



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:17 AM UTC

PDB ID : 7Z5N / pdb_00007z5n
Title : Crystal structure of DYRK1A in complex with CX-4945
Authors : Pustelny, K.; Grygier, P.; Golik, P.; Dubin, G.; Czarna, A.
Deposited on : 2022-03-09
Resolution : 2.77 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

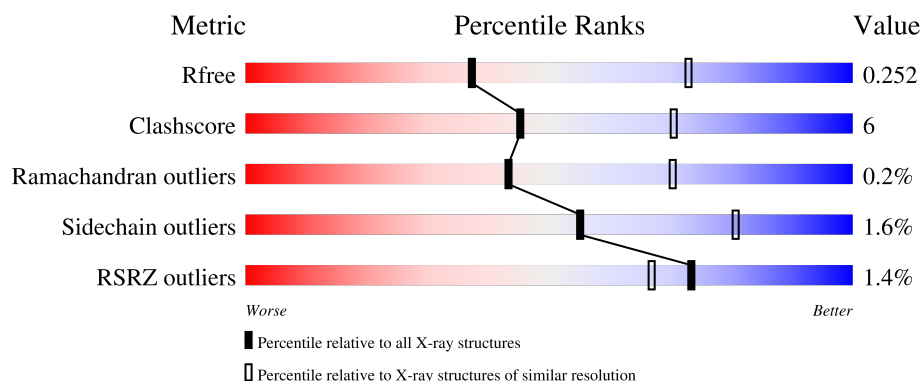
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	370	
1	B	370	
1	C	370	
1	D	370	
1	E	370	

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Mol	Chain	Length	Quality of chain
1	F	370	% 79% 14% 6%
1	G	370	2% 71% 18% • 10%
1	H	370	2% 65% 17% • 17%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21926 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 Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	P	S	0	0	0
			2766	1779	471	498	1	17			
1	B	343	Total	C	N	O	P	S	0	0	0
			2724	1752	461	493	1	17			
1	C	344	Total	C	N	O	P	S	0	0	0
			2741	1768	462	493	1	17			
1	D	338	Total	C	N	O	P	S	0	0	0
			2658	1710	449	481	1	17			
1	E	340	Total	C	N	O	P	S	0	0	0
			2714	1747	459	490	1	17			
1	F	346	Total	C	N	O	P	S	0	0	0
			2675	1710	463	484	1	17			
1	G	333	Total	C	N	O	P	S	0	0	0
			2587	1671	430	469	1	16			
1	H	307	Total	C	N	O	P	S	0	0	0
			2341	1482	409	433	1	16			

There are 48 discrepancies between the modelled and reference sequences:

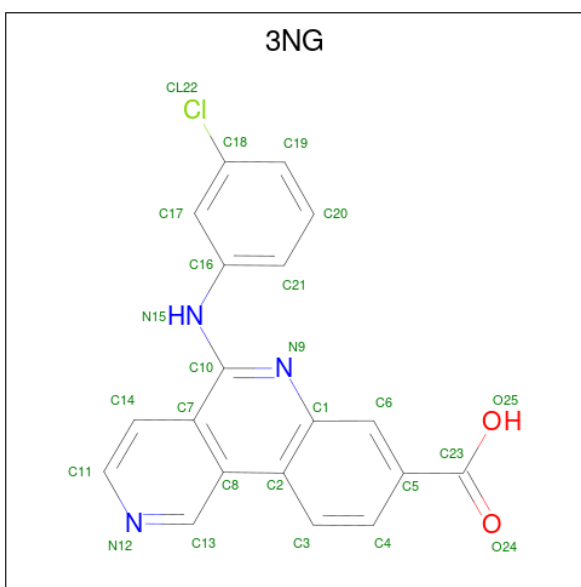
Chain	Residue	Modelled	Actual	Comment	Reference
A	490	HIS	-	expression tag	UNP Q13627
A	491	HIS	-	expression tag	UNP Q13627
A	492	HIS	-	expression tag	UNP Q13627
A	493	HIS	-	expression tag	UNP Q13627
A	494	HIS	-	expression tag	UNP Q13627
A	495	HIS	-	expression tag	UNP Q13627
B	490	HIS	-	expression tag	UNP Q13627
B	491	HIS	-	expression tag	UNP Q13627
B	492	HIS	-	expression tag	UNP Q13627
B	493	HIS	-	expression tag	UNP Q13627
B	494	HIS	-	expression tag	UNP Q13627
B	495	HIS	-	expression tag	UNP Q13627
C	490	HIS	-	expression tag	UNP Q13627

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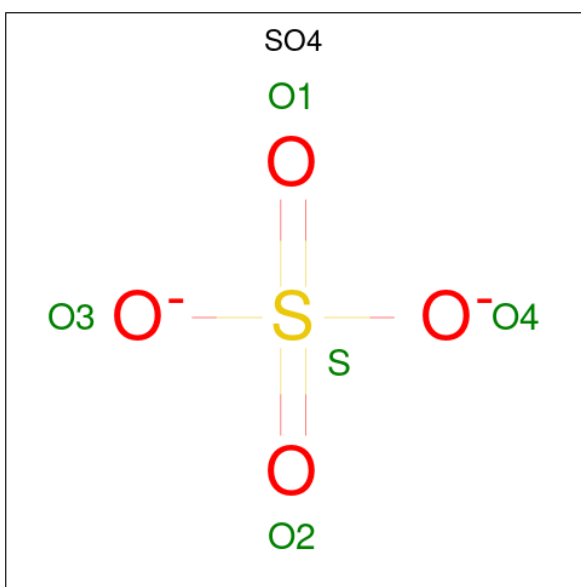
Chain	Residue	Modelled	Actual	Comment	Reference
C	491	HIS	-	expression tag	UNP Q13627
C	492	HIS	-	expression tag	UNP Q13627
C	493	HIS	-	expression tag	UNP Q13627
C	494	HIS	-	expression tag	UNP Q13627
C	495	HIS	-	expression tag	UNP Q13627
D	490	HIS	-	expression tag	UNP Q13627
D	491	HIS	-	expression tag	UNP Q13627
D	492	HIS	-	expression tag	UNP Q13627
D	493	HIS	-	expression tag	UNP Q13627
D	494	HIS	-	expression tag	UNP Q13627
D	495	HIS	-	expression tag	UNP Q13627
E	490	HIS	-	expression tag	UNP Q13627
E	491	HIS	-	expression tag	UNP Q13627
E	492	HIS	-	expression tag	UNP Q13627
E	493	HIS	-	expression tag	UNP Q13627
E	494	HIS	-	expression tag	UNP Q13627
E	495	HIS	-	expression tag	UNP Q13627
F	490	HIS	-	expression tag	UNP Q13627
F	491	HIS	-	expression tag	UNP Q13627
F	492	HIS	-	expression tag	UNP Q13627
F	493	HIS	-	expression tag	UNP Q13627
F	494	HIS	-	expression tag	UNP Q13627
F	495	HIS	-	expression tag	UNP Q13627
G	490	HIS	-	expression tag	UNP Q13627
G	491	HIS	-	expression tag	UNP Q13627
G	492	HIS	-	expression tag	UNP Q13627
G	493	HIS	-	expression tag	UNP Q13627
G	494	HIS	-	expression tag	UNP Q13627
G	495	HIS	-	expression tag	UNP Q13627
H	490	HIS	-	expression tag	UNP Q13627
H	491	HIS	-	expression tag	UNP Q13627
H	492	HIS	-	expression tag	UNP Q13627
H	493	HIS	-	expression tag	UNP Q13627
H	494	HIS	-	expression tag	UNP Q13627
H	495	HIS	-	expression tag	UNP Q13627

- Molecule 2 is 5-[(3-chlorophenyl)amino]benzo[c][2,6]naphthyridine-8-carboxylic acid (CCD ID: 3NG) (formula: C₁₉H₁₂ClN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	B	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	D	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	E	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	F	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	G	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	H	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		

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



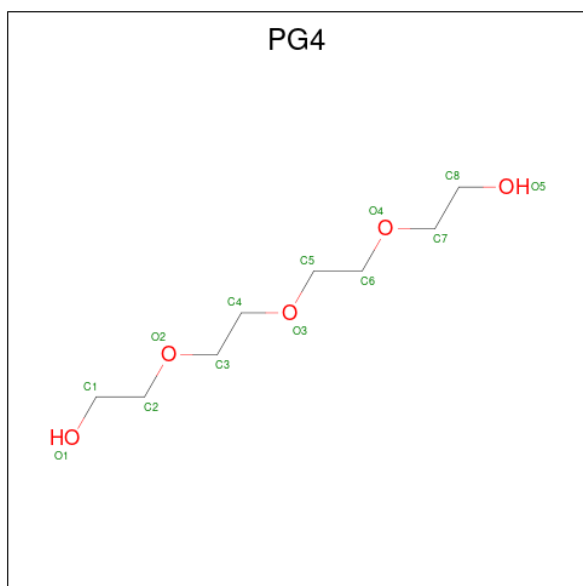
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



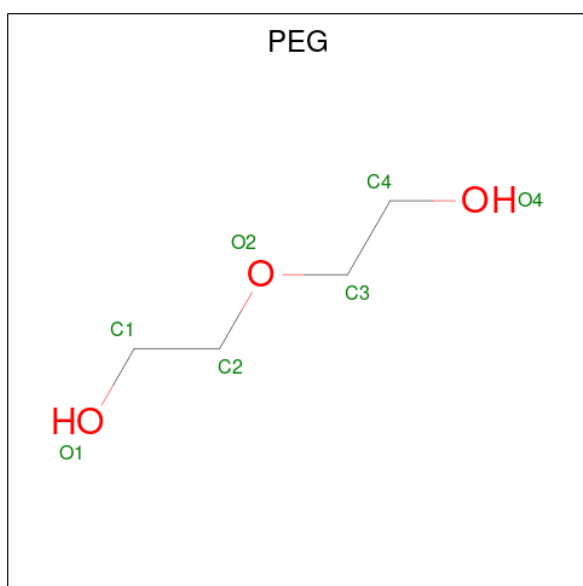
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

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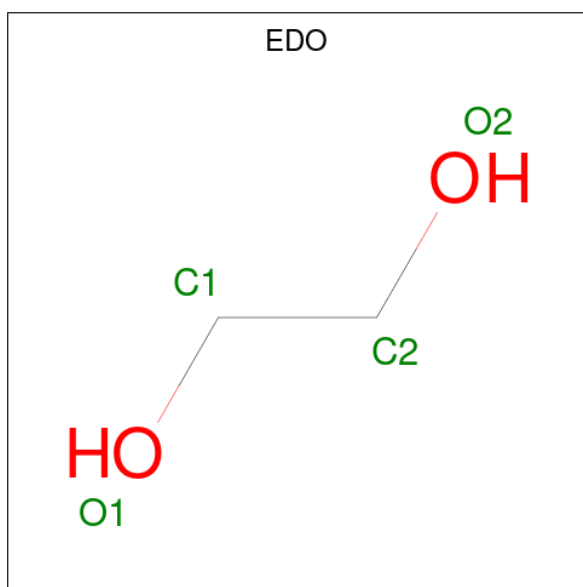
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



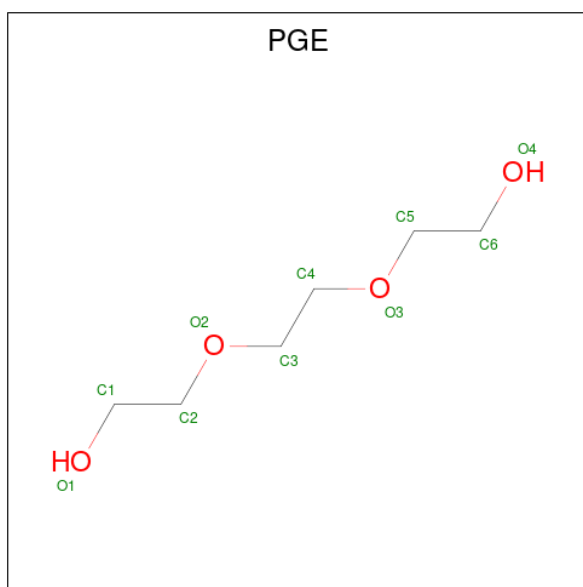
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	H	1	Total	C	O	0	0
			10	6	4		

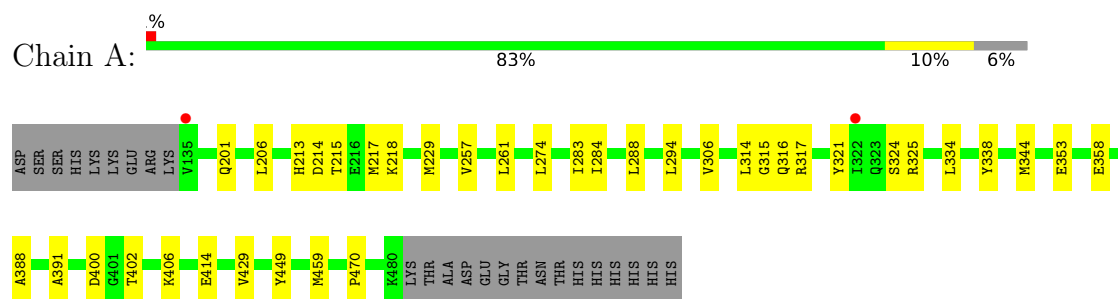
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	53	Total	O	0	0
			53	53		
8	B	31	Total	O	0	0
			31	31		
8	C	38	Total	O	0	0
			38	38		
8	D	21	Total	O	0	0
			21	21		
8	E	26	Total	O	0	0
			26	26		
8	F	8	Total	O	0	0
			8	8		
8	G	12	Total	O	0	0
			12	12		
8	H	17	Total	O	0	0
			17	17		

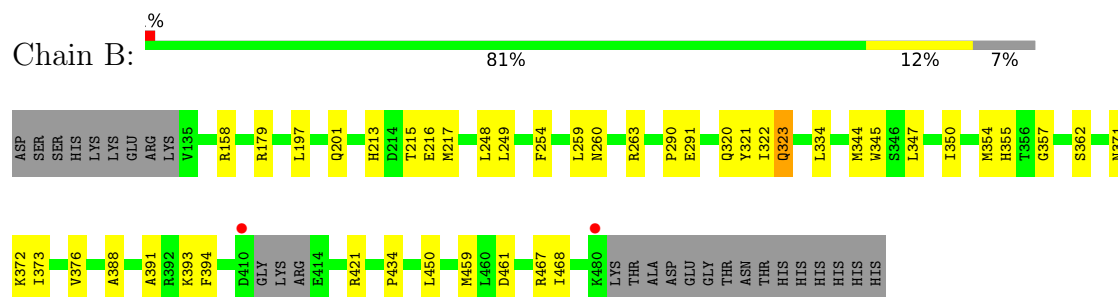
3 Residue-property plots [i](#)

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.

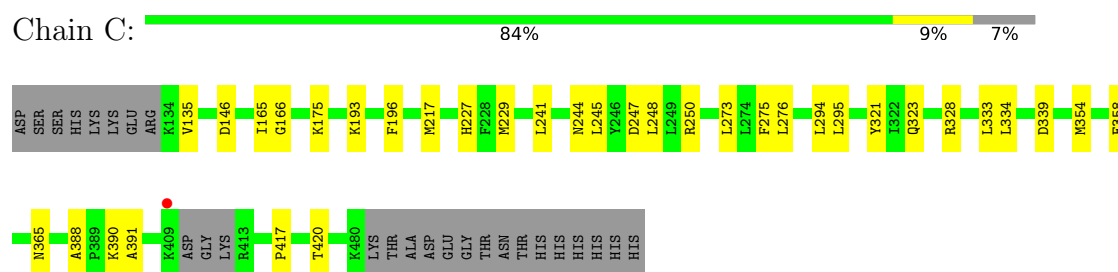
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



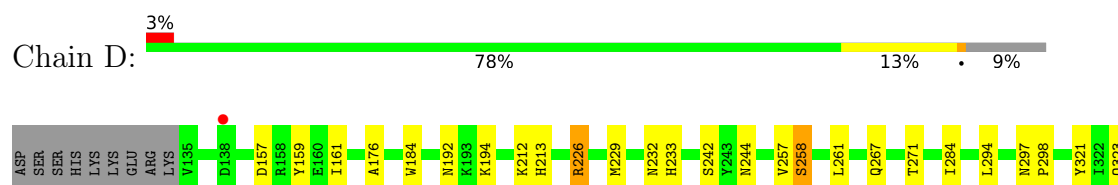
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

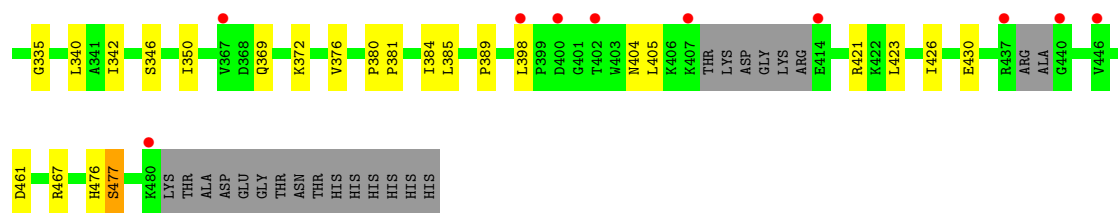


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



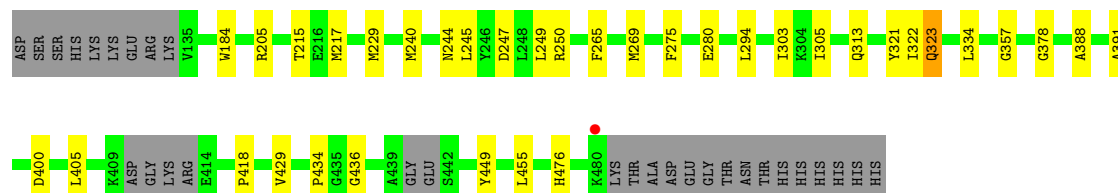
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





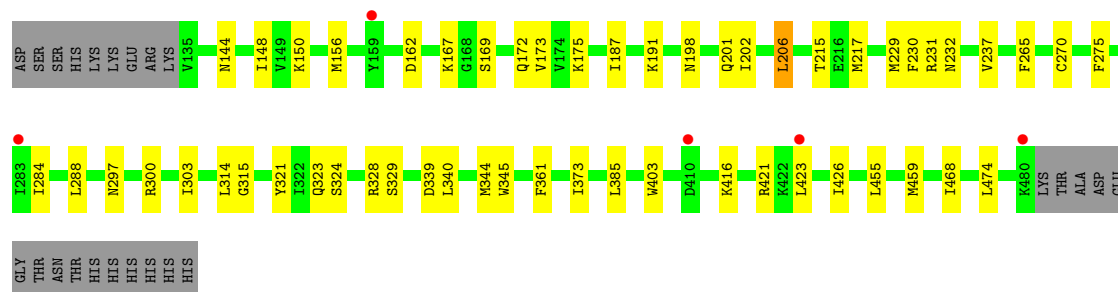
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain E: 82% 9% 8%



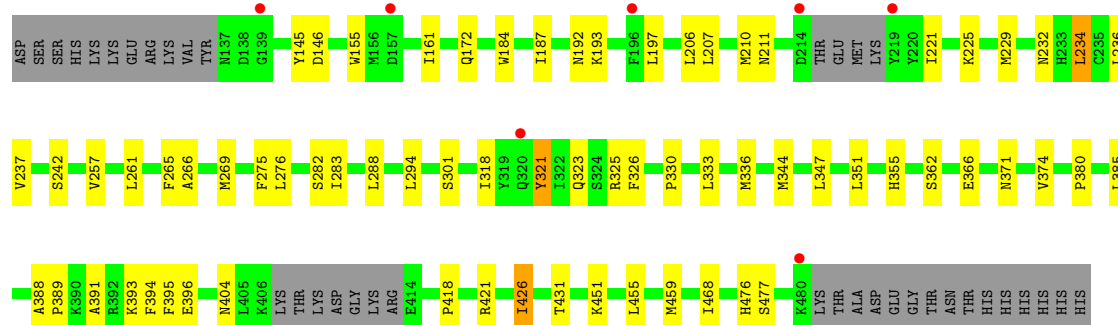
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain F: 79% 14% 6%



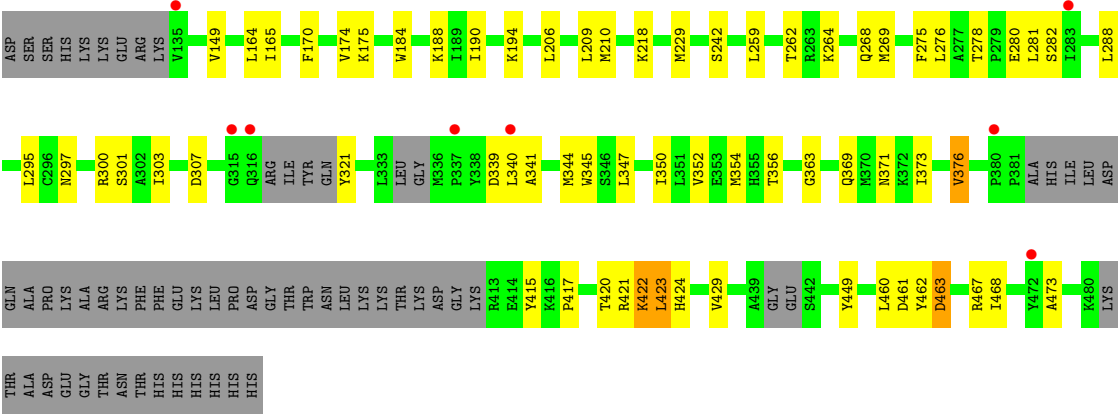
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain G: 71% 18% 10%



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain H: 65% 17% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.68Å 134.32Å 121.72Å 90.00° 96.48° 90.00°	Depositor
Resolution (Å)	26.14 – 2.77 26.14 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.14-2.77) 99.7 (26.14-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.205 , 0.252 0.205 , 0.252	Depositor DCC
R_{free} test set	5112 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21926	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 3NG, PG4, PTR, EDO, PGE, PEG

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	0.21	0/2815	0.35	0/3805
1	B	0.14	0/2772	0.31	0/3751
1	C	0.18	0/2789	0.33	0/3773
1	D	0.18	0/2704	0.36	0/3662
1	E	0.20	0/2761	0.35	0/3733
1	F	0.18	0/2721	0.36	0/3686
1	G	0.21	0/2632	0.40	0/3567
1	H	0.28	0/2374	0.47	1/3213 (0.0%)
All	All	0.20	0/21568	0.37	1/29190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	460	LEU	N-CA-C	-5.61	106.32	112.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2766	0	2692	24	0
1	B	2724	0	2615	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2741	0	2658	20	0
1	D	2658	0	2522	36	0
1	E	2714	0	2618	25	0
1	F	2675	0	2488	38	0
1	G	2587	0	2434	44	0
1	H	2341	0	2105	41	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
2	C	25	0	11	1	0
2	D	25	0	11	0	0
2	E	25	0	11	1	0
2	F	25	0	11	1	0
2	G	25	0	11	0	0
2	H	25	0	11	1	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	15	0	0	1	0
3	D	15	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
3	G	10	0	0	0	0
3	H	5	0	0	0	0
4	A	26	0	36	1	0
4	B	26	0	36	0	0
4	C	13	0	18	1	0
4	D	13	0	18	1	0
4	E	13	0	18	3	0
4	H	13	0	18	0	0
5	A	7	0	10	0	0
5	E	7	0	10	0	0
5	G	14	0	20	2	0
6	A	12	0	18	0	0
6	B	12	0	18	0	0
6	C	12	0	18	0	0
6	E	4	0	6	0	0
6	F	4	0	6	0	0
6	G	8	0	12	3	0
7	B	10	0	14	1	0
7	H	10	0	14	1	0
8	A	53	0	0	1	0
8	B	31	0	0	0	0
8	C	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	21	0	0	1	0
8	E	26	0	0	0	0
8	F	8	0	0	0	0
8	G	12	0	0	1	0
8	H	17	0	0	0	0
All	All	21926	0	20510	251	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (251) 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:D:257:VAL:CG1	1:D:261:LEU:HD23	1.67	1.23
1:D:257:VAL:HG11	1:D:261:LEU:CD2	1.74	1.16
1:D:257:VAL:HG11	1:D:261:LEU:HD23	0.90	0.88
1:A:215:THR:HG22	1:A:217:MET:H	1.39	0.88
1:B:215:THR:HG22	1:B:217:MET:H	1.46	0.80
1:E:247:ASP:OD1	1:E:250:ARG:NH2	2.21	0.73
1:D:257:VAL:HG12	1:D:258:SER:N	2.03	0.73
1:E:215:THR:HG22	1:E:217:MET:H	1.54	0.72
1:G:155:TRP:CE2	1:G:161:ILE:HD11	2.26	0.70
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.73	0.70
1:D:423:LEU:HA	1:D:426:ILE:HG12	1.74	0.70
1:D:159:TYR:OH	1:D:226:ARG:NH1	2.26	0.68
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.75	0.67
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.76	0.67
1:D:346:SER:O	1:D:350:ILE:HG13	1.95	0.67
1:G:388:ALA:HB3	1:G:391:ALA:HB2	1.77	0.66
1:G:355:HIS:NE2	8:G:601:HOH:O	2.28	0.66
1:E:269:MET:HE1	1:E:305:ILE:HG13	1.76	0.66
1:F:215:THR:HG22	1:F:217:MET:H	1.61	0.66
1:D:421:ARG:HG2	1:D:426:ILE:HD11	1.80	0.64
1:D:257:VAL:HG12	1:D:261:LEU:HB3	1.79	0.63
1:E:388:ALA:HB3	1:E:391:ALA:HB2	1.81	0.62
1:E:269:MET:HA	1:E:269:MET:HE2	1.82	0.62
1:D:257:VAL:HG11	1:D:261:LEU:CG	2.30	0.61
1:E:429:VAL:HG13	1:E:449:TYR:HB3	1.82	0.61
1:G:366:GLU:HB3	6:G:507:EDO:H12	1.81	0.61
1:G:192:ASN:OD1	1:G:232:ASN:HB3	2.00	0.61
1:G:321:PTR:HE2	6:G:507:EDO:H11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:LYS:HG2	1:F:172:GLN:HG2	1.82	0.60
1:F:323:GLN:HB3	1:F:328:ARG:HA	1.83	0.60
1:H:206:LEU:HA	1:H:209:LEU:HD12	1.83	0.60
1:H:164:LEU:HA	1:H:174:VAL:HG12	1.84	0.59
1:B:322:ILE:HG23	1:B:323:GLN:HG3	1.84	0.59
1:D:257:VAL:CG1	1:D:258:SER:N	2.66	0.58
1:F:265:PHE:HD1	1:F:303:ILE:HD13	1.68	0.58
1:H:218:LYS:HB3	1:H:275:PHE:HE2	1.68	0.58
1:B:461:ASP:O	1:B:467:ARG:NH1	2.37	0.58
1:D:381:PRO:HG2	1:D:384:ILE:HD12	1.85	0.57
1:G:380:PRO:HG2	1:G:385:LEU:HD21	1.85	0.57
1:D:194:LYS:NZ	8:D:602:HOH:O	2.36	0.57
1:D:257:VAL:HG12	1:D:258:SER:H	1.66	0.57
1:D:257:VAL:CG1	1:D:258:SER:H	2.18	0.57
1:C:229:MET:HE2	1:H:229:MET:HE2	1.85	0.57
1:F:297:ASN:HB2	1:F:300:ARG:HB2	1.87	0.57
1:B:344:MET:HE1	1:B:347:LEU:HD23	1.87	0.56
1:H:339:ASP:OD1	1:H:341:ALA:N	2.34	0.56
1:F:455:LEU:HG	1:F:459:MET:HE3	1.88	0.56
1:G:336:MET:HG2	1:G:389:PRO:HD2	1.88	0.56
1:G:197:LEU:HD12	1:G:234:LEU:HD12	1.88	0.55
1:E:240:MET:HE2	4:E:504:PG4:H51	1.88	0.55
1:G:344:MET:HE1	1:G:347:LEU:HD23	1.89	0.55
1:C:244:ASN:OD1	1:C:247:ASP:N	2.35	0.55
1:H:345:TRP:CZ2	1:H:373:ILE:HD13	2.41	0.55
1:F:148:ILE:HD12	1:F:148:ILE:O	2.07	0.55
1:F:423:LEU:HA	1:F:426:ILE:HD13	1.89	0.55
1:A:294:LEU:HD22	1:A:306:VAL:HG11	1.90	0.54
1:D:257:VAL:CG1	1:D:261:LEU:HB3	2.38	0.54
1:G:321:PTR:CE2	6:G:507:EDO:H11	2.38	0.54
1:A:334:LEU:HB3	1:A:388:ALA:HB1	1.90	0.54
1:G:210:MET:HE1	1:G:221:ILE:HG12	1.88	0.54
1:B:376:VAL:HG22	1:B:421:ARG:HG2	1.89	0.53
1:D:461:ASP:O	1:D:467:ARG:NH1	2.42	0.53
1:F:426:ILE:H	1:F:426:ILE:HD12	1.72	0.53
1:H:345:TRP:HZ2	1:H:373:ILE:HD13	1.72	0.53
1:C:334:LEU:HB3	1:C:388:ALA:HB1	1.90	0.53
1:H:297:ASN:HB3	1:H:300:ARG:HB2	1.89	0.53
1:C:193:LYS:HB3	1:C:196:PHE:HD1	1.74	0.52
1:H:278:THR:HG22	1:H:280:GLU:HG2	1.91	0.52
1:H:462:TYR:O	1:H:463:ASP:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:PHE:CD1	1:F:303:ILE:HD13	2.44	0.52
1:G:184:TRP:CE2	5:G:505:PEG:H32	2.43	0.52
1:F:314:LEU:HD12	1:F:315:GLY:H	1.75	0.52
1:G:431:THR:HG22	1:G:431:THR:O	2.10	0.52
1:D:476:HIS:CD2	1:D:477:SER:H	2.28	0.52
1:F:344:MET:HE3	1:F:468:ILE:HG23	1.92	0.52
1:E:205:ARG:NH2	1:E:313:GLN:OE1	2.38	0.52
1:G:421:ARG:O	1:G:421:ARG:HG3	2.10	0.51
1:E:280:GLU:OE1	1:E:280:GLU:N	2.33	0.51
1:F:270:CYS:HB3	1:F:474:LEU:HD22	1.92	0.51
1:H:461:ASP:HB3	1:H:467:ARG:HA	1.91	0.51
1:G:266:ALA:HB2	1:G:351:LEU:HD21	1.92	0.51
1:A:400:ASP:HB3	1:A:402:THR:HG22	1.92	0.51
1:C:175:LYS:HD3	4:C:505:PG4:H12	1.93	0.51
1:E:269:MET:HE1	1:E:305:ILE:CG1	2.39	0.51
1:H:429:VAL:HG22	1:H:449:TYR:HB3	1.92	0.50
1:G:394:PHE:HB2	1:G:395:PHE:CD1	2.45	0.50
1:F:284:ILE:HD11	1:F:339:ASP:C	2.36	0.50
1:G:455:LEU:O	1:G:459:MET:HG3	2.11	0.50
1:D:267:GLN:O	1:D:271:THR:OG1	2.29	0.50
1:F:323:GLN:O	1:F:324:SER:C	2.55	0.49
1:F:148:ILE:HD13	1:F:150:LYS:HE3	1.93	0.49
1:F:202:ILE:O	1:F:206:LEU:HD12	2.12	0.49
1:D:323:GLN:OE1	1:D:342:ILE:HB	2.11	0.49
1:H:184:TRP:CE2	7:H:504:PGE:H42	2.48	0.49
1:B:249:LEU:HD22	1:B:357:GLY:HA2	1.95	0.49
1:E:184:TRP:CZ2	4:E:504:PG4:H21	2.48	0.49
1:G:146:ASP:HB3	1:G:172:GLN:HE21	1.78	0.49
1:B:344:MET:HE2	1:B:459:MET:HG2	1.95	0.49
1:E:322:ILE:HG13	1:E:323:GLN:HG3	1.94	0.49
1:A:284:ILE:HD11	1:A:314:LEU:HD13	1.95	0.48
1:B:254:PHE:CD2	1:F:416:LYS:HD3	2.48	0.48
1:D:184:TRP:CE2	4:D:505:PG4:H82	2.48	0.48
1:G:206:LEU:O	1:G:210:MET:HG3	2.12	0.48
1:A:213:HIS:O	1:A:218:LYS:HE2	2.14	0.48
1:C:165:ILE:HD11	1:C:175:LYS:HB2	1.95	0.48
1:F:230:PHE:CE2	1:F:231:ARG:HG3	2.48	0.48
1:A:317:ARG:HG2	1:A:338:TYR:CE2	2.49	0.48
1:B:158:ARG:O	1:B:179:ARG:HG2	2.14	0.48
1:A:344:MET:SD	1:A:459:MET:HE2	2.54	0.48
1:E:334:LEU:HB3	1:E:388:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLY:C	1:A:317:ARG:H	2.21	0.48
1:G:184:TRP:CZ2	5:G:505:PEG:H32	2.49	0.48
1:G:326:PHE:CD1	1:G:362:SER:HA	2.49	0.48
1:A:317:ARG:NH1	8:A:604:HOH:O	2.47	0.47
1:D:297:ASN:ND2	1:D:298:PRO:HD2	2.29	0.47
1:B:350:ILE:O	1:B:354:MET:HG2	2.14	0.47
1:D:244:ASN:HA	1:D:294:LEU:HA	1.97	0.47
1:A:214:ASP:HA	1:A:218:LYS:NZ	2.29	0.47
1:D:380:PRO:HB2	1:D:385:LEU:HD21	1.95	0.47
1:G:145:TYR:CG	1:G:193:LYS:HG3	2.50	0.47
1:G:265:PHE:O	1:G:269:MET:HG2	2.15	0.47
1:H:275:PHE:HD1	1:H:275:PHE:C	2.23	0.47
1:B:259:LEU:HB2	1:B:355:HIS:HE1	1.80	0.47
1:C:390:LYS:NZ	8:C:602:HOH:O	2.38	0.47
1:H:259:LEU:HA	1:H:262:THR:OG1	2.15	0.47
1:B:291:GLU:OE1	1:B:291:GLU:N	2.46	0.46
1:B:344:MET:HA	1:B:344:MET:HE3	1.96	0.46
1:B:362:SER:O	1:B:372:LYS:NZ	2.47	0.46
1:C:247:ASP:OD1	1:C:250:ARG:NH2	2.47	0.46
1:C:273:LEU:HA	1:C:276:LEU:HD23	1.97	0.46
1:F:198:ASN:HA	1:F:201:GLN:HE21	1.80	0.46
1:H:188:LYS:HD3	1:H:190:ILE:HD11	1.96	0.46
1:F:217:MET:HB2	1:F:275:PHE:HB2	1.96	0.46
1:G:225:LYS:HB2	1:G:237:VAL:HG12	1.98	0.46
1:H:417:PRO:O	1:H:420:THR:OG1	2.29	0.46
1:F:187:ILE:HG12	1:F:237:VAL:HG22	1.97	0.46
1:C:217:MET:HB3	1:C:275:PHE:HB2	1.98	0.46
1:H:275:PHE:HE1	1:H:281:LEU:HD11	1.81	0.46
1:G:242:SER:O	1:G:294:LEU:HD12	2.16	0.46
7:B:512:PGE:H3	7:B:512:PGE:H52	1.73	0.46
1:F:321:PTR:HE2	1:F:328:ARG:NH1	2.31	0.46
1:G:207:LEU:O	1:G:211:ASN:ND2	2.48	0.46
1:H:275:PHE:C	1:H:275:PHE:CD1	2.93	0.46
1:H:423:LEU:O	1:H:424:HIS:C	2.58	0.46
1:A:229:MET:HE2	1:E:229:MET:HE2	1.97	0.46
1:E:265:PHE:CD1	1:E:303:ILE:HD13	2.50	0.46
1:G:421:ARG:HH21	1:G:426:ILE:HG21	1.81	0.46
1:G:374:VAL:HG13	1:G:418:PRO:HB3	1.98	0.45
1:H:295:LEU:HD23	1:H:303:ILE:HG22	1.98	0.45
1:A:353:GLU:HG3	1:A:358:GLU:C	2.41	0.45
1:F:173:VAL:HG21	2:F:501:3NG:H17	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:GLU:N	1:G:404:ASN:O	2.44	0.45
1:H:352:VAL:O	1:H:356:THR:HG23	2.16	0.45
1:F:361:PHE:CD2	1:F:373:ILE:HD13	2.51	0.45
1:G:451:LYS:HD3	1:G:477:SER:C	2.42	0.45
1:H:264:LYS:O	1:H:268:GLN:HG3	2.15	0.45
1:H:165:ILE:HD11	1:H:175:LYS:HB2	1.98	0.45
1:D:192:ASN:HB2	1:D:233:HIS:CE1	2.52	0.45
1:D:369:GLN:O	1:D:372:LYS:N	2.49	0.45
1:D:257:VAL:CG1	1:D:261:LEU:CD2	2.57	0.45
1:F:385:LEU:HD13	1:F:403:TRP:CD2	2.52	0.45
1:B:344:MET:HG2	1:B:468:ILE:O	2.16	0.44
1:D:404:ASN:OD1	1:D:405:LEU:N	2.49	0.44
1:E:184:TRP:CD1	4:E:504:PG4:H31	2.52	0.44
1:H:363:GLY:H	1:H:369:GLN:NE2	2.15	0.44
1:A:414:GLU:OE2	1:G:325:ARG:NH2	2.51	0.44
1:D:284:ILE:HG12	1:D:340:LEU:HA	1.99	0.44
1:C:417:PRO:HB2	1:C:420:THR:HG21	1.99	0.44
1:F:416:LYS:HE3	1:F:421:ARG:HD2	1.99	0.44
1:G:266:ALA:HB2	1:G:351:LEU:CD2	2.48	0.44
1:H:170:PHE:CE1	1:H:188:LYS:HG3	2.52	0.44
1:H:350:ILE:O	1:H:354:MET:HG2	2.17	0.44
1:G:276:LEU:CD2	1:G:283:ILE:HB	2.48	0.44
1:C:241:LEU:HB2	1:C:294:LEU:HD23	1.99	0.44
1:G:318:ILE:O	1:G:318:ILE:HG13	2.18	0.44
1:G:455:LEU:HB2	1:G:476:HIS:CE1	2.53	0.44
1:A:406:LYS:HE3	1:A:406:LYS:HB3	1.73	0.44
1:D:376:VAL:HG22	1:D:421:ARG:HD3	2.00	0.44
1:G:275:PHE:CD1	1:G:275:PHE:C	2.95	0.44
1:B:290:PRO:HD3	1:B:350:ILE:HG12	1.98	0.43
1:C:248:LEU:HD11	1:C:295:LEU:HD11	2.00	0.43
2:E:501:3NG:H17	2:E:501:3NG:N9	2.33	0.43
1:H:339:ASP:OD1	1:H:339:ASP:C	2.61	0.43
1:D:161:ILE:HD13	1:D:176:ALA:HB2	1.99	0.43
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.84	0.43
1:E:249:LEU:HD11	1:E:357:GLY:HA2	1.99	0.43
1:E:215:THR:HG22	1:E:217:MET:N	2.27	0.43
1:B:355:HIS:HD2	1:B:434:PRO:HG2	1.82	0.43
1:H:468:ILE:HG13	1:H:473:ALA:HB2	1.99	0.43
1:H:269:MET:HG3	1:H:347:LEU:HD11	2.01	0.43
1:C:166:GLY:HA3	2:C:501:3NG:C19	2.49	0.43
1:F:144:ASN:O	1:F:191:LYS:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:SER:O	1:F:191:LYS:NZ	2.51	0.43
1:H:339:ASP:OD1	1:H:340:LEU:N	2.52	0.43
1:F:329:SER:HA	1:F:345:TRP:CD1	2.54	0.43
1:H:376:VAL:HG12	1:H:421:ARG:HB3	2.00	0.43
1:F:229:MET:HE3	1:F:229:MET:HB3	1.79	0.42
1:A:274:LEU:HB2	1:A:470:PRO:HB2	2.01	0.42
1:B:344:MET:HE2	1:B:459:MET:SD	2.59	0.42
1:E:455:LEU:HD13	1:E:476:HIS:CD2	2.54	0.42
1:F:201:GLN:H	1:F:201:GLN:HG2	1.65	0.42
1:H:468:ILE:CG1	1:H:473:ALA:HB2	2.49	0.42
1:F:229:MET:HE1	1:F:232:ASN:HA	2.00	0.42
1:B:393:LYS:HG2	1:B:394:PHE:CE1	2.54	0.42
1:D:192:ASN:OD1	1:D:232:ASN:ND2	2.50	0.42
1:F:162:ASP:HB3	1:F:175:LYS:HG2	2.02	0.42
1:G:330:PRO:HA	1:G:333:LEU:HB2	2.01	0.42
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.80	0.42
1:C:339:ASP:OD1	1:C:339:ASP:N	2.49	0.42
1:E:244:ASN:HA	1:E:294:LEU:HA	2.01	0.42
1:E:405:LEU:HD12	1:E:405:LEU:H	1.85	0.42
1:G:366:GLU:HG3	1:G:393:LYS:NZ	2.34	0.42
1:H:344:MET:HE3	1:H:468:ILE:HG23	2.01	0.42
1:A:429:VAL:HG22	1:A:449:TYR:HB3	2.01	0.42
1:F:288:LEU:HD23	1:F:288:LEU:HA	1.81	0.42
1:C:328:ARG:HD2	1:C:333:LEU:HD13	2.01	0.42
1:D:421:ARG:HG2	1:D:426:ILE:CD1	2.50	0.42
1:A:324:SER:O	1:A:325:ARG:C	2.63	0.41
1:F:284:ILE:HG12	1:F:340:LEU:HA	2.02	0.41
1:H:206:LEU:O	1:H:210:MET:HG3	2.20	0.41
1:E:280:GLU:H	1:E:280:GLU:CD	2.26	0.41
1:G:257:VAL:HB	1:G:261:LEU:HD23	2.02	0.41
1:G:388:ALA:CB	1:G:391:ALA:HB2	2.49	0.41
1:H:149:VAL:HG11	1:H:174:VAL:HG11	2.02	0.41
1:H:288:LEU:HD23	1:H:288:LEU:HA	1.84	0.41
1:H:307:ASP:H	2:H:501:3NG:C23	2.34	0.41
1:H:420:THR:O	1:H:422:LYS:N	2.54	0.41
1:B:450:LEU:HD23	1:B:450:LEU:HA	1.92	0.41
1:C:227:HIS:O	1:H:194:LYS:HE3	2.19	0.41
1:A:257:VAL:HB	1:A:261:LEU:HD23	2.03	0.41
1:G:421:ARG:NH2	1:G:426:ILE:HG21	2.35	0.41
1:C:245:LEU:HB3	1:C:354:MET:SD	2.60	0.41
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:TRP:HZ2	1:B:373:ILE:HD13	1.86	0.41
1:A:206:LEU:HD22	1:A:283:ILE:HG12	2.03	0.41
1:E:217:MET:HB3	1:E:275:PHE:HB2	2.02	0.41
1:A:201:GLN:HA	4:A:507:PG4:H82	2.01	0.41
1:B:260:ASN:HA	1:B:263:ARG:NH1	2.36	0.41
1:D:192:ASN:CG	1:D:232:ASN:HD22	2.29	0.41
1:E:378:GLY:HA2	1:E:418:PRO:HB3	2.03	0.41
1:F:385:LEU:HD23	1:F:385:LEU:HA	1.82	0.41
1:G:187:ILE:HA	1:G:236:LEU:O	2.21	0.41
1:B:334:LEU:HB3	1:B:388:ALA:HB1	2.03	0.41
1:F:156:MET:HE2	1:F:156:MET:HB3	1.81	0.41
1:D:335:GLY:O	1:D:389:PRO:HG2	2.21	0.40
1:G:344:MET:HG2	1:G:468:ILE:O	2.20	0.40
1:H:371:ASN:ND2	1:H:415:TYR:CD2	2.90	0.40
1:B:197:LEU:O	1:B:201:GLN:HG3	2.22	0.40
1:D:229:MET:HE3	1:D:229:MET:HB3	1.92	0.40
1:E:434:PRO:C	1:E:436:GLY:H	2.29	0.40
1:C:365:ASN:HB2	3:C:504:SO4:S	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/370 (93%)	330 (96%)	12 (4%)	1 (0%)	36	63
1	B	338/370 (91%)	320 (95%)	17 (5%)	1 (0%)	36	63
1	C	339/370 (92%)	322 (95%)	16 (5%)	1 (0%)	36	63
1	D	331/370 (90%)	311 (94%)	20 (6%)	0	100	100
1	E	333/370 (90%)	311 (93%)	20 (6%)	2 (1%)	21	47
1	F	343/370 (93%)	324 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	326/370 (88%)	305 (94%)	21 (6%)	0	100	100
1	H	297/370 (80%)	279 (94%)	18 (6%)	0	100	100
All	All	2650/2960 (90%)	2502 (94%)	143 (5%)	5 (0%)	43	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	E	323	GLN
1	E	400	ASP
1	B	323	GLN
1	C	323	GLN

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	287/328 (88%)	287 (100%)	0	100	100
1	B	279/328 (85%)	275 (99%)	4 (1%)	59	82
1	C	283/328 (86%)	280 (99%)	3 (1%)	65	85
1	D	268/328 (82%)	259 (97%)	9 (3%)	32	65
1	E	280/328 (85%)	279 (100%)	1 (0%)	84	93
1	F	259/328 (79%)	258 (100%)	1 (0%)	84	93
1	G	256/328 (78%)	248 (97%)	8 (3%)	35	68
1	H	220/328 (67%)	212 (96%)	8 (4%)	31	63
All	All	2132/2624 (81%)	2098 (98%)	34 (2%)	55	81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	213	HIS
1	B	216	GLU

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	371	ASN
1	C	135	VAL
1	C	146	ASP
1	C	358	GLU
1	D	157	ASP
1	D	212	LYS
1	D	213	HIS
1	D	226	ARG
1	D	242	SER
1	D	258	SER
1	D	398	LEU
1	D	430	GLU
1	D	477	SER
1	E	245	LEU
1	F	206	LEU
1	G	229	MET
1	G	234	LEU
1	G	282	SER
1	G	288	LEU
1	G	301	SER
1	G	323	GLN
1	G	371	ASN
1	G	426	ILE
1	H	242	SER
1	H	276	LEU
1	H	282	SER
1	H	301	SER
1	H	376	VAL
1	H	422	LYS
1	H	423	LEU
1	H	463	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	425	ASN
1	A	475	GLN
1	B	213	HIS
1	B	313	GLN
1	B	369	GLN

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Mol	Chain	Res	Type
1	C	251	ASN
1	D	213	HIS
1	D	297	ASN
1	D	320	GLN
1	D	371	ASN
1	E	172	GLN
1	E	297	ASN
1	F	144	ASN
1	F	213	HIS
1	F	371	ASN
1	G	151	ASN
1	G	172	GLN
1	G	297	ASN
1	G	369	GLN
1	H	137	ASN
1	H	199	GLN
1	H	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	C	321	1	15,16,17	1.15	1 (6%)	17,22,24	0.71	0
1	PTR	E	321	1	15,16,17	1.30	1 (6%)	17,22,24	0.50	0
1	PTR	G	321	1	15,16,17	1.31	1 (6%)	17,22,24	0.47	0
1	PTR	D	321	1	15,16,17	1.34	1 (6%)	17,22,24	0.48	0
1	PTR	A	321	1	15,16,17	1.31	1 (6%)	17,22,24	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PTR	F	321	1	15,16,17	0.54	0	17,22,24	0.57	0
1	PTR	B	321	1	15,16,17	1.32	1 (6%)	17,22,24	0.58	0
1	PTR	H	321	1	15,16,17	1.34	1 (6%)	17,22,24	0.53	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
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1
1	PTR	E	321	1	-	0/10/11/13	0/1/1/1
1	PTR	G	321	1	-	1/10/11/13	0/1/1/1
1	PTR	D	321	1	-	2/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1
1	PTR	F	321	1	-	3/10/11/13	0/1/1/1
1	PTR	B	321	1	-	4/10/11/13	0/1/1/1
1	PTR	H	321	1	-	2/10/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	321	PTR	OH-CZ	-4.48	1.30	1.40
1	D	321	PTR	OH-CZ	-4.45	1.30	1.40
1	B	321	PTR	OH-CZ	-4.34	1.30	1.40
1	G	321	PTR	OH-CZ	-4.27	1.31	1.40
1	E	321	PTR	OH-CZ	-4.25	1.31	1.40
1	A	321	PTR	OH-CZ	-4.23	1.31	1.40
1	C	321	PTR	OH-CZ	-3.92	1.31	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	O-C-CA-CB
1	F	321	PTR	O-C-CA-CB
1	H	321	PTR	N-CA-CB-CG
1	H	321	PTR	C-CA-CB-CG
1	F	321	PTR	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
1	F	321	PTR	CA-CB-CG-CD1
1	A	321	PTR	CZ-OH-P-O1P
1	B	321	PTR	CZ-OH-P-O1P
1	D	321	PTR	CA-CB-CG-CD2
1	D	321	PTR	CA-CB-CG-CD1
1	G	321	PTR	CZ-OH-P-O3P
1	B	321	PTR	CA-CB-CG-CD1
1	B	321	PTR	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	321	PTR	2	0
1	F	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

57 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	$\# Z > 2$
6	EDO	F	503	-	3,3,3	0.43	0	2,2,2	0.34	0
3	SO4	H	502	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	E	502	-	4,4,4	0.24	0	6,6,6	0.09	0
6	EDO	A	512	-	3,3,3	0.44	0	2,2,2	0.34	0
4	PG4	A	508	-	12,12,12	0.15	0	11,11,11	0.62	0
3	SO4	B	506	-	4,4,4	0.34	0	6,6,6	0.15	0
2	3NG	F	501	-	28,28,28	0.62	1 (3%)	39,40,40	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	G	506	-	3,3,3	0.09	0	2,2,2	0.07	0
4	PG4	E	504	-	12,12,12	0.14	0	11,11,11	0.60	0
3	SO4	B	502	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.10	0
2	3NG	G	501	-	28,28,28	0.64	1 (3%)	39,40,40	0.79	0
5	PEG	G	505	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PEG	E	505	-	6,6,6	0.15	0	5,5,5	0.08	0
6	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	B	509	-	3,3,3	0.44	0	2,2,2	0.33	0
4	PG4	H	503	-	12,12,12	0.16	0	11,11,11	0.59	0
3	SO4	C	504	-	4,4,4	0.25	0	6,6,6	0.12	0
5	PEG	G	504	-	6,6,6	0.16	0	5,5,5	0.07	0
3	SO4	C	502	-	4,4,4	0.25	0	6,6,6	0.16	0
6	EDO	C	507	-	3,3,3	0.40	0	2,2,2	0.52	0
6	EDO	A	510	-	3,3,3	0.45	0	2,2,2	0.34	0
2	3NG	E	501	-	28,28,28	0.65	1 (3%)	39,40,40	0.77	0
6	EDO	C	506	-	3,3,3	0.43	0	2,2,2	0.33	0
3	SO4	G	503	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	505	-	4,4,4	0.24	0	6,6,6	0.06	0
2	3NG	H	501	-	28,28,28	0.64	1 (3%)	39,40,40	0.76	0
3	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	506	-	4,4,4	0.36	0	6,6,6	0.09	0
6	EDO	E	506	-	3,3,3	0.44	0	2,2,2	0.37	0
3	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	E	503	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.07	0
6	EDO	B	511	-	3,3,3	0.45	0	2,2,2	0.34	0
2	3NG	A	501	-	28,28,28	0.65	1 (3%)	39,40,40	0.75	0
2	3NG	B	501	-	28,28,28	0.65	1 (3%)	39,40,40	0.76	0
6	EDO	C	508	-	3,3,3	0.09	0	2,2,2	0.11	0
7	PGE	H	504	-	9,9,9	0.36	0	8,8,8	0.23	0
3	SO4	D	504	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	B	504	-	4,4,4	0.28	0	6,6,6	0.11	0
5	PEG	A	509	-	6,6,6	0.15	0	5,5,5	0.08	0
4	PG4	B	507	-	12,12,12	0.14	0	11,11,11	0.60	0
6	EDO	B	510	-	3,3,3	0.44	0	2,2,2	0.33	0
3	SO4	A	505	-	4,4,4	0.26	0	6,6,6	0.21	0
4	PG4	A	507	-	12,12,12	0.12	0	11,11,11	0.60	0
3	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO4	G	502	-	4,4,4	0.24	0	6,6,6	0.08	0
4	PG4	B	508	-	12,12,12	0.12	0	11,11,11	0.54	0
6	EDO	G	507	-	3,3,3	0.08	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3NG	C	501	-	28,28,28	0.65	1 (3%)	39,40,40	0.77	0
2	3NG	D	501	-	28,28,28	0.63	1 (3%)	39,40,40	0.75	0
3	SO4	B	503	-	4,4,4	0.23	0	6,6,6	0.06	0
4	PG4	D	505	-	12,12,12	0.17	0	11,11,11	0.55	0
3	SO4	A	503	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	F	502	-	4,4,4	0.24	0	6,6,6	0.12	0
7	PGE	B	512	-	9,9,9	0.32	0	8,8,8	0.29	0
4	PG4	C	505	-	12,12,12	0.13	0	11,11,11	0.58	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
6	EDO	F	503	-	-	0/1/1/1	-
6	EDO	A	512	-	-	1/1/1/1	-
4	PG4	A	508	-	-	5/10/10/10	-
6	EDO	G	506	-	-	0/1/1/1	-
2	3NG	F	501	-	-	4/8/8/8	0/4/4/4
4	PG4	E	504	-	-	3/10/10/10	-
2	3NG	G	501	-	-	0/8/8/8	0/4/4/4
5	PEG	G	505	-	-	1/4/4/4	-
5	PEG	E	505	-	-	3/4/4/4	-
6	EDO	A	511	-	-	0/1/1/1	-
6	EDO	B	509	-	-	0/1/1/1	-
4	PG4	H	503	-	-	2/10/10/10	-
5	PEG	G	504	-	-	0/4/4/4	-
6	EDO	C	507	-	-	0/1/1/1	-
6	EDO	A	510	-	-	0/1/1/1	-
2	3NG	E	501	-	-	0/8/8/8	0/4/4/4
6	EDO	C	506	-	-	0/1/1/1	-
2	3NG	H	501	-	-	1/8/8/8	0/4/4/4
6	EDO	E	506	-	-	0/1/1/1	-
6	EDO	B	511	-	-	0/1/1/1	-
7	PGE	H	504	-	-	0/7/7/7	-
2	3NG	A	501	-	-	0/8/8/8	0/4/4/4
2	3NG	B	501	-	-	0/8/8/8	0/4/4/4
6	EDO	C	508	-	-	1/1/1/1	-
5	PEG	A	509	-	-	2/4/4/4	-
4	PG4	B	507	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	510	-	-	0/1/1/1	-
4	PG4	A	507	-	-	1/10/10/10	-
6	EDO	G	507	-	-	1/1/1/1	-
2	3NG	C	501	-	-	0/8/8/8	0/4/4/4
2	3NG	D	501	-	-	0/8/8/8	0/4/4/4
4	PG4	B	508	-	-	4/10/10/10	-
4	PG4	D	505	-	-	4/10/10/10	-
7	PGE	B	512	-	-	3/7/7/7	-
4	PG4	C	505	-	-	3/10/10/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	3NG	O25-C23	-2.20	1.24	1.30
2	H	501	3NG	O25-C23	-2.18	1.24	1.30
2	A	501	3NG	O25-C23	-2.17	1.24	1.30
2	E	501	3NG	O25-C23	-2.16	1.24	1.30
2	D	501	3NG	O25-C23	-2.14	1.24	1.30
2	C	501	3NG	O25-C23	-2.14	1.24	1.30
2	G	501	3NG	O25-C23	-2.07	1.24	1.30
2	F	501	3NG	O25-C23	-2.04	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	507	PG4	O3-C5-C6-O4
4	B	508	PG4	O2-C3-C4-O3
4	C	505	PG4	O4-C7-C8-O5
4	A	508	PG4	O3-C5-C6-O4
4	B	507	PG4	O1-C1-C2-O2
5	E	505	PEG	O2-C3-C4-O4
4	B	507	PG4	O2-C3-C4-O3
4	D	505	PG4	O4-C7-C8-O5
4	E	504	PG4	O2-C3-C4-O3
4	A	508	PG4	O4-C7-C8-O5
5	E	505	PEG	O1-C1-C2-O2
6	A	512	EDO	O1-C1-C2-O2
7	B	512	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
7	B	512	PGE	C3-C4-O3-C5
4	H	503	PG4	O3-C5-C6-O4
5	G	505	PEG	O1-C1-C2-O2
4	A	508	PG4	C5-C6-O4-C7
4	D	505	PG4	C5-C6-O4-C7
4	D	505	PG4	C4-C3-O2-C2
4	C	505	PG4	C1-C2-O2-C3
5	A	509	PEG	O2-C3-C4-O4
4	A	508	PG4	O2-C3-C4-O3
4	A	507	PG4	O3-C5-C6-O4
4	H	503	PG4	C1-C2-O2-C3
4	B	507	PG4	C6-C5-O3-C4
4	D	505	PG4	O1-C1-C2-O2
4	B	508	PG4	C5-C6-O4-C7
6	G	507	EDO	O1-C1-C2-O2
5	E	505	PEG	C4-C3-O2-C2
7	B	512	PGE	C6-C5-O3-C4
4	B	507	PG4	C4-C3-O2-C2
4	B	508	PG4	C1-C2-O2-C3
4	E	504	PG4	O4-C7-C8-O5
2	F	501	3NG	O24-C23-C5-C6
2	F	501	3NG	O24-C23-C5-C4
2	F	501	3NG	O25-C23-C5-C6
4	B	508	PG4	C3-C4-O3-C5
6	C	508	EDO	O1-C1-C2-O2
4	A	508	PG4	O1-C1-C2-O2
2	F	501	3NG	O25-C23-C5-C4
5	A	509	PEG	C1-C2-O2-C3
4	C	505	PG4	O2-C3-C4-O3
4	E	504	PG4	C5-C6-O4-C7
4	B	507	PG4	O4-C7-C8-O5
2	H	501	3NG	C21-C16-N15-C10

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	3NG	1	0
4	E	504	PG4	3	0
5	G	505	PEG	2	0
3	C	504	SO4	1	0
2	E	501	3NG	1	0

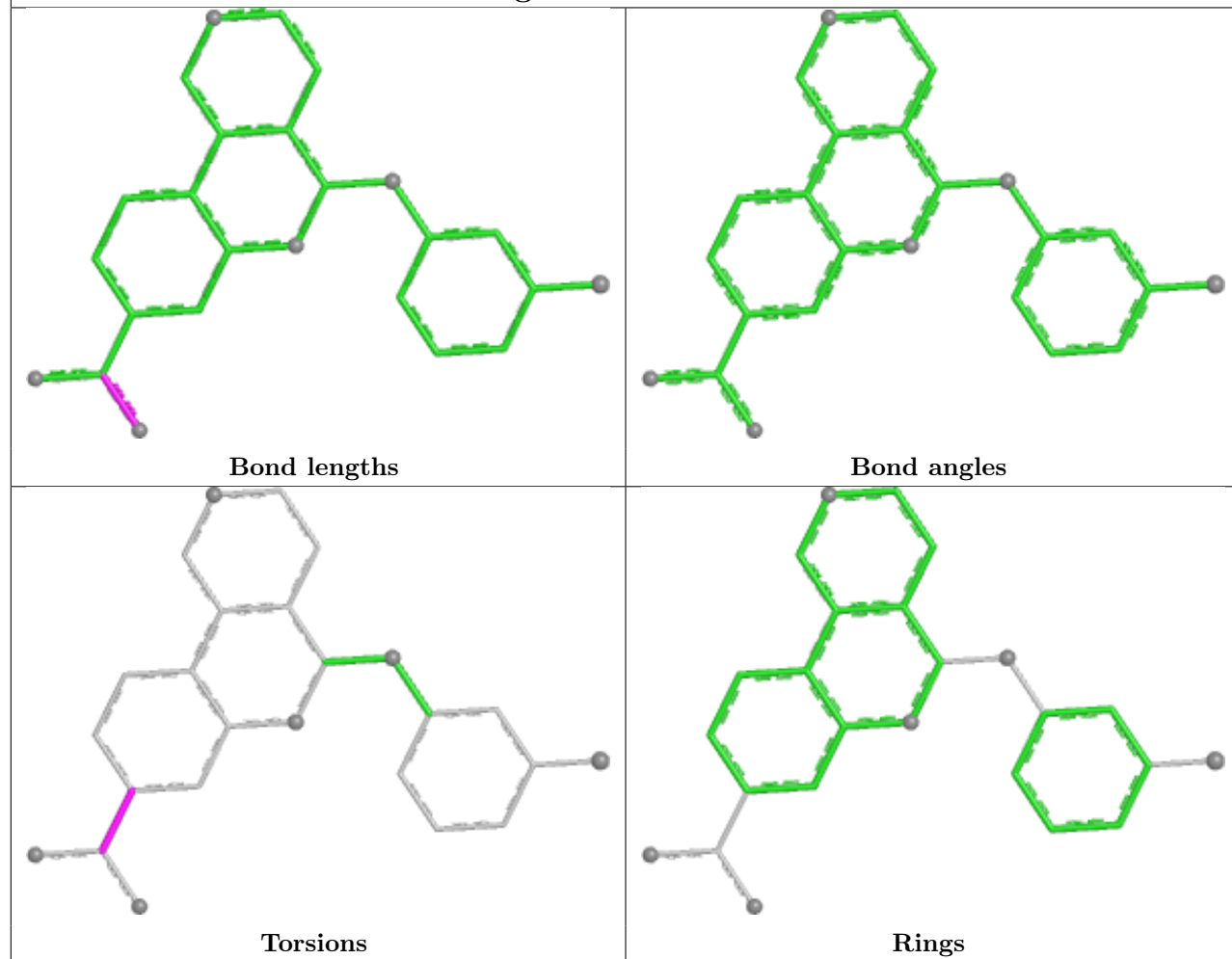
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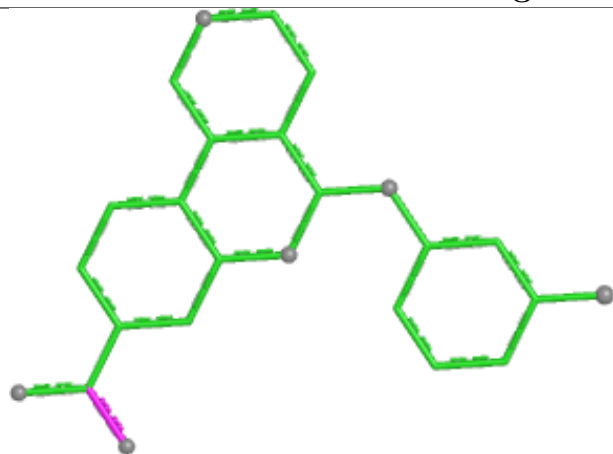
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	3NG	1	0
7	H	504	PGE	1	0
4	A	507	PG4	1	0
6	G	507	EDO	3	0
2	C	501	3NG	1	0
4	D	505	PG4	1	0
7	B	512	PGE	1	0
4	C	505	PG4	1	0

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.

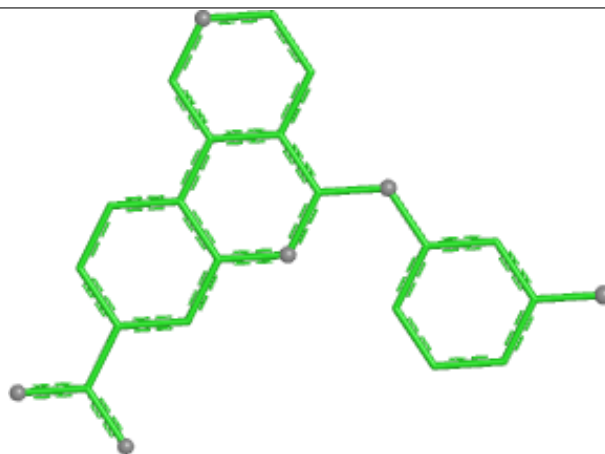
Ligand 3NG F 501



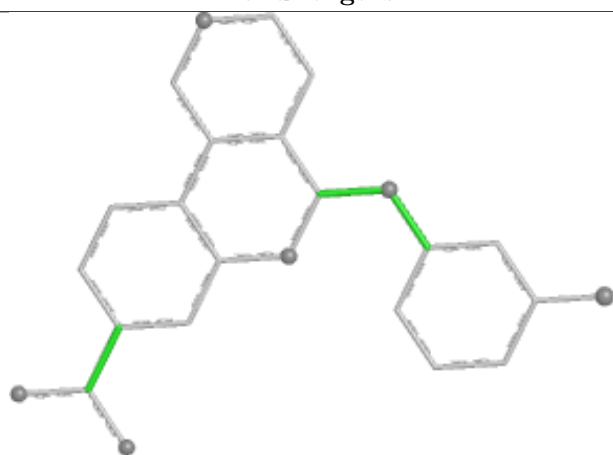
Ligand 3NG G 501



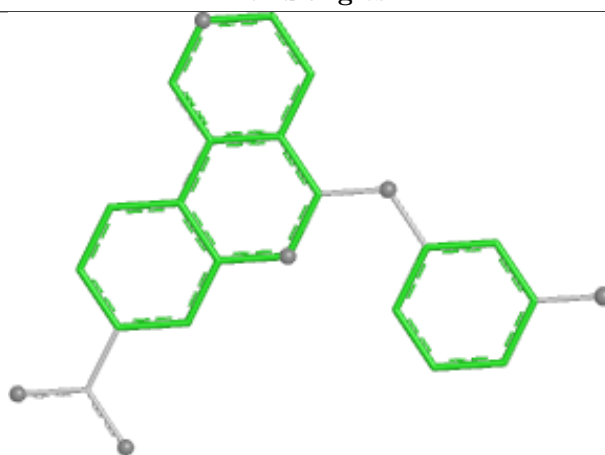
Bond lengths



Bond angles

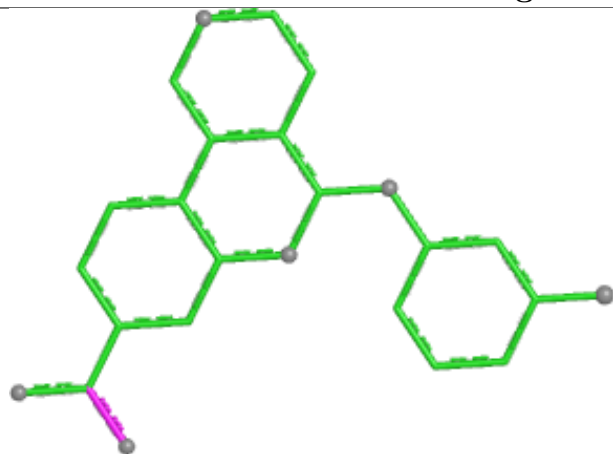


Torsions

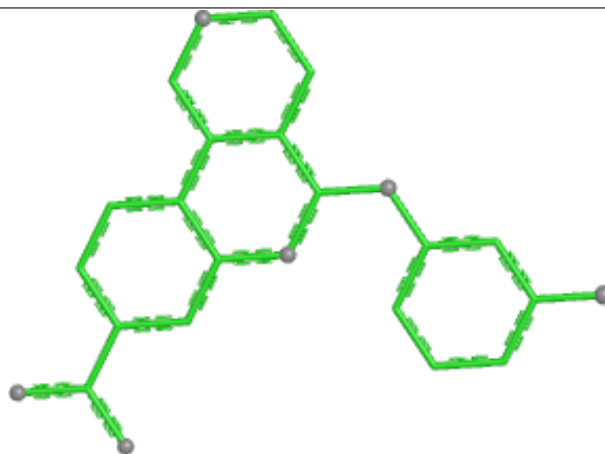


Rings

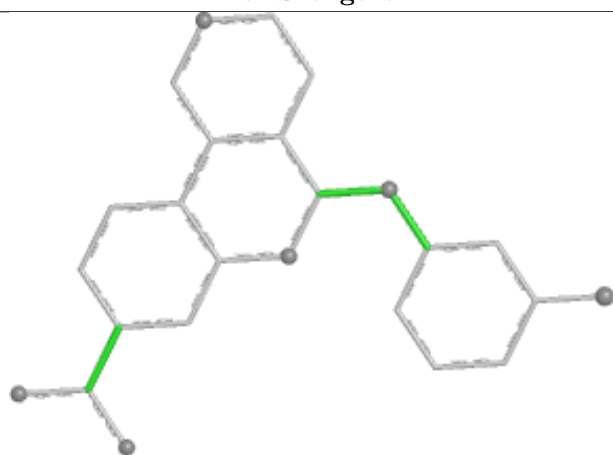
Ligand 3NG E 501



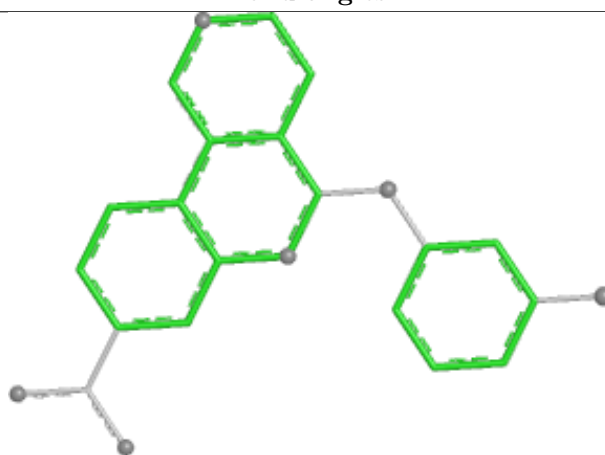
Bond lengths



Bond angles

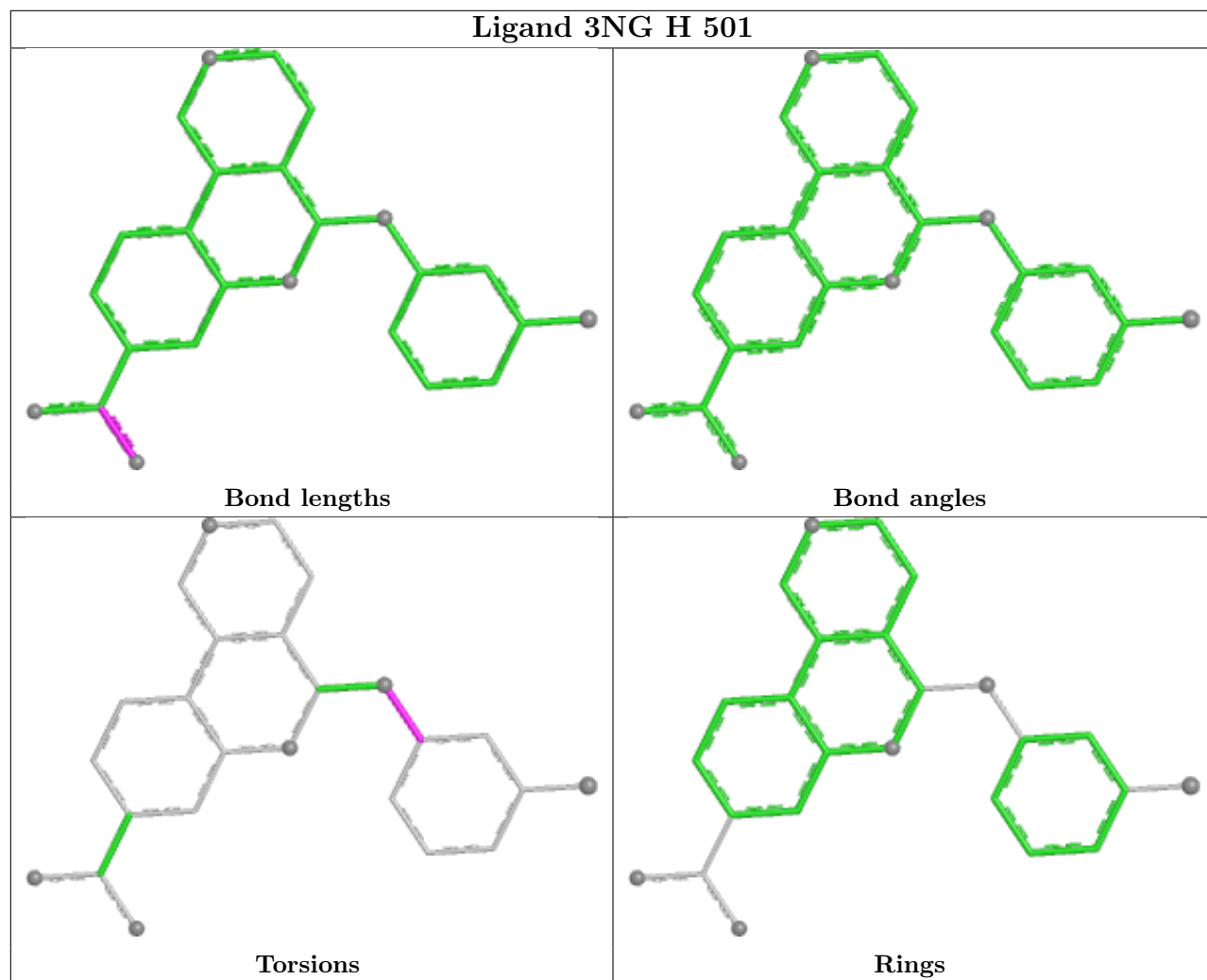


Torsions

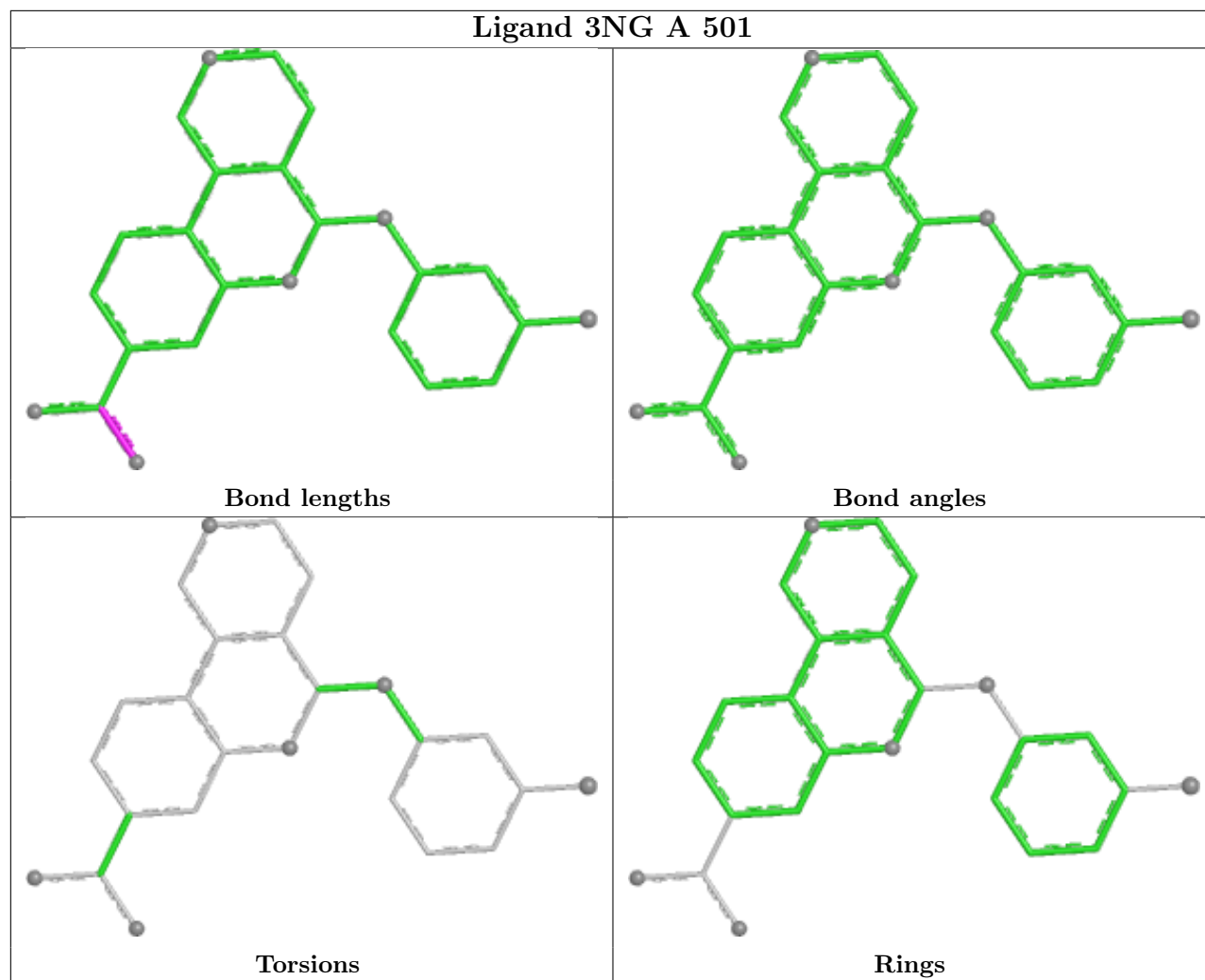


Rings

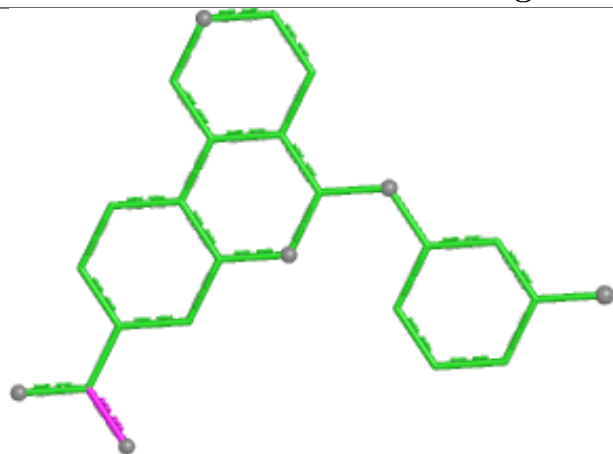
Ligand 3NG H 501



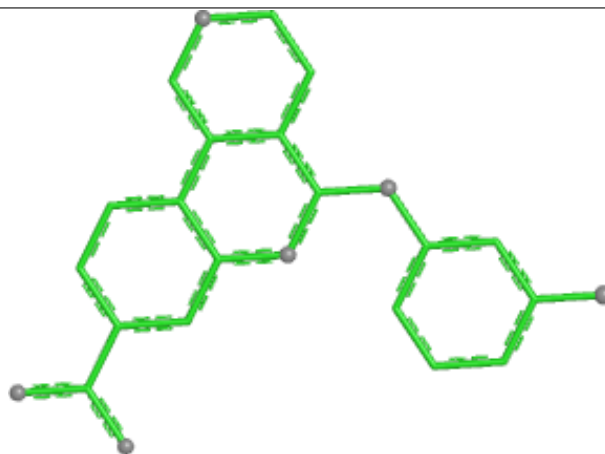
Ligand 3NG A 501



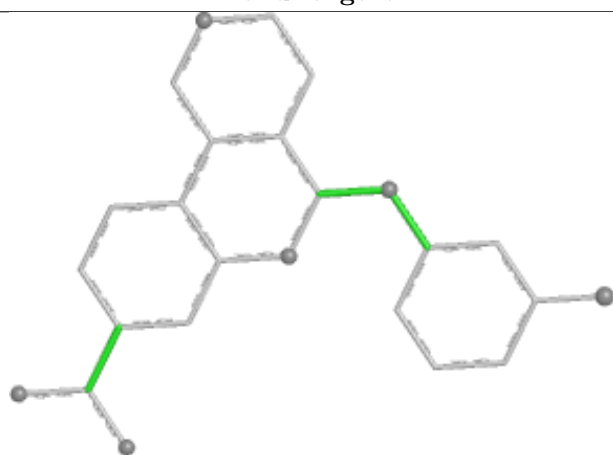
Ligand 3NG B 501



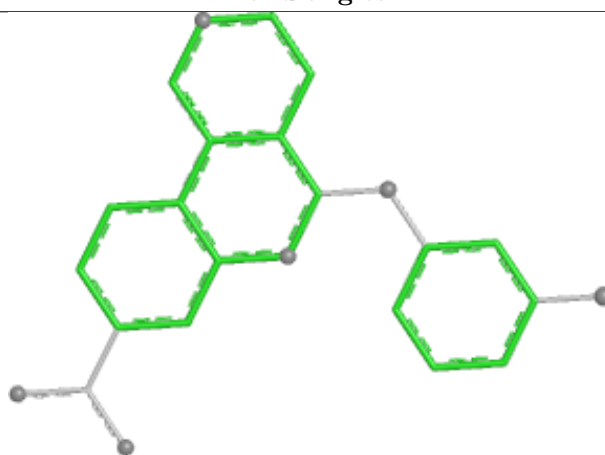
Bond lengths



Bond angles

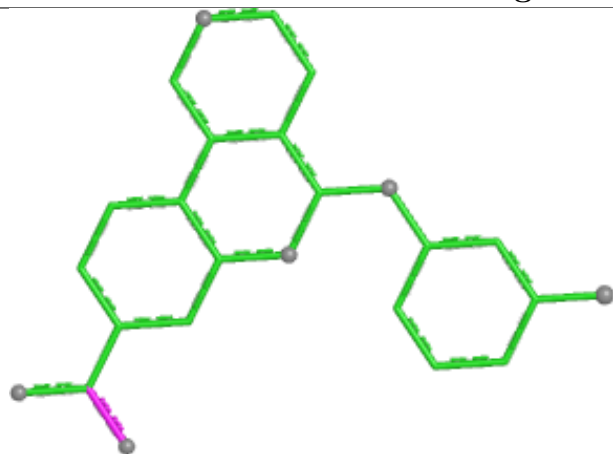


Torsions

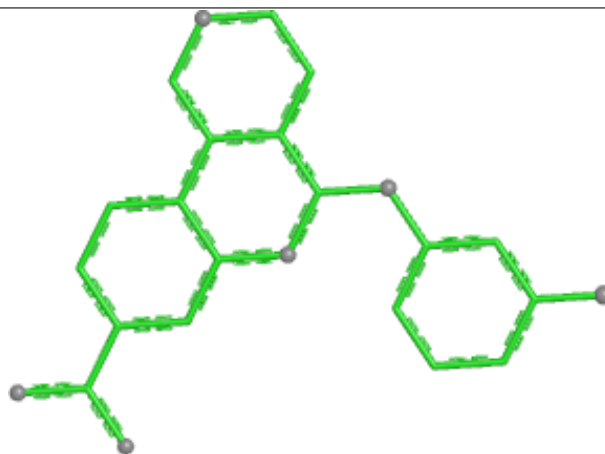


Rings

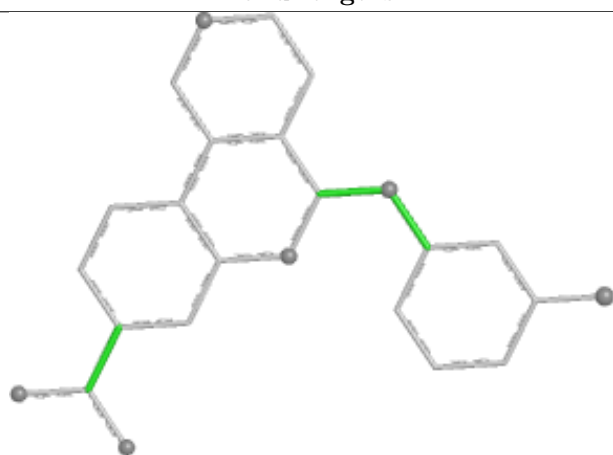
Ligand 3NG C 501



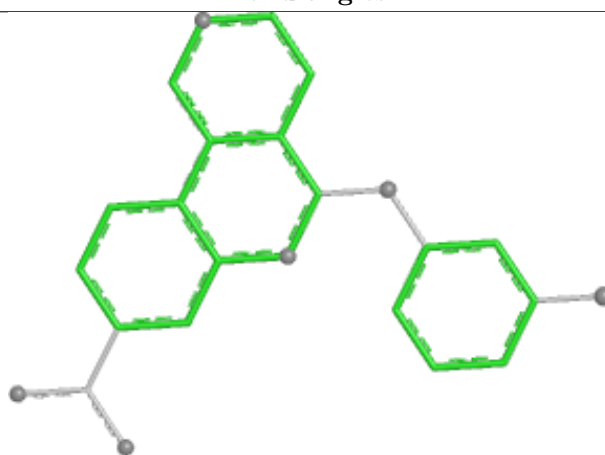
Bond lengths



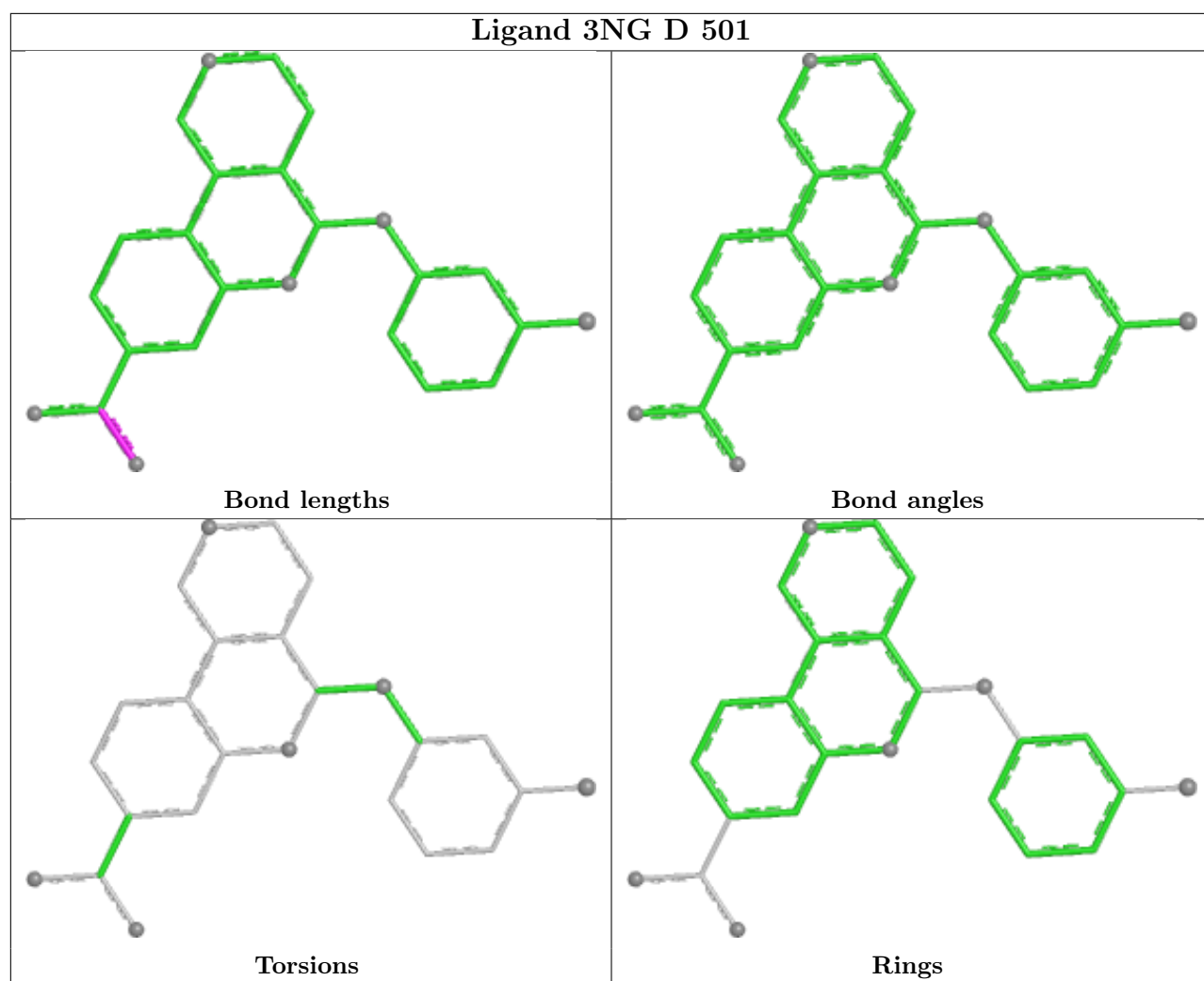
Bond angles



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	345/370 (93%)	-0.38	2 (0%) 85 81	46, 62, 97, 140	0
1	B	342/370 (92%)	-0.25	2 (0%) 85 81	49, 73, 107, 142	0
1	C	343/370 (92%)	-0.35	1 (0%) 90 88	52, 68, 99, 127	0
1	D	337/370 (91%)	0.08	11 (3%) 49 42	51, 93, 134, 167	0
1	E	339/370 (91%)	-0.14	1 (0%) 90 88	51, 80, 112, 133	0
1	F	345/370 (93%)	0.18	5 (1%) 73 67	80, 100, 127, 162	0
1	G	332/370 (89%)	0.21	7 (2%) 63 56	69, 92, 127, 145	0
1	H	306/370 (82%)	0.30	8 (2%) 57 49	64, 102, 134, 160	0
All	All	2689/2960 (90%)	-0.05	37 (1%) 73 67	46, 84, 125, 167	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	410	ASP	4.6
1	G	320	GLN	3.3
1	B	410	ASP	3.3
1	D	400	ASP	3.3
1	D	407	LYS	3.0
1	H	340	LEU	2.9
1	G	214	ASP	2.9
1	D	480	LYS	2.8
1	H	283	ILE	2.6
1	H	316	GLN	2.6
1	D	414	GLU	2.6
1	G	157	ASP	2.6
1	H	337	PRO	2.5
1	G	480	LYS	2.4
1	H	472	TYR	2.4
1	H	135	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	380	PRO	2.3
1	D	402	THR	2.3
1	D	446	VAL	2.3
1	G	219	TYR	2.3
1	D	367	VAL	2.3
1	A	135	VAL	2.2
1	C	409	LYS	2.2
1	G	196	PHE	2.2
1	F	480	LYS	2.2
1	D	398	LEU	2.2
1	F	283	ILE	2.2
1	D	138	ASP	2.1
1	E	480	LYS	2.1
1	F	159	TYR	2.1
1	D	440	GLY	2.1
1	H	315	GLY	2.1
1	G	139	GLY	2.1
1	D	437	ARG	2.0
1	B	480	LYS	2.0
1	F	423	LEU	2.0
1	A	322	ILE	2.0

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

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
1	PTR	H	321	16/17	0.76	0.15	117,136,148,157	0
1	PTR	C	321	16/17	0.89	0.12	68,80,97,100	0
1	PTR	D	321	16/17	0.90	0.10	96,108,117,127	0
1	PTR	G	321	16/17	0.91	0.11	91,105,109,112	0
1	PTR	E	321	16/17	0.91	0.10	80,92,104,106	0
1	PTR	B	321	16/17	0.92	0.12	69,77,85,92	0
1	PTR	A	321	16/17	0.93	0.12	58,68,78,85	0
1	PTR	F	321	16/17	0.93	0.08	93,111,118,119	0

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(Å ²)	Q<0.9
6	EDO	F	503	4/4	0.39	0.27	98,106,107,110	0
3	SO4	A	506	5/5	0.64	0.15	118,122,149,152	0
6	EDO	G	507	4/4	0.71	0.17	80,98,101,105	0
5	PEG	E	505	7/7	0.72	0.17	65,85,91,95	0
3	SO4	G	503	5/5	0.73	0.13	115,125,129,145	0
3	SO4	B	503	5/5	0.73	0.09	123,130,155,161	0
6	EDO	E	506	4/4	0.74	0.24	94,99,110,110	0
6	EDO	B	511	4/4	0.75	0.17	81,87,89,90	0
3	SO4	H	502	5/5	0.77	0.18	114,118,126,189	0
3	SO4	D	503	5/5	0.79	0.16	97,107,125,127	0
3	SO4	D	502	5/5	0.81	0.18	89,101,109,112	0
6	EDO	G	506	4/4	0.82	0.15	67,72,75,86	0
3	SO4	F	502	5/5	0.82	0.11	101,111,113,113	0
3	SO4	B	502	5/5	0.84	0.13	88,95,110,124	0
3	SO4	G	502	5/5	0.85	0.17	106,112,122,144	0
4	PG4	A	508	13/13	0.85	0.11	84,91,102,103	0
5	PEG	G	505	7/7	0.86	0.12	113,117,134,152	0
6	EDO	A	510	4/4	0.86	0.13	64,69,69,69	0
3	SO4	D	504	5/5	0.86	0.12	86,93,98,117	0
3	SO4	E	503	5/5	0.86	0.14	97,100,124,127	0
3	SO4	B	504	5/5	0.86	0.17	78,87,106,136	0
5	PEG	A	509	7/7	0.86	0.14	68,75,82,87	0
3	SO4	B	505	5/5	0.86	0.23	104,108,124,124	0
4	PG4	C	505	13/13	0.87	0.11	82,96,108,109	0
2	3NG	F	501	25/25	0.87	0.12	85,95,107,108	0
6	EDO	B	509	4/4	0.88	0.17	64,66,77,87	0
6	EDO	A	512	4/4	0.88	0.10	70,75,78,82	0
6	EDO	C	507	4/4	0.89	0.12	71,71,78,85	0
6	EDO	C	508	4/4	0.89	0.11	67,73,79,86	0
3	SO4	E	502	5/5	0.89	0.08	83,86,103,106	0
3	SO4	A	502	5/5	0.89	0.12	76,78,100,113	0
5	PEG	G	504	7/7	0.89	0.13	73,86,95,96	0

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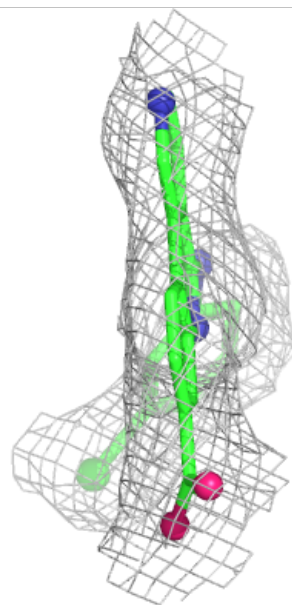
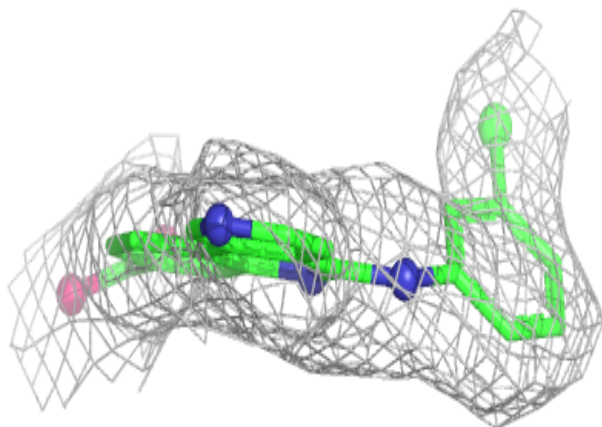
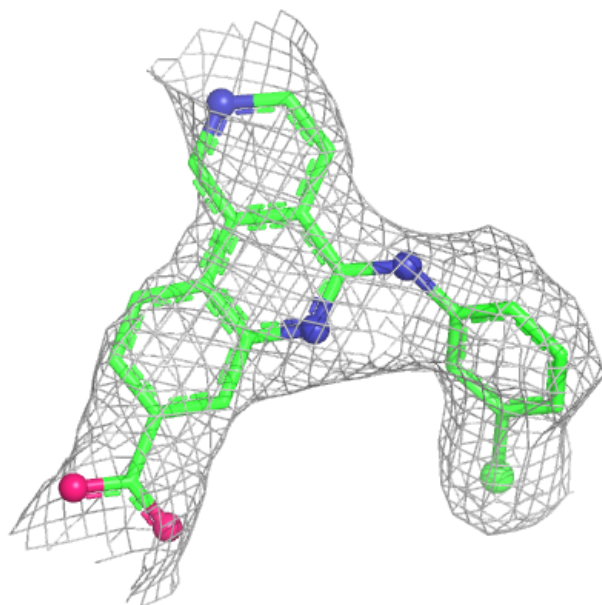
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	D	505	13/13	0.89	0.11	67,82,99,100	0
7	PGE	B	512	10/10	0.89	0.11	72,77,87,88	0
2	3NG	D	501	25/25	0.90	0.11	63,78,91,96	0
6	EDO	A	511	4/4	0.90	0.10	70,76,80,86	0
7	PGE	H	504	10/10	0.90	0.11	59,68,76,79	0
4	PG4	E	504	13/13	0.91	0.09	59,72,80,82	0
6	EDO	C	506	4/4	0.91	0.11	65,70,76,78	0
3	SO4	A	505	5/5	0.91	0.13	80,83,95,126	0
3	SO4	B	506	5/5	0.91	0.18	111,124,132,247	0
6	EDO	B	510	4/4	0.91	0.11	75,77,89,91	0
4	PG4	H	503	13/13	0.92	0.10	51,65,76,78	0
3	SO4	A	504	5/5	0.92	0.08	73,85,93,98	0
2	3NG	G	501	25/25	0.94	0.09	66,72,87,91	0
2	3NG	H	501	25/25	0.94	0.09	62,73,82,88	0
2	3NG	B	501	25/25	0.95	0.08	50,56,65,71	0
2	3NG	C	501	25/25	0.95	0.08	54,60,67,73	0
2	3NG	A	501	25/25	0.95	0.08	45,59,70,71	0
4	PG4	B	507	13/13	0.95	0.06	46,53,59,66	0
4	PG4	B	508	13/13	0.95	0.08	44,55,68,77	0
2	3NG	E	501	25/25	0.95	0.09	50,58,73,75	0
3	SO4	A	503	5/5	0.95	0.12	77,90,105,107	0
3	SO4	C	504	5/5	0.96	0.08	77,84,98,109	0
3	SO4	C	503	5/5	0.96	0.08	79,80,87,92	0
4	PG4	A	507	13/13	0.97	0.07	47,57,65,67	0
3	SO4	C	502	5/5	0.98	0.05	73,75,85,87	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.

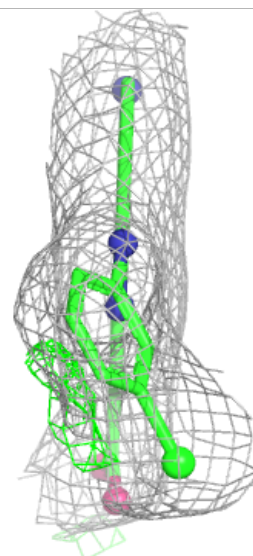
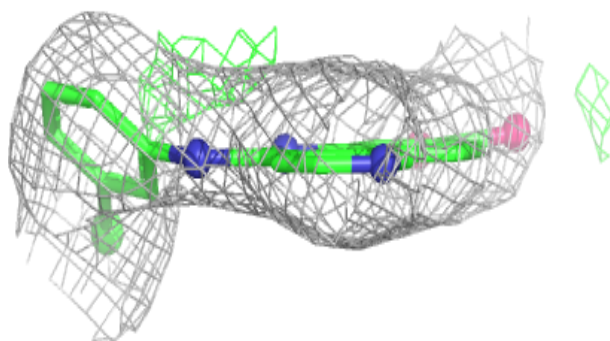
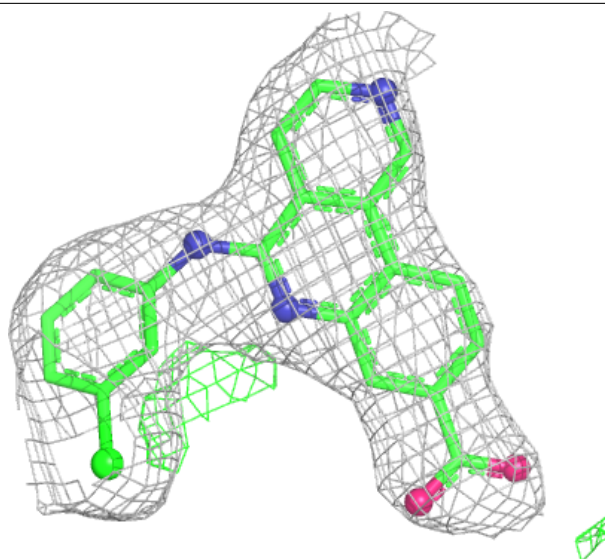
Electron density around 3NG F 501:

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



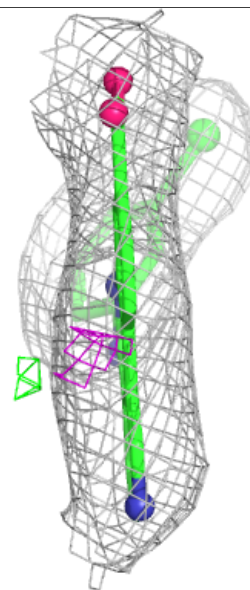
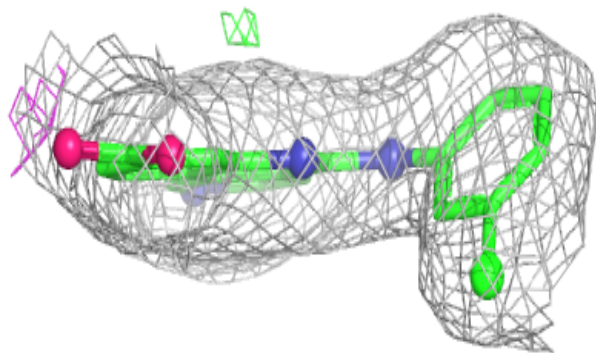
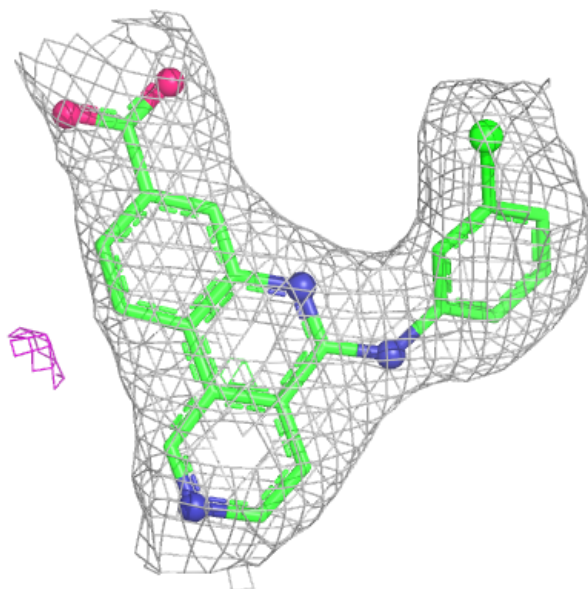
Electron density around 3NG D 501:

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



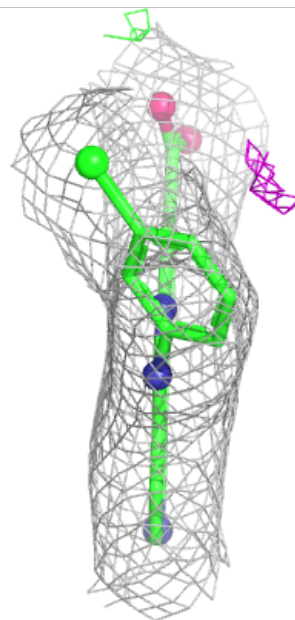
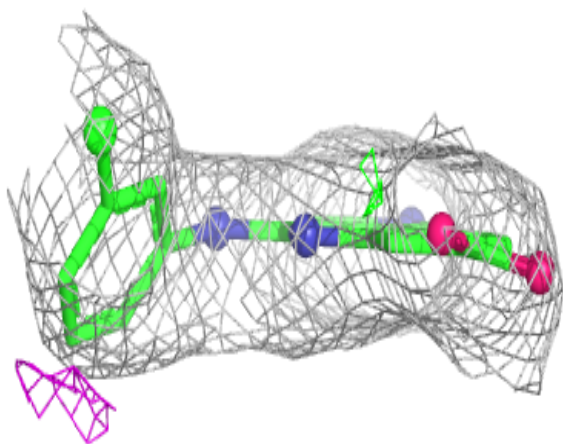
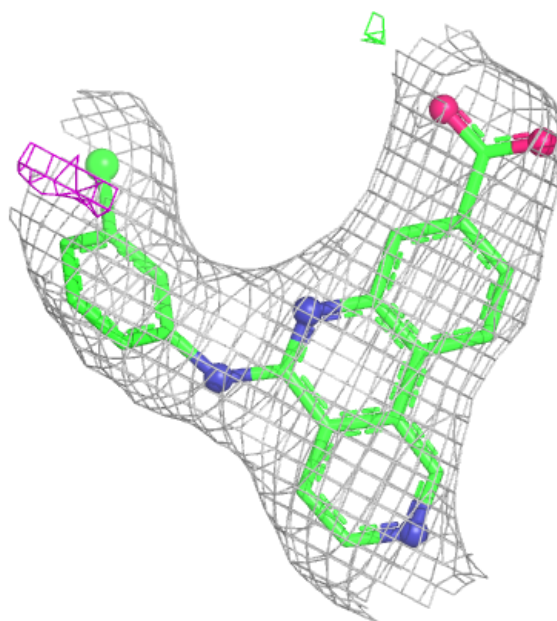
Electron density around 3NG G 501:

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



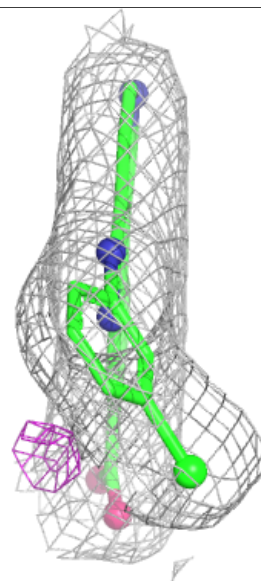
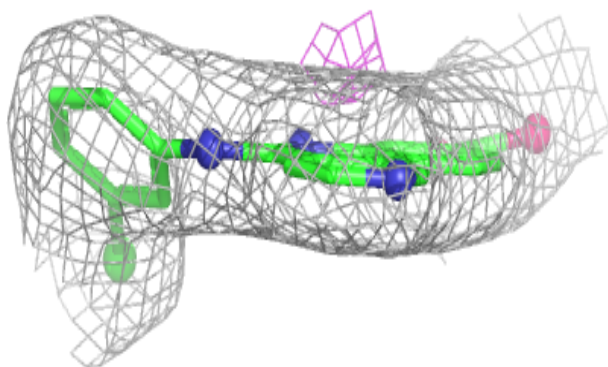
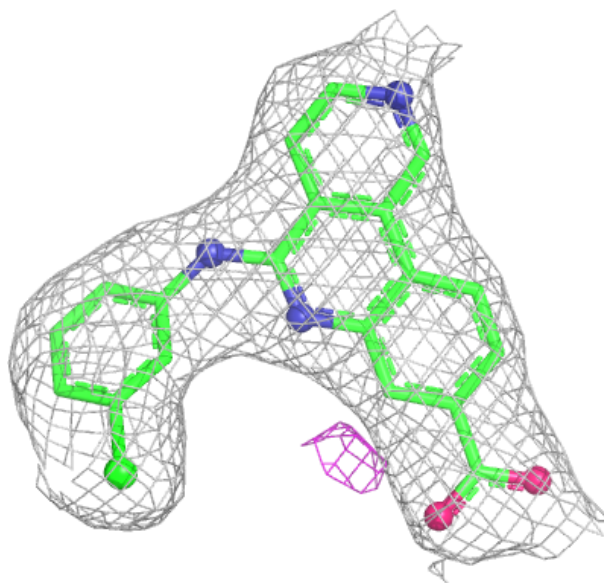
Electron density around 3NG H 501:

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



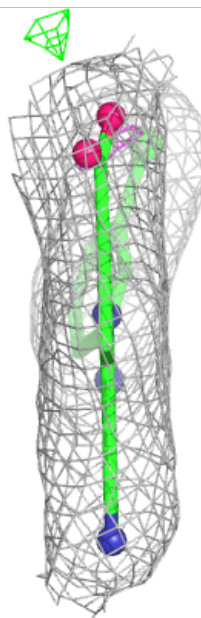
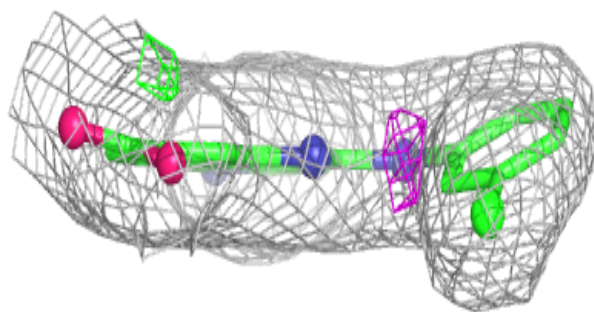
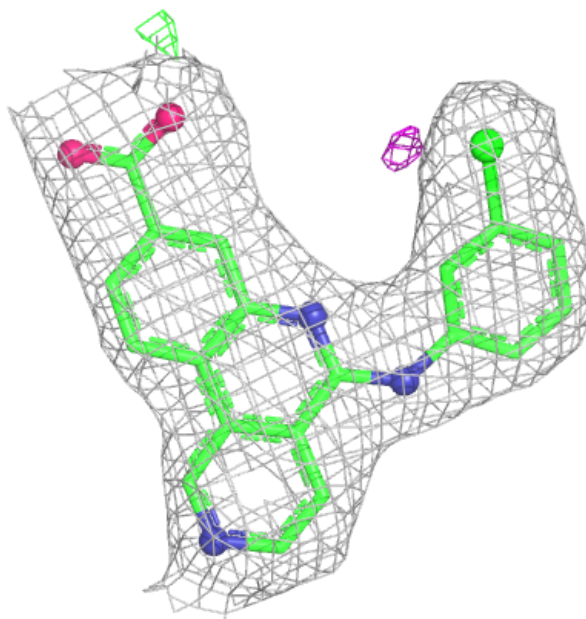
Electron density around 3NG B 501:

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and green (positive)



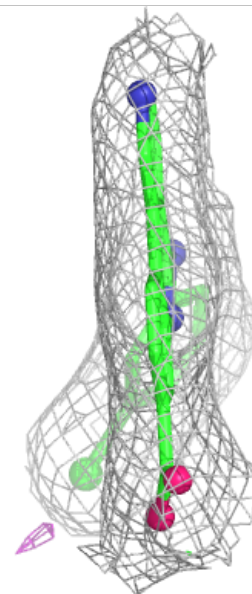
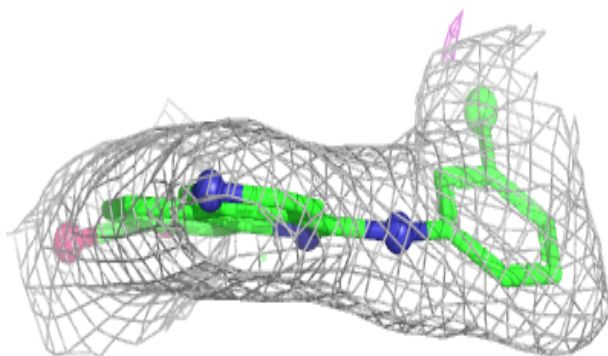
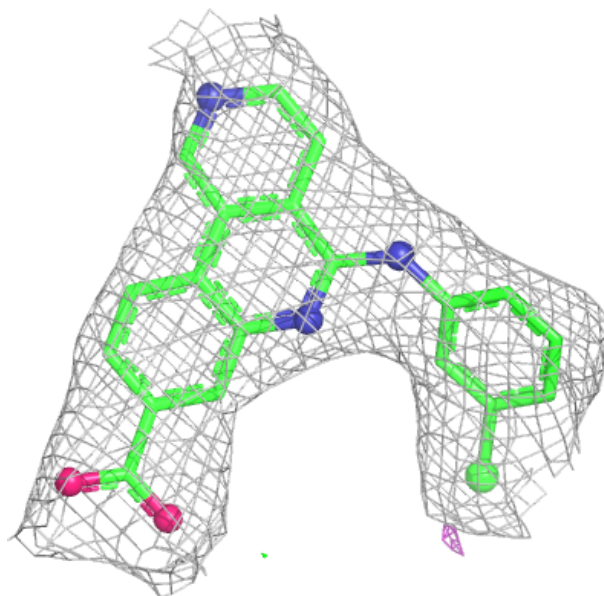
Electron density around 3NG C 501:

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



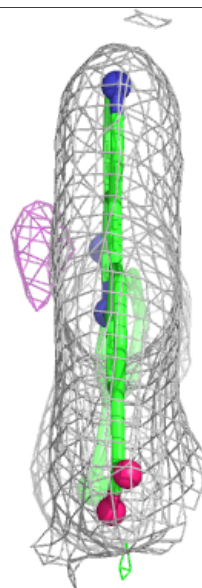
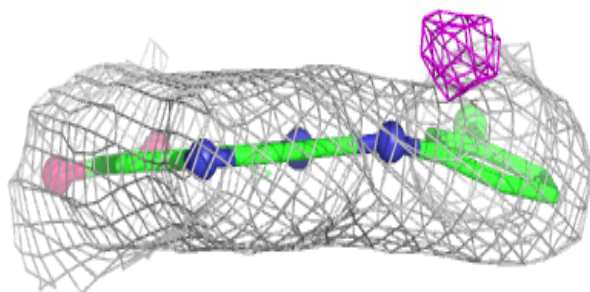
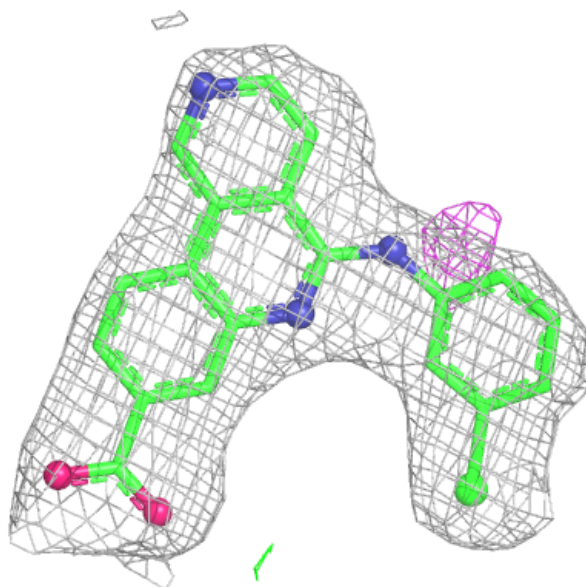
Electron density around 3NG A 501:

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



Electron density around 3NG E 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.