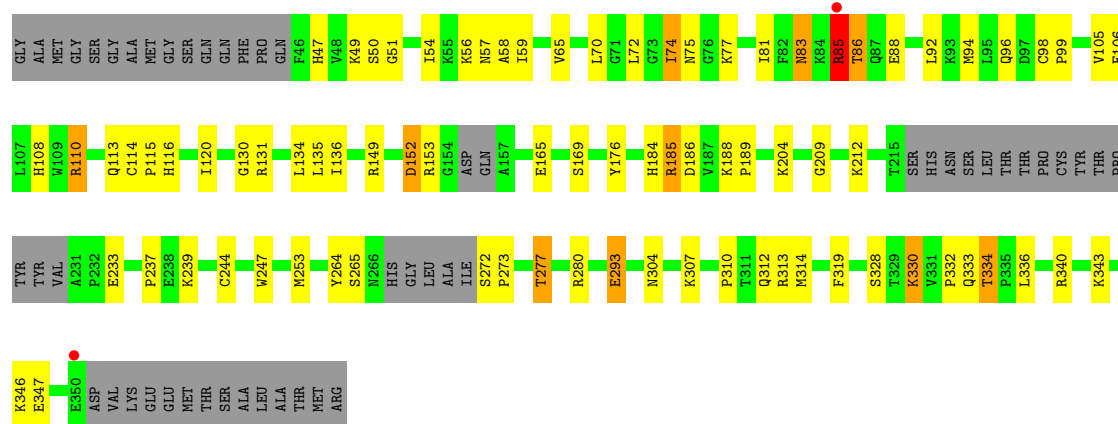
- Molecule 1: MAP kinase-activated protein kinase 2



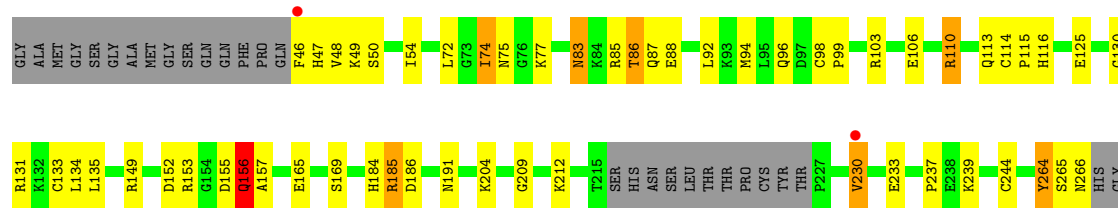




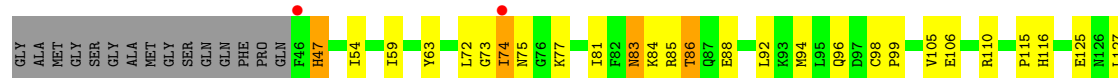
- Molecule 1: MAP kinase-activated protein kinase 2

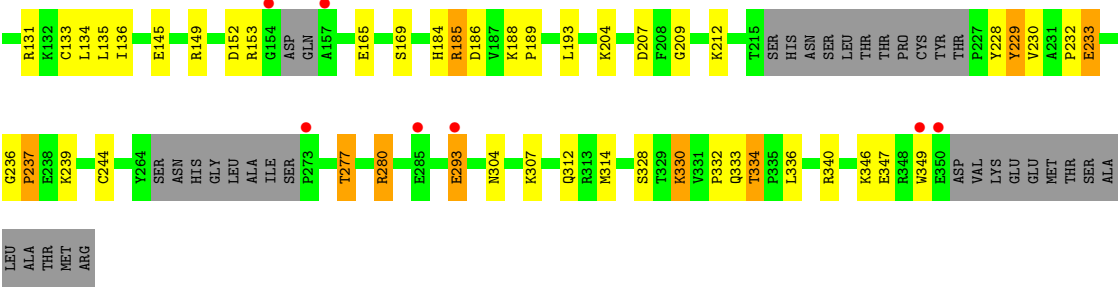


- Molecule 1: MAP kinase-activated protein kinase 2



- Molecule 1: MAP kinase-activated protein kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.21Å 183.19Å 217.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 3.20 46.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.73-3.20) 99.7 (46.73-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.238 , 0.258 (Not available) , 0.259	Depositor DCC
R_{free} test set	4642 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	91.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 96.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28332	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: P4O

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	0.95	0/2366	1.05	7/3188 (0.2%)
1	B	0.86	0/2413	1.05	8/3254 (0.2%)
1	C	0.89	0/2373	1.10	14/3197 (0.4%)
1	D	0.91	0/2346	1.08	14/3160 (0.4%)
1	E	0.82	1/2413 (0.0%)	1.08	14/3254 (0.4%)
1	F	0.92	0/2367	1.10	13/3189 (0.4%)
1	G	0.86	0/2379	1.07	8/3206 (0.2%)
1	H	0.80	0/2413	1.06	8/3254 (0.2%)
1	I	0.87	0/2367	1.12	15/3189 (0.5%)
1	J	0.77	0/2346	1.05	9/3160 (0.3%)
1	K	0.78	0/2413	1.06	10/3254 (0.3%)
1	L	0.82	2/2367 (0.1%)	1.11	15/3189 (0.5%)
All	All	0.86	3/28563 (0.0%)	1.08	135/38494 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	230	VAL	CA-CB	5.92	1.60	1.54
1	E	272	SER	CA-C	5.38	1.59	1.52
1	L	47	HIS	CA-CB	5.06	1.59	1.53

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	47	HIS	CB-CA-C	-10.55	93.90	110.78
1	L	47	HIS	CB-CA-C	-10.17	94.50	110.78
1	E	272	SER	CA-C-N	10.07	130.35	119.87
1	E	272	SER	C-N-CA	10.07	130.35	119.87
1	I	280	ARG	NE-CZ-NH2	9.98	128.19	119.20
1	L	280	ARG	NE-CZ-NH2	9.98	128.19	119.20
1	C	280	ARG	NE-CZ-NH2	9.95	128.16	119.20
1	F	280	ARG	NE-CZ-NH2	9.81	128.03	119.20
1	C	47	HIS	CB-CA-C	-9.78	95.13	110.78
1	J	85	ARG	CA-CB-CG	9.57	133.24	114.10
1	F	280	ARG	NE-CZ-NH1	-9.44	112.06	121.50
1	C	280	ARG	NE-CZ-NH1	-9.41	112.09	121.50
1	G	47	HIS	CB-CA-C	-9.41	95.50	111.31
1	D	47	HIS	CB-CA-C	-9.37	96.04	111.68
1	L	280	ARG	NE-CZ-NH1	-9.34	112.16	121.50
1	F	47	HIS	CB-CA-C	-9.16	95.91	111.31
1	K	103	ARG	NE-CZ-NH2	8.99	127.29	119.20
1	H	47	HIS	CB-CA-C	-8.99	96.21	111.31
1	H	272	SER	CA-C-N	8.99	128.63	119.82
1	H	272	SER	C-N-CA	8.99	128.63	119.82
1	K	103	ARG	NE-CZ-NH1	-8.96	112.54	121.50
1	B	47	HIS	CB-CA-C	-8.90	96.36	111.31
1	B	103	ARG	NE-CZ-NH1	-8.83	112.67	121.50
1	A	47	HIS	CB-CA-C	-8.80	96.53	111.31
1	I	280	ARG	NE-CZ-NH1	-8.74	112.76	121.50
1	H	103	ARG	NE-CZ-NH1	-8.71	112.79	121.50
1	E	340	ARG	NE-CZ-NH2	8.71	127.04	119.20
1	B	103	ARG	NE-CZ-NH2	8.63	126.97	119.20
1	H	103	ARG	NE-CZ-NH2	8.63	126.97	119.20
1	K	47	HIS	CB-CA-C	-8.59	96.87	111.31
1	L	149	ARG	NE-CZ-NH2	8.43	126.78	119.20
1	E	103	ARG	NE-CZ-NH1	-8.41	113.09	121.50
1	E	47	HIS	CB-CA-C	-8.29	97.38	111.31
1	I	47	HIS	N-CA-C	8.09	122.03	108.20
1	I	149	ARG	NE-CZ-NH2	7.91	126.32	119.20
1	E	103	ARG	NE-CZ-NH2	7.85	126.26	119.20
1	J	85	ARG	N-CA-C	7.75	121.23	111.69
1	C	280	ARG	CD-NE-CZ	7.70	135.19	124.40
1	I	280	ARG	CD-NE-CZ	7.69	135.17	124.40
1	D	149	ARG	CB-CG-CD	7.69	128.99	111.30
1	J	47	HIS	CB-CA-C	-7.64	98.48	111.31
1	J	85	ARG	N-CA-CB	7.52	121.40	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	340	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	C	340	ARG	NE-CZ-NH2	-7.49	112.46	119.20
1	F	340	ARG	CD-NE-CZ	7.49	134.88	124.40
1	L	340	ARG	CD-NE-CZ	7.37	134.72	124.40
1	L	280	ARG	CD-NE-CZ	7.37	134.72	124.40
1	G	132	LYS	CG-CD-CE	7.33	128.16	111.30
1	L	149	ARG	NE-CZ-NH1	-7.31	114.19	121.50
1	F	149	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	F	280	ARG	CD-NE-CZ	7.29	134.61	124.40
1	I	340	ARG	CD-NE-CZ	7.25	134.55	124.40
1	L	340	ARG	NE-CZ-NH2	-7.16	112.76	119.20
1	C	340	ARG	CD-NE-CZ	7.07	134.30	124.40
1	I	149	ARG	NE-CZ-NH1	-6.80	114.70	121.50
1	D	272	SER	CA-C-N	-6.75	112.82	119.64
1	D	272	SER	C-N-CA	-6.75	112.82	119.64
1	I	84	LYS	CG-CD-CE	6.74	126.80	111.30
1	F	340	ARG	NE-CZ-NH2	-6.63	113.24	119.20
1	I	47	HIS	N-CA-CB	6.55	121.18	110.37
1	C	149	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	K	264	TYR	N-CA-C	6.44	118.45	109.31
1	A	293	GLU	N-CA-CB	-6.43	100.41	110.44
1	F	84	LYS	CB-CG-CD	6.41	126.04	111.30
1	F	84	LYS	CG-CD-CE	6.41	126.04	111.30
1	I	84	LYS	CB-CG-CD	6.39	125.99	111.30
1	L	340	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	E	340	ARG	CD-NE-CZ	6.34	133.27	124.40
1	J	340	ARG	NE-CZ-NH2	6.33	124.90	119.20
1	D	149	ARG	CD-NE-CZ	6.31	133.24	124.40
1	D	47	HIS	N-CA-C	6.29	119.78	107.57
1	K	103	ARG	CD-NE-CZ	6.26	133.16	124.40
1	F	149	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	G	293	GLU	CA-CB-CG	6.25	126.60	114.10
1	C	47	HIS	N-CA-C	6.22	118.84	108.20
1	H	103	ARG	CD-NE-CZ	6.20	133.09	124.40
1	J	131	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	J	293	GLU	CA-CB-CG	6.18	126.47	114.10
1	C	340	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	C	149	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	E	103	ARG	CD-NE-CZ	6.02	132.82	124.40
1	B	103	ARG	CD-NE-CZ	5.95	132.74	124.40
1	H	131	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	I	340	ARG	NE-CZ-NH1	5.91	127.41	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	293	GLU	CA-CB-CG	5.87	125.84	114.10
1	D	346	LYS	CG-CD-CE	5.83	124.70	111.30
1	F	340	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	J	264	TYR	N-CA-C	5.81	119.36	110.36
1	C	47	HIS	N-CA-CB	5.80	119.94	110.37
1	G	346	LYS	CG-CD-CE	5.80	124.63	111.30
1	A	293	GLU	CA-CB-CG	5.77	125.65	114.10
1	L	346	LYS	CG-CD-CE	5.74	124.50	111.30
1	L	47	HIS	N-CA-C	5.74	118.01	108.20
1	B	340	ARG	NE-CZ-NH2	5.72	124.34	119.20
1	K	131	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	D	340	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	A	150	ILE	N-CA-C	-5.63	105.03	110.72
1	K	340	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	D	340	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	L	47	HIS	N-CA-CB	5.56	119.55	110.37
1	I	152	ASP	N-CA-C	5.55	116.37	108.54
1	G	229	TYR	N-CA-C	-5.51	103.96	111.56
1	E	131	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	D	149	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	K	230	VAL	CA-C-N	5.39	129.49	120.86
1	K	230	VAL	C-N-CA	5.39	129.49	120.86
1	E	114	CYS	CA-C-N	5.38	125.04	119.56
1	E	114	CYS	C-N-CA	5.38	125.04	119.56
1	K	272	SER	N-CA-C	5.37	121.67	109.81
1	G	340	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	C	188	LYS	CA-C-N	5.33	126.50	119.84
1	C	188	LYS	C-N-CA	5.33	126.50	119.84
1	B	340	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	G	340	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	B	152	ASP	N-CA-C	5.29	116.00	108.54
1	E	229	TYR	N-CA-C	-5.29	105.53	113.89
1	J	152	ASP	N-CA-C	5.25	115.95	108.54
1	D	181	ASN	N-CA-C	5.25	118.86	111.52
1	H	340	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	340	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	E	154	GLY	N-CA-C	-5.18	100.91	113.18
1	L	293	GLU	N-CA-CB	-5.16	102.60	110.33
1	I	228	TYR	N-CA-C	5.10	121.26	113.61
1	D	330	LYS	CB-CG-CD	5.09	123.02	111.30
1	L	131	ARG	CD-NE-CZ	5.08	131.50	124.40
1	D	304	ASN	N-CA-C	5.07	119.18	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	149	ARG	CD-NE-CZ	5.06	131.48	124.40
1	A	340	ARG	NE-CZ-NH1	-5.05	116.44	121.50
1	F	47	HIS	N-CA-CB	5.05	118.72	110.39
1	D	131	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	C	239	LYS	CG-CD-CE	5.03	122.87	111.30
1	G	239	LYS	CG-CD-CE	5.03	122.86	111.30
1	B	131	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	131	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	E	239	LYS	CG-CD-CE	5.01	122.82	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	272	SER	Peptide
1	E	154	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2317	0	2344	35	2
1	B	2361	0	2385	54	2
1	C	2322	0	2351	41	1
1	D	2298	0	2326	50	1
1	E	2361	0	2385	55	8
1	F	2316	0	2346	50	1
1	G	2329	0	2353	48	0
1	H	2361	0	2385	43	2
1	I	2316	0	2346	48	3
1	J	2298	0	2326	52	8
1	K	2361	0	2385	43	0
1	L	2316	0	2346	42	2
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	26	0	16	2	0
2	F	26	0	16	3	0
2	G	26	0	16	0	0
2	H	26	0	16	1	0
2	I	26	0	16	0	0
2	J	26	0	16	2	0
2	K	26	0	16	1	0
2	L	26	0	16	1	0
3	A	3	0	0	1	0
3	B	8	0	0	2	0
3	C	6	0	0	0	0
3	D	8	0	0	3	0
3	E	5	0	0	1	0
3	F	2	0	0	0	0
3	G	6	0	0	1	0
3	H	7	0	0	0	0
3	I	2	0	0	0	0
3	J	6	0	0	1	0
3	K	4	0	0	1	0
3	L	7	0	0	1	0
All	All	28332	0	28470	498	15

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 9.

All (498) 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:A:47:HIS:HA	3:A:366:HOH:O	1.52	1.08
1:H:265:SER:O	1:H:272:SER:HA	1.71	0.88
1:H:271:ILE:HG12	1:H:274:GLY:HA3	1.53	0.88
1:F:332:PRO:HB2	1:F:334:THR:HG22	1.55	0.88
1:I:332:PRO:HB2	1:I:334:THR:HG22	1.53	0.87
1:B:48:VAL:HG21	1:J:59:ILE:HG22	1.57	0.87
1:B:59:ILE:HG22	1:I:48:VAL:HG21	1.59	0.84
1:G:332:PRO:HB2	1:G:334:THR:HG22	1.57	0.84
1:C:332:PRO:HB2	1:C:334:THR:HG22	1.60	0.83
1:A:83:ASN:HB3	1:A:86:THR:HG22	1.60	0.83
1:A:110:ARG:NH1	1:G:130:GLY:O	2.13	0.82
1:D:83:ASN:HB3	1:D:86:THR:HG22	1.60	0.82
1:J:83:ASN:HB3	1:J:86:THR:HG22	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:332:PRO:HB2	1:J:334:THR:HG22	1.60	0.82
1:L:332:PRO:HB2	1:L:334:THR:HG22	1.60	0.82
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.60	0.81
1:K:266:ASN:HB2	1:K:271:ILE:HA	1.62	0.81
1:B:127:LEU:HD13	1:I:113:GLN:HE21	1.46	0.80
1:E:332:PRO:HB2	1:E:334:THR:HG22	1.61	0.80
1:D:332:PRO:HB2	1:D:334:THR:HG22	1.61	0.79
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.62	0.79
1:I:116:HIS:CE1	1:I:169:SER:HB2	2.17	0.79
1:K:332:PRO:HB2	1:K:334:THR:HG22	1.62	0.79
1:L:83:ASN:HB3	1:L:86:THR:HG22	1.63	0.79
1:H:83:ASN:HB3	1:H:86:THR:HG22	1.61	0.79
1:B:83:ASN:HB3	1:B:86:THR:HG22	1.65	0.79
1:E:83:ASN:HB3	1:E:86:THR:HG22	1.63	0.77
1:F:83:ASN:HB3	1:F:86:THR:HG22	1.65	0.77
1:B:110:ARG:NH1	1:J:130:GLY:O	2.17	0.77
1:C:83:ASN:HB3	1:C:86:THR:HG22	1.65	0.77
1:K:83:ASN:HB3	1:K:86:THR:HG22	1.65	0.77
1:I:83:ASN:HB3	1:I:86:THR:HG22	1.66	0.76
1:H:332:PRO:HB2	1:H:334:THR:HG22	1.67	0.76
1:A:83:ASN:CB	1:A:86:THR:HG22	2.16	0.76
1:D:83:ASN:CB	1:D:86:THR:HG22	2.16	0.75
1:D:48:VAL:HG21	1:L:59:ILE:HG22	1.68	0.74
1:B:50:SER:HB2	1:J:57:ASN:HA	1.70	0.74
1:G:83:ASN:HB3	1:G:86:THR:HG22	1.70	0.73
1:F:330:LYS:HG3	1:F:330:LYS:O	1.85	0.73
1:B:184:HIS:HD2	1:B:186:ASP:H	1.37	0.73
1:B:116:HIS:CE1	1:B:169:SER:HB2	2.25	0.72
1:B:233:GLU:HG2	1:C:310:PRO:HG3	1.72	0.72
1:E:83:ASN:CB	1:E:86:THR:HG22	2.20	0.72
1:D:235:LEU:O	1:E:280:ARG:NH2	2.23	0.72
1:J:83:ASN:CB	1:J:86:THR:HG22	2.19	0.71
1:K:116:HIS:CE1	1:K:169:SER:HB2	2.25	0.71
1:G:266:ASN:HB2	1:G:272:SER:N	2.05	0.71
1:E:116:HIS:CE1	1:E:169:SER:HB2	2.26	0.71
1:D:272:SER:HB2	1:D:273:PRO:HD2	1.73	0.70
1:K:155:ASP:O	1:K:156:GLN:HB2	1.88	0.70
1:H:83:ASN:CB	1:H:86:THR:HG22	2.21	0.70
1:D:46:PHE:N	3:D:372:HOH:O	2.24	0.69
1:C:83:ASN:CB	1:C:86:THR:HG22	2.23	0.69
1:C:330:LYS:O	1:C:330:LYS:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:HIS:CE1	1:D:169:SER:HB2	2.26	0.69
1:D:310:PRO:HG3	1:F:233:GLU:HG2	1.75	0.69
1:E:265:SER:O	1:E:272:SER:HA	1.92	0.68
1:K:98:CYS:HB2	1:K:99:PRO:HD2	1.75	0.68
1:L:184:HIS:HD2	1:L:186:ASP:H	1.41	0.68
1:K:330:LYS:HG3	1:K:330:LYS:O	1.94	0.67
1:E:227:PRO:HB2	1:E:230:VAL:HB	1.77	0.67
1:D:330:LYS:O	1:D:330:LYS:HG3	1.95	0.66
1:B:56:LYS:O	1:I:50:SER:HB2	1.95	0.66
1:A:184:HIS:HD2	1:A:186:ASP:H	1.42	0.66
1:G:152:ASP:O	1:G:153:ARG:HG3	1.96	0.66
1:K:152:ASP:O	1:K:153:ARG:HG3	1.95	0.66
1:B:83:ASN:CB	1:B:86:THR:HG22	2.24	0.66
1:F:128:TYR:HD1	1:G:47:HIS:O	1.78	0.66
1:J:116:HIS:CE1	1:J:169:SER:HB2	2.31	0.66
1:H:330:LYS:HG3	1:H:330:LYS:O	1.93	0.66
1:K:83:ASN:CB	1:K:86:THR:HG22	2.25	0.66
1:H:184:HIS:HD2	1:H:186:ASP:H	1.44	0.66
1:J:185:ARG:HH21	1:J:212:LYS:HD2	1.61	0.66
1:F:83:ASN:CB	1:F:86:THR:HG22	2.25	0.65
1:L:116:HIS:CE1	1:L:169:SER:HB2	2.31	0.65
1:G:188:LYS:HE2	1:I:229:TYR:OH	1.96	0.64
1:L:98:CYS:HB2	1:L:99:PRO:HD2	1.79	0.64
1:I:83:ASN:CB	1:I:86:THR:HG22	2.27	0.64
1:E:184:HIS:HD2	1:E:186:ASP:H	1.46	0.64
1:L:83:ASN:CB	1:L:86:THR:HG22	2.28	0.64
1:E:59:ILE:HG22	1:K:48:VAL:HG21	1.81	0.63
1:A:115:PRO:O	1:A:204:LYS:HE2	1.98	0.63
1:F:127:LEU:N	1:G:49:LYS:O	2.27	0.63
1:E:48:VAL:HG21	1:H:59:ILE:HG22	1.80	0.62
1:G:46:PHE:N	3:G:368:HOH:O	2.31	0.62
1:H:98:CYS:HB2	1:H:99:PRO:HD2	1.81	0.62
1:E:152:ASP:O	1:E:153:ARG:HG3	2.00	0.62
1:H:185:ARG:HH21	1:H:212:LYS:HD2	1.62	0.62
1:G:83:ASN:CB	1:G:86:THR:HG22	2.30	0.62
1:E:113:GLN:HE21	1:H:127:LEU:HD13	1.63	0.62
1:L:74:ILE:HG12	1:L:209:GLY:HA3	1.81	0.62
1:A:98:CYS:HB2	1:A:99:PRO:HD2	1.80	0.62
1:A:185:ARG:HH21	1:A:212:LYS:HD2	1.64	0.62
1:F:116:HIS:CE1	1:F:169:SER:HB2	2.35	0.61
1:D:184:HIS:HD2	1:D:186:ASP:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:HIS:CE1	1:A:169:SER:HB2	2.36	0.61
1:J:92:LEU:HD11	1:J:135:LEU:HB3	1.83	0.61
1:D:92:LEU:HD11	1:D:135:LEU:HB3	1.83	0.61
1:F:184:HIS:HD2	1:F:186:ASP:H	1.49	0.61
1:D:152:ASP:O	1:D:153:ARG:HG3	2.01	0.60
1:G:94:MET:HG2	1:G:135:LEU:HD22	1.84	0.60
1:G:98:CYS:HB2	1:G:99:PRO:HD2	1.82	0.60
1:J:152:ASP:O	1:J:153:ARG:HG3	2.02	0.60
1:H:272:SER:HB3	1:H:273:PRO:HD2	1.83	0.60
1:I:57:ASN:HA	1:J:50:SER:HB2	1.84	0.60
1:J:313:ARG:NH1	1:L:233:GLU:OE1	2.33	0.60
1:J:110:ARG:HH11	1:J:110:ARG:HG2	1.67	0.60
1:H:92:LEU:HD11	1:H:135:LEU:HB3	1.84	0.59
1:K:185:ARG:HH21	1:K:212:LYS:HD2	1.65	0.59
1:K:271:ILE:HG23	1:K:273:PRO:HD2	1.83	0.59
1:K:184:HIS:HD2	1:K:186:ASP:H	1.48	0.59
1:F:98:CYS:HB2	1:F:99:PRO:HD2	1.83	0.59
1:D:232:PRO:HB3	1:E:280:ARG:HA	1.84	0.59
1:E:330:LYS:O	1:E:330:LYS:HG2	2.03	0.59
1:I:184:HIS:HD2	1:I:186:ASP:H	1.47	0.59
1:G:184:HIS:HD2	1:G:186:ASP:H	1.51	0.59
1:B:98:CYS:HB2	1:B:99:PRO:HD2	1.83	0.59
1:E:333:GLN:HG3	3:E:366:HOH:O	2.02	0.58
1:F:185:ARG:HH21	1:F:212:LYS:HD2	1.67	0.58
1:I:330:LYS:HG2	1:I:330:LYS:O	2.03	0.58
1:B:185:ARG:HH21	1:B:212:LYS:HD2	1.68	0.58
1:D:98:CYS:HB2	1:D:99:PRO:HD2	1.85	0.58
1:F:127:LEU:HD13	1:G:113:GLN:HE21	1.69	0.58
1:D:272:SER:HB2	1:D:273:PRO:CD	2.33	0.58
1:G:185:ARG:HH21	1:G:212:LYS:HD2	1.68	0.58
1:B:127:LEU:HB2	1:I:49:LYS:HB2	1.85	0.58
1:G:330:LYS:O	1:G:330:LYS:HG2	2.03	0.58
1:K:46:PHE:N	3:K:366:HOH:O	2.36	0.58
1:I:92:LEU:HD11	1:I:135:LEU:HB3	1.86	0.58
1:E:98:CYS:HB2	1:E:99:PRO:HD2	1.85	0.57
1:L:330:LYS:O	1:L:330:LYS:HG2	2.04	0.57
1:H:228:TYR:HD1	1:H:228:TYR:O	1.87	0.57
1:H:116:HIS:CE1	1:H:169:SER:HB2	2.39	0.57
1:C:73:GLY:HA2	2:C:1:P4O:H8C1	1.86	0.57
1:C:184:HIS:HD2	1:C:186:ASP:H	1.52	0.57
1:J:98:CYS:HB2	1:J:99:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD11	1:A:135:LEU:HB3	1.86	0.57
1:C:185:ARG:HH21	1:C:212:LYS:HD2	1.69	0.57
1:C:116:HIS:CE1	1:C:169:SER:HB2	2.40	0.57
1:I:98:CYS:HB2	1:I:99:PRO:HD2	1.86	0.57
1:I:130:GLY:O	1:J:110:ARG:NH1	2.38	0.57
1:F:128:TYR:CD1	1:G:47:HIS:O	2.58	0.57
1:A:229:TYR:CD1	1:A:229:TYR:N	2.70	0.56
1:L:92:LEU:HD11	1:L:135:LEU:HB3	1.87	0.56
1:G:92:LEU:HD11	1:G:135:LEU:HB3	1.88	0.56
1:K:94:MET:HG2	1:K:135:LEU:HD22	1.88	0.56
1:H:110:ARG:NH1	1:K:130:GLY:O	2.39	0.56
1:B:152:ASP:O	1:B:153:ARG:HG3	2.05	0.56
1:C:98:CYS:HB2	1:C:99:PRO:HD2	1.88	0.56
1:B:50:SER:HB3	1:J:58:ALA:N	2.21	0.56
1:G:116:HIS:CE1	1:G:169:SER:HB2	2.41	0.56
1:H:74:ILE:HG12	1:H:209:GLY:HA3	1.87	0.56
1:B:127:LEU:HD13	1:I:113:GLN:NE2	2.19	0.55
1:D:185:ARG:HH21	1:D:212:LYS:HD2	1.71	0.55
1:E:185:ARG:HH21	1:E:212:LYS:HD2	1.71	0.55
1:J:184:HIS:HD2	1:J:186:ASP:H	1.53	0.55
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.87	0.55
1:E:266:ASN:HB3	1:E:271:ILE:HG23	1.88	0.55
1:G:272:SER:N	1:G:273:PRO:HD2	2.22	0.55
1:A:330:LYS:O	1:A:330:LYS:HG2	2.06	0.55
1:B:50:SER:CB	1:J:57:ASN:HA	2.36	0.55
1:C:83:ASN:C	1:C:83:ASN:HD22	2.15	0.55
1:J:330:LYS:O	1:J:330:LYS:HG2	2.06	0.55
1:A:83:ASN:CG	1:A:86:THR:HG22	2.32	0.54
1:B:350:GLU:O	3:B:369:HOH:O	2.18	0.54
1:L:115:PRO:O	1:L:204:LYS:HE2	2.07	0.54
1:D:310:PRO:CG	1:F:233:GLU:HG2	2.38	0.54
1:A:152:ASP:O	1:A:153:ARG:HG3	2.08	0.54
1:D:115:PRO:O	1:D:204:LYS:HE2	2.08	0.54
1:G:86:THR:HG23	1:G:88:GLU:HB2	1.89	0.54
1:H:152:ASP:O	1:H:153:ARG:HG3	2.08	0.54
1:L:152:ASP:O	1:L:153:ARG:HG3	2.09	0.53
1:L:185:ARG:HH21	1:L:212:LYS:HD2	1.74	0.53
1:B:50:SER:HB3	1:J:58:ALA:H	1.73	0.53
1:I:152:ASP:O	1:I:153:ARG:HG3	2.09	0.53
1:F:92:LEU:HD11	1:F:135:LEU:HB3	1.91	0.53
1:E:47:HIS:O	1:H:128:TYR:HD1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:SER:N	1:G:273:PRO:CD	2.72	0.53
1:L:94:MET:HG2	1:L:135:LEU:HD22	1.91	0.53
1:K:307:LYS:HD3	1:K:312:GLN:HB3	1.91	0.53
1:C:92:LEU:HD11	1:C:135:LEU:HB3	1.90	0.52
1:F:74:ILE:HG12	1:F:209:GLY:HA3	1.91	0.52
1:B:94:MET:HG2	1:B:135:LEU:HD22	1.91	0.52
1:F:73:GLY:HA2	2:F:1:P4O:C8	2.39	0.52
1:H:272:SER:HB3	1:H:273:PRO:CD	2.39	0.52
1:I:94:MET:HG2	1:I:135:LEU:HD22	1.91	0.52
1:J:188:LYS:HD3	1:L:229:TYR:CZ	2.43	0.52
1:C:94:MET:HG2	1:C:135:LEU:HD22	1.91	0.52
1:E:74:ILE:HG12	1:E:209:GLY:HA3	1.90	0.52
1:B:230:VAL:HB	3:B:370:HOH:O	2.09	0.52
1:I:185:ARG:HH21	1:I:212:LYS:HD2	1.74	0.52
1:J:74:ILE:HG12	1:J:209:GLY:HA3	1.91	0.52
1:I:83:ASN:C	1:I:83:ASN:HD22	2.18	0.52
1:L:86:THR:HG23	1:L:88:GLU:H	1.75	0.52
1:B:105:VAL:HG22	1:B:136:ILE:HD11	1.92	0.52
1:B:233:GLU:HG2	1:C:310:PRO:CG	2.38	0.52
1:B:74:ILE:HG12	1:B:209:GLY:HA3	1.91	0.52
1:B:115:PRO:O	1:B:204:LYS:HE2	2.10	0.52
1:D:73:GLY:HA2	2:D:1:P4O:C8	2.40	0.52
1:F:74:ILE:HG23	1:F:207:ASP:OD2	2.10	0.51
1:E:191:ASN:ND2	2:E:1:P4O:H8C2	2.25	0.51
1:F:83:ASN:ND2	1:F:86:THR:H	2.08	0.51
1:G:115:PRO:O	1:G:204:LYS:HE2	2.11	0.51
1:K:115:PRO:O	1:K:204:LYS:HE2	2.10	0.51
1:D:73:GLY:HA2	2:D:1:P4O:H8C1	1.92	0.51
1:F:110:ARG:HG2	1:F:110:ARG:HH11	1.75	0.51
1:K:92:LEU:HD11	1:K:135:LEU:HB3	1.93	0.51
1:G:283:GLN:HG3	1:I:317:THR:HG21	1.93	0.51
1:C:115:PRO:O	1:C:204:LYS:HE2	2.11	0.51
1:G:277:THR:HA	1:G:280:ARG:HG2	1.93	0.51
1:J:115:PRO:O	1:J:204:LYS:HE2	2.10	0.51
1:J:272:SER:N	3:J:367:HOH:O	2.44	0.51
1:E:92:LEU:HD11	1:E:135:LEU:HB3	1.93	0.51
1:G:307:LYS:HD3	1:G:312:GLN:HB3	1.93	0.51
1:L:83:ASN:HD22	1:L:83:ASN:C	2.19	0.51
1:F:83:ASN:C	1:F:83:ASN:HD22	2.19	0.50
1:H:105:VAL:HG22	1:H:136:ILE:HD11	1.93	0.50
1:I:74:ILE:HG12	1:I:209:GLY:HA3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:ASN:ND2	2:K:1:P4O:H8C2	2.27	0.50
1:L:74:ILE:HG23	1:L:207:ASP:OD2	2.12	0.50
1:J:70:LEU:HD13	2:J:1:P4O:C17	2.42	0.50
1:A:304:ASN:HD22	1:A:314:MET:HB2	1.76	0.50
1:D:281:MET:HE2	1:F:179:SER:HB3	1.92	0.50
1:E:127:LEU:HD13	1:K:113:GLN:HE21	1.76	0.50
1:D:86:THR:HG23	1:D:88:GLU:HB2	1.94	0.50
1:E:83:ASN:CG	1:E:86:THR:HG22	2.36	0.50
1:E:307:LYS:HD3	1:E:312:GLN:HB3	1.93	0.50
1:B:128:TYR:HD1	1:I:47:HIS:O	1.95	0.50
1:E:188:LYS:HB2	1:E:189:PRO:HD2	1.94	0.50
1:F:105:VAL:HG22	1:F:136:ILE:HD11	1.93	0.50
1:C:110:ARG:NH1	1:D:130:GLY:O	2.45	0.49
1:E:110:ARG:HH11	1:E:110:ARG:HG2	1.76	0.49
1:E:94:MET:HG2	1:E:135:LEU:HD22	1.94	0.49
1:G:86:THR:O	1:G:87:GLN:HB2	2.13	0.49
1:I:332:PRO:HB2	1:I:334:THR:CG2	2.34	0.49
1:K:165:GLU:HG3	1:K:328:SER:HB3	1.95	0.49
1:E:56:LYS:O	1:K:50:SER:HB2	2.12	0.49
1:G:266:ASN:CB	1:G:272:SER:N	2.73	0.49
1:L:83:ASN:ND2	1:L:86:THR:H	2.11	0.49
1:F:332:PRO:HB2	1:F:334:THR:CG2	2.35	0.49
1:E:235:LEU:HD13	1:F:276:LYS:HG3	1.95	0.49
1:E:266:ASN:CB	1:E:271:ILE:HG23	2.43	0.49
1:A:307:LYS:HD3	1:A:312:GLN:HB3	1.94	0.49
1:C:330:LYS:O	1:C:330:LYS:CG	2.60	0.49
1:E:265:SER:O	1:E:271:ILE:O	2.31	0.49
1:I:321:ASN:OD1	1:I:326:MET:HE2	2.12	0.49
1:K:266:ASN:HB2	1:K:271:ILE:CA	2.40	0.49
1:G:304:ASN:HD22	1:G:314:MET:HB2	1.78	0.49
1:H:233:GLU:HG2	1:I:310:PRO:HG3	1.95	0.49
1:J:247:TRP:CD2	1:L:232:PRO:HD3	2.48	0.49
1:G:74:ILE:HG12	1:G:209:GLY:HA3	1.95	0.48
1:H:74:ILE:HG23	1:H:207:ASP:OD2	2.13	0.48
1:L:86:THR:HG23	1:L:88:GLU:HB2	1.95	0.48
1:H:228:TYR:O	1:H:228:TYR:CD1	2.66	0.48
1:C:307:LYS:HD3	1:C:312:GLN:HB3	1.96	0.48
1:E:277:THR:HA	1:E:280:ARG:HG2	1.95	0.48
1:F:115:PRO:O	1:F:204:LYS:HE2	2.13	0.48
1:D:141:LEU:HD13	1:D:193:LEU:HB2	1.96	0.48
1:J:310:PRO:HB3	1:L:233:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:THR:HG23	1:C:88:GLU:HB2	1.95	0.48
1:J:94:MET:HG2	1:J:135:LEU:HD22	1.96	0.48
1:J:307:LYS:HD3	1:J:312:GLN:HB3	1.95	0.48
1:D:153:ARG:HB3	3:D:371:HOH:O	2.13	0.48
1:E:165:GLU:HG3	1:E:328:SER:HB3	1.96	0.48
1:B:179:SER:HB3	1:C:281:MET:HE2	1.95	0.48
1:C:83:ASN:CG	1:C:86:THR:HG22	2.39	0.48
1:C:50:SER:HB2	1:D:57:ASN:HA	1.96	0.47
1:E:115:PRO:O	1:E:204:LYS:HE2	2.14	0.47
1:B:272:SER:N	1:B:273:PRO:HD2	2.29	0.47
1:I:307:LYS:HD3	1:I:312:GLN:HB3	1.96	0.47
1:J:310:PRO:HG3	1:L:233:GLU:HG2	1.96	0.47
1:D:65:VAL:HA	1:D:81:ILE:HG22	1.96	0.47
1:D:74:ILE:HG12	1:D:209:GLY:HA3	1.95	0.47
1:I:115:PRO:O	1:I:204:LYS:HE2	2.14	0.47
1:L:73:GLY:HA2	2:L:1:P4O:H8C1	1.96	0.47
1:B:86:THR:HG23	1:B:88:GLU:HB2	1.96	0.47
1:B:330:LYS:O	1:B:330:LYS:HG2	2.14	0.47
1:E:86:THR:HG23	1:E:88:GLU:H	1.80	0.47
1:I:65:VAL:HA	1:I:81:ILE:HG22	1.95	0.47
1:D:272:SER:N	1:D:275:MET:H	2.12	0.47
1:J:70:LEU:HD22	2:J:1:P4O:N16	2.30	0.47
1:D:83:ASN:CG	1:D:86:THR:HG22	2.39	0.47
1:F:165:GLU:HG3	1:F:328:SER:HB3	1.97	0.47
1:K:321:ASN:OD1	1:K:326:MET:HE2	2.14	0.47
1:H:155:ASP:O	1:H:156:GLN:HB2	2.15	0.47
1:I:86:THR:HG23	1:I:88:GLU:H	1.80	0.47
1:K:74:ILE:HG12	1:K:209:GLY:HA3	1.96	0.47
1:G:86:THR:HG23	1:G:88:GLU:CB	2.45	0.46
1:I:74:ILE:HG23	1:I:207:ASP:OD2	2.15	0.46
1:I:288:ASN:HB3	1:I:289:PRO:HA	1.97	0.46
1:G:332:PRO:HB2	1:G:334:THR:CG2	2.37	0.46
1:G:321:ASN:OD1	1:G:326:MET:HE2	2.15	0.46
1:J:110:ARG:HG2	1:J:110:ARG:NH1	2.29	0.46
1:J:277:THR:HA	1:J:280:ARG:HG2	1.98	0.46
1:F:145:GLU:HA	1:F:193:LEU:HD23	1.97	0.46
1:F:307:LYS:HD3	1:F:312:GLN:HB3	1.96	0.46
1:H:94:MET:HG2	1:H:135:LEU:HD22	1.98	0.46
1:A:186:ASP:OD1	1:A:188:LYS:HE3	2.15	0.46
1:B:83:ASN:C	1:B:83:ASN:HD22	2.23	0.46
1:D:307:LYS:HD3	1:D:312:GLN:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:THR:HG23	1:H:88:GLU:H	1.81	0.46
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.81	0.46
1:B:184:HIS:CD2	1:B:186:ASP:H	2.26	0.46
1:B:288:ASN:HB3	1:B:289:PRO:HA	1.97	0.46
1:C:152:ASP:O	1:C:153:ARG:HG3	2.16	0.46
1:D:86:THR:HG23	1:D:88:GLU:H	1.80	0.46
1:H:86:THR:HG23	1:H:88:GLU:HB2	1.97	0.46
1:H:191:ASN:ND2	2:H:1:P4O:H8C2	2.31	0.46
1:J:86:THR:HG23	1:J:88:GLU:HB2	1.98	0.46
1:K:125:GLU:HA	1:K:133:CYS:O	2.16	0.46
1:A:74:ILE:HG12	1:A:209:GLY:HA3	1.97	0.46
1:H:83:ASN:CG	1:H:86:THR:HG22	2.40	0.46
1:J:83:ASN:CG	1:J:86:THR:HG22	2.41	0.46
1:A:229:TYR:N	1:A:229:TYR:HD1	2.14	0.45
1:C:86:THR:HG23	1:C:88:GLU:H	1.80	0.45
1:C:188:LYS:HB2	1:C:189:PRO:HD2	1.98	0.45
1:G:276:LYS:HG3	1:I:235:LEU:HD13	1.97	0.45
1:G:279:ILE:HG22	1:I:232:PRO:HG3	1.99	0.45
1:H:307:LYS:HD3	1:H:312:GLN:HB3	1.97	0.45
1:K:110:ARG:HG2	1:K:110:ARG:HH11	1.81	0.45
1:K:277:THR:HA	1:K:280:ARG:HG2	1.97	0.45
1:C:86:THR:HG23	1:C:88:GLU:CB	2.47	0.45
1:C:264:TYR:HB3	1:C:265:SER:H	1.50	0.45
1:E:153:ARG:HB3	1:E:155:ASP:O	2.17	0.45
1:H:184:HIS:CD2	1:H:186:ASP:H	2.28	0.45
1:H:277:THR:HA	1:H:280:ARG:HG2	1.98	0.45
1:L:188:LYS:HB2	1:L:189:PRO:HD2	1.99	0.45
1:L:307:LYS:HD3	1:L:312:GLN:HB3	1.96	0.45
1:C:332:PRO:HB2	1:C:334:THR:CG2	2.41	0.45
1:L:165:GLU:HG3	1:L:328:SER:HB3	1.97	0.45
1:A:184:HIS:HD2	1:A:186:ASP:N	2.13	0.45
1:A:321:ASN:OD1	1:A:326:MET:HE2	2.17	0.45
1:B:83:ASN:CG	1:B:86:THR:HG22	2.42	0.45
1:H:65:VAL:HA	1:H:81:ILE:HG22	1.97	0.45
1:J:332:PRO:HB2	1:J:334:THR:CG2	2.41	0.45
1:B:149:ARG:NH2	1:B:201:ALA:HB3	2.32	0.45
1:F:83:ASN:CG	1:F:86:THR:HG22	2.42	0.45
1:G:239:LYS:NZ	1:G:239:LYS:HB3	2.31	0.45
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.80	0.45
1:E:74:ILE:HG23	1:E:207:ASP:OD2	2.17	0.45
1:F:200:ASN:ND2	1:F:200:ASN:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:VAL:HG22	1:L:136:ILE:HD11	1.99	0.45
1:F:127:LEU:HB2	1:G:49:LYS:HB2	1.98	0.45
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.81	0.44
1:C:321:ASN:OD1	1:C:326:MET:HE2	2.17	0.44
1:I:141:LEU:HD13	1:I:193:LEU:HB2	1.97	0.44
1:J:272:SER:HB3	1:J:273:PRO:HD3	1.98	0.44
1:I:239:LYS:HB3	1:I:239:LYS:NZ	2.33	0.44
1:J:304:ASN:HD22	1:J:314:MET:HB2	1.83	0.44
1:I:110:ARG:HG2	1:I:110:ARG:HH11	1.81	0.44
1:E:272:SER:H	1:E:273:PRO:HD2	1.83	0.44
1:F:277:THR:HA	1:F:280:ARG:HG2	2.00	0.44
1:G:110:ARG:HG2	1:G:110:ARG:HH11	1.83	0.44
1:H:115:PRO:O	1:H:204:LYS:HE2	2.17	0.44
1:K:83:ASN:CG	1:K:86:THR:HG22	2.42	0.44
1:H:110:ARG:HH11	1:H:110:ARG:HG2	1.82	0.44
1:I:86:THR:HG23	1:I:88:GLU:HB2	2.00	0.44
1:B:83:ASN:ND2	1:B:86:THR:H	2.15	0.44
1:B:140:CYS:SG	2:B:1:P4O:H17	2.58	0.44
1:E:127:LEU:N	1:K:49:LYS:O	2.34	0.44
1:E:239:LYS:NZ	1:E:239:LYS:HB3	2.33	0.44
1:F:73:GLY:HA2	2:F:1:P4O:H8C1	1.98	0.44
1:A:74:ILE:HG23	1:A:207:ASP:OD2	2.17	0.44
1:D:321:ASN:OD1	1:D:326:MET:HE2	2.18	0.44
1:E:49:LYS:O	1:H:127:LEU:N	2.43	0.44
1:E:65:VAL:HA	1:E:81:ILE:HG22	2.00	0.44
1:E:271:ILE:HG12	1:E:278:ARG:HH12	1.82	0.44
1:B:51:GLY:N	1:J:56:LYS:O	2.48	0.43
1:C:86:THR:O	1:C:87:GLN:HB2	2.18	0.43
1:F:114:CYS:HB2	1:F:176:TYR:CD2	2.53	0.43
1:H:86:THR:O	1:H:87:GLN:HB2	2.16	0.43
1:J:272:SER:HB3	1:J:273:PRO:CD	2.48	0.43
1:B:272:SER:H	1:B:273:PRO:HD2	1.83	0.43
1:D:239:LYS:NZ	1:D:239:LYS:HB3	2.33	0.43
1:L:125:GLU:HA	1:L:133:CYS:O	2.18	0.43
1:C:145:GLU:HA	1:C:193:LEU:HD23	2.00	0.43
1:D:94:MET:HG2	1:D:135:LEU:HD22	2.00	0.43
1:E:321:ASN:OD1	1:E:326:MET:HE2	2.19	0.43
1:G:86:THR:HG23	1:G:88:GLU:H	1.83	0.43
1:J:108:HIS:CG	1:J:120:ILE:HD11	2.54	0.43
1:J:114:CYS:HB2	1:J:176:TYR:CD2	2.53	0.43
1:A:86:THR:HG23	1:A:88:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:HIS:HD2	1:B:186:ASP:N	2.11	0.43
1:F:59:ILE:HG22	1:G:48:VAL:HG21	2.00	0.43
1:C:114:CYS:HA	1:C:115:PRO:HD3	1.90	0.43
1:C:200:ASN:H	1:C:200:ASN:ND2	2.15	0.43
1:C:239:LYS:NZ	1:C:239:LYS:HB3	2.33	0.43
1:D:142:ASP:HA	2:D:1:P4O:N16	2.33	0.43
1:E:237:PRO:HB2	1:E:238:GLU:H	1.73	0.43
1:K:264:TYR:HB3	1:K:265:SER:H	1.56	0.43
1:L:277:THR:HA	1:L:280:ARG:HG2	2.00	0.43
1:L:304:ASN:HD22	1:L:314:MET:HB2	1.83	0.43
1:F:114:CYS:HA	1:F:115:PRO:HD3	1.90	0.43
1:J:165:GLU:HG3	1:J:328:SER:HB3	1.99	0.43
1:A:125:GLU:HA	1:A:133:CYS:O	2.19	0.43
1:A:277:THR:HA	1:A:280:ARG:HG2	2.01	0.43
1:B:277:THR:HA	1:B:280:ARG:HG2	2.01	0.43
1:D:332:PRO:HB2	1:D:334:THR:CG2	2.42	0.43
1:E:110:ARG:HG2	1:E:110:ARG:NH1	2.34	0.43
1:F:94:MET:HG2	1:F:135:LEU:HD22	2.00	0.43
1:L:228:TYR:CD2	1:L:228:TYR:N	2.87	0.43
1:E:86:THR:O	1:E:87:GLN:HB2	2.18	0.42
1:G:165:GLU:HG3	1:G:328:SER:HB3	2.01	0.42
1:J:105:VAL:HG22	1:J:136:ILE:HD11	2.01	0.42
1:J:253:MET:HE1	1:J:319:PHE:HE2	1.84	0.42
1:K:86:THR:HG23	1:K:88:GLU:HB2	2.00	0.42
1:E:130:GLY:O	1:K:110:ARG:HG2	2.19	0.42
1:E:142:ASP:HA	2:E:1:P4O:N16	2.34	0.42
1:B:86:THR:HG23	1:B:88:GLU:H	1.85	0.42
1:D:188:LYS:HB2	1:D:189:PRO:HD2	2.01	0.42
1:H:83:ASN:C	1:H:83:ASN:HD22	2.27	0.42
1:H:83:ASN:ND2	1:H:86:THR:H	2.17	0.42
1:H:186:ASP:OD1	1:H:188:LYS:HE3	2.20	0.42
1:I:184:HIS:CD2	1:I:186:ASP:H	2.33	0.42
1:K:152:ASP:C	1:K:153:ARG:HG3	2.44	0.42
1:L:74:ILE:CG1	1:L:209:GLY:HA3	2.49	0.42
1:L:86:THR:HG23	1:L:88:GLU:CB	2.49	0.42
1:C:277:THR:HA	1:C:280:ARG:HG2	2.01	0.42
1:F:49:LYS:HG3	1:F:113:GLN:OE1	2.19	0.42
1:G:281:MET:HE3	1:I:317:THR:OG1	2.19	0.42
1:D:125:GLU:C	1:D:126:ASN:HD22	2.28	0.42
1:I:236:GLY:HA2	1:I:237:PRO:HD3	1.94	0.42
1:K:266:ASN:CB	1:K:271:ILE:HA	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:ASN:C	1:G:83:ASN:HD22	2.28	0.42
1:H:304:ASN:HD22	1:H:314:MET:HB2	1.85	0.42
1:I:83:ASN:CG	1:I:86:THR:HG22	2.45	0.42
1:I:304:ASN:HD22	1:I:314:MET:HB2	1.85	0.42
1:B:233:GLU:OE1	1:C:313:ARG:NH1	2.49	0.42
1:B:271:ILE:HG23	1:B:273:PRO:HG2	2.02	0.42
1:D:86:THR:HG23	1:D:88:GLU:CB	2.50	0.42
1:I:94:MET:HE2	1:I:94:MET:HB3	1.98	0.42
1:K:288:ASN:HB3	1:K:289:PRO:HA	2.02	0.42
1:L:332:PRO:HB2	1:L:334:THR:CG2	2.41	0.42
1:C:74:ILE:HG12	1:C:209:GLY:HA3	2.00	0.42
1:F:125:GLU:HA	1:F:133:CYS:O	2.19	0.42
1:A:83:ASN:ND2	1:A:86:THR:H	2.18	0.41
1:B:86:THR:O	1:B:87:GLN:HB2	2.20	0.41
1:B:186:ASP:OD1	1:B:188:LYS:HE3	2.20	0.41
1:I:86:THR:HG23	1:I:88:GLU:CB	2.49	0.41
1:K:86:THR:O	1:K:87:GLN:HB2	2.19	0.41
1:A:130:GLY:O	1:F:110:ARG:NH1	2.53	0.41
1:B:188:LYS:HB2	1:B:189:PRO:HD2	2.01	0.41
1:G:242:LYS:C	1:G:244:CYS:H	2.27	0.41
1:J:65:VAL:HA	1:J:81:ILE:HG22	2.02	0.41
1:D:47:HIS:HA	3:D:370:HOH:O	2.19	0.41
1:D:165:GLU:HG3	1:D:328:SER:HB3	2.02	0.41
1:F:149:ARG:HH22	1:F:201:ALA:HB3	1.85	0.41
1:G:188:LYS:HB2	1:G:189:PRO:HD2	2.02	0.41
1:B:86:THR:HG23	1:B:88:GLU:CB	2.50	0.41
1:F:86:THR:HG23	1:F:88:GLU:HB2	2.01	0.41
1:I:114:CYS:HA	1:I:115:PRO:HD3	1.96	0.41
1:E:86:THR:HG23	1:E:88:GLU:HB2	2.02	0.41
1:F:70:LEU:HD13	2:F:1:P4O:C17	2.51	0.41
1:K:86:THR:HG23	1:K:88:GLU:CB	2.51	0.41
1:A:49:LYS:HG3	1:A:113:GLN:OE1	2.20	0.41
1:A:73:GLY:HA2	2:A:1:P4O:C8	2.50	0.41
1:F:191:ASN:HD22	1:F:191:ASN:HA	1.72	0.41
1:J:114:CYS:HA	1:J:115:PRO:HD3	1.90	0.41
1:A:94:MET:HG2	1:A:135:LEU:HD22	2.02	0.41
1:C:114:CYS:HB2	1:C:176:TYR:CD2	2.55	0.41
1:D:277:THR:HA	1:D:280:ARG:HG2	2.02	0.41
1:B:49:LYS:HG3	1:B:113:GLN:OE1	2.21	0.41
1:A:188:LYS:HD3	1:C:229:TYR:CZ	2.56	0.41
1:A:237:PRO:O	1:A:238:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLU:HA	1:B:133:CYS:O	2.20	0.41
1:D:145:GLU:HA	1:D:193:LEU:HD23	2.01	0.41
1:E:235:LEU:HD13	1:F:276:LYS:CG	2.50	0.41
1:F:188:LYS:HB2	1:F:189:PRO:HD2	2.01	0.41
1:I:56:LYS:O	1:J:51:GLY:N	2.49	0.41
1:I:347:GLU:C	1:I:349:TRP:H	2.29	0.41
1:L:184:HIS:CD2	1:L:186:ASP:H	2.29	0.41
1:L:349:TRP:HE3	3:L:370:HOH:O	2.04	0.41
1:D:236:GLY:HA2	1:D:237:PRO:HD3	1.94	0.41
1:E:86:THR:HG23	1:E:88:GLU:CB	2.51	0.41
1:E:230:VAL:HG22	1:E:231:ALA:H	1.86	0.41
1:E:235:LEU:HD22	1:F:276:LYS:HE3	2.02	0.41
1:F:56:LYS:O	1:G:50:SER:HB2	2.21	0.41
1:H:141:LEU:HD13	1:H:193:LEU:HB2	2.02	0.41
1:J:49:LYS:HG3	1:J:113:GLN:OE1	2.21	0.41
1:D:111:ALA:HB1	1:D:117:ILE:HD13	2.03	0.40
1:F:86:THR:HG23	1:F:88:GLU:H	1.85	0.40
1:J:83:ASN:C	1:J:83:ASN:HD22	2.28	0.40
1:K:114:CYS:HA	1:K:115:PRO:HD3	1.94	0.40
1:K:272:SER:N	1:K:273:PRO:HD2	2.35	0.40
1:L:145:GLU:HA	1:L:193:LEU:HD23	2.02	0.40
1:G:94:MET:HE2	1:G:94:MET:HB3	1.98	0.40
1:G:152:ASP:C	1:G:153:ARG:HG3	2.46	0.40
1:J:188:LYS:HB2	1:J:189:PRO:HD2	2.02	0.40
1:L:236:GLY:HA2	1:L:237:PRO:HD3	1.93	0.40
1:A:338:THR:O	1:A:342:LEU:HB2	2.22	0.40
1:D:113:GLN:HE21	1:L:127:LEU:HD13	1.86	0.40
1:K:83:ASN:ND2	1:K:86:THR:H	2.19	0.40
1:L:63:TYR:CD1	1:L:81:ILE:HD12	2.56	0.40
1:C:83:ASN:ND2	1:C:86:THR:H	2.19	0.40
1:D:74:ILE:HG23	1:D:207:ASP:OD2	2.21	0.40
1:D:114:CYS:HB3	1:D:117:ILE:HD12	2.03	0.40
1:J:86:THR:HG23	1:J:88:GLU:CB	2.51	0.40
1:K:83:ASN:HD22	1:K:83:ASN:C	2.30	0.40

All (15) 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)
1:I:198:ARG:NH2	1:L:84:LYS:O[2_555]	1.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ARG:NE	1:J:85:ARG:NE[2_554]	1.50	0.70
1:E:340:ARG:NH1	1:J:85:ARG:CZ[2_554]	1.57	0.63
1:E:340:ARG:CB	1:J:85:ARG:CD[2_554]	1.66	0.54
1:E:340:ARG:NH1	1:J:85:ARG:NH2[2_554]	1.70	0.50
1:A:68:GLN:OE1	1:C:85:ARG:NH1[4_455]	1.75	0.45
1:E:340:ARG:CZ	1:J:85:ARG:NE[2_554]	1.83	0.37
1:E:340:ARG:CB	1:J:85:ARG:CG[2_554]	1.87	0.33
1:D:68:GLN:OE1	1:F:85:ARG:NH1[4_555]	1.92	0.28
1:A:168:LYS:NZ	1:I:293:GLU:OE1[3_555]	2.01	0.19
1:E:340:ARG:CZ	1:J:85:ARG:CZ[2_554]	2.08	0.12
1:I:198:ARG:CZ	1:L:84:LYS:O[2_555]	2.09	0.11
1:B:293:GLU:OE1	1:H:168:LYS:NZ[3_555]	2.10	0.10
1:E:340:ARG:CD	1:J:85:ARG:CG[2_554]	2.11	0.09
1:B:344:GLU:O	1:H:47:HIS:CE1[3_555]	2.13	0.07

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	277/334 (83%)	257 (93%)	18 (6%)	2 (1%)	18	52
1	B	284/334 (85%)	260 (92%)	21 (7%)	3 (1%)	11	43
1	C	277/334 (83%)	259 (94%)	17 (6%)	1 (0%)	30	62
1	D	275/334 (82%)	258 (94%)	16 (6%)	1 (0%)	30	62
1	E	284/334 (85%)	260 (92%)	21 (7%)	3 (1%)	11	43
1	F	276/334 (83%)	257 (93%)	18 (6%)	1 (0%)	30	62
1	G	278/334 (83%)	260 (94%)	17 (6%)	1 (0%)	30	62
1	H	284/334 (85%)	258 (91%)	23 (8%)	3 (1%)	11	43
1	I	276/334 (83%)	260 (94%)	15 (5%)	1 (0%)	30	62
1	J	275/334 (82%)	258 (94%)	16 (6%)	1 (0%)	30	62
1	K	284/334 (85%)	260 (92%)	21 (7%)	3 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	276/334 (83%)	258 (94%)	17 (6%)	1 (0%)	30	62
All	All	3346/4008 (84%)	3105 (93%)	220 (7%)	21 (1%)	21	56

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	VAL
1	A	237	PRO
1	B	157	ALA
1	B	237	PRO
1	C	237	PRO
1	D	237	PRO
1	E	237	PRO
1	F	237	PRO
1	G	237	PRO
1	H	156	GLN
1	H	237	PRO
1	I	237	PRO
1	J	237	PRO
1	K	156	GLN
1	K	157	ALA
1	K	237	PRO
1	L	237	PRO
1	B	156	GLN
1	E	155	ASP
1	E	272	SER
1	H	272	SER

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	257/297 (86%)	231 (90%)	26 (10%)	7	30
1	B	262/297 (88%)	238 (91%)	24 (9%)	8	33
1	C	257/297 (86%)	233 (91%)	24 (9%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	255/297 (86%)	229 (90%)	26 (10%)	7	29
1	E	262/297 (88%)	236 (90%)	26 (10%)	7	31
1	F	256/297 (86%)	229 (90%)	27 (10%)	6	28
1	G	258/297 (87%)	229 (89%)	29 (11%)	6	25
1	H	262/297 (88%)	234 (89%)	28 (11%)	6	27
1	I	256/297 (86%)	231 (90%)	25 (10%)	7	31
1	J	255/297 (86%)	228 (89%)	27 (11%)	6	27
1	K	262/297 (88%)	234 (89%)	28 (11%)	6	27
1	L	256/297 (86%)	231 (90%)	25 (10%)	7	31
All	All	3098/3564 (87%)	2783 (90%)	315 (10%)	7	29

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	72	LEU
1	A	74	ILE
1	A	75	ASN
1	A	77	LYS
1	A	83	ASN
1	A	85	ARG
1	A	86	THR
1	A	106	GLU
1	A	110	ARG
1	A	134	LEU
1	A	149	ARG
1	A	185	ARG
1	A	229	TYR
1	A	233	GLU
1	A	239	LYS
1	A	265	SER
1	A	277	THR
1	A	293	GLU
1	A	330	LYS
1	A	333	GLN
1	A	334	THR
1	A	336	LEU
1	A	343	LYS
1	A	346	LYS

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Mol	Chain	Res	Type
1	A	347	GLU
1	B	54	ILE
1	B	66	THR
1	B	74	ILE
1	B	75	ASN
1	B	77	LYS
1	B	83	ASN
1	B	85	ARG
1	B	86	THR
1	B	106	GLU
1	B	110	ARG
1	B	134	LEU
1	B	149	ARG
1	B	156	GLN
1	B	185	ARG
1	B	233	GLU
1	B	239	LYS
1	B	277	THR
1	B	293	GLU
1	B	330	LYS
1	B	333	GLN
1	B	334	THR
1	B	336	LEU
1	B	346	LYS
1	B	347	GLU
1	C	47	HIS
1	C	54	ILE
1	C	72	LEU
1	C	74	ILE
1	C	75	ASN
1	C	83	ASN
1	C	85	ARG
1	C	86	THR
1	C	96	GLN
1	C	106	GLU
1	C	110	ARG
1	C	134	LEU
1	C	185	ARG
1	C	233	GLU
1	C	239	LYS
1	C	244	CYS
1	C	277	THR

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Mol	Chain	Res	Type
1	C	293	GLU
1	C	330	LYS
1	C	333	GLN
1	C	334	THR
1	C	336	LEU
1	C	346	LYS
1	C	347	GLU
1	D	54	ILE
1	D	72	LEU
1	D	74	ILE
1	D	75	ASN
1	D	77	LYS
1	D	83	ASN
1	D	85	ARG
1	D	86	THR
1	D	106	GLU
1	D	110	ARG
1	D	134	LEU
1	D	149	ARG
1	D	185	ARG
1	D	233	GLU
1	D	239	LYS
1	D	244	CYS
1	D	272	SER
1	D	277	THR
1	D	293	GLU
1	D	330	LYS
1	D	333	GLN
1	D	334	THR
1	D	336	LEU
1	D	343	LYS
1	D	346	LYS
1	D	347	GLU
1	E	54	ILE
1	E	72	LEU
1	E	74	ILE
1	E	75	ASN
1	E	83	ASN
1	E	85	ARG
1	E	86	THR
1	E	96	GLN
1	E	106	GLU

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Mol	Chain	Res	Type
1	E	110	ARG
1	E	134	LEU
1	E	149	ARG
1	E	155	ASP
1	E	185	ARG
1	E	233	GLU
1	E	239	LYS
1	E	244	CYS
1	E	272	SER
1	E	277	THR
1	E	293	GLU
1	E	330	LYS
1	E	333	GLN
1	E	334	THR
1	E	336	LEU
1	E	346	LYS
1	E	347	GLU
1	F	47	HIS
1	F	54	ILE
1	F	72	LEU
1	F	74	ILE
1	F	75	ASN
1	F	77	LYS
1	F	83	ASN
1	F	84	LYS
1	F	85	ARG
1	F	86	THR
1	F	96	GLN
1	F	106	GLU
1	F	110	ARG
1	F	134	LEU
1	F	185	ARG
1	F	230	VAL
1	F	233	GLU
1	F	239	LYS
1	F	244	CYS
1	F	277	THR
1	F	293	GLU
1	F	330	LYS
1	F	333	GLN
1	F	334	THR
1	F	336	LEU

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Mol	Chain	Res	Type
1	F	346	LYS
1	F	347	GLU
1	G	54	ILE
1	G	66	THR
1	G	72	LEU
1	G	74	ILE
1	G	75	ASN
1	G	77	LYS
1	G	83	ASN
1	G	85	ARG
1	G	86	THR
1	G	96	GLN
1	G	106	GLU
1	G	110	ARG
1	G	132	LYS
1	G	134	LEU
1	G	149	ARG
1	G	185	ARG
1	G	230	VAL
1	G	233	GLU
1	G	239	LYS
1	G	244	CYS
1	G	277	THR
1	G	293	GLU
1	G	330	LYS
1	G	333	GLN
1	G	334	THR
1	G	336	LEU
1	G	343	LYS
1	G	346	LYS
1	G	347	GLU
1	H	54	ILE
1	H	74	ILE
1	H	75	ASN
1	H	77	LYS
1	H	83	ASN
1	H	85	ARG
1	H	86	THR
1	H	96	GLN
1	H	106	GLU
1	H	110	ARG
1	H	134	LEU

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Mol	Chain	Res	Type
1	H	149	ARG
1	H	155	ASP
1	H	185	ARG
1	H	228	TYR
1	H	229	TYR
1	H	233	GLU
1	H	239	LYS
1	H	244	CYS
1	H	277	THR
1	H	293	GLU
1	H	330	LYS
1	H	333	GLN
1	H	334	THR
1	H	336	LEU
1	H	343	LYS
1	H	346	LYS
1	H	347	GLU
1	I	47	HIS
1	I	54	ILE
1	I	72	LEU
1	I	74	ILE
1	I	75	ASN
1	I	83	ASN
1	I	84	LYS
1	I	85	ARG
1	I	86	THR
1	I	106	GLU
1	I	110	ARG
1	I	134	LEU
1	I	185	ARG
1	I	230	VAL
1	I	233	GLU
1	I	239	LYS
1	I	244	CYS
1	I	277	THR
1	I	293	GLU
1	I	330	LYS
1	I	333	GLN
1	I	334	THR
1	I	336	LEU
1	I	346	LYS
1	I	347	GLU

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Mol	Chain	Res	Type
1	J	54	ILE
1	J	72	LEU
1	J	74	ILE
1	J	75	ASN
1	J	77	LYS
1	J	83	ASN
1	J	85	ARG
1	J	86	THR
1	J	96	GLN
1	J	106	GLU
1	J	110	ARG
1	J	134	LEU
1	J	149	ARG
1	J	185	ARG
1	J	233	GLU
1	J	239	LYS
1	J	244	CYS
1	J	265	SER
1	J	277	THR
1	J	293	GLU
1	J	330	LYS
1	J	333	GLN
1	J	334	THR
1	J	336	LEU
1	J	343	LYS
1	J	346	LYS
1	J	347	GLU
1	K	54	ILE
1	K	72	LEU
1	K	74	ILE
1	K	75	ASN
1	K	77	LYS
1	K	83	ASN
1	K	85	ARG
1	K	86	THR
1	K	96	GLN
1	K	106	GLU
1	K	110	ARG
1	K	134	LEU
1	K	149	ARG
1	K	156	GLN
1	K	185	ARG

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Mol	Chain	Res	Type
1	K	230	VAL
1	K	233	GLU
1	K	239	LYS
1	K	244	CYS
1	K	271	ILE
1	K	277	THR
1	K	293	GLU
1	K	330	LYS
1	K	333	GLN
1	K	334	THR
1	K	336	LEU
1	K	346	LYS
1	K	347	GLU
1	L	47	HIS
1	L	54	ILE
1	L	72	LEU
1	L	74	ILE
1	L	75	ASN
1	L	77	LYS
1	L	83	ASN
1	L	85	ARG
1	L	86	THR
1	L	96	GLN
1	L	106	GLU
1	L	110	ARG
1	L	134	LEU
1	L	185	ARG
1	L	229	TYR
1	L	233	GLU
1	L	239	LYS
1	L	244	CYS
1	L	277	THR
1	L	293	GLU
1	L	330	LYS
1	L	333	GLN
1	L	334	THR
1	L	336	LEU
1	L	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	83	ASN
1	A	116	HIS
1	A	151	GLN
1	A	184	HIS
1	A	191	ASN
1	A	200	ASN
1	A	304	ASN
1	A	333	GLN
1	B	83	ASN
1	B	116	HIS
1	B	151	GLN
1	B	156	GLN
1	B	184	HIS
1	B	191	ASN
1	B	200	ASN
1	B	304	ASN
1	B	333	GLN
1	C	83	ASN
1	C	116	HIS
1	C	184	HIS
1	C	191	ASN
1	C	200	ASN
1	C	304	ASN
1	C	333	GLN
1	D	75	ASN
1	D	83	ASN
1	D	116	HIS
1	D	184	HIS
1	D	191	ASN
1	D	200	ASN
1	D	304	ASN
1	D	333	GLN
1	E	83	ASN
1	E	113	GLN
1	E	151	GLN
1	E	184	HIS
1	E	191	ASN
1	E	200	ASN
1	E	333	GLN
1	F	75	ASN
1	F	83	ASN
1	F	116	HIS

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Mol	Chain	Res	Type
1	F	184	HIS
1	F	191	ASN
1	F	200	ASN
1	F	304	ASN
1	F	333	GLN
1	G	83	ASN
1	G	113	GLN
1	G	184	HIS
1	G	191	ASN
1	G	200	ASN
1	G	304	ASN
1	G	333	GLN
1	H	83	ASN
1	H	181	ASN
1	H	184	HIS
1	H	191	ASN
1	H	200	ASN
1	H	266	ASN
1	H	304	ASN
1	H	333	GLN
1	I	83	ASN
1	I	113	GLN
1	I	151	GLN
1	I	184	HIS
1	I	191	ASN
1	I	200	ASN
1	I	304	ASN
1	I	333	GLN
1	J	75	ASN
1	J	83	ASN
1	J	184	HIS
1	J	191	ASN
1	J	200	ASN
1	J	304	ASN
1	J	333	GLN
1	K	83	ASN
1	K	151	GLN
1	K	184	HIS
1	K	191	ASN
1	K	200	ASN
1	K	266	ASN
1	K	304	ASN

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Mol	Chain	Res	Type
1	K	333	GLN
1	L	83	ASN
1	L	184	HIS
1	L	191	ASN
1	L	304	ASN
1	L	333	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	P4O	D	1	-	29,30,30	1.59	3 (10%)	39,43,43	1.55	8 (20%)
2	P4O	I	1	-	29,30,30	1.43	5 (17%)	39,43,43	1.98	13 (33%)
2	P4O	A	1	-	29,30,30	1.38	4 (13%)	39,43,43	1.76	10 (25%)
2	P4O	B	1	-	29,30,30	1.39	2 (6%)	39,43,43	1.80	11 (28%)
2	P4O	F	1	-	29,30,30	1.50	4 (13%)	39,43,43	1.94	9 (23%)
2	P4O	H	1	-	29,30,30	1.45	2 (6%)	39,43,43	1.77	12 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P4O	J	1	-	29,30,30	1.50	3 (10%)	39,43,43	2.02	11 (28%)
2	P4O	K	1	-	29,30,30	1.55	3 (10%)	39,43,43	1.54	6 (15%)
2	P4O	E	1	-	29,30,30	1.43	4 (13%)	39,43,43	1.62	8 (20%)
2	P4O	G	1	-	29,30,30	1.45	3 (10%)	39,43,43	1.79	9 (23%)
2	P4O	L	1	-	29,30,30	1.45	4 (13%)	39,43,43	2.11	13 (33%)
2	P4O	C	1	-	29,30,30	1.42	4 (13%)	39,43,43	1.81	8 (20%)

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	P4O	D	1	-	-	0/8/18/18	0/5/5/5
2	P4O	I	1	-	-	0/8/18/18	0/5/5/5
2	P4O	A	1	-	-	0/8/18/18	0/5/5/5
2	P4O	B	1	-	-	0/8/18/18	0/5/5/5
2	P4O	F	1	-	-	0/8/18/18	0/5/5/5
2	P4O	H	1	-	-	0/8/18/18	0/5/5/5
2	P4O	J	1	-	-	0/8/18/18	0/5/5/5
2	P4O	K	1	-	-	0/8/18/18	0/5/5/5
2	P4O	E	1	-	-	0/8/18/18	0/5/5/5
2	P4O	G	1	-	-	0/8/18/18	0/5/5/5
2	P4O	L	1	-	-	0/8/18/18	0/5/5/5
2	P4O	C	1	-	-	0/8/18/18	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	P4O	C20-C21	6.02	1.51	1.42
2	D	1	P4O	C20-C21	5.87	1.50	1.42
2	F	1	P4O	C20-C21	5.25	1.50	1.42
2	H	1	P4O	C20-C21	5.21	1.49	1.42
2	C	1	P4O	C20-C21	5.19	1.49	1.42
2	L	1	P4O	C20-C21	5.13	1.49	1.42
2	K	1	P4O	C20-C21	5.13	1.49	1.42
2	I	1	P4O	C20-C21	5.11	1.49	1.42
2	A	1	P4O	C20-C21	4.95	1.49	1.42
2	B	1	P4O	C20-C21	4.88	1.49	1.42
2	G	1	P4O	C20-C21	4.82	1.49	1.42
2	E	1	P4O	C20-C21	4.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	P4O	C4-C6	2.81	1.50	1.45
2	G	1	P4O	C4-C6	2.72	1.50	1.45
2	D	1	P4O	C17-N16	2.64	1.36	1.31
2	K	1	P4O	C4-C6	2.62	1.49	1.45
2	G	1	P4O	C17-N16	2.59	1.36	1.31
2	D	1	P4O	C4-C6	2.57	1.49	1.45
2	F	1	P4O	C4-C6	2.56	1.49	1.45
2	J	1	P4O	C3-C4	-2.54	1.36	1.42
2	H	1	P4O	C4-C6	2.50	1.49	1.45
2	B	1	P4O	C4-C6	2.38	1.49	1.45
2	L	1	P4O	C17-N16	2.36	1.35	1.31
2	A	1	P4O	C17-N16	2.33	1.35	1.31
2	L	1	P4O	C4-C6	2.32	1.49	1.45
2	E	1	P4O	C12-C2	2.27	1.51	1.47
2	K	1	P4O	C17-N16	2.23	1.35	1.31
2	I	1	P4O	C3-C4	-2.22	1.37	1.42
2	L	1	P4O	C23-C22	2.19	1.41	1.36
2	F	1	P4O	C3-C4	-2.15	1.37	1.42
2	C	1	P4O	C23-C22	2.14	1.41	1.36
2	I	1	P4O	C17-N16	2.12	1.35	1.31
2	C	1	P4O	C4-C6	2.08	1.48	1.45
2	C	1	P4O	C17-N16	2.08	1.35	1.31
2	J	1	P4O	C17-N16	2.06	1.35	1.31
2	A	1	P4O	C3-C4	-2.04	1.37	1.42
2	I	1	P4O	C23-C22	2.04	1.41	1.36
2	A	1	P4O	C4-C6	2.04	1.48	1.45
2	I	1	P4O	C4-C6	2.02	1.48	1.45
2	E	1	P4O	C17-N16	2.02	1.35	1.31
2	F	1	P4O	C23-C22	2.00	1.41	1.36

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	P4O	C19-C18-C17	5.29	122.82	116.26
2	C	1	P4O	C18-C17-N16	-5.23	120.87	125.48
2	F	1	P4O	C12-C2-C3	-4.95	123.42	131.03
2	J	1	P4O	C18-C17-N16	-4.80	121.25	125.48
2	J	1	P4O	C19-C18-C17	4.79	122.20	116.26
2	L	1	P4O	C18-C17-N16	-4.70	121.34	125.48
2	J	1	P4O	C12-C2-C3	-4.54	124.05	131.03
2	A	1	P4O	C18-C17-N16	-4.40	121.60	125.48
2	L	1	P4O	C12-C2-C3	-4.36	124.33	131.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	P4O	C12-C2-C3	-4.22	124.55	131.03
2	A	1	P4O	C19-C18-C17	4.17	121.43	116.26
2	I	1	P4O	C12-C2-C3	-4.13	124.68	131.03
2	C	1	P4O	C19-C18-C17	4.08	121.32	116.26
2	F	1	P4O	C18-C17-N16	-4.06	121.90	125.48
2	B	1	P4O	C12-C2-C3	-4.04	124.82	131.03
2	B	1	P4O	C10-N15-C14	4.02	122.86	117.24
2	B	1	P4O	C11-C10-N15	-3.98	119.09	123.97
2	I	1	P4O	C18-C17-N16	-3.88	122.06	125.48
2	H	1	P4O	C19-C18-C17	3.88	121.07	116.26
2	C	1	P4O	C12-C2-C3	-3.72	125.31	131.03
2	E	1	P4O	C18-C17-N16	-3.68	122.23	125.48
2	E	1	P4O	C10-N15-C14	3.68	122.38	117.24
2	L	1	P4O	C17-N16-C21	3.66	121.19	116.96
2	I	1	P4O	C10-N15-C14	3.65	122.35	117.24
2	L	1	P4O	C12-C2-N1	3.64	127.37	122.76
2	C	1	P4O	C17-N16-C21	3.61	121.14	116.96
2	G	1	P4O	C18-C17-N16	-3.58	122.33	125.48
2	G	1	P4O	C19-C18-C17	3.55	120.67	116.26
2	H	1	P4O	C18-C17-N16	-3.46	122.43	125.48
2	I	1	P4O	C19-C18-C17	3.42	120.50	116.26
2	D	1	P4O	C10-N15-C14	3.41	122.01	117.24
2	L	1	P4O	C9-C5-C4	-3.40	123.08	125.13
2	E	1	P4O	C11-C10-N15	-3.38	119.84	123.97
2	E	1	P4O	C17-N16-C21	3.35	120.84	116.96
2	H	1	P4O	C10-N15-C14	3.31	121.87	117.24
2	D	1	P4O	C11-C10-N15	-3.28	119.96	123.97
2	G	1	P4O	C10-N15-C14	3.25	121.79	117.24
2	J	1	P4O	C11-C10-N15	-3.24	120.01	123.97
2	I	1	P4O	C11-C10-N15	-3.23	120.02	123.97
2	L	1	P4O	C11-C10-N15	-3.20	120.05	123.97
2	A	1	P4O	C3-C4-C5	3.18	110.13	107.65
2	L	1	P4O	C10-N15-C14	3.17	121.67	117.24
2	D	1	P4O	C19-C18-C17	3.15	120.16	116.26
2	I	1	P4O	C3-C4-C5	3.14	110.10	107.65
2	F	1	P4O	C11-C10-N15	-3.14	120.13	123.97
2	J	1	P4O	C10-N15-C14	3.13	121.62	117.24
2	K	1	P4O	C19-C18-C17	3.04	120.03	116.26
2	H	1	P4O	C11-C10-N15	-3.03	120.26	123.97
2	L	1	P4O	C19-C18-C17	2.99	119.97	116.26
2	K	1	P4O	C3-C4-C5	2.99	109.99	107.65
2	J	1	P4O	C3-C4-C5	2.98	109.98	107.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	P4O	C4-C5-N1	-2.94	106.61	109.75
2	K	1	P4O	C18-C17-N16	-2.88	122.94	125.48
2	B	1	P4O	C17-N16-C21	2.78	120.18	116.96
2	G	1	P4O	C11-C10-N15	-2.78	120.56	123.97
2	D	1	P4O	C18-C17-N16	-2.77	123.04	125.48
2	E	1	P4O	C19-C18-C17	2.76	119.68	116.26
2	A	1	P4O	C10-N15-C14	2.76	121.10	117.24
2	K	1	P4O	C4-C5-N1	-2.75	106.81	109.75
2	L	1	P4O	O26-C6-C4	-2.75	119.91	125.98
2	H	1	P4O	C9-C5-C4	2.75	126.78	125.13
2	J	1	P4O	C17-N16-C21	2.74	120.13	116.96
2	L	1	P4O	C4-C5-N1	-2.72	106.85	109.75
2	B	1	P4O	O26-C6-C4	-2.69	120.05	125.98
2	B	1	P4O	C12-C2-N1	2.69	126.17	122.76
2	F	1	P4O	C12-C2-N1	2.68	126.16	122.76
2	F	1	P4O	C18-C19-C20	-2.66	116.89	121.61
2	B	1	P4O	C4-C5-N1	-2.64	106.93	109.75
2	B	1	P4O	C18-C17-N16	-2.62	123.18	125.48
2	I	1	P4O	C3-C2-N1	2.61	110.84	107.51
2	B	1	P4O	C3-C4-C5	2.57	109.66	107.65
2	C	1	P4O	C11-C10-N15	-2.57	120.83	123.97
2	H	1	P4O	C12-C2-C3	-2.55	127.12	131.03
2	F	1	P4O	C10-N15-C14	2.54	120.79	117.24
2	A	1	P4O	C12-C2-C3	-2.52	127.16	131.03
2	C	1	P4O	C10-N15-C14	2.51	120.76	117.24
2	I	1	P4O	C4-C5-N1	-2.50	107.08	109.75
2	J	1	P4O	O26-C6-C4	-2.49	120.49	125.98
2	K	1	P4O	O26-C6-C4	-2.49	120.50	125.98
2	B	1	P4O	C19-C18-C17	2.48	119.34	116.26
2	G	1	P4O	C22-C21-N16	2.47	122.53	118.55
2	H	1	P4O	C3-C4-C5	2.47	109.58	107.65
2	L	1	P4O	C22-C21-N16	2.46	122.51	118.55
2	A	1	P4O	O26-C6-C4	-2.46	120.57	125.98
2	H	1	P4O	C4-C5-N1	-2.43	107.15	109.75
2	L	1	P4O	C3-C4-C5	2.43	109.55	107.65
2	I	1	P4O	C17-N16-C21	2.42	119.76	116.96
2	I	1	P4O	O26-C6-C4	-2.40	120.69	125.98
2	F	1	P4O	C8-C9-C5	2.39	112.75	108.37
2	A	1	P4O	C17-N16-C21	2.38	119.71	116.96
2	E	1	P4O	C4-C5-N1	-2.37	107.22	109.75
2	G	1	P4O	C3-C2-N1	2.36	110.52	107.51
2	I	1	P4O	C25-C20-C21	2.35	121.60	118.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	P4O	C22-C21-N16	2.32	122.28	118.55
2	A	1	P4O	C22-C21-N16	2.31	122.27	118.55
2	H	1	P4O	C3-C2-N1	2.30	110.44	107.51
2	H	1	P4O	C17-N16-C21	2.29	119.61	116.96
2	F	1	P4O	C3-C2-N1	2.29	110.42	107.51
2	J	1	P4O	C4-C5-N1	-2.28	107.31	109.75
2	E	1	P4O	C8-C9-C5	2.27	112.53	108.37
2	J	1	P4O	C3-C2-N1	2.27	110.40	107.51
2	G	1	P4O	C22-C21-C20	-2.26	116.78	119.04
2	I	1	P4O	C24-C23-C22	2.24	123.40	120.40
2	C	1	P4O	C22-C21-N16	2.23	122.13	118.55
2	L	1	P4O	C9-C8-N7	-2.22	105.02	110.95
2	D	1	P4O	C4-C5-N1	-2.21	107.39	109.75
2	C	1	P4O	C8-C9-C5	2.19	112.38	108.37
2	D	1	P4O	C12-C2-C3	-2.19	127.67	131.03
2	J	1	P4O	C12-C2-N1	2.18	125.52	122.76
2	A	1	P4O	C11-C10-N15	-2.15	121.34	123.97
2	D	1	P4O	C13-C14-N15	-2.11	119.47	122.13
2	K	1	P4O	C24-C23-C22	2.10	123.22	120.40
2	G	1	P4O	C25-C20-C21	2.10	121.26	118.43
2	D	1	P4O	C24-C23-C22	2.10	123.21	120.40
2	B	1	P4O	C20-C21-N16	-2.09	119.15	122.03
2	E	1	P4O	C20-C21-N16	-2.04	119.22	122.03
2	H	1	P4O	C18-C19-C20	-2.03	118.00	121.61
2	H	1	P4O	C8-C9-C5	2.02	112.07	108.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

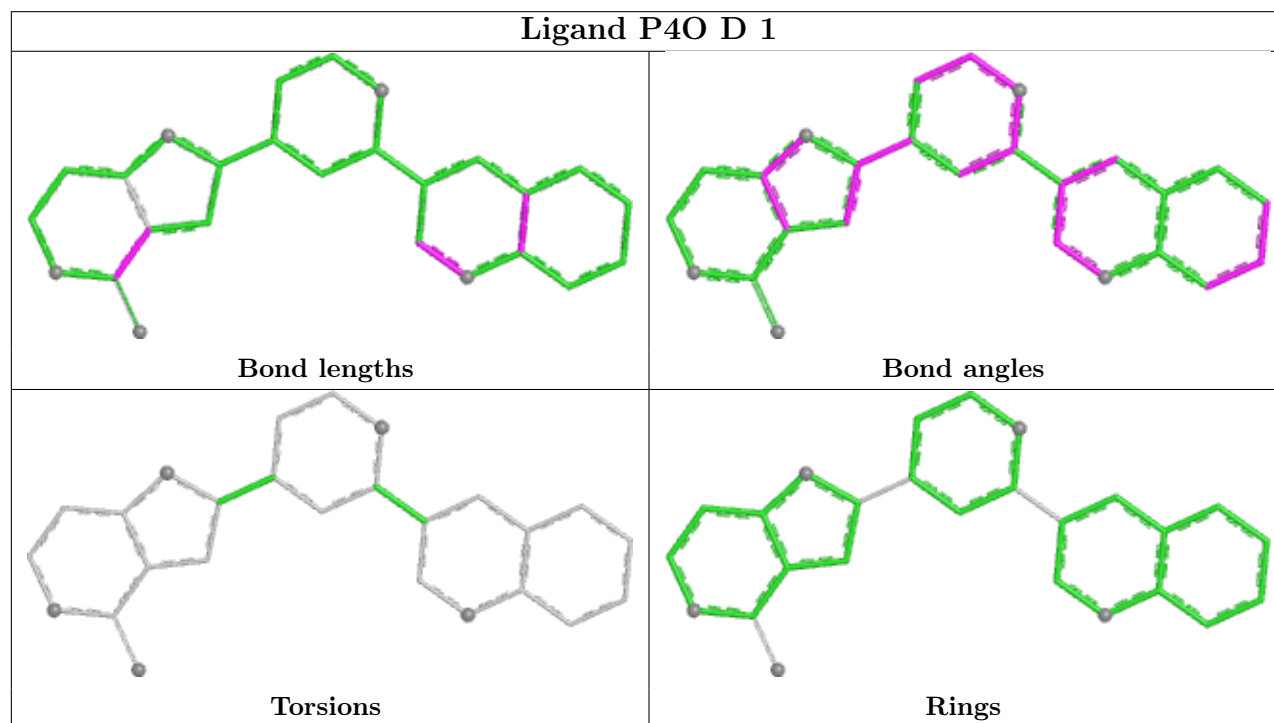
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	P4O	3	0
2	A	1	P4O	1	0
2	B	1	P4O	1	0
2	F	1	P4O	3	0
2	H	1	P4O	1	0
2	J	1	P4O	2	0
2	K	1	P4O	1	0
2	E	1	P4O	2	0
2	L	1	P4O	1	0

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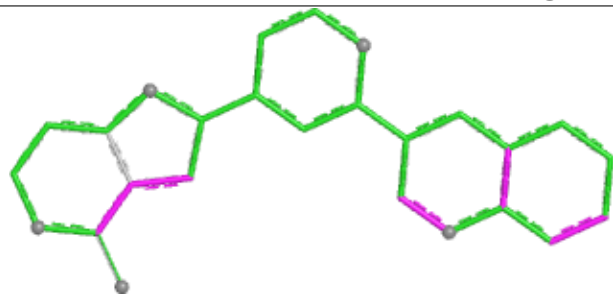
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	P4O	1	0

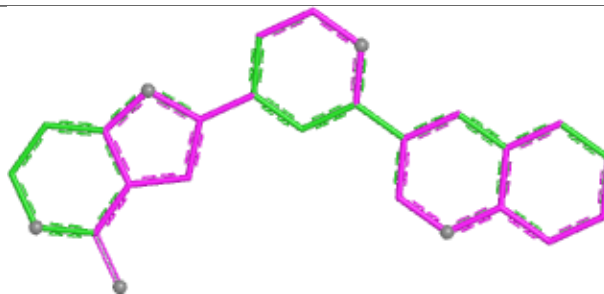
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



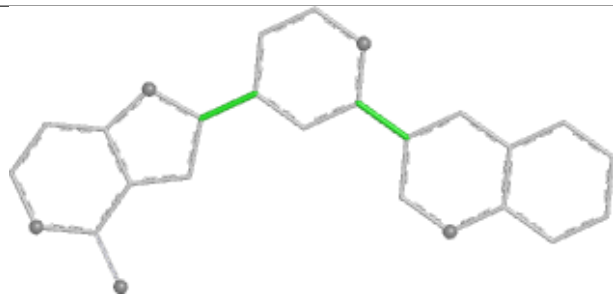
Ligand P4O I 1



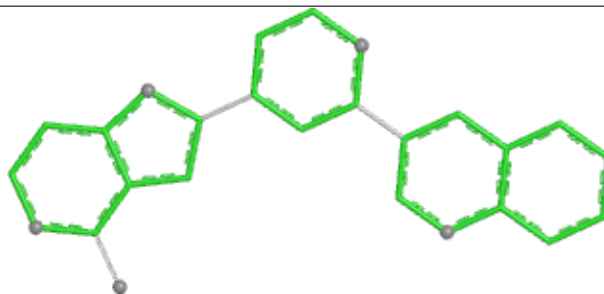
Bond lengths



Bond angles

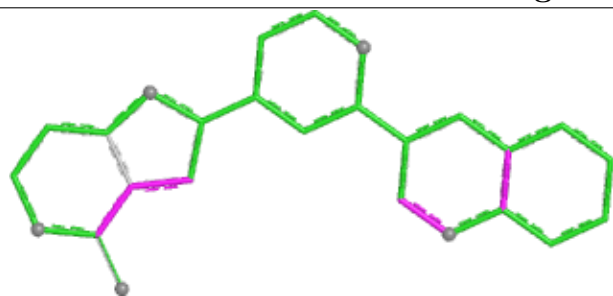


Torsions

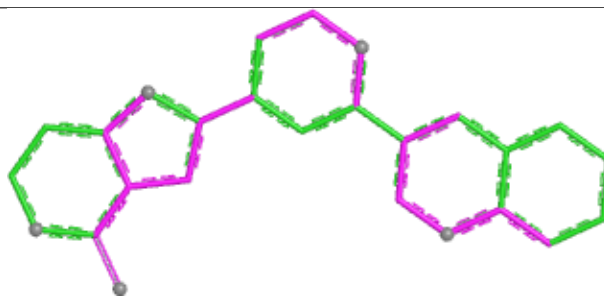


Rings

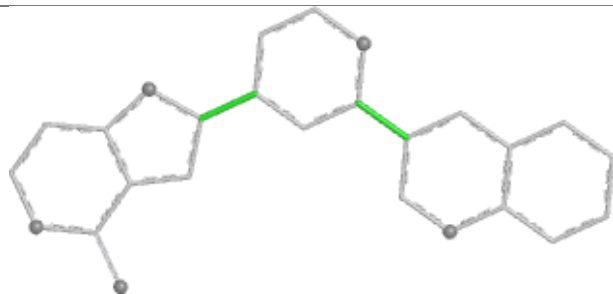
Ligand P4O A 1



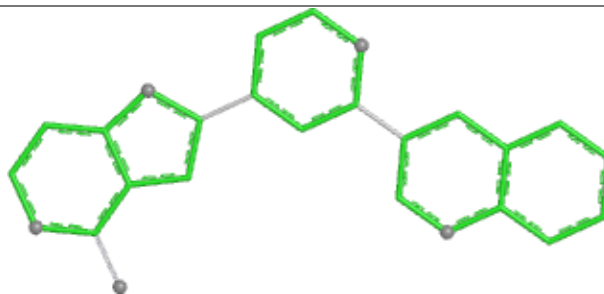
Bond lengths



Bond angles

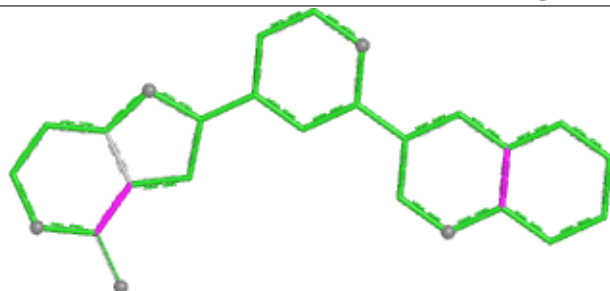


Torsions

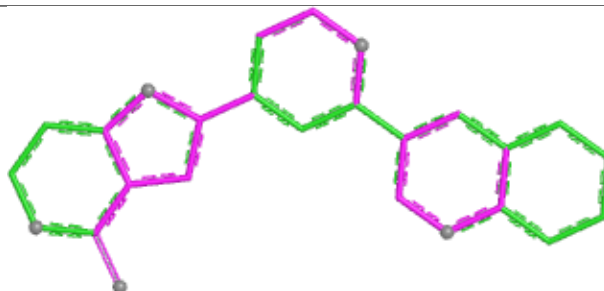


Rings

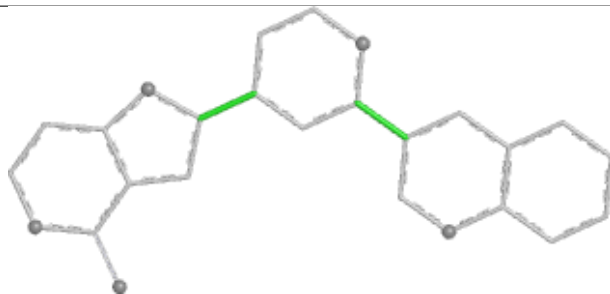
Ligand P4O B 1



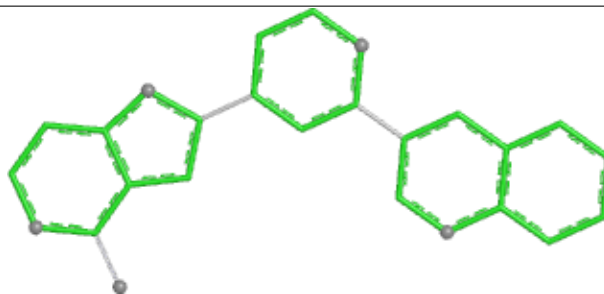
Bond lengths



Bond angles

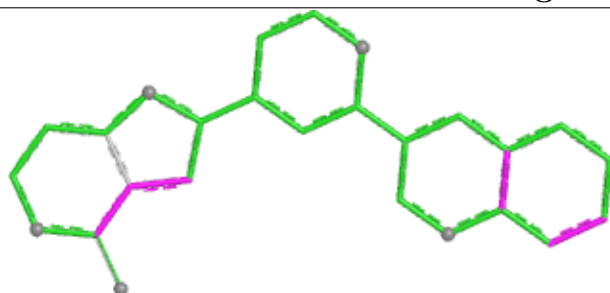


Torsions

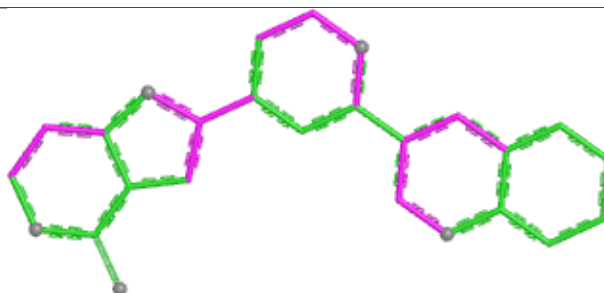


Rings

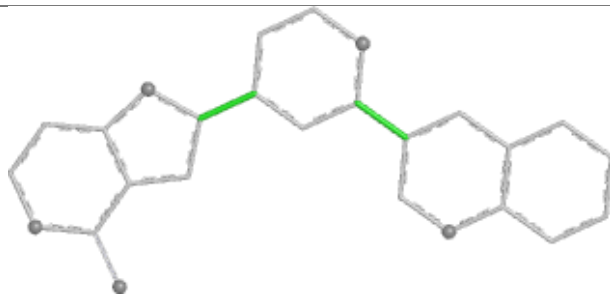
Ligand P4O F 1



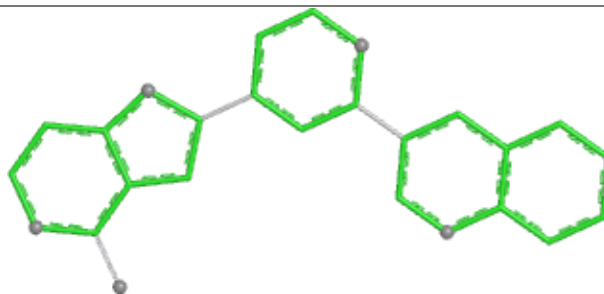
Bond lengths



Bond angles

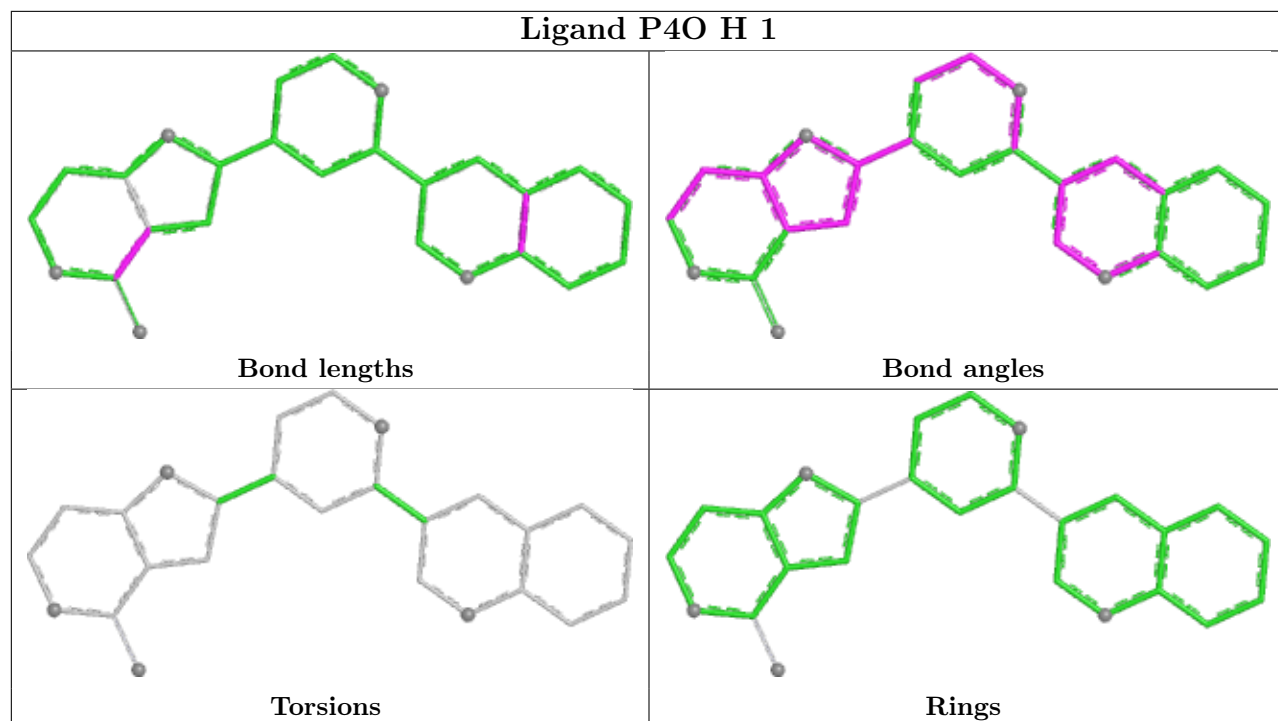


Torsions

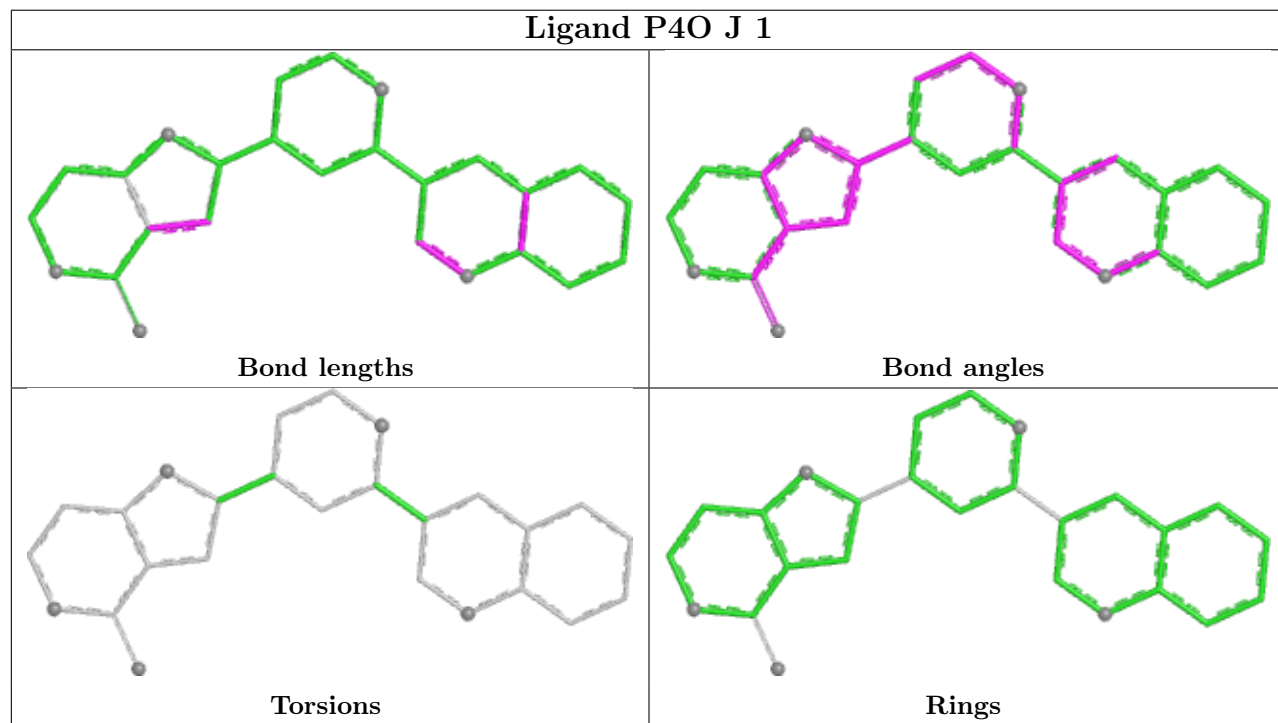


Rings

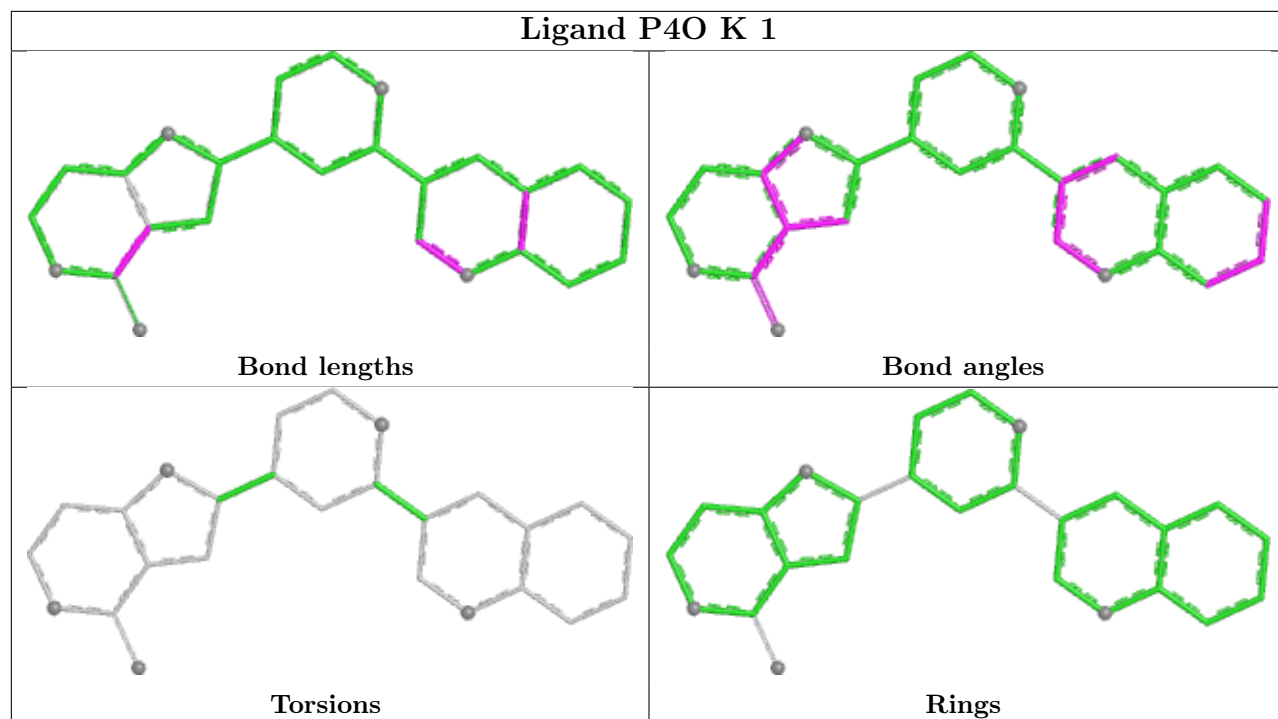
Ligand P4O H 1



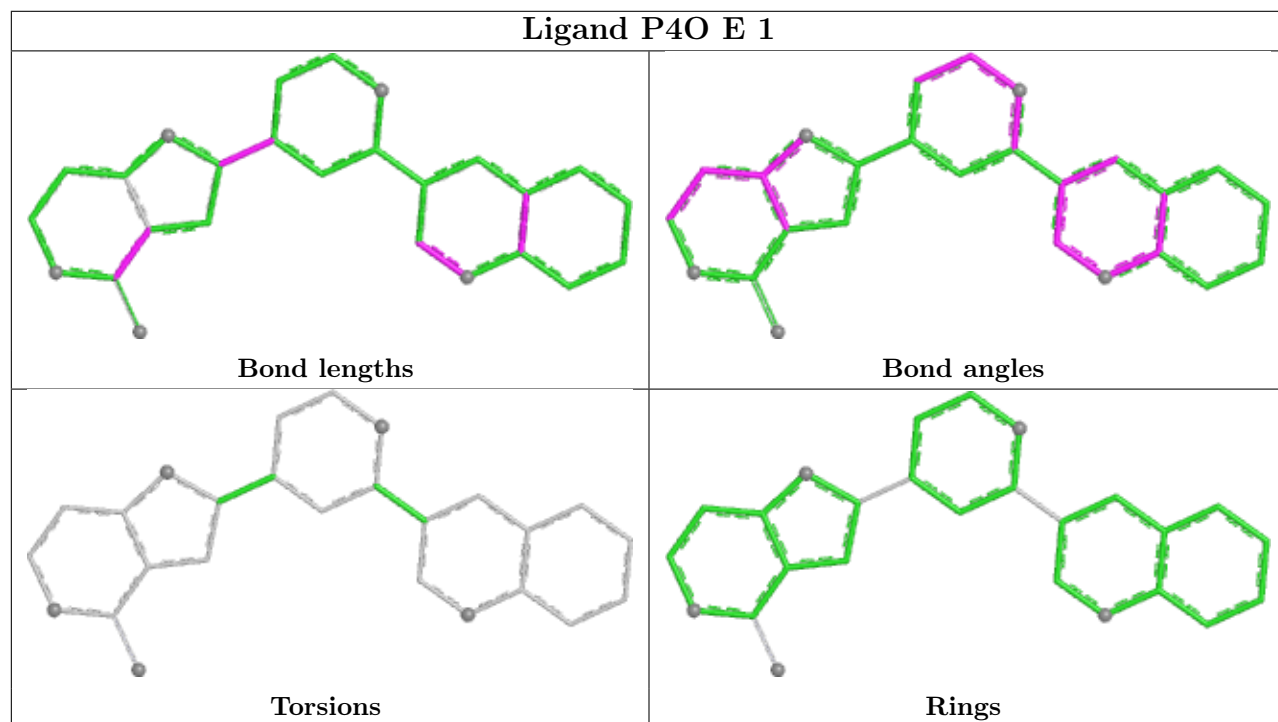
Ligand P4O J 1



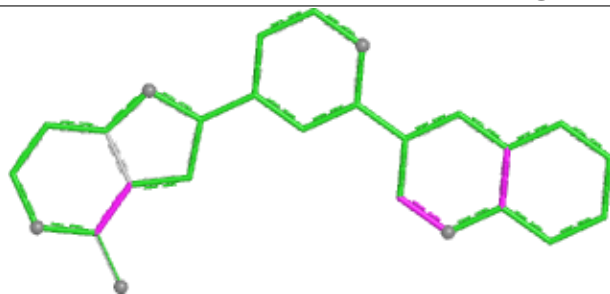
Ligand P4O K 1



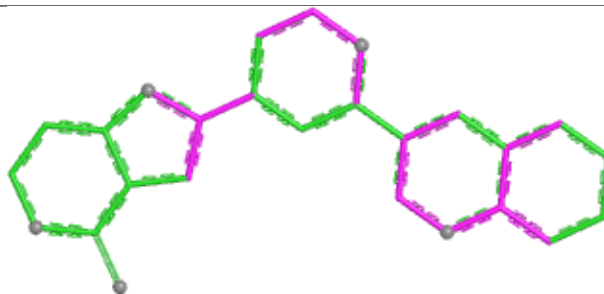
Ligand P4O E 1



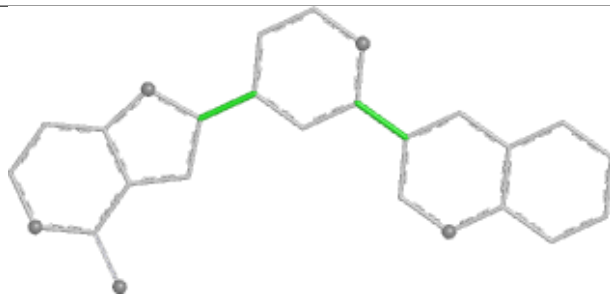
Ligand P4O G 1



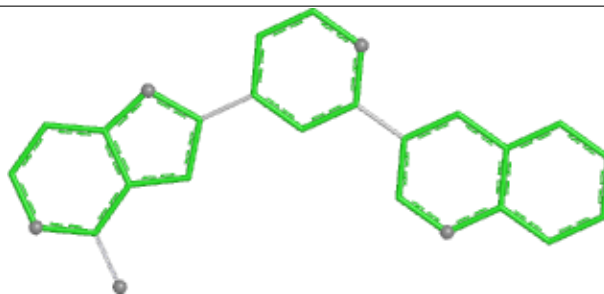
Bond lengths



Bond angles

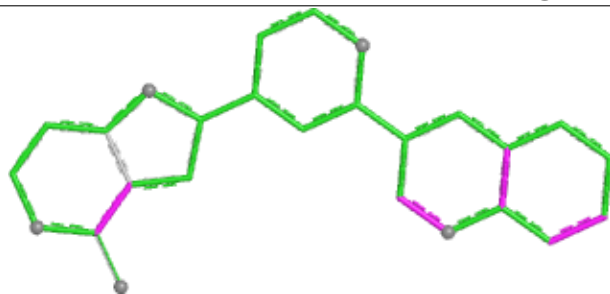


Torsions

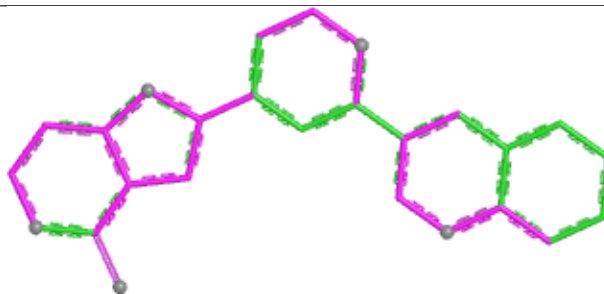


Rings

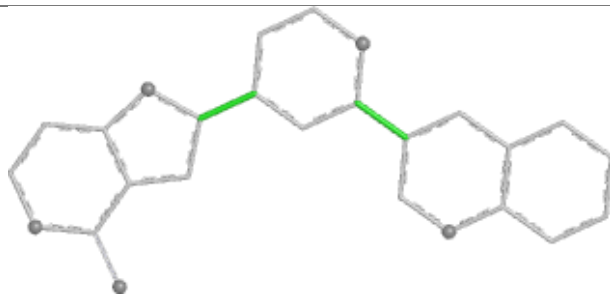
Ligand P4O L 1



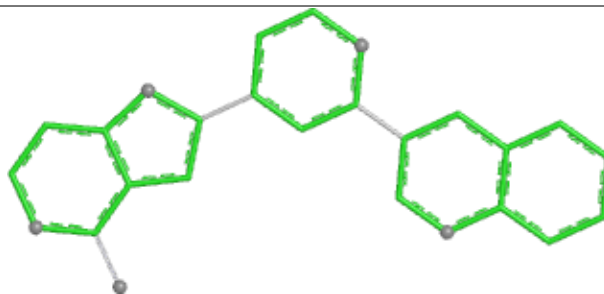
Bond lengths



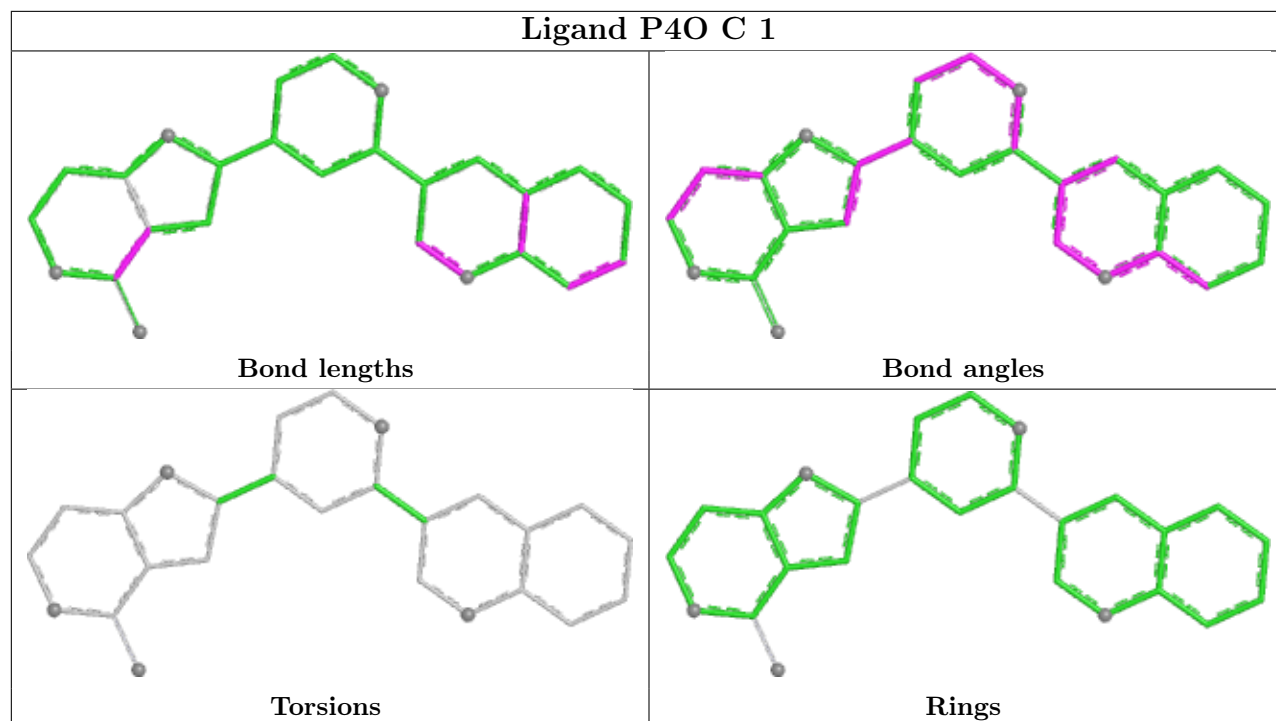
Bond angles



Torsions



Rings



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	285/334 (85%)	0.19	10 (3%)	47	29	42, 63, 95, 119	0
1	B	290/334 (86%)	0.12	8 (2%)	55	35	42, 64, 94, 118	0
1	C	285/334 (85%)	0.20	12 (4%)	40	25	42, 63, 93, 118	0
1	D	283/334 (84%)	0.22	9 (3%)	50	31	42, 63, 93, 118	0
1	E	290/334 (86%)	0.04	6 (2%)	63	43	42, 64, 95, 118	0
1	F	284/334 (85%)	0.29	12 (4%)	40	25	42, 63, 93, 118	0
1	G	286/334 (85%)	0.20	13 (4%)	38	24	42, 63, 93, 118	0
1	H	290/334 (86%)	-0.03	7 (2%)	59	40	42, 64, 94, 118	0
1	I	284/334 (85%)	0.18	13 (4%)	37	23	42, 63, 93, 118	0
1	J	283/334 (84%)	-0.04	2 (0%)	84	69	42, 63, 93, 119	0
1	K	290/334 (86%)	0.02	5 (1%)	69	49	42, 64, 95, 119	0
1	L	284/334 (85%)	0.06	9 (3%)	50	31	42, 63, 93, 118	0
All	All	3434/4008 (85%)	0.12	106 (3%)	51	32	42, 63, 95, 119	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	157	ALA	6.3
1	C	157	ALA	5.3
1	I	154	GLY	4.9
1	C	154	GLY	4.9
1	F	154	GLY	4.4
1	B	350	GLU	4.3
1	G	154	GLY	4.2
1	G	46	PHE	3.9
1	J	350	GLU	3.9
1	C	67	SER	3.5
1	C	329	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	157	ALA	3.3
1	I	113	GLN	3.3
1	B	157	ALA	3.2
1	A	264	TYR	3.2
1	C	350	GLU	3.1
1	H	155	ASP	3.1
1	F	329	THR	3.0
1	I	230	VAL	3.0
1	F	350	GLU	3.0
1	E	232	PRO	3.0
1	G	232	PRO	3.0
1	K	271	ILE	3.0
1	I	350	GLU	2.9
1	F	46	PHE	2.9
1	H	271	ILE	2.9
1	C	199	PRO	2.9
1	H	350	GLU	2.9
1	C	293	GLU	2.9
1	I	157	ALA	2.9
1	E	350	GLU	2.8
1	F	48	VAL	2.8
1	C	328	SER	2.8
1	E	230	VAL	2.7
1	C	46	PHE	2.7
1	J	85	ARG	2.7
1	B	48	VAL	2.7
1	A	289	PRO	2.6
1	C	230	VAL	2.6
1	H	235	LEU	2.6
1	I	46	PHE	2.6
1	G	274	GLY	2.6
1	D	350	GLU	2.6
1	I	293	GLU	2.6
1	L	157	ALA	2.6
1	L	46	PHE	2.6
1	D	46	PHE	2.6
1	F	232	PRO	2.6
1	I	48	VAL	2.6
1	F	328	SER	2.5
1	A	154	GLY	2.5
1	E	271	ILE	2.5
1	H	230	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	231	ALA	2.5
1	K	46	PHE	2.5
1	A	232	PRO	2.4
1	D	157	ALA	2.4
1	C	229	TYR	2.4
1	G	47	HIS	2.4
1	E	231	ALA	2.4
1	D	94	MET	2.4
1	H	48	VAL	2.4
1	L	349	TRP	2.4
1	F	130	GLY	2.3
1	I	233	GLU	2.3
1	D	85	ARG	2.3
1	A	229	TYR	2.3
1	A	46	PHE	2.3
1	B	293	GLU	2.3
1	A	350	GLU	2.3
1	B	261	PRO	2.3
1	F	199	PRO	2.3
1	G	152	ASP	2.3
1	K	230	VAL	2.3
1	G	48	VAL	2.3
1	D	154	GLY	2.2
1	D	289	PRO	2.2
1	I	264	TYR	2.2
1	G	231	ALA	2.2
1	H	229	TYR	2.2
1	I	74	ILE	2.2
1	A	47	HIS	2.2
1	G	350	GLU	2.2
1	L	273	PRO	2.2
1	G	349	TRP	2.2
1	E	340	ARG	2.1
1	I	329	THR	2.1
1	B	228	TYR	2.1
1	G	229	TYR	2.1
1	D	292	SER	2.1
1	L	293	GLU	2.1
1	K	339	SER	2.1
1	G	113	GLN	2.1
1	K	273	PRO	2.1
1	C	48	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	242	LYS	2.1
1	D	231	ALA	2.1
1	B	46	PHE	2.1
1	L	74	ILE	2.0
1	L	350	GLU	2.0
1	F	60	ILE	2.0
1	A	231	ALA	2.0
1	B	241	ASP	2.0
1	L	154	GLY	2.0
1	A	293	GLU	2.0
1	L	285	GLU	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](#)

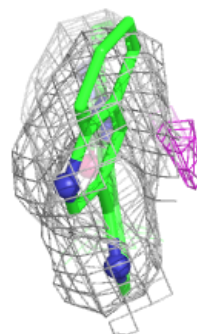
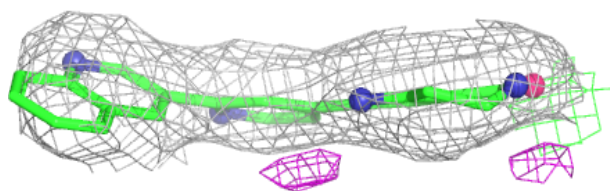
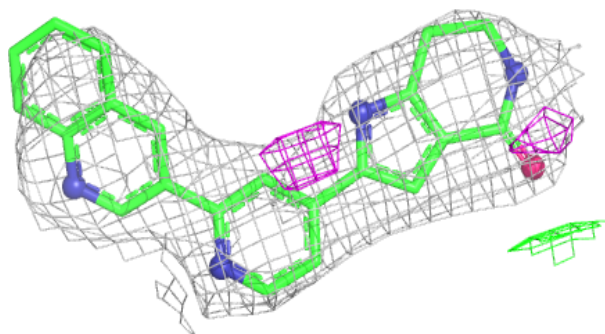
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	P4O	K	1	26/26	0.90	0.14	95,97,106,107	0
2	P4O	J	1	26/26	0.92	0.11	97,110,120,120	0
2	P4O	G	1	26/26	0.92	0.11	71,77,88,88	0
2	P4O	L	1	26/26	0.92	0.11	93,97,105,106	0
2	P4O	F	1	26/26	0.93	0.09	70,74,86,88	0
2	P4O	B	1	26/26	0.93	0.09	70,77,95,96	0
2	P4O	H	1	26/26	0.93	0.10	78,82,92,93	0
2	P4O	I	1	26/26	0.95	0.09	83,86,93,95	0
2	P4O	E	1	26/26	0.96	0.08	87,91,98,100	0
2	P4O	A	1	26/26	0.96	0.08	62,68,78,78	0
2	P4O	C	1	26/26	0.96	0.08	70,79,93,95	0
2	P4O	D	1	26/26	0.96	0.08	62,71,80,81	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.

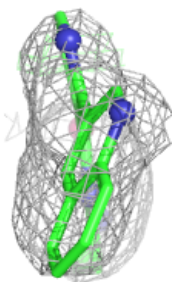
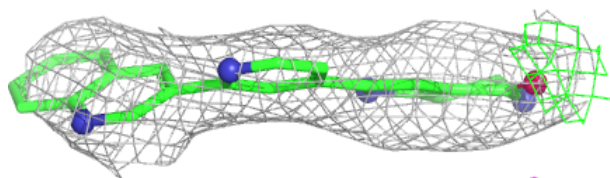
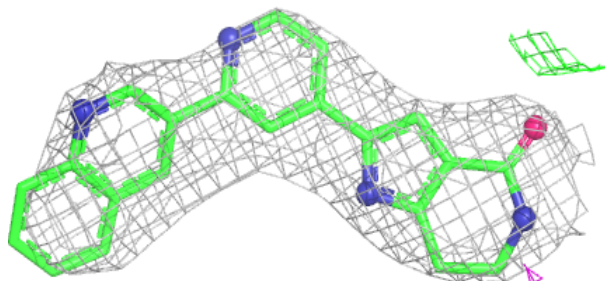
Electron density around P4O K 1:

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

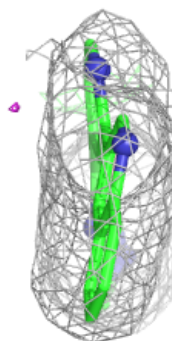
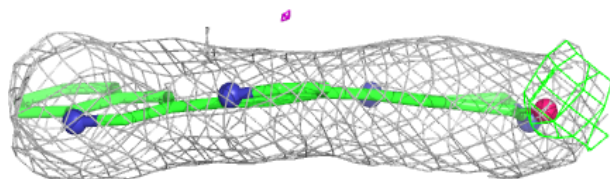
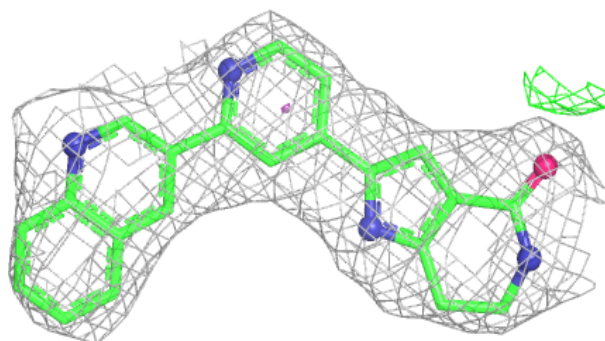


Electron density around P4O J 1:

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

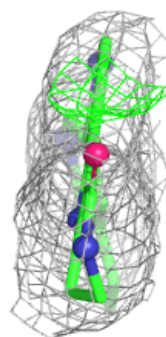
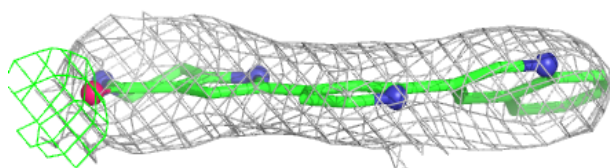
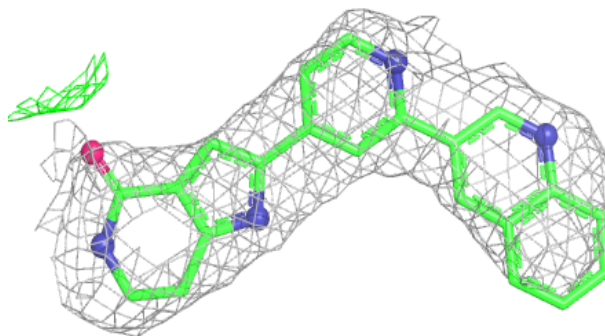
**Electron density around P4O G 1:**

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

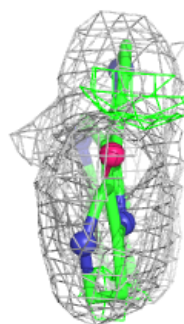
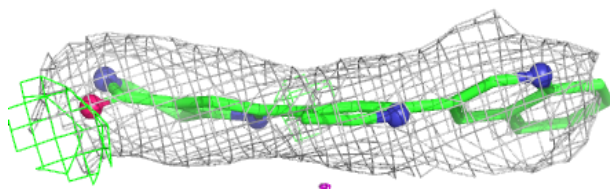
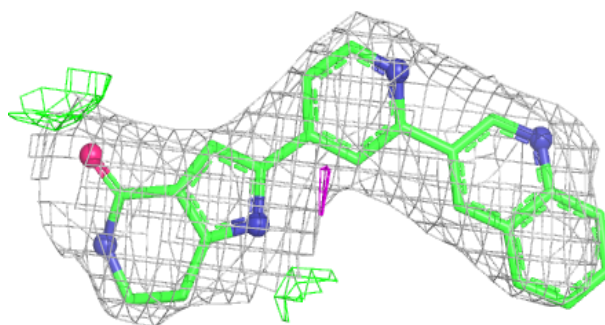


Electron density around P4O L 1:

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

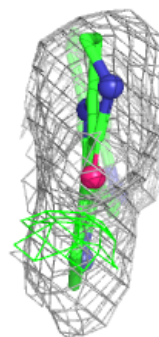
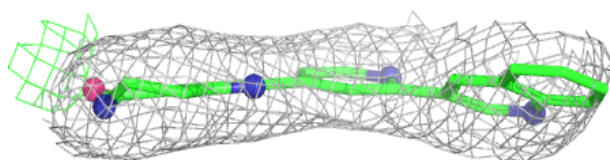
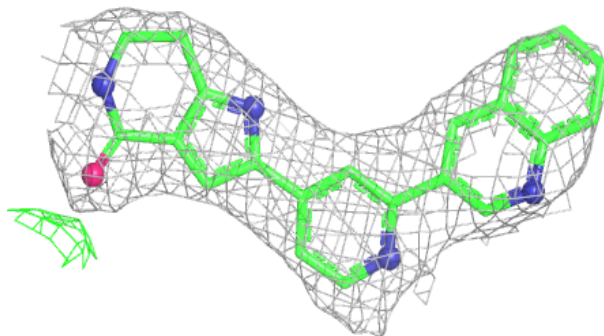
**Electron density around P4O F 1:**

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

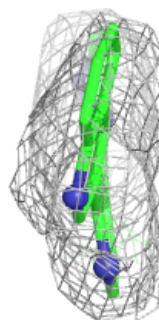
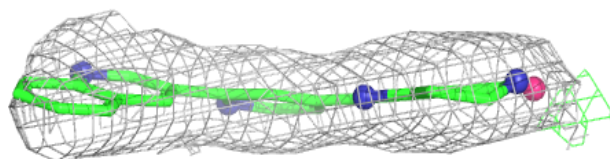


Electron density around P4O B 1:

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

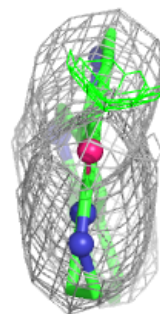
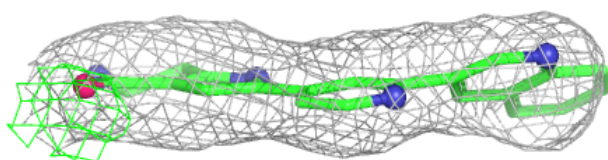
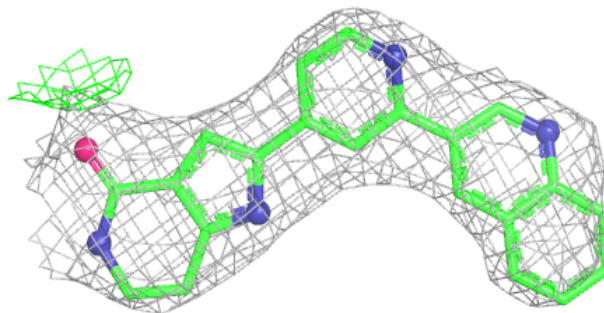
**Electron density around P4O H 1:**

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

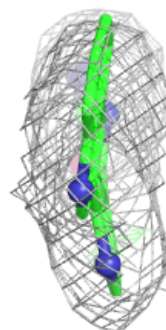
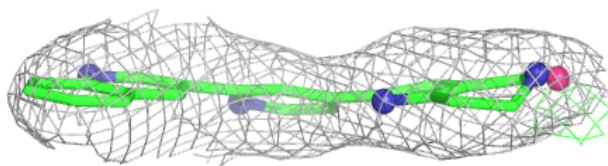
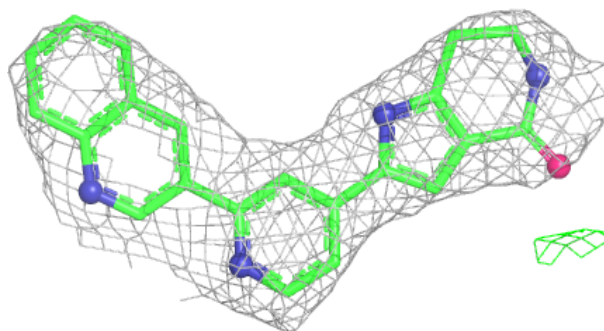


Electron density around P4O I 1:

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

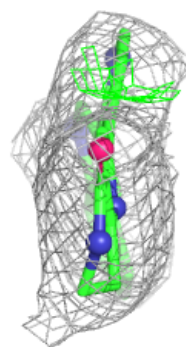
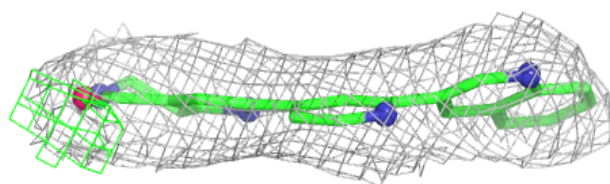
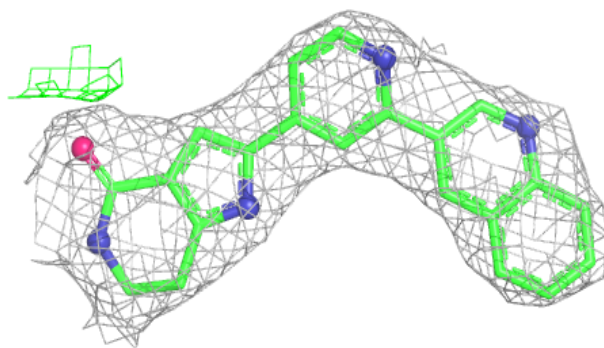
**Electron density around P4O E 1:**

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

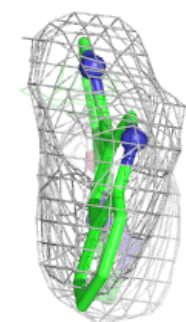
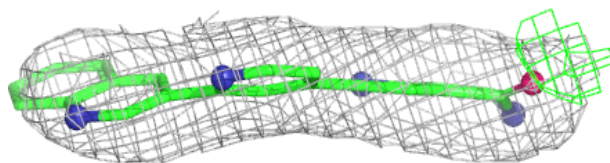
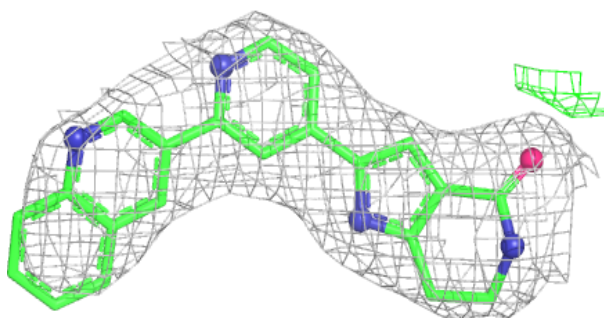


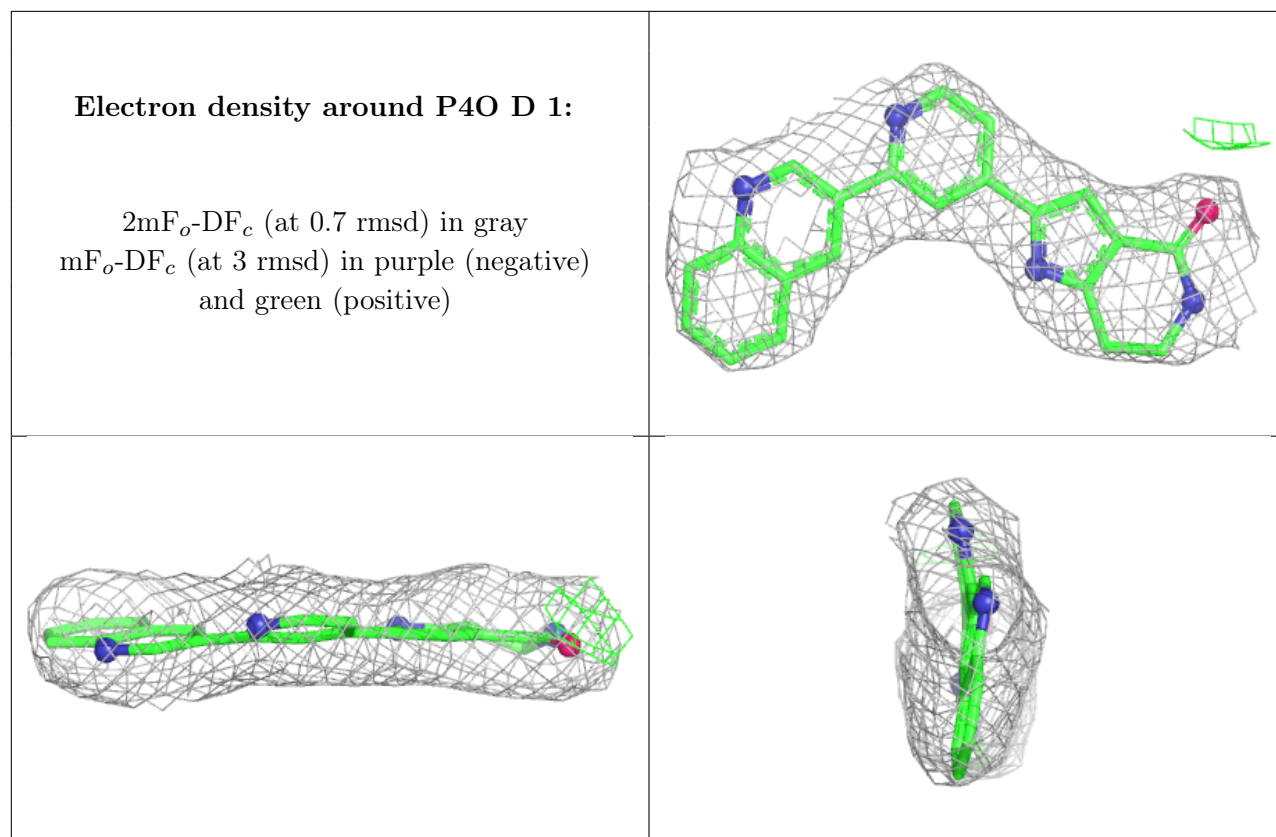
Electron density around P4O A 1:

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

**Electron density around P4O C 1:**

$2mF_o-DF_c$ (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.