Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 08:54 PM BST

PDB ID	:	6QSH
Title	:	Crystal structure of the hybrid bioinorganic complex of Pizza6S linked by the 1:2 Ce-substituted Keggin
Authors	:	Noguchi, H.; Vandebroek, L.; Kamata, K.; Tame, J.R.H.; Van Meervelt, L.; Parac-Vogt, T.N.; Voet, A.R.D.
Deposited on	:	2019-02-20
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.324
Clashscore		78
Ramachandran outliers		0.8%
Sidechain outliers		1.5%
RSRZ outliers		33.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
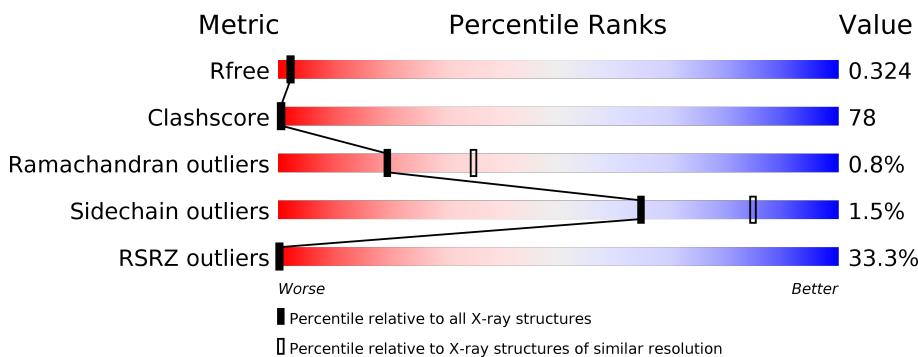
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 <=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	256	32% — 73% — 21% — · ·
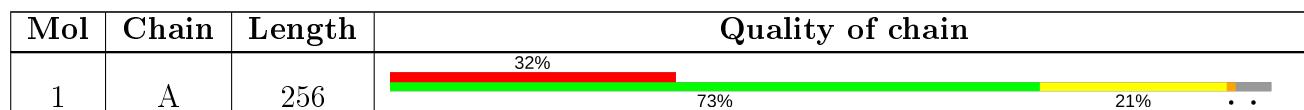
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JGH	A	401	-	-	X	-
2	JGH	A	402[A]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JGH	A	402[B]	-	-	X	-
2	JGH	A	402[C]	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2182 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 Pizza6S.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	0	0	0
			1749	1081	311	357			

- Molecule 2 is 1:2 Ce-substituted Keggin (three-letter code: JGH) (formula: $CeH_2O_{78}P_2W_{22}$).
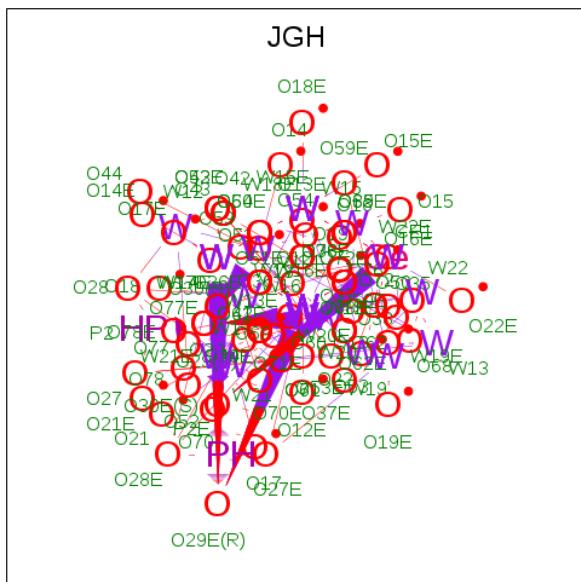
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Ce	O	P	W	0	0
			103	1	78	2	22		
2	A	1	Total	Ce	O	P	W	0	1
			309	3	234	6	66		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		

3 Residue-property plots ⓘ

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

• Molecule 1: Pizza6S
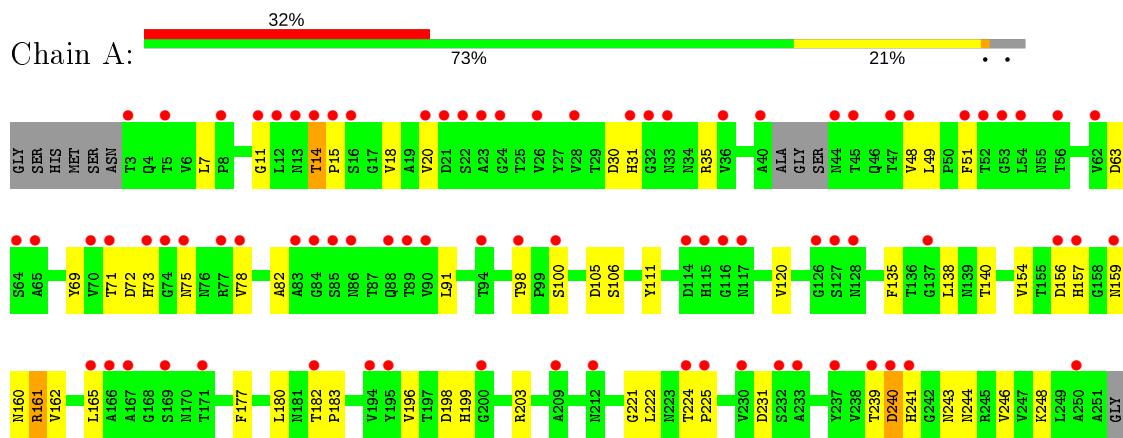
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.37Å 67.26Å 69.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.37 – 2.50 42.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.37-2.50) 99.8 (42.37-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.258 , 0.323 0.259 , 0.324	Depositor DCC
R_{free} test set	479 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.850	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.7	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.040 for -h,l,k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	2182	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: JGH

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	0.26	0/1777	0.47	0/2446

There are no bond length outliers.

There are no bond angle outliers.

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	1749	0	1729	40	0
2	A	412	0	0	269	0
3	A	21	0	0	0	0
All	All	2182	0	1729	305	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 78.

All (305) 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)
2:A:402[C]:JGH:O14E	2:A:402[C]:JGH:W14E	1.66	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402[A]:JGH:O14E	2:A:402[A]:JGH:W14E	1.66	1.42
2:A:402[B]:JGH:W14E	2:A:402[B]:JGH:O14E	1.67	1.41
2:A:401:JGH:W14E	2:A:401:JGH:O14E	1.66	1.41
2:A:402[C]:JGH:W21E	2:A:402[C]:JGH:O21E	1.69	1.40
2:A:402[C]:JGH:W16E	2:A:402[C]:JGH:O16E	1.69	1.40
2:A:402[B]:JGH:O17E	2:A:402[B]:JGH:W17E	1.69	1.40
2:A:402[B]:JGH:O16E	2:A:402[B]:JGH:W16E	1.69	1.40
2:A:402[C]:JGH:O17E	2:A:402[C]:JGH:W17E	1.69	1.40
2:A:402[A]:JGH:W21E	2:A:402[A]:JGH:O21E	1.69	1.39
2:A:401:JGH:W21E	2:A:401:JGH:O21E	1.69	1.39
2:A:402[A]:JGH:W17E	2:A:402[A]:JGH:O17E	1.68	1.39
2:A:401:JGH:O17E	2:A:401:JGH:W17E	1.68	1.38
2:A:402[A]:JGH:O16E	2:A:402[A]:JGH:W16E	1.69	1.38
2:A:401:JGH:W16E	2:A:401:JGH:O16E	1.69	1.38
2:A:402[B]:JGH:O12E	2:A:402[B]:JGH:W12E	1.70	1.38
2:A:402[B]:JGH:O21E	2:A:402[B]:JGH:W21E	1.69	1.38
2:A:402[A]:JGH:W12E	2:A:402[A]:JGH:O12E	1.70	1.38
2:A:401:JGH:W19E	2:A:401:JGH:O19E	1.72	1.37
2:A:402[C]:JGH:O12E	2:A:402[C]:JGH:W12E	1.70	1.37
2:A:401:JGH:W22E	2:A:401:JGH:O22E	1.73	1.36
2:A:402[A]:JGH:O22E	2:A:402[A]:JGH:W22E	1.72	1.36
2:A:401:JGH:W12E	2:A:401:JGH:O12E	1.70	1.36
2:A:402[C]:JGH:O19E	2:A:402[C]:JGH:W19E	1.72	1.36
2:A:402[B]:JGH:W22E	2:A:402[B]:JGH:O22E	1.73	1.36
2:A:402[C]:JGH:W22E	2:A:402[C]:JGH:O22E	1.73	1.35
2:A:402[A]:JGH:O19E	2:A:402[A]:JGH:W19E	1.73	1.35
2:A:402[B]:JGH:O13E	2:A:402[B]:JGH:W13E	1.75	1.35
2:A:401:JGH:O18E	2:A:401:JGH:W18E	1.75	1.35
2:A:401:JGH:O15E	2:A:401:JGH:W15E	1.74	1.35
2:A:402[A]:JGH:O18E	2:A:402[A]:JGH:W18E	1.75	1.35
2:A:402[B]:JGH:W19E	2:A:402[B]:JGH:O19E	1.73	1.34
2:A:402[A]:JGH:O13E	2:A:402[A]:JGH:W13E	1.75	1.34
2:A:402[B]:JGH:O18E	2:A:402[B]:JGH:W18E	1.75	1.34
2:A:402[C]:JGH:W15E	2:A:402[C]:JGH:O15E	1.74	1.34
2:A:402[B]:JGH:O15E	2:A:402[B]:JGH:W15E	1.74	1.34
2:A:402[C]:JGH:W18E	2:A:402[C]:JGH:O18E	1.74	1.34
2:A:402[C]:JGH:O20E	2:A:402[C]:JGH:W20E	1.76	1.34
2:A:402[A]:JGH:W15E	2:A:402[A]:JGH:O15E	1.74	1.34
2:A:402[B]:JGH:O20E	2:A:402[B]:JGH:W20E	1.76	1.34
2:A:401:JGH:O36E	2:A:401:JGH:W20E	1.76	1.33
2:A:402[C]:JGH:W13E	2:A:402[C]:JGH:O13E	1.75	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:JGH:W13E	2:A:401:JGH:O13E	1.75	1.33
2:A:401:JGH:O20E	2:A:401:JGH:W20E	1.76	1.32
2:A:402[A]:JGH:O36E	2:A:402[A]:JGH:W20E	1.75	1.32
2:A:402[B]:JGH:O36E	2:A:402[B]:JGH:W20E	1.75	1.32
2:A:402[A]:JGH:O20E	2:A:402[A]:JGH:W20E	1.76	1.31
2:A:402[C]:JGH:O36E	2:A:402[C]:JGH:W20E	1.76	1.30
2:A:402[B]:JGH:O38E	2:A:402[B]:JGH:W13E	1.80	1.30
2:A:402[A]:JGH:O35E	2:A:402[A]:JGH:W15E	1.80	1.29
2:A:402[C]:JGH:O35E	2:A:402[C]:JGH:W15E	1.81	1.29
2:A:402[C]:JGH:O38E	2:A:402[C]:JGH:W13E	1.80	1.28
2:A:401:JGH:W13E	2:A:401:JGH:O38E	1.80	1.28
2:A:401:JGH:W15E	2:A:401:JGH:O35E	1.81	1.28
2:A:402[B]:JGH:O35E	2:A:402[B]:JGH:W15E	1.80	1.28
2:A:402[A]:JGH:O38E	2:A:402[A]:JGH:W13E	1.80	1.27
2:A:402[B]:JGH:O44E	2:A:402[B]:JGH:W12E	1.84	1.26
2:A:402[A]:JGH:O44E	2:A:402[A]:JGH:W12E	1.83	1.26
2:A:402[B]:JGH:O37E	2:A:402[B]:JGH:W19E	1.84	1.25
2:A:402[C]:JGH:O44E	2:A:402[C]:JGH:W12E	1.84	1.25
2:A:401:JGH:O44E	2:A:401:JGH:W12E	1.84	1.24
2:A:402[A]:JGH:O37E	2:A:402[A]:JGH:W19E	1.85	1.24
2:A:402[C]:JGH:W19E	2:A:402[C]:JGH:O37E	1.85	1.23
2:A:402[B]:JGH:O62E	2:A:402[B]:JGH:W16E	1.87	1.23
2:A:401:JGH:W19E	2:A:401:JGH:O37E	1.85	1.23
2:A:402[C]:JGH:W16E	2:A:402[C]:JGH:O62E	1.87	1.22
2:A:401:JGH:W22E	2:A:401:JGH:O68E	1.88	1.22
2:A:402[A]:JGH:O68E	2:A:402[A]:JGH:W22E	1.88	1.22
2:A:402[A]:JGH:O59E	2:A:402[A]:JGH:W18E	1.88	1.22
2:A:402[A]:JGH:O62E	2:A:402[A]:JGH:W16E	1.87	1.22
2:A:401:JGH:O59E	2:A:401:JGH:W18E	1.88	1.22
2:A:402[B]:JGH:W22E	2:A:402[B]:JGH:O68E	1.88	1.22
2:A:402[A]:JGH:W12E	2:A:402[A]:JGH:O42E	1.89	1.21
2:A:401:JGH:W16E	2:A:401:JGH:O62E	1.87	1.21
2:A:402[C]:JGH:W12E	2:A:402[C]:JGH:O42E	1.88	1.21
2:A:402[C]:JGH:O68E	2:A:402[C]:JGH:W22E	1.88	1.21
2:A:402[C]:JGH:W18E	2:A:402[C]:JGH:O59E	1.88	1.21
2:A:402[B]:JGH:O59E	2:A:402[B]:JGH:W18E	1.88	1.21
2:A:402[C]:JGH:W13E	2:A:402[C]:JGH:O43E	1.88	1.21
2:A:402[B]:JGH:O43E	2:A:402[B]:JGH:W13E	1.89	1.21
2:A:401:JGH:W16E	2:A:401:JGH:O53E	1.89	1.21
2:A:401:JGH:O72E	2:A:401:JGH:W20E	1.89	1.21
2:A:402[C]:JGH:W16E	2:A:402[C]:JGH:O53E	1.89	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402[A]:JGH:O43E	2:A:402[A]:JGH:W13E	1.89	1.20
2:A:402[C]:JGH:O72E	2:A:402[C]:JGH:W20E	1.89	1.20
2:A:402[A]:JGH:O72E	2:A:402[A]:JGH:W20E	1.90	1.20
2:A:402[A]:JGH:W21E	2:A:402[A]:JGH:O71E	1.90	1.20
2:A:401:JGH:O42E	2:A:401:JGH:W12E	1.88	1.20
2:A:402[B]:JGH:W21E	2:A:402[B]:JGH:O71E	1.90	1.20
2:A:402[B]:JGH:O53E	2:A:402[B]:JGH:W16E	1.89	1.19
2:A:401:JGH:W13E	2:A:401:JGH:O43E	1.88	1.19
2:A:402[C]:JGH:W22E	2:A:402[C]:JGH:O69E	1.91	1.19
2:A:402[B]:JGH:O54E	2:A:402[B]:JGH:W14E	1.91	1.19
2:A:402[B]:JGH:O72E	2:A:402[B]:JGH:W20E	1.90	1.19
2:A:401:JGH:W22E	2:A:401:JGH:O69E	1.91	1.19
2:A:401:JGH:O71E	2:A:401:JGH:W21E	1.89	1.19
2:A:401:JGH:W16E	2:A:401:JGH:O71E	1.91	1.19
2:A:402[C]:JGH:O54E	2:A:402[C]:JGH:W14E	1.91	1.19
2:A:402[B]:JGH:W16E	2:A:402[B]:JGH:O71E	1.91	1.19
2:A:402[A]:JGH:O53E	2:A:402[A]:JGH:W16E	1.89	1.19
2:A:402[B]:JGH:O42E	2:A:402[B]:JGH:W12E	1.89	1.18
2:A:402[B]:JGH:W19E	2:A:402[B]:JGH:O50E	1.92	1.18
2:A:402[B]:JGH:W17E	2:A:402[B]:JGH:O70E	1.91	1.18
2:A:402[A]:JGH:W18E	2:A:402[A]:JGH:O51E	1.90	1.18
2:A:401:JGH:O52E	2:A:401:JGH:W17E	1.91	1.18
2:A:402[B]:JGH:W22E	2:A:402[B]:JGH:O77E	1.92	1.18
2:A:402[B]:JGH:W22E	2:A:402[B]:JGH:O69E	1.91	1.18
2:A:402[B]:JGH:W21E	2:A:402[B]:JGH:O78E	1.91	1.18
2:A:401:JGH:O70E	2:A:401:JGH:W17E	1.91	1.18
2:A:401:JGH:O78E	2:A:401:JGH:W21E	1.92	1.18
2:A:401:JGH:W19E	2:A:401:JGH:O50E	1.92	1.18
2:A:402[C]:JGH:O51E	2:A:402[C]:JGH:W18E	1.91	1.18
2:A:402[C]:JGH:W16E	2:A:402[C]:JGH:O71E	1.92	1.18
2:A:402[C]:JGH:O70E	2:A:402[C]:JGH:W17E	1.91	1.18
2:A:402[A]:JGH:W19E	2:A:402[A]:JGH:O50E	1.92	1.18
2:A:402[C]:JGH:W21E	2:A:402[C]:JGH:O78E	1.92	1.18
2:A:402[B]:JGH:W18E	2:A:402[B]:JGH:O51E	1.90	1.18
2:A:402[A]:JGH:O52E	2:A:402[A]:JGH:W17E	1.91	1.18
2:A:402[C]:JGH:O52E	2:A:402[C]:JGH:W17E	1.91	1.18
2:A:402[A]:JGH:W16E	2:A:402[A]:JGH:O71E	1.92	1.18
2:A:402[C]:JGH:O50E	2:A:402[C]:JGH:W19E	1.91	1.18
2:A:402[C]:JGH:W21E	2:A:402[C]:JGH:O71E	1.90	1.18
2:A:402[B]:JGH:O61E	2:A:402[B]:JGH:W17E	1.92	1.18
2:A:402[A]:JGH:O69E	2:A:402[A]:JGH:W22E	1.91	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402[B]:JGH:W14E	2:A:402[B]:JGH:O43E	1.92	1.18
2:A:402[A]:JGH:O77E	2:A:402[A]:JGH:W22E	1.92	1.18
2:A:401:JGH:W14E	2:A:401:JGH:O54E	1.91	1.17
2:A:402[C]:JGH:O43E	2:A:402[C]:JGH:W14E	1.91	1.17
2:A:401:JGH:O76E	2:A:401:JGH:W22E	1.92	1.17
2:A:402[B]:JGH:O52E	2:A:402[B]:JGH:W17E	1.91	1.17
2:A:401:JGH:W18E	2:A:401:JGH:O51E	1.91	1.17
2:A:401:JGH:O60E	2:A:401:JGH:W17E	1.93	1.17
2:A:402[A]:JGH:O76E	2:A:402[A]:JGH:W22E	1.92	1.17
2:A:402[A]:JGH:W17E	2:A:402[A]:JGH:O70E	1.90	1.17
2:A:402[A]:JGH:W17E	2:A:402[A]:JGH:O60E	1.93	1.17
2:A:402[B]:JGH:W22E	2:A:402[B]:JGH:O76E	1.92	1.17
2:A:402[A]:JGH:O54E	2:A:402[A]:JGH:W14E	1.91	1.17
2:A:402[C]:JGH:O76E	2:A:402[C]:JGH:W22E	1.92	1.17
2:A:402[A]:JGH:W17E	2:A:402[A]:JGH:O61E	1.92	1.17
2:A:401:JGH:W22E	2:A:401:JGH:O77E	1.92	1.16
2:A:402[C]:JGH:W22E	2:A:402[C]:JGH:O77E	1.92	1.16
2:A:401:JGH:W17E	2:A:401:JGH:O61E	1.92	1.16
2:A:402[C]:JGH:O61E	2:A:402[C]:JGH:W17E	1.92	1.16
2:A:401:JGH:W14E	2:A:401:JGH:O43E	1.92	1.16
2:A:401:JGH:W18E	2:A:401:JGH:O69E	1.93	1.16
2:A:402[A]:JGH:O78E	2:A:402[A]:JGH:W21E	1.91	1.16
2:A:402[A]:JGH:O43E	2:A:402[A]:JGH:W14E	1.92	1.16
2:A:402[C]:JGH:O60E	2:A:402[C]:JGH:W17E	1.93	1.16
2:A:402[C]:JGH:W13E	2:A:402[C]:JGH:O50E	1.94	1.15
2:A:401:JGH:W13E	2:A:401:JGH:O50E	1.95	1.15
2:A:402[B]:JGH:O61E	2:A:402[B]:JGH:W16E	1.95	1.15
2:A:402[B]:JGH:W17E	2:A:402[B]:JGH:O60E	1.93	1.15
2:A:402[A]:JGH:O61E	2:A:402[A]:JGH:W16E	1.95	1.15
2:A:402[A]:JGH:O50E	2:A:402[A]:JGH:W13E	1.94	1.15
2:A:402[A]:JGH:W18E	2:A:402[A]:JGH:O69E	1.93	1.15
2:A:402[B]:JGH:O77E	2:A:402[B]:JGH:W21E	1.95	1.15
2:A:402[B]:JGH:W19E	2:A:402[B]:JGH:O68E	1.96	1.14
2:A:402[B]:JGH:O69E	2:A:402[B]:JGH:W18E	1.94	1.14
2:A:402[C]:JGH:W18E	2:A:402[C]:JGH:O69E	1.93	1.14
2:A:402[A]:JGH:W21E	2:A:402[A]:JGH:O77E	1.95	1.14
2:A:401:JGH:W19E	2:A:401:JGH:O68E	1.95	1.14
2:A:401:JGH:W21E	2:A:401:JGH:O77E	1.95	1.14
2:A:402[A]:JGH:W12E	2:A:402[A]:JGH:O51E	1.96	1.14
2:A:402[C]:JGH:W21E	2:A:402[C]:JGH:O77E	1.96	1.14
2:A:402[C]:JGH:W16E	2:A:402[C]:JGH:O61E	1.95	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402[B]:JGH:W21E	2:A:402[B]:JGH:O70E	1.96	1.14
2:A:402[C]:JGH:O68E	2:A:402[C]:JGH:W19E	1.95	1.14
2:A:401:JGH:W12E	2:A:401:JGH:O51E	1.96	1.14
2:A:402[A]:JGH:W21E	2:A:402[A]:JGH:O70E	1.95	1.14
2:A:401:JGH:W16E	2:A:401:JGH:O61E	1.95	1.14
2:A:402[B]:JGH:W12E	2:A:402[B]:JGH:O51E	1.96	1.14
2:A:402[B]:JGH:O50E	2:A:402[B]:JGH:W13E	1.95	1.14
2:A:402[A]:JGH:O52E	2:A:402[A]:JGH:W12E	1.97	1.13
2:A:402[C]:JGH:O42E	2:A:402[C]:JGH:W14E	1.96	1.13
2:A:401:JGH:O70E	2:A:401:JGH:W21E	1.96	1.13
2:A:402[A]:JGH:O68E	2:A:402[A]:JGH:W19E	1.95	1.13
2:A:401:JGH:O52E	2:A:401:JGH:W12E	1.97	1.13
2:A:401:JGH:W14E	2:A:401:JGH:O53E	1.97	1.13
2:A:401:JGH:O42E	2:A:401:JGH:W14E	1.97	1.13
2:A:402[A]:JGH:O53E	2:A:402[A]:JGH:W14E	1.97	1.13
2:A:402[C]:JGH:O51E	2:A:402[C]:JGH:W12E	1.96	1.13
2:A:401:JGH:W15E	2:A:401:JGH:O72E	1.97	1.12
2:A:402[C]:JGH:O53E	2:A:402[C]:JGH:W14E	1.97	1.12
2:A:402[B]:JGH:O52E	2:A:402[B]:JGH:W12E	1.97	1.12
2:A:402[C]:JGH:W21E	2:A:402[C]:JGH:O70E	1.96	1.12
2:A:402[B]:JGH:W15E	2:A:402[B]:JGH:O72E	1.98	1.12
2:A:402[B]:JGH:O76E	2:A:402[B]:JGH:W20E	1.97	1.12
2:A:402[A]:JGH:O76E	2:A:402[A]:JGH:W20E	1.97	1.12
2:A:402[B]:JGH:W14E	2:A:402[B]:JGH:O42E	1.97	1.12
2:A:402[A]:JGH:O42E	2:A:402[A]:JGH:W14E	1.97	1.12
2:A:401:JGH:O60E	2:A:401:JGH:W18E	1.98	1.12
2:A:402[B]:JGH:W14E	2:A:402[B]:JGH:O53E	1.97	1.11
2:A:402[C]:JGH:W12E	2:A:402[C]:JGH:O52E	1.97	1.11
2:A:402[C]:JGH:O76E	2:A:402[C]:JGH:W20E	1.98	1.11
2:A:402[B]:JGH:O78E	2:A:402[B]:JGH:W20E	1.99	1.11
2:A:402[A]:JGH:W18E	2:A:402[A]:JGH:O60E	1.98	1.11
2:A:402[A]:JGH:W15E	2:A:402[A]:JGH:O72E	1.98	1.11
2:A:402[C]:JGH:O60E	2:A:402[C]:JGH:W18E	1.98	1.10
2:A:402[A]:JGH:O78E	2:A:402[A]:JGH:W20E	1.99	1.10
2:A:402[C]:JGH:W20E	2:A:402[C]:JGH:O78E	1.99	1.10
2:A:401:JGH:O76E	2:A:401:JGH:W20E	1.97	1.10
2:A:402[C]:JGH:O59E	2:A:402[C]:JGH:W19E	2.00	1.10
2:A:401:JGH:O54E	2:A:401:JGH:W15E	2.00	1.10
2:A:401:JGH:W19E	2:A:401:JGH:O59E	1.99	1.10
2:A:402[B]:JGH:O60E	2:A:402[B]:JGH:W18E	1.98	1.10
2:A:402[A]:JGH:O59E	2:A:402[A]:JGH:W19E	1.99	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:JGH:O78E	2:A:401:JGH:W20E	1.99	1.10
2:A:402[C]:JGH:W15E	2:A:402[C]:JGH:O72E	1.97	1.10
2:A:402[B]:JGH:W19E	2:A:402[B]:JGH:O59E	1.99	1.09
2:A:402[A]:JGH:W15E	2:A:402[A]:JGH:O54E	2.00	1.09
2:A:402[B]:JGH:O54E	2:A:402[B]:JGH:W15E	2.00	1.08
2:A:402[C]:JGH:O54E	2:A:402[C]:JGH:W15E	2.00	1.08
2:A:402[A]:JGH:W15E	2:A:402[A]:JGH:O62E	2.06	1.04
2:A:402[B]:JGH:O44E	2:A:402[B]:JGH:W13E	2.06	1.03
2:A:402[A]:JGH:O44E	2:A:402[A]:JGH:W13E	2.06	1.03
2:A:402[B]:JGH:O62E	2:A:402[B]:JGH:W15E	2.06	1.02
2:A:401:JGH:W15E	2:A:401:JGH:O62E	2.06	1.02
2:A:402[C]:JGH:W13E	2:A:402[C]:JGH:O44E	2.06	1.02
2:A:402[C]:JGH:W15E	2:A:402[C]:JGH:O62E	2.06	1.02
2:A:401:JGH:O44E	2:A:401:JGH:W13E	2.06	1.02
2:A:402[A]:JGH:O36E	2:A:402[A]:JGH:O38	1.96	0.83
2:A:402[C]:JGH:W13E	2:A:402[C]:JGH:O27E	2.35	0.74
2:A:401:JGH:W13E	2:A:401:JGH:O27E	2.35	0.74
2:A:402[A]:JGH:O27E	2:A:402[A]:JGH:W13E	2.35	0.73
2:A:402[B]:JGH:W13E	2:A:402[B]:JGH:O27E	2.35	0.73
1:A:135:PHE:HB3	1:A:138:LEU:HD11	1.71	0.70
2:A:402[A]:JGH:W22E	2:A:402[A]:JGH:O30E	2.40	0.70
2:A:402[C]:JGH:W22E	2:A:402[C]:JGH:O30E	2.40	0.70
2:A:401:JGH:O30E	2:A:401:JGH:W22E	2.40	0.69
2:A:401:JGH:W14E	2:A:401:JGH:O29E	2.40	0.69
2:A:402[B]:JGH:W14E	2:A:402[B]:JGH:O29E	2.40	0.69
2:A:402[A]:JGH:O29E	2:A:402[A]:JGH:W14E	2.40	0.69
2:A:402[C]:JGH:O29E	2:A:402[C]:JGH:W14E	2.40	0.69
2:A:402[C]:JGH:O28E	2:A:402[C]:JGH:W17E	2.41	0.69
2:A:401:JGH:O28E	2:A:401:JGH:W17E	2.41	0.69
2:A:402[C]:JGH:O27E	2:A:402[C]:JGH:W19E	2.41	0.69
2:A:402[B]:JGH:O30E	2:A:402[B]:JGH:W22E	2.40	0.69
2:A:401:JGH:W19E	2:A:401:JGH:O27E	2.41	0.68
2:A:402[A]:JGH:O27E	2:A:402[A]:JGH:W19E	2.42	0.68
2:A:402[B]:JGH:W19E	2:A:402[B]:JGH:O27E	2.41	0.68
2:A:402[A]:JGH:W17E	2:A:402[A]:JGH:O28E	2.41	0.68
2:A:402[B]:JGH:O30E	2:A:402[B]:JGH:W20E	2.42	0.68
2:A:402[B]:JGH:W17E	2:A:402[B]:JGH:O28E	2.41	0.68
2:A:402[C]:JGH:O30E	2:A:402[C]:JGH:W20E	2.42	0.67
2:A:402[A]:JGH:W20E	2:A:402[A]:JGH:O30E	2.42	0.67
2:A:401:JGH:O30E	2:A:401:JGH:W20E	2.42	0.67
2:A:401:JGH:W12E	2:A:401:JGH:O28E	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402[C]:JGH:O28E	2:A:402[C]:JGH:W18E	2.43	0.67
2:A:402[A]:JGH:W12E	2:A:402[A]:JGH:O28E	2.43	0.67
2:A:402[B]:JGH:W12E	2:A:402[B]:JGH:O28E	2.43	0.67
2:A:402[B]:JGH:O28E	2:A:402[B]:JGH:W18E	2.43	0.67
2:A:401:JGH:W18E	2:A:401:JGH:O28E	2.43	0.66
2:A:402[A]:JGH:W18E	2:A:402[A]:JGH:O28E	2.43	0.66
2:A:402[C]:JGH:O28E	2:A:402[C]:JGH:W12E	2.43	0.66
1:A:73:HIS:CE1	1:A:98:THR:HB	2.32	0.65
2:A:402[C]:JGH:W15E	2:A:402[C]:JGH:O29E	2.45	0.64
2:A:401:JGH:W15E	2:A:401:JGH:O29E	2.45	0.64
2:A:402[B]:JGH:W15E	2:A:402[B]:JGH:O29E	2.46	0.64
2:A:402[A]:JGH:W15E	2:A:402[A]:JGH:O29E	2.46	0.64
2:A:401:JGH:W16E	2:A:401:JGH:O29E	2.46	0.64
2:A:402[C]:JGH:W16E	2:A:402[C]:JGH:O29E	2.46	0.64
2:A:402[A]:JGH:O29E	2:A:402[A]:JGH:W16E	2.46	0.64
2:A:402[B]:JGH:W16E	2:A:402[B]:JGH:O29E	2.46	0.64
1:A:49:LEU:HD12	1:A:51:PHE:HE2	1.64	0.62
1:A:30:ASP:OD2	1:A:35:ARG:NH2	2.32	0.61
2:A:401:JGH:O30E	2:A:401:JGH:W21E	2.50	0.60
1:A:30:ASP:HB3	1:A:35:ARG:HB3	1.82	0.60
1:A:73:HIS:NE2	2:A:402[C]:JGH:O76	2.34	0.60
2:A:402[C]:JGH:W21E	2:A:402[C]:JGH:O30E	2.50	0.59
2:A:402[A]:JGH:W21E	2:A:402[A]:JGH:O30E	2.51	0.59
1:A:239:THR:HG22	1:A:246:VAL:HG22	1.85	0.58
2:A:402[B]:JGH:O30E	2:A:402[B]:JGH:W21E	2.50	0.58
1:A:177:PHE:HB3	1:A:180:LEU:HG	1.85	0.57
1:A:162:VAL:HG21	1:A:196:VAL:HG21	1.87	0.57
1:A:73:HIS:NE2	2:A:402[B]:JGH:O19	2.38	0.57
1:A:18:VAL:HB	1:A:239:THR:HG23	1.87	0.57
1:A:105:ASP:OD1	1:A:106:SER:N	2.38	0.56
1:A:198:ASP:HB3	1:A:203:ARG:HG3	1.87	0.55
1:A:225:PRO:HA	1:A:240:ASP:HA	1.88	0.55
1:A:7:LEU:HD21	1:A:248:LYS:HG2	1.88	0.55
1:A:63:ASP:HB2	1:A:69:TYR:HE1	1.74	0.53
1:A:20:VAL:HG21	1:A:231:ASP:HB3	1.91	0.52
1:A:100:SER:OG	2:A:402[A]:JGH:O21	2.27	0.50
1:A:156:ASP:HB3	1:A:161:ARG:HG2	1.97	0.47
1:A:222:LEU:HD23	1:A:225:PRO:HG3	1.95	0.47
1:A:15:PRO:HD3	1:A:244:ASN:HA	1.95	0.47
1:A:14:THR:O	1:A:31:HIS:HB3	2.14	0.47
1:A:160:ASN:HA	1:A:183:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:HG21	1:A:100:SER:O	2.16	0.45
1:A:120:VAL:HG21	1:A:154:VAL:HG21	1.98	0.45
1:A:221:GLY:O	1:A:243:ASN:ND2	2.50	0.45
1:A:73:HIS:HE1	1:A:98:THR:HB	1.82	0.44
1:A:157:HIS:CD2	1:A:182:THR:HA	2.53	0.44
1:A:182:THR:O	1:A:199:HIS:HB3	2.18	0.44
1:A:105:ASP:HB2	1:A:111:TYR:HE2	1.83	0.43
1:A:140:THR:O	1:A:157:HIS:HB3	2.18	0.43
1:A:199:HIS:NE2	1:A:224:THR:HB	2.34	0.42
1:A:160:ASN:HA	1:A:183:PRO:CD	2.51	0.41
1:A:14:THR:HB	1:A:241:HIS:CD2	2.56	0.41
1:A:11:GLY:O	1:A:35:ARG:NH2	2.52	0.41
1:A:35:ARG:CG	1:A:48:VAL:HG21	2.51	0.41
1:A:72:ASP:HB3	1:A:75:ASN:HB2	2.03	0.41
1:A:78:VAL:HG23	1:A:91:LEU:HB2	2.02	0.41
1:A:73:HIS:HD2	2:A:402[C]:JGH:O78	2.04	0.40
1:A:159:ASN:HB2	1:A:161:ARG:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/256 (94%)	213 (88%)	27 (11%)	2 (1%)	19	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	14	THR

5.3.2 Protein sidechains (i)

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	195/201 (97%)	192 (98%)	3 (2%)	65 85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ARG
1	A	165	LEU
1	A	240	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	JGH	A	402[A]	-	44,148,148	1.36	4 (9%)	12,460,460	1.18	0
2	JGH	A	401	3	44,148,148	1.34	4 (9%)	12,460,460	1.04	2 (16%)
2	JGH	A	402[C]	-	44,148,148	1.34	4 (9%)	12,460,460	0.97	0
2	JGH	A	402[B]	-	44,148,148	1.35	4 (9%)	12,460,460	1.00	0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	JGH	W14E-O14E	-2.10	1.66	2.16
2	A	402[C]	JGH	W14E-O14E	-2.10	1.66	2.16
2	A	402[B]	JGH	W14-O14	-2.10	1.66	2.16
2	A	402[A]	JGH	W14-O14	-2.10	1.66	2.16
2	A	401	JGH	W14-O14	-2.09	1.66	2.16
2	A	402[C]	JGH	W14-O14	-2.09	1.66	2.16
2	A	402[A]	JGH	W14E-O14E	-2.09	1.67	2.16
2	A	402[B]	JGH	W14E-O14E	-2.09	1.67	2.16
2	A	402[B]	JGH	W17-O17	-2.02	1.68	2.16
2	A	402[A]	JGH	W17-O17	-2.01	1.68	2.16
2	A	402[A]	JGH	W17E-O17E	-2.01	1.68	2.16
2	A	401	JGH	W17E-O17E	-2.01	1.68	2.16
2	A	402[C]	JGH	W17-O17	-2.01	1.68	2.16
2	A	401	JGH	W17-O17	-2.01	1.68	2.16
2	A	402[B]	JGH	W17E-O17E	-2.01	1.69	2.16
2	A	402[C]	JGH	W17E-O17E	-2.01	1.69	2.16

All (2) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	JGH	O30-P2-O28	2.11	110.73	108.39
2	A	401	JGH	O30E-P2E-O28E	2.01	110.62	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402[A]	JGH	68	0
2	A	401	JGH	66	0
2	A	402[C]	JGH	68	0
2	A	402[B]	JGH	67	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 then 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 JGH A 402 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand JGH A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand JGH A 402 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand JGH A 402 (B)

Bond lengths

Bond angles

Torsions

Rings
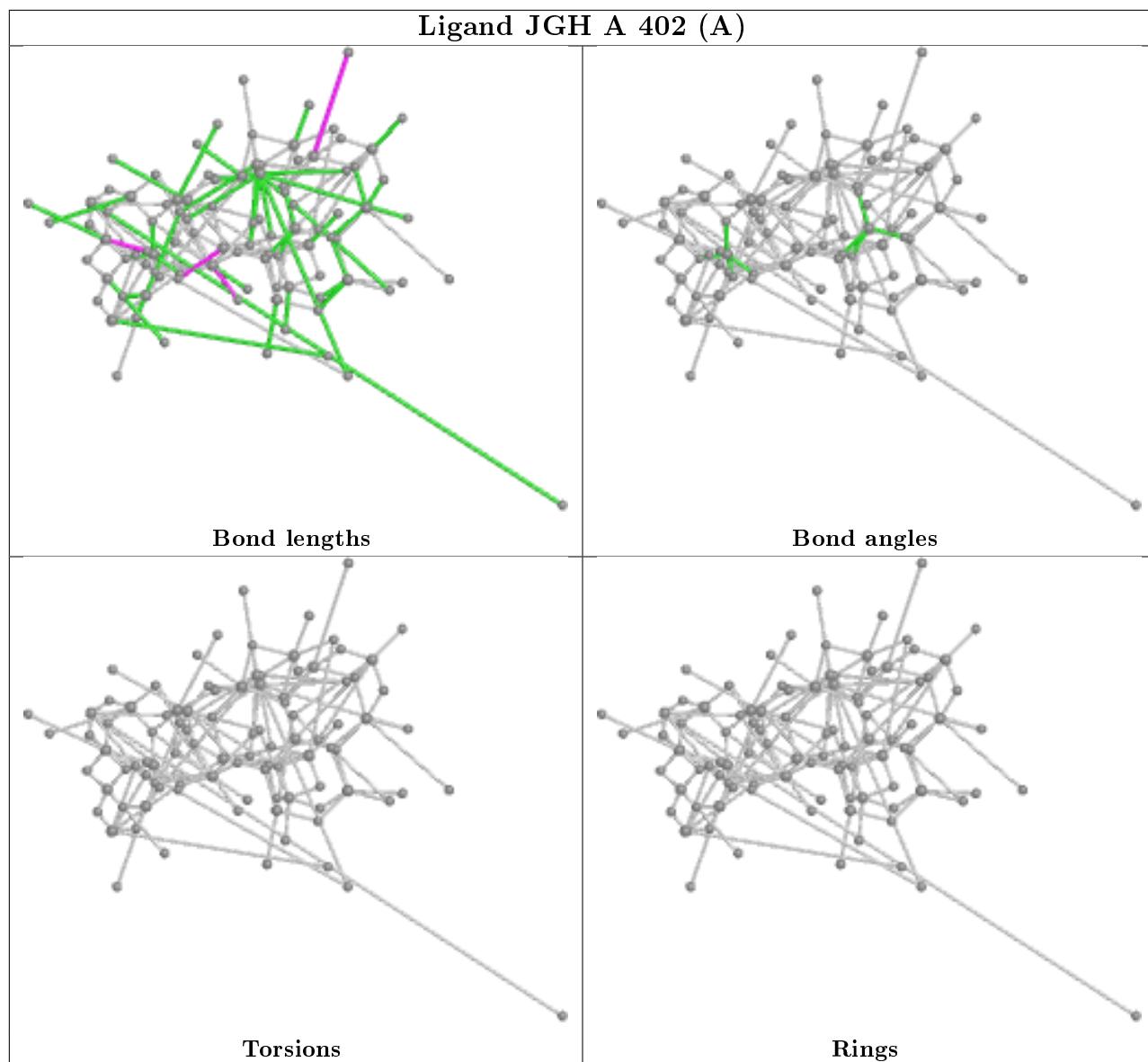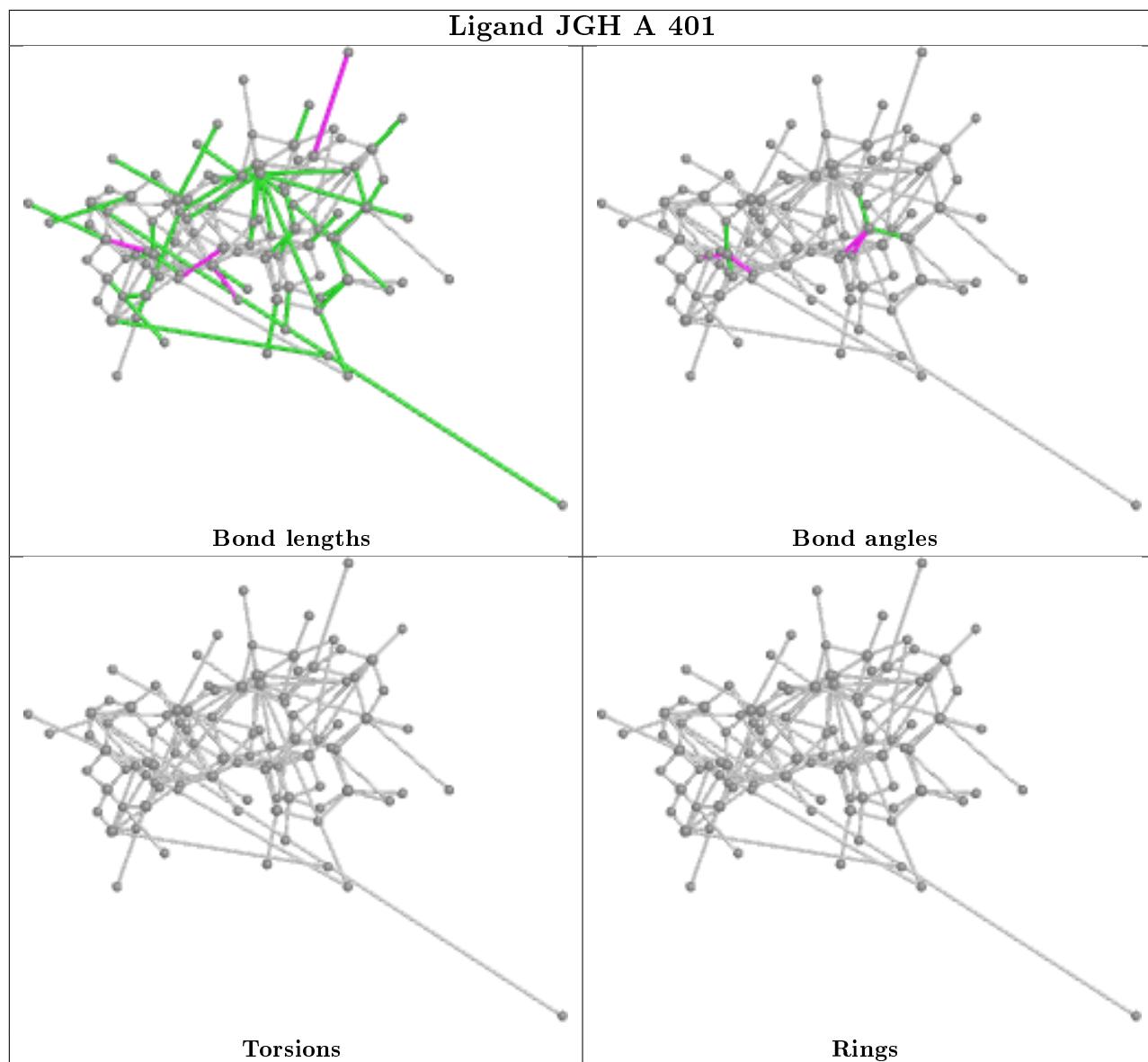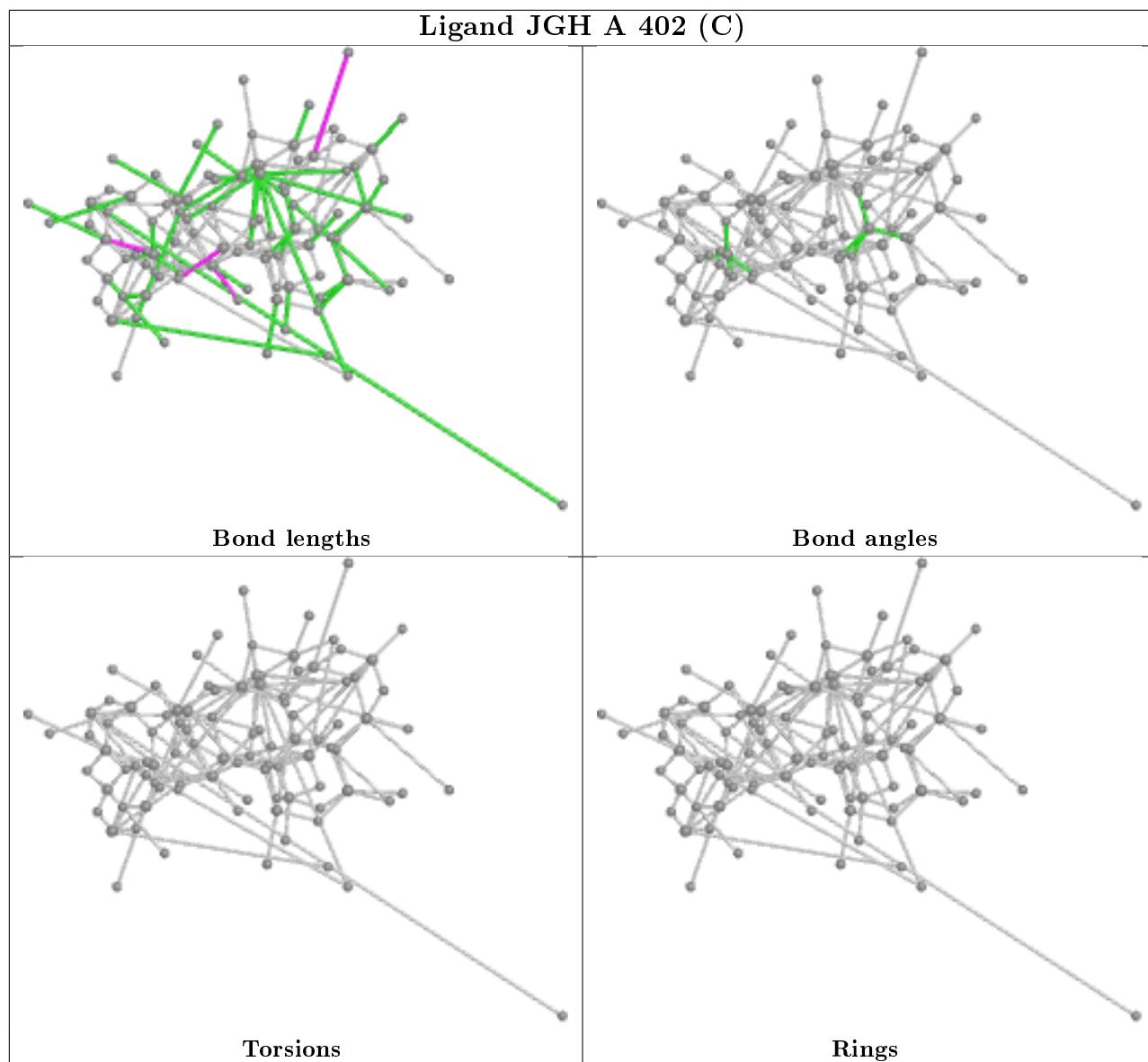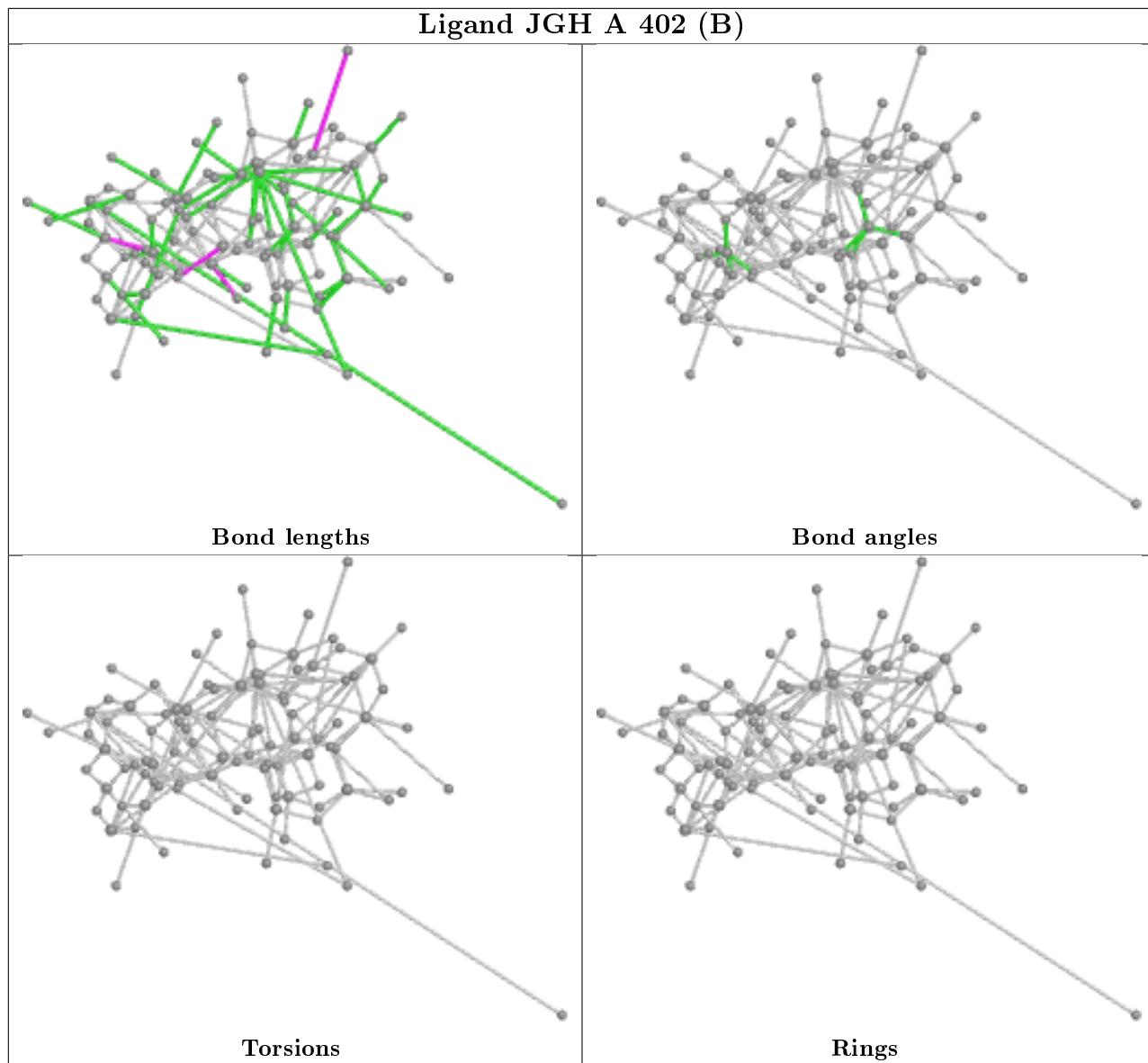
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	246/256 (96%)	1.73	82 (33%)	0	0	9, 31, 54, 73	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	9.2
1	A	44	ASN	6.5
1	A	88	GLN	6.1
1	A	52	THR	5.7
1	A	45	THR	5.3
1	A	167	ALA	4.8
1	A	13	ASN	4.8
1	A	126	GLY	4.8
1	A	157	HIS	4.6
1	A	62	VAL	4.5
1	A	3	THR	4.4
1	A	83	ALA	4.4
1	A	74	GLY	4.3
1	A	32	GLY	4.2
1	A	16	SER	4.2
1	A	47	THR	4.0
1	A	14	THR	4.0
1	A	115	HIS	3.8
1	A	21	ASP	3.8
1	A	84	GLY	3.6
1	A	40	ALA	3.5
1	A	64	SER	3.5
1	A	33	ASN	3.4
1	A	169	SER	3.4
1	A	48	VAL	3.4
1	A	225	PRO	3.3
1	A	171	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	20	VAL	3.2
1	A	240	ASP	3.0
1	A	15	PRO	3.0
1	A	117	ASN	3.0
1	A	241	HIS	3.0
1	A	232	SER	2.9
1	A	230	VAL	2.9
1	A	166	ALA	2.8
1	A	237	TYR	2.8
1	A	71	THR	2.8
1	A	89	THR	2.8
1	A	239	THR	2.7
1	A	94	THR	2.7
1	A	26	VAL	2.7
1	A	165	LEU	2.7
1	A	11	GLY	2.7
1	A	194	VAL	2.6
1	A	53	GLY	2.6
1	A	8	PRO	2.6
1	A	36	VAL	2.6
1	A	65	ALA	2.6
1	A	54	LEU	2.5
1	A	24	GLY	2.5
1	A	209	ALA	2.5
1	A	212	ASN	2.5
1	A	224	THR	2.5
1	A	31	HIS	2.5
1	A	73	HIS	2.5
1	A	22	SER	2.5
1	A	98	THR	2.4
1	A	182	THR	2.4
1	A	116	GLY	2.3
1	A	127	SER	2.3
1	A	90	VAL	2.3
1	A	56	THR	2.3
1	A	51	PHE	2.3
1	A	159	ASN	2.3
1	A	85	SER	2.3
1	A	75	ASN	2.3
1	A	250	ALA	2.2
1	A	70	VAL	2.2
1	A	28	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	78	VAL	2.2
1	A	23	ALA	2.1
1	A	137	GLY	2.1
1	A	12	LEU	2.1
1	A	156	ASP	2.1
1	A	200	GLY	2.1
1	A	5	THR	2.1
1	A	77	ARG	2.1
1	A	100	SER	2.1
1	A	86	ASN	2.0
1	A	128	ASN	2.0
1	A	114	ASP	2.0
1	A	195	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å²)	Q<0.9
2	JGH	A	402[A]	103/103	0.94	0.18	12,12,12,12	103
2	JGH	A	402[C]	103/103	0.94	0.18	12,12,12,12	103
2	JGH	A	402[B]	103/103	0.94	0.18	12,12,12,12	103
2	JGH	A	401	103/103	0.96	0.18	5,45,87,149	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 JGH A 402 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
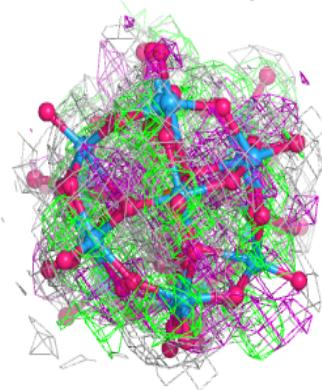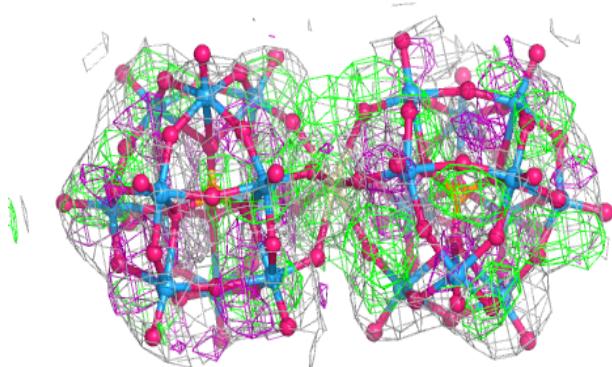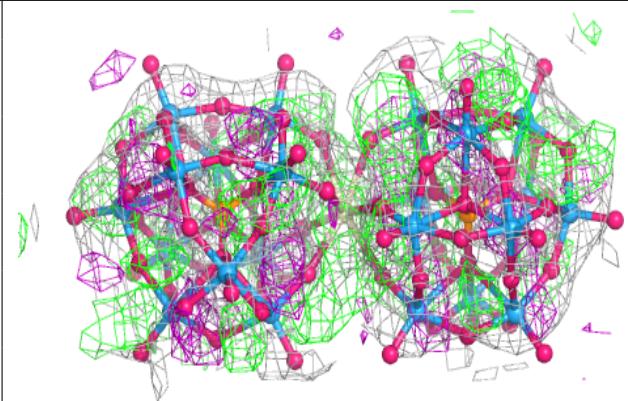
Electron density around JGH A 402 (C):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
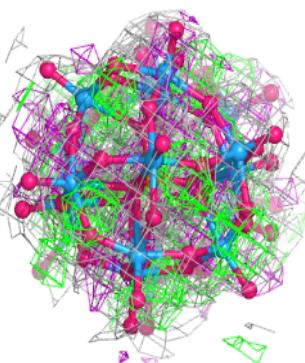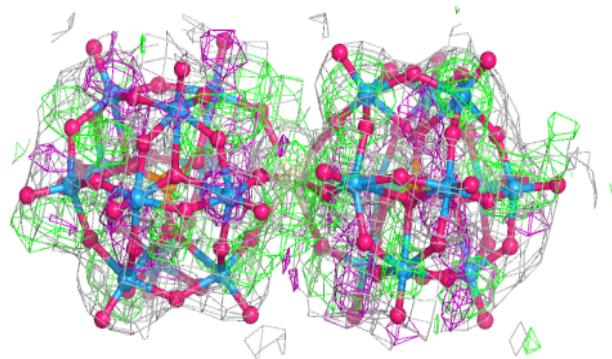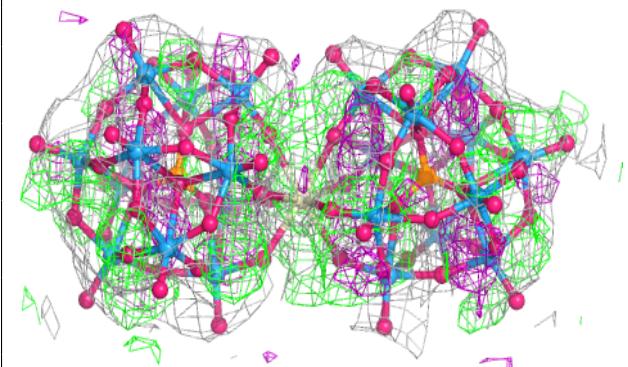
Electron density around JGH A 402 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
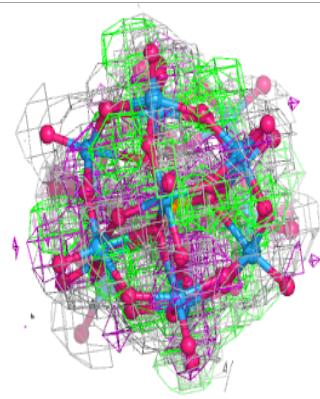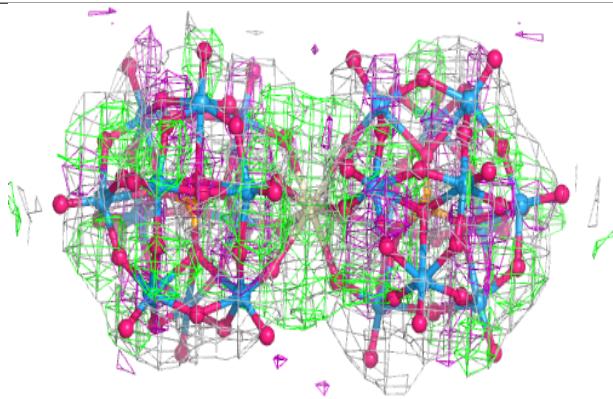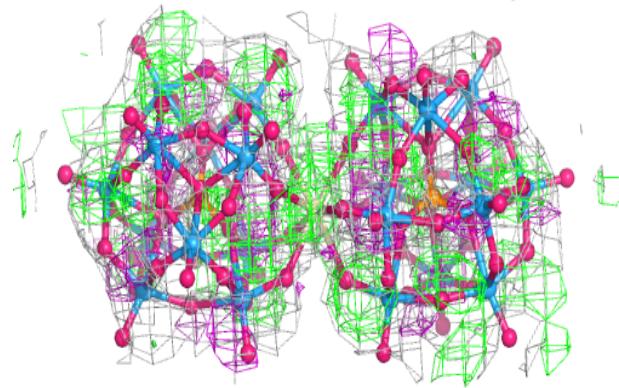
Electron density around JGH A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
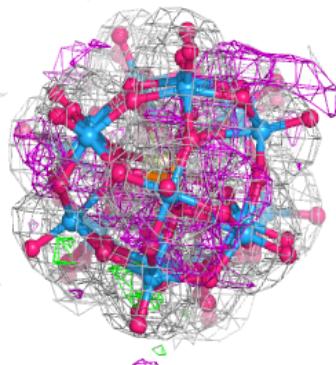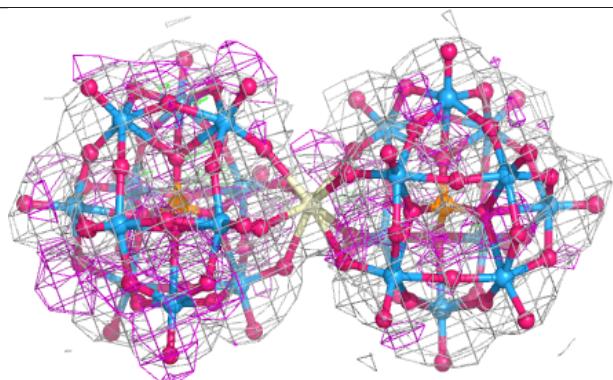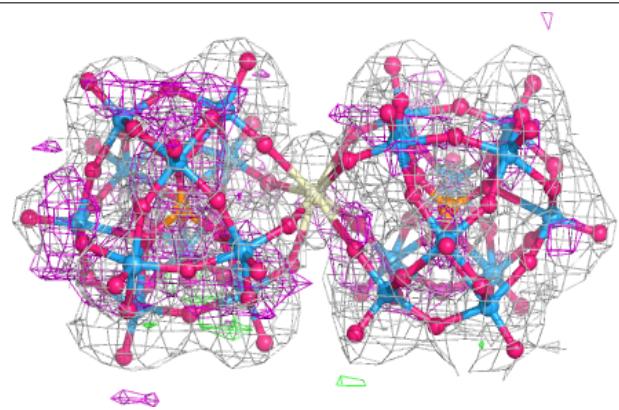
6.5 Other polymers (i)

There are no such residues in this entry.