



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:44 am BST

PDB ID : 2A3X  
Title : Decameric crystal structure of human serum amyloid P-component bound to Bis-1,2-[[[(Z)-2carboxy- 2-methyl-1,3-dioxane]- 5-yloxy carbonyl]-piperazine  
Authors : Ho, J.G.; Kitov, P.I.; Paszkiewicz, E.; Sadowska, J.; Bundle, D.R.; Ng, K.K.  
Deposited on : 2005-06-27  
Resolution : 3.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

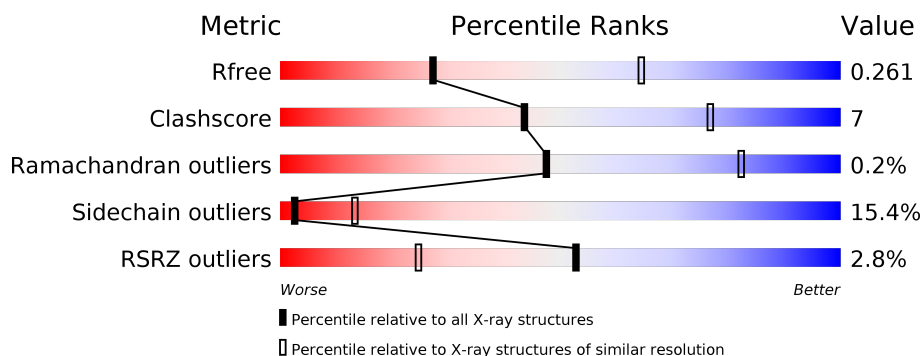
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	204	<div> <div>5%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>
1	B	204	<div> <div>8%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>
1	C	204	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	D	204	<div> <div>78%</div> <div>17%</div> <div>5%</div> </div>
1	E	204	<div> <div>70%</div> <div>25%</div> <div>5%</div> </div>
1	F	204	<div> <div>5%</div> <div>64%</div> <div>30%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	204	<div><div></div><div>8%</div><div>68%</div><div>29%</div><div></div></div>
1	H	204	<div><div></div><div>66%</div><div>29%</div><div></div></div>
1	I	204	<div><div></div><div>71%</div><div>24%</div><div>5%</div></div>
1	J	204	<div><div></div><div>%</div><div>65%</div><div>31%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16606 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 Serum amyloid P-component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	B	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	C	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	D	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	E	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	F	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	G	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	H	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	I	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			
1	J	204	Total	C	N	O	S	0	0	0
			1649	1071	272	303	3			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

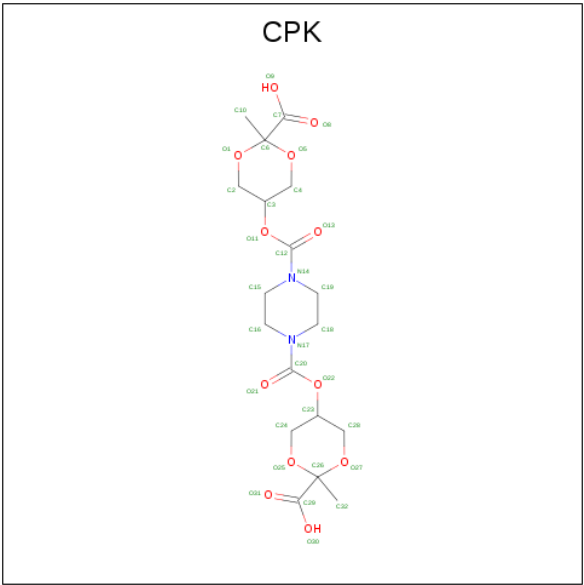
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Ca	0	0
			2	2		
2	J	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	E	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	I	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	F	2	Total	Ca	0	0
			2	2		

- Molecule 3 is BIS-1,2-{[(Z)-2CARBOXY-2-METHYL-1,3-DIOXANE]-5-YLOXYCARBONYL}-PIPERAZINE (three-letter code: CPK) (formula: C<sub>18</sub>H<sub>26</sub>N<sub>2</sub>O<sub>12</sub>).

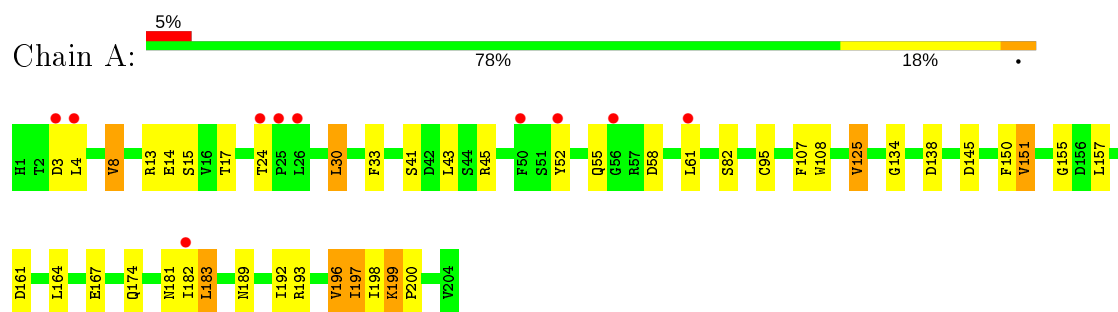


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			32	18	2	12		
3	H	1	Total	C	N	O	0	0
			32	18	2	12		
3	I	1	Total	C	N	O	0	0
			32	18	2	12		

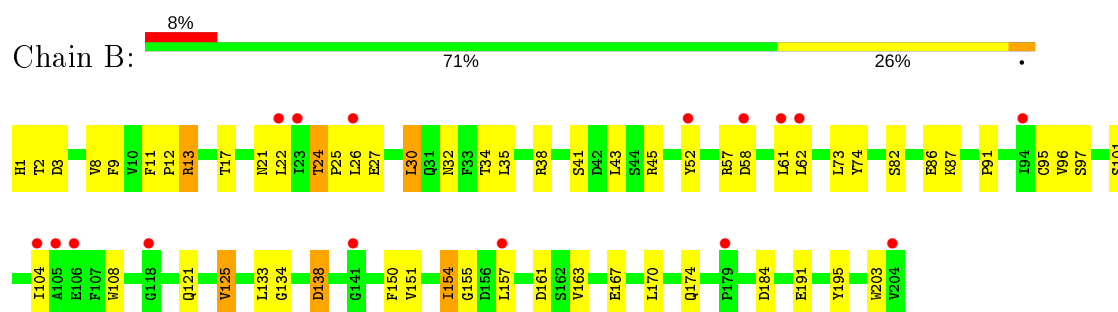
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

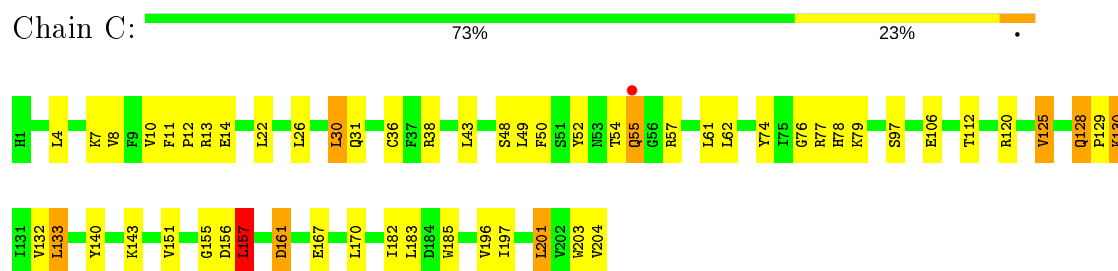
#### • Molecule 1: Serum amyloid P-component



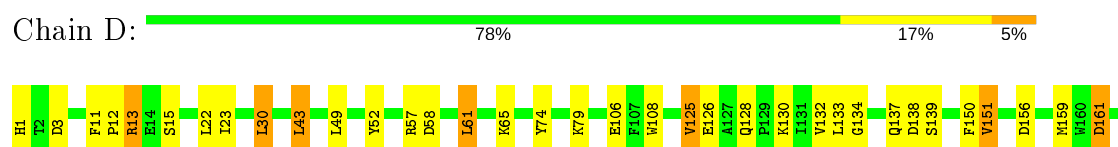
#### • Molecule 1: Serum amyloid P-component

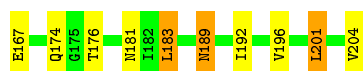


#### • Molecule 1: Serum amyloid P-component

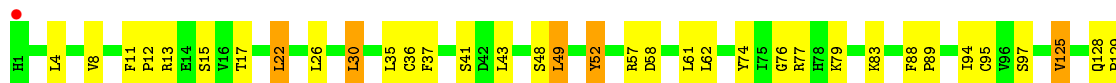


#### • Molecule 1: Serum amyloid P-component

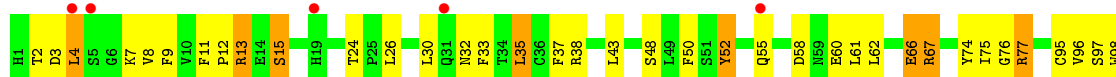




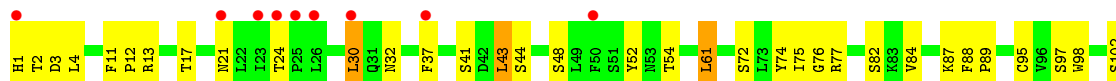
- Molecule 1: Serum amyloid P-component



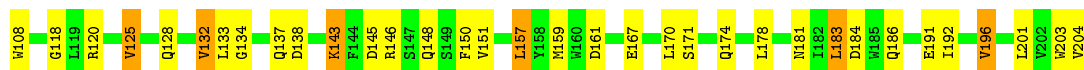
- Molecule 1: Serum amyloid P-component



- Molecule 1: Serum amyloid P-component

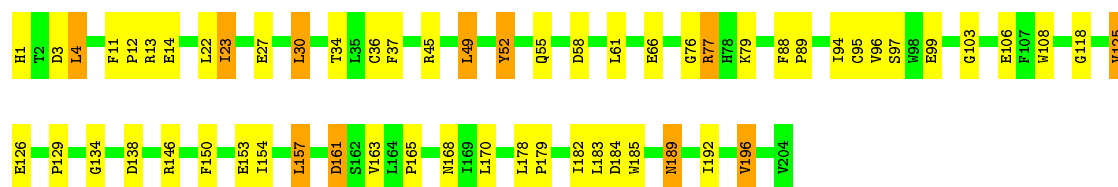


- Molecule 1: Serum amyloid P-component



- Molecule 1: Serum amyloid P-component

Chain I:  71% 24% 5%



• Molecule 1: Serum amyloid P-component

Chain J:  65% 31% 4%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.86 Å 95.05 Å 164.26 Å 90.00° 98.74° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 76.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-3.00) 95.0 (76.96-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.228 , 0.282 0.212 , 0.261	Depositor DCC
$R_{free}$ test set	2298 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.4	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CPK

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	0.32	0/1696	0.62	3/2306 (0.1%)
1	B	0.32	0/1696	0.61	5/2306 (0.2%)
1	C	0.33	0/1696	0.69	3/2306 (0.1%)
1	D	0.36	0/1696	0.69	5/2306 (0.2%)
1	E	0.33	0/1696	0.67	3/2306 (0.1%)
1	F	0.43	0/1696	0.65	5/2306 (0.2%)
1	G	0.41	1/1696 (0.1%)	0.64	3/2306 (0.1%)
1	H	0.34	0/1696	0.69	3/2306 (0.1%)
1	I	0.37	0/1696	0.68	4/2306 (0.2%)
1	J	0.34	0/1696	0.67	2/2306 (0.1%)
All	All	0.36	1/16960 (0.0%)	0.66	36/23060 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	82	SER	CB-OG	7.17	1.51	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	LEU	CA-CB-CG	6.67	130.63	115.30
1	H	157	LEU	CA-CB-CG	6.43	130.08	115.30
1	G	145	ASP	CB-CG-OD2	5.64	123.37	118.30
1	J	157	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	138	ASP	CB-CG-OD2	5.59	123.33	118.30
1	F	58	ASP	CB-CG-OD2	5.52	123.27	118.30
1	I	184	ASP	CB-CG-OD2	5.47	123.23	118.30
1	D	156	ASP	CB-CG-OD2	5.47	123.22	118.30
1	G	156	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	156	ASP	CB-CG-OD2	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	184	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	138	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	3	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	58	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	3	ASP	CB-CG-OD2	5.35	123.12	118.30
1	I	138	ASP	CB-CG-OD2	5.32	123.09	118.30
1	I	161	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	3	ASP	CB-CG-OD2	5.23	123.00	118.30
1	I	3	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	138	ASP	CB-CG-OD2	5.18	122.96	118.30
1	G	161	ASP	CB-CG-OD2	5.16	122.95	118.30
1	E	184	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	3	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	58	ASP	CB-CG-OD2	5.13	122.91	118.30
1	J	138	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	58	ASP	CB-CG-OD2	5.08	122.87	118.30
1	F	138	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	161	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	184	ASP	CB-CG-OD2	5.05	122.85	118.30
1	H	3	ASP	CB-CG-OD2	5.04	122.84	118.30
1	F	156	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	138	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	58	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	161	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	184	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	161	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1649	0	1624	13	0
1	B	1649	0	1624	19	0
1	C	1649	0	1624	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1649	0	1624	17	0
1	E	1649	0	1624	26	0
1	F	1649	0	1624	28	0
1	G	1649	0	1624	22	0
1	H	1649	0	1624	29	0
1	I	1649	0	1624	28	0
1	J	1649	0	1624	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
3	C	32	0	24	0	0
3	H	32	0	24	0	0
3	I	32	0	24	0	0
All	All	16606	0	16312	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD11	1:A:151:VAL:HG13	1.53	0.91
1:A:30:LEU:HD21	1:A:33:PHE:HB3	1.51	0.91
1:H:138:ASP:HB2	1:H:143:LYS:HB3	1.59	0.84
1:C:52:TYR:HB3	1:C:61:LEU:O	1.91	0.71
1:C:30:LEU:HB2	1:C:125:VAL:HG22	1.73	0.70
1:I:23:ILE:HG13	1:I:189:ASN:HB3	1.75	0.69
1:H:201:LEU:HD11	1:H:204:VAL:HG23	1.76	0.68
1:F:30:LEU:HB2	1:F:125:VAL:HG22	1.77	0.67
1:J:95:CYS:HB2	1:J:108:TRP:HB2	1.77	0.66
1:C:62:LEU:HB3	1:C:74:TYR:HB2	1.77	0.66
1:D:159:MET:HB3	1:D:183:LEU:HB2	1.78	0.66
1:G:161:ASP:HB3	1:G:182:ILE:HD11	1.78	0.65
1:A:52:TYR:HB3	1:A:61:LEU:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:LEU:O	1:E:95:CYS:HA	1.97	0.65
1:I:192:ILE:HG23	1:I:196:VAL:HG13	1.79	0.65
1:F:32:ASN:HB3	1:F:163:VAL:HG23	1.79	0.64
1:D:201:LEU:HD21	1:D:204:VAL:HB	1.80	0.64
1:I:30:LEU:HB2	1:I:125:VAL:HG22	1.78	0.64
1:I:76:GLY:O	1:I:77:ARG:HB2	1.98	0.63
1:C:8:VAL:HG13	1:C:201:LEU:HB2	1.81	0.62
1:G:30:LEU:HB2	1:G:125:VAL:HG22	1.80	0.62
1:H:132:VAL:HG13	1:H:137:GLN:NE2	2.13	0.62
1:F:201:LEU:HD21	1:F:204:VAL:HB	1.81	0.62
1:I:52:TYR:HB3	1:I:61:LEU:O	2.00	0.62
1:J:99:GLU:HB2	1:J:163:VAL:HG21	1.82	0.61
1:E:192:ILE:HG23	1:E:196:VAL:HG13	1.83	0.61
1:F:52:TYR:HB3	1:F:61:LEU:O	2.01	0.61
1:H:134:GLY:HA2	1:H:150:PHE:HB3	1.83	0.61
1:B:21:ASN:HB2	1:B:191:GLU:HB2	1.83	0.60
1:G:84:VAL:HB	1:G:114:LEU:HD21	1.83	0.60
1:H:77:ARG:HG3	1:H:77:ARG:HH11	1.66	0.60
1:D:192:ILE:HG23	1:D:196:VAL:HG13	1.83	0.60
1:F:62:LEU:HB3	1:F:74:TYR:HB2	1.82	0.60
1:J:60:GLU:OE2	1:J:123:TYR:OH	2.19	0.60
1:F:118:GLY:HA3	1:J:12:PRO:HB2	1.82	0.59
1:F:37:PHE:HB3	1:F:157:LEU:HD22	1.83	0.59
1:G:52:TYR:HB3	1:G:61:LEU:O	2.01	0.59
1:A:161:ASP:H	1:A:181:ASN:HD21	1.51	0.58
1:J:34:THR:HG21	1:J:164:LEU:HB2	1.86	0.58
1:I:37:PHE:HB3	1:I:157:LEU:HD22	1.84	0.57
1:C:76:GLY:O	1:C:77:ARG:HB2	2.05	0.57
1:I:95:CYS:HB2	1:I:108:TRP:HB2	1.85	0.57
1:I:99:GLU:HB2	1:I:163:VAL:HG21	1.87	0.57
1:I:165:PRO:HG2	1:I:168:ASN:HD22	1.68	0.56
1:A:182:ILE:HG22	1:A:183:LEU:HD22	1.86	0.56
1:H:21:ASN:HB2	1:H:191:GLU:HB2	1.87	0.56
1:F:33:PHE:CE1	1:F:98:TRP:HB3	2.40	0.56
1:G:37:PHE:HB3	1:G:157:LEU:HD22	1.87	0.56
1:E:8:VAL:HG12	1:E:155:GLY:HA3	1.88	0.56
1:G:95:CYS:HB2	1:G:108:TRP:HB2	1.88	0.55
1:G:43:LEU:HD21	1:G:151:VAL:HG13	1.88	0.55
1:B:95:CYS:HB2	1:B:108:TRP:HB2	1.87	0.55
1:F:195:TYR:HE1	1:G:121:GLN:NE2	2.04	0.55
1:F:35:LEU:O	1:F:95:CYS:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:ARG:HG3	1:H:77:ARG:NH1	2.21	0.55
1:D:57:ARG:HG3	1:D:126:GLU:OE1	2.07	0.54
1:G:75:ILE:HB	1:G:119:LEU:HD11	1.88	0.54
1:J:145:ASP:HB3	1:J:148:GLN:HB2	1.89	0.54
1:J:192:ILE:HG23	1:J:196:VAL:HG13	1.89	0.54
1:E:76:GLY:O	1:E:77:ARG:HB2	2.07	0.54
1:J:52:TYR:CZ	1:J:129:PRO:HG3	2.43	0.54
1:E:145:ASP:HB3	1:E:148:GLN:HB2	1.88	0.54
1:G:21:ASN:HB2	1:G:191:GLU:HB2	1.90	0.54
1:A:30:LEU:HB3	1:A:125:VAL:HG13	1.91	0.53
1:E:37:PHE:HB3	1:E:157:LEU:HD22	1.91	0.52
1:H:95:CYS:HB2	1:H:108:TRP:HB2	1.91	0.52
1:H:30:LEU:HB2	1:H:125:VAL:HG22	1.92	0.52
1:H:192:ILE:HG23	1:H:196:VAL:HG13	1.92	0.52
1:J:199:LYS:HD2	1:J:200:PRO:HD2	1.92	0.51
1:H:52:TYR:HB3	1:H:61:LEU:O	2.11	0.51
1:I:37:PHE:CE2	1:I:49:LEU:HG	2.45	0.51
1:F:8:VAL:HG21	1:F:153:GLU:OE1	2.10	0.51
1:G:134:GLY:HA2	1:G:150:PHE:HB3	1.92	0.51
1:H:145:ASP:HB3	1:H:148:GLN:HB2	1.91	0.51
1:E:36:CYS:HA	1:E:94:ILE:O	2.11	0.51
1:C:130:LYS:HD3	1:C:140:TYR:CZ	2.47	0.50
1:B:8:VAL:HG12	1:B:155:GLY:HA3	1.94	0.50
1:F:60:GLU:O	1:F:75:ILE:HA	2.11	0.50
1:A:197:ILE:HG13	1:B:104:ILE:HD11	1.93	0.50
1:D:192:ILE:HG23	1:D:196:VAL:CG1	2.42	0.50
1:G:32:ASN:HB3	1:G:163:VAL:HG23	1.94	0.50
1:J:32:ASN:HB3	1:J:163:VAL:HG23	1.93	0.50
1:J:38:ARG:HB3	1:J:203:TRP:HH2	1.77	0.49
1:F:4:LEU:HD12	1:F:7:LYS:HD2	1.93	0.49
1:H:103:GLY:O	1:H:118:GLY:HA2	2.12	0.49
1:D:52:TYR:HB3	1:D:61:LEU:O	2.12	0.49
1:E:157:LEU:O	1:E:185:TRP:HB2	2.12	0.49
1:H:32:ASN:OD1	1:H:99:GLU:HA	2.13	0.49
1:H:161:ASP:OD1	1:H:181:ASN:ND2	2.46	0.49
1:E:22:LEU:HD21	1:E:133:LEU:HD22	1.95	0.49
1:A:30:LEU:CD2	1:A:33:PHE:HB3	2.33	0.49
1:D:23:ILE:HB	1:D:189:ASN:HB3	1.94	0.49
1:B:13:ARG:HG2	1:B:195:TYR:HD2	1.78	0.48
1:F:9:PHE:HD2	1:F:185:TRP:HH2	1.61	0.48
1:I:14:GLU:HG3	1:I:45:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:13:ARG:HD2	1:J:15:SER:HB3	1.95	0.48
1:H:91:PRO:HB3	1:H:203:TRP:CE3	2.49	0.48
1:E:182:ILE:HG22	1:E:183:LEU:HD13	1.95	0.48
1:E:8:VAL:HG13	1:E:201:LEU:HB2	1.94	0.47
1:J:62:LEU:HB3	1:J:74:TYR:HB2	1.96	0.47
1:E:52:TYR:HB3	1:E:61:LEU:O	2.14	0.47
1:H:76:GLY:O	1:H:77:ARG:HB2	2.13	0.47
1:F:98:TRP:HA	1:F:104:ILE:O	2.14	0.47
1:I:134:GLY:HA2	1:I:150:PHE:HB3	1.97	0.47
1:I:161:ASP:HB3	1:I:182:ILE:HD11	1.96	0.47
1:B:32:ASN:HB3	1:B:163:VAL:HG23	1.97	0.47
1:E:159:MET:HB2	1:E:183:LEU:HB2	1.97	0.47
1:E:52:TYR:CE1	1:E:129:PRO:HB3	2.50	0.47
1:C:50:PHE:HD1	1:C:133:LEU:HD11	1.79	0.46
1:D:43:LEU:HD21	1:D:151:VAL:HG13	1.96	0.46
1:E:199:LYS:HD2	1:E:200:PRO:HD2	1.96	0.46
1:C:8:VAL:HG12	1:C:155:GLY:HA3	1.97	0.46
1:C:36:CYS:O	1:C:157:LEU:HA	2.16	0.46
1:A:192:ILE:HG23	1:A:196:VAL:HG13	1.95	0.46
1:J:91:PRO:HB3	1:J:203:TRP:CE3	2.50	0.46
1:I:88:PHE:HA	1:I:89:PRO:HA	1.76	0.46
1:I:34:THR:HG23	1:I:97:SER:HB3	1.98	0.46
1:B:91:PRO:HB3	1:B:203:TRP:CE3	2.51	0.46
1:H:36:CYS:HA	1:H:94:ILE:O	2.16	0.46
1:A:199:LYS:HD3	1:A:200:PRO:HD2	1.98	0.45
1:D:61:LEU:HA	1:D:74:TYR:O	2.16	0.45
1:J:170:LEU:O	1:J:174:GLN:HB2	2.15	0.45
1:B:34:THR:HG23	1:B:97:SER:HB3	1.98	0.45
1:B:62:LEU:HB3	1:B:74:TYR:HB2	1.99	0.45
1:I:150:PHE:CE2	1:I:154:ILE:HG13	2.51	0.45
1:E:52:TYR:CZ	1:E:129:PRO:HB3	2.52	0.45
1:D:132:VAL:HG13	1:D:137:GLN:NE2	2.31	0.45
1:H:88:PHE:HA	1:H:89:PRO:HA	1.81	0.45
1:J:134:GLY:HA2	1:J:150:PHE:HB3	1.99	0.45
1:I:103:GLY:O	1:I:118:GLY:HA2	2.16	0.45
1:J:33:PHE:CE2	1:J:98:TRP:HB3	2.51	0.45
1:F:13:ARG:HH21	1:F:15:SER:HB2	1.82	0.45
1:F:199:LYS:HD3	1:F:200:PRO:HD2	1.97	0.45
1:E:26:LEU:HD11	1:E:30:LEU:HD13	1.98	0.45
1:D:106:GLU:HG2	1:D:108:TRP:HE1	1.82	0.45
1:D:134:GLY:HA2	1:D:150:PHE:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:TRP:HD1	1:G:105:ALA:HB2	1.81	0.44
1:I:178:LEU:HD12	1:I:178:LEU:N	2.32	0.44
1:C:161:ASP:HB3	1:C:182:ILE:HD11	2.00	0.44
1:I:178:LEU:H	1:I:178:LEU:HD12	1.82	0.44
1:E:62:LEU:HB3	1:E:74:TYR:HB2	2.00	0.44
1:J:52:TYR:CE2	1:J:129:PRO:HG3	2.52	0.44
1:D:167:GLU:CD	1:D:167:GLU:H	2.21	0.44
1:F:13:ARG:HG2	1:F:195:TYR:HD2	1.83	0.44
1:J:24:THR:HA	1:J:25:PRO:HD3	1.82	0.44
1:J:61:LEU:HA	1:J:74:TYR:O	2.17	0.44
1:F:156:ASP:HA	1:F:185:TRP:CD1	2.53	0.44
1:B:43:LEU:HD21	1:B:45:ARG:NH1	2.33	0.44
1:C:201:LEU:HD11	1:C:204:VAL:HG23	2.00	0.44
1:E:128:GLN:N	1:E:129:PRO:HD3	2.32	0.44
1:E:37:PHE:CE1	1:E:49:LEU:HG	2.53	0.44
1:A:134:GLY:HA2	1:A:150:PHE:HB3	2.00	0.43
1:G:114:LEU:HD23	1:G:114:LEU:HA	1.83	0.43
1:D:13:ARG:HD2	1:D:15:SER:HB3	1.99	0.43
1:H:22:LEU:HD22	1:H:133:LEU:HD13	2.00	0.43
1:I:153:GLU:OE1	1:J:116:LYS:NZ	2.51	0.43
1:B:30:LEU:HB3	1:B:125:VAL:HG13	2.00	0.43
1:B:73:LEU:HD13	1:B:96:VAL:HG21	1.99	0.43
1:D:11:PHE:HA	1:D:12:PRO:HD3	1.81	0.43
1:I:96:VAL:HA	1:I:106:GLU:O	2.19	0.43
1:I:58:ASP:O	1:I:77:ARG:NH1	2.49	0.43
1:G:192:ILE:HG23	1:G:196:VAL:HG13	1.99	0.43
1:C:97:SER:OG	1:C:106:GLU:HB3	2.19	0.43
1:C:61:LEU:HA	1:C:74:TYR:O	2.18	0.43
1:G:61:LEU:HA	1:G:74:TYR:O	2.18	0.43
1:H:74:TYR:CE2	1:H:79:LYS:HB3	2.54	0.43
1:A:8:VAL:HG12	1:A:155:GLY:HA3	2.01	0.43
1:F:11:PHE:HA	1:F:12:PRO:HD3	1.83	0.43
1:H:70:GLU:HG3	1:H:83:LYS:HG2	2.00	0.43
1:D:30:LEU:HB2	1:D:125:VAL:HG22	2.01	0.43
1:I:11:PHE:HA	1:I:12:PRO:HD3	1.81	0.43
1:J:43:LEU:HD13	1:J:151:VAL:HG22	2.01	0.43
1:J:38:ARG:HB3	1:J:203:TRP:CH2	2.54	0.43
1:B:9:PHE:HB2	1:B:154:ILE:HG22	2.01	0.42
1:F:50:PHE:CZ	1:F:131:ILE:HG21	2.55	0.42
1:B:13:ARG:HE	1:B:195:TYR:HD2	1.68	0.42
1:E:11:PHE:HA	1:E:12:PRO:HD3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:THR:O	1:G:176:THR:OG1	2.37	0.42
1:B:52:TYR:HB3	1:B:61:LEU:O	2.19	0.42
1:D:161:ASP:CG	1:D:181:ASN:HD21	2.21	0.42
1:H:8:VAL:HG13	1:H:201:LEU:HB2	2.01	0.42
1:I:36:CYS:HA	1:I:94:ILE:O	2.19	0.42
1:G:97:SER:OG	1:G:106:GLU:HB2	2.20	0.42
1:E:88:PHE:HA	1:E:89:PRO:HA	1.81	0.42
1:F:136:GLU:OE2	1:F:137:GLN:O	2.38	0.42
1:F:156:ASP:HA	1:F:185:TRP:CG	2.55	0.42
1:I:4:LEU:HB3	1:I:185:TRP:NE1	2.34	0.41
1:B:35:LEU:HD11	1:B:157:LEU:HD11	2.01	0.41
1:C:11:PHE:HA	1:C:12:PRO:HD3	1.89	0.41
1:G:132:VAL:HG22	1:G:137:GLN:NE2	2.35	0.41
1:I:52:TYR:CE1	1:I:129:PRO:HB3	2.55	0.41
1:C:157:LEU:HB3	1:C:185:TRP:CE3	2.55	0.41
1:E:30:LEU:HB3	1:E:125:VAL:HG13	2.01	0.41
1:F:76:GLY:O	1:F:77:ARG:HB2	2.18	0.41
1:E:37:PHE:CE1	1:E:94:ILE:HD12	2.55	0.41
1:A:95:CYS:HB2	1:A:108:TRP:HB2	2.03	0.41
1:B:11:PHE:HA	1:B:12:PRO:HD3	1.86	0.41
1:F:128:GLN:N	1:F:129:PRO:HD3	2.36	0.41
1:B:134:GLY:HA2	1:B:150:PHE:HB3	2.02	0.41
1:H:77:ARG:CG	1:H:77:ARG:HH11	2.32	0.41
1:C:10:VAL:HG12	1:C:197:ILE:O	2.20	0.41
1:I:23:ILE:CG1	1:I:189:ASN:HB3	2.46	0.41
1:E:157:LEU:HB3	1:E:185:TRP:CE3	2.56	0.41
1:G:88:PHE:HA	1:G:89:PRO:HA	1.68	0.41
1:H:26:LEU:HD21	1:H:30:LEU:HD13	2.02	0.41
1:J:52:TYR:HB3	1:J:61:LEU:O	2.21	0.41
1:F:99:GLU:HB3	1:F:102:SER:OG	2.21	0.40
1:F:96:VAL:HA	1:F:106:GLU:O	2.21	0.40
1:G:76:GLY:HA3	1:G:120:ARG:HH11	1.85	0.40
1:H:146:ARG:C	1:H:148:GLN:H	2.24	0.40
1:C:128:GLN:N	1:C:129:PRO:HD3	2.36	0.40
1:I:30:LEU:CB	1:I:125:VAL:HG22	2.48	0.40
1:J:157:LEU:HB3	1:J:185:TRP:CE3	2.57	0.40
1:J:13:ARG:HG2	1:J:195:TYR:HD2	1.86	0.40
1:B:24:THR:C	1:B:26:LEU:H	2.24	0.40
1:C:74:TYR:HA	1:C:78:HIS:O	2.20	0.40
1:E:159:MET:O	1:E:180:ALA:HB1	2.22	0.40
1:G:11:PHE:HA	1:G:12:PRO:HD3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:MET:HB3	1:H:183:LEU:HB2	2.02	0.40
1:F:66:GLU:HB2	1:F:67:ARG:HG2	2.04	0.40
1:H:11:PHE:HA	1:H:12:PRO:HD3	1.83	0.40
1:H:186:GLN:HE21	1:H:186:GLN:HB2	1.77	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	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
1	B	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	29	68
1	C	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	29	68
1	D	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
1	E	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
1	F	202/204 (99%)	189 (94%)	13 (6%)	0	100	100
1	G	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
1	H	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
1	I	202/204 (99%)	192 (95%)	8 (4%)	2 (1%)	15	53
1	J	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
All	All	2020/2040 (99%)	1913 (95%)	103 (5%)	4 (0%)	47	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	GLN
1	I	77	ARG
1	B	25	PRO

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Mol	Chain	Res	Type
1	I	179	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/181 (100%)	154 (85%)	27 (15%)	3	14
1	B	181/181 (100%)	157 (87%)	24 (13%)	4	17
1	C	181/181 (100%)	149 (82%)	32 (18%)	2	9
1	D	181/181 (100%)	161 (89%)	20 (11%)	6	25
1	E	181/181 (100%)	151 (83%)	30 (17%)	2	11
1	F	181/181 (100%)	148 (82%)	33 (18%)	1	9
1	G	181/181 (100%)	152 (84%)	29 (16%)	2	12
1	H	181/181 (100%)	154 (85%)	27 (15%)	3	14
1	I	181/181 (100%)	161 (89%)	20 (11%)	6	25
1	J	181/181 (100%)	144 (80%)	37 (20%)	1	6
All	All	1810/1810 (100%)	1531 (85%)	279 (15%)	2	13

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	8	VAL
1	A	13	ARG
1	A	14	GLU
1	A	15	SER
1	A	17	THR
1	A	24	THR
1	A	30	LEU
1	A	41	SER
1	A	45	ARG
1	A	55	GLN
1	A	82	SER

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Mol	Chain	Res	Type
1	A	107	PHE
1	A	125	VAL
1	A	145	ASP
1	A	151	VAL
1	A	157	LEU
1	A	164	LEU
1	A	167	GLU
1	A	174	GLN
1	A	183	LEU
1	A	189	ASN
1	A	193	ARG
1	A	196	VAL
1	A	197	ILE
1	A	198	ILE
1	A	199	LYS
1	B	1	HIS
1	B	2	THR
1	B	13	ARG
1	B	17	THR
1	B	22	LEU
1	B	24	THR
1	B	27	GLU
1	B	30	LEU
1	B	38	ARG
1	B	41	SER
1	B	57	ARG
1	B	82	SER
1	B	86	GLU
1	B	87	LYS
1	B	101	SER
1	B	121	GLN
1	B	125	VAL
1	B	133	LEU
1	B	138	ASP
1	B	151	VAL
1	B	154	ILE
1	B	167	GLU
1	B	170	LEU
1	B	174	GLN
1	C	4	LEU
1	C	7	LYS
1	C	13	ARG

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Mol	Chain	Res	Type
1	C	14	GLU
1	C	22	LEU
1	C	26	LEU
1	C	30	LEU
1	C	31	GLN
1	C	38	ARG
1	C	43	LEU
1	C	48	SER
1	C	49	LEU
1	C	54	THR
1	C	55	GLN
1	C	57	ARG
1	C	79	LYS
1	C	112	THR
1	C	120	ARG
1	C	125	VAL
1	C	128	GLN
1	C	130	LYS
1	C	132	VAL
1	C	133	LEU
1	C	143	LYS
1	C	151	VAL
1	C	157	LEU
1	C	167	GLU
1	C	170	LEU
1	C	183	LEU
1	C	196	VAL
1	C	201	LEU
1	C	203	TRP
1	D	1	HIS
1	D	13	ARG
1	D	22	LEU
1	D	30	LEU
1	D	43	LEU
1	D	49	LEU
1	D	61	LEU
1	D	65	LYS
1	D	79	LYS
1	D	125	VAL
1	D	128	GLN
1	D	130	LYS
1	D	133	LEU

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Mol	Chain	Res	Type
1	D	139	SER
1	D	151	VAL
1	D	174	GLN
1	D	176	THR
1	D	183	LEU
1	D	189	ASN
1	D	201	LEU
1	E	4	LEU
1	E	13	ARG
1	E	15	SER
1	E	17	THR
1	E	22	LEU
1	E	30	LEU
1	E	41	SER
1	E	43	LEU
1	E	48	SER
1	E	49	LEU
1	E	52	TYR
1	E	57	ARG
1	E	79	LYS
1	E	83	LYS
1	E	97	SER
1	E	125	VAL
1	E	130	LYS
1	E	133	LEU
1	E	138	ASP
1	E	151	VAL
1	E	157	LEU
1	E	159	MET
1	E	162	SER
1	E	164	LEU
1	E	167	GLU
1	E	171	SER
1	E	178	LEU
1	E	189	ASN
1	E	193	ARG
1	E	196	VAL
1	F	2	THR
1	F	4	LEU
1	F	13	ARG
1	F	15	SER
1	F	24	THR

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Mol	Chain	Res	Type
1	F	26	LEU
1	F	35	LEU
1	F	38	ARG
1	F	43	LEU
1	F	48	SER
1	F	52	TYR
1	F	55	GLN
1	F	66	GLU
1	F	67	ARG
1	F	77	ARG
1	F	97	SER
1	F	112	THR
1	F	120	ARG
1	F	128	GLN
1	F	130	LYS
1	F	154	ILE
1	F	157	LEU
1	F	170	LEU
1	F	174	GLN
1	F	176	THR
1	F	178	LEU
1	F	181	ASN
1	F	183	LEU
1	F	189	ASN
1	F	193	ARG
1	F	198	ILE
1	F	199	LYS
1	F	203	TRP
1	G	1	HIS
1	G	2	THR
1	G	3	ASP
1	G	4	LEU
1	G	13	ARG
1	G	17	THR
1	G	24	THR
1	G	30	LEU
1	G	41	SER
1	G	43	LEU
1	G	44	SER
1	G	48	SER
1	G	54	THR
1	G	61	LEU

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Mol	Chain	Res	Type
1	G	72	SER
1	G	77	ARG
1	G	87	LYS
1	G	102	SER
1	G	116	LYS
1	G	133	LEU
1	G	138	ASP
1	G	146	ARG
1	G	164	LEU
1	G	170	LEU
1	G	174	GLN
1	G	176	THR
1	G	181	ASN
1	G	183	LEU
1	G	196	VAL
1	H	4	LEU
1	H	5	SER
1	H	10	VAL
1	H	22	LEU
1	H	30	LEU
1	H	31	GLN
1	H	43	LEU
1	H	44	SER
1	H	49	LEU
1	H	54	THR
1	H	61	LEU
1	H	101	SER
1	H	107	PHE
1	H	120	ARG
1	H	125	VAL
1	H	128	GLN
1	H	132	VAL
1	H	143	LYS
1	H	151	VAL
1	H	157	LEU
1	H	167	GLU
1	H	170	LEU
1	H	171	SER
1	H	174	GLN
1	H	178	LEU
1	H	183	LEU
1	H	196	VAL

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Mol	Chain	Res	Type
1	I	1	HIS
1	I	4	LEU
1	I	13	ARG
1	I	22	LEU
1	I	23	ILE
1	I	27	GLU
1	I	30	LEU
1	I	49	LEU
1	I	52	TYR
1	I	55	GLN
1	I	66	GLU
1	I	79	LYS
1	I	125	VAL
1	I	126	GLU
1	I	146	ARG
1	I	157	LEU
1	I	170	LEU
1	I	183	LEU
1	I	189	ASN
1	I	196	VAL
1	J	1	HIS
1	J	4	LEU
1	J	7	LYS
1	J	13	ARG
1	J	18	ASP
1	J	22	LEU
1	J	26	LEU
1	J	27	GLU
1	J	28	LYS
1	J	30	LEU
1	J	38	ARG
1	J	40	TYR
1	J	44	SER
1	J	49	LEU
1	J	55	GLN
1	J	57	ARG
1	J	61	LEU
1	J	65	LYS
1	J	79	LYS
1	J	82	SER
1	J	97	SER
1	J	101	SER

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Mol	Chain	Res	Type
1	J	114	LEU
1	J	125	VAL
1	J	128	GLN
1	J	130	LYS
1	J	133	LEU
1	J	138	ASP
1	J	143	LYS
1	J	151	VAL
1	J	164	LEU
1	J	167	GLU
1	J	171	SER
1	J	183	LEU
1	J	189	ASN
1	J	193	ARG
1	J	196	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	181	ASN
1	B	53	ASN
1	B	186	GLN
1	C	31	GLN
1	C	55	GLN
1	C	110	ASN
1	C	186	GLN
1	D	1	HIS
1	D	128	GLN
1	F	21	ASN
1	F	189	ASN
1	G	93	HIS
1	G	121	GLN
1	H	186	GLN
1	I	1	HIS
1	I	128	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 20 are monoatomic - leaving 3 for Mogul analysis.

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$
3	CPK	C	402	2	28,34,34	4.61	6 (21%)	32,50,50	2.96	16 (50%)
3	CPK	H	403	2	28,34,34	4.56	6 (21%)	32,50,50	3.13	19 (59%)
3	CPK	I	401	2	28,34,34	4.50	6 (21%)	32,50,50	3.41	23 (71%)

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
3	CPK	C	402	2	-	6/16/62/62	0/3/3/3
3	CPK	H	403	2	-	8/16/62/62	0/3/3/3
3	CPK	I	401	2	-	8/16/62/62	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	CPK	O21-C20	15.18	1.43	1.21
3	C	402	CPK	O13-C12	14.93	1.43	1.21
3	H	403	CPK	O21-C20	14.82	1.43	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	403	CPK	O13-C12	14.71	1.43	1.21
3	I	401	CPK	O21-C20	14.69	1.43	1.21
3	I	401	CPK	O13-C12	14.32	1.42	1.21
3	I	401	CPK	C12-N14	6.69	1.46	1.35
3	H	403	CPK	C12-N14	6.60	1.46	1.35
3	H	403	CPK	C20-N17	6.47	1.46	1.35
3	I	401	CPK	C20-N17	6.47	1.46	1.35
3	C	402	CPK	C12-N14	6.34	1.45	1.35
3	C	402	CPK	C20-N17	6.18	1.45	1.35
3	H	403	CPK	O22-C20	4.77	1.43	1.34
3	C	402	CPK	O22-C20	4.75	1.43	1.34
3	I	401	CPK	O11-C12	4.71	1.43	1.34
3	H	403	CPK	O11-C12	4.60	1.43	1.34
3	C	402	CPK	O11-C12	4.59	1.43	1.34
3	I	401	CPK	O22-C20	4.49	1.43	1.34

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	401	CPK	O11-C12-N14	9.43	119.73	111.27
3	H	403	CPK	O11-C12-N14	8.16	118.59	111.27
3	I	401	CPK	O22-C20-N17	7.47	117.97	111.27
3	C	402	CPK	O11-C12-N14	7.21	117.74	111.27
3	H	403	CPK	O22-C20-N17	6.74	117.31	111.27
3	C	402	CPK	C18-N17-C20	-5.07	107.25	121.77
3	C	402	CPK	C16-N17-C20	-4.78	108.10	121.77
3	C	402	CPK	C19-N14-C12	-4.73	108.23	121.77
3	I	401	CPK	C19-N14-C12	-4.62	108.56	121.77
3	I	401	CPK	O25-C26-C32	4.58	112.00	106.24
3	C	402	CPK	C18-N17-C16	4.54	121.36	112.62
3	I	401	CPK	O1-C6-C10	4.24	111.57	106.24
3	H	403	CPK	C18-N17-C16	4.14	120.60	112.62
3	H	403	CPK	C18-N17-C20	-4.09	110.06	121.77
3	H	403	CPK	C16-N17-C20	-4.06	110.14	121.77
3	I	401	CPK	C18-N17-C16	4.03	120.37	112.62
3	C	402	CPK	O22-C20-N17	3.96	114.82	111.27
3	I	401	CPK	C18-N17-C20	-3.95	110.48	121.77
3	I	401	CPK	C19-N14-C15	3.90	120.14	112.62
3	H	403	CPK	C19-N14-C12	-3.88	110.67	121.77
3	C	402	CPK	C15-N14-C12	-3.88	110.68	121.77
3	H	403	CPK	C19-N14-C15	3.77	119.88	112.62
3	H	403	CPK	O25-C26-C32	3.70	110.90	106.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	403	CPK	O1-C6-C10	3.68	110.87	106.24
3	H	403	CPK	C15-N14-C12	-3.50	111.75	121.77
3	C	402	CPK	O27-C26-C32	3.45	110.58	106.24
3	C	402	CPK	C19-N14-C15	3.45	119.26	112.62
3	C	402	CPK	O25-C26-C32	3.41	110.53	106.24
3	C	402	CPK	O1-C6-C10	3.40	110.51	106.24
3	I	401	CPK	O13-C12-N14	-3.26	118.86	124.32
3	C	402	CPK	O13-C12-N14	-3.19	118.98	124.32
3	H	403	CPK	O21-C20-N17	-3.18	119.00	124.32
3	H	403	CPK	O13-C12-N14	-3.00	119.31	124.32
3	I	401	CPK	C16-N17-C20	-3.00	113.20	121.77
3	I	401	CPK	C19-C18-N17	-2.94	104.15	110.44
3	I	401	CPK	C2-O1-C6	2.93	116.50	113.94
3	I	401	CPK	O21-C20-N17	-2.90	119.47	124.32
3	H	403	CPK	O5-C6-C10	2.77	109.72	106.24
3	I	401	CPK	C15-N14-C12	-2.77	113.86	121.77
3	I	401	CPK	C32-C26-C29	-2.70	106.71	111.11
3	I	401	CPK	C16-C15-N14	-2.67	104.72	110.44
3	I	401	CPK	O11-C12-O13	-2.67	119.23	124.86
3	C	402	CPK	O21-C20-N17	-2.57	120.02	124.32
3	I	401	CPK	O27-C26-C32	2.56	109.46	106.24
3	H	403	CPK	C16-C15-N14	-2.51	105.05	110.44
3	C	402	CPK	C2-O1-C6	2.51	116.13	113.94
3	I	401	CPK	C4-O5-C6	2.49	116.11	113.94
3	I	401	CPK	C15-C16-N17	-2.46	105.18	110.44
3	H	403	CPK	O11-C12-O13	-2.39	119.82	124.86
3	I	401	CPK	O22-C20-O21	-2.32	119.97	124.86
3	C	402	CPK	O5-C6-C10	2.24	109.06	106.24
3	I	401	CPK	O5-C6-C10	2.23	109.05	106.24
3	H	403	CPK	C28-O27-C26	2.22	115.88	113.94
3	H	403	CPK	C18-C19-N14	-2.20	105.73	110.44
3	H	403	CPK	C19-C18-N17	-2.19	105.75	110.44
3	I	401	CPK	C18-C19-N14	-2.14	105.86	110.44
3	H	403	CPK	C10-C6-C7	-2.13	107.64	111.11
3	C	402	CPK	C18-C19-N14	-2.08	105.97	110.44

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	401	CPK	O22-C20-N17-C16
3	I	401	CPK	O22-C20-N17-C18

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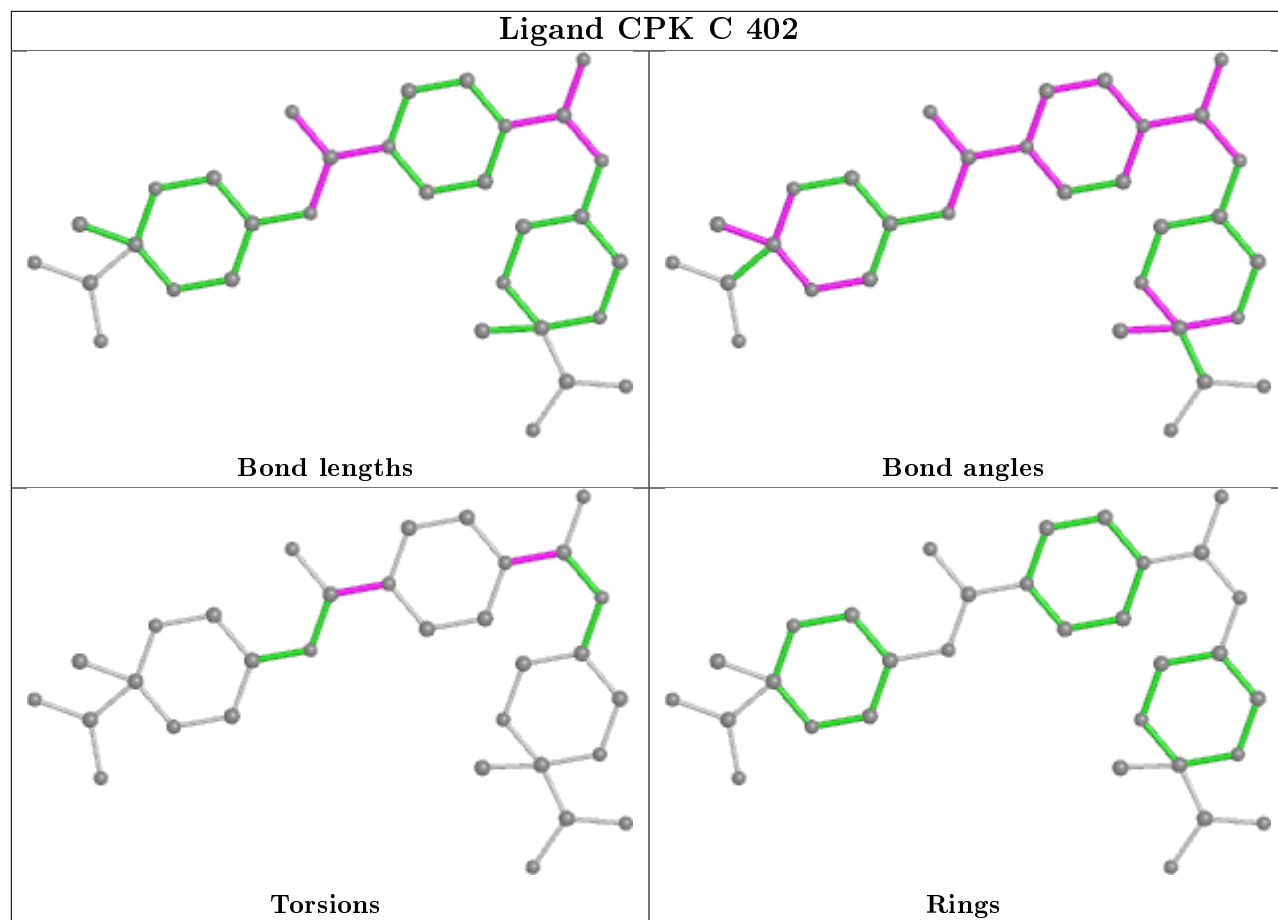
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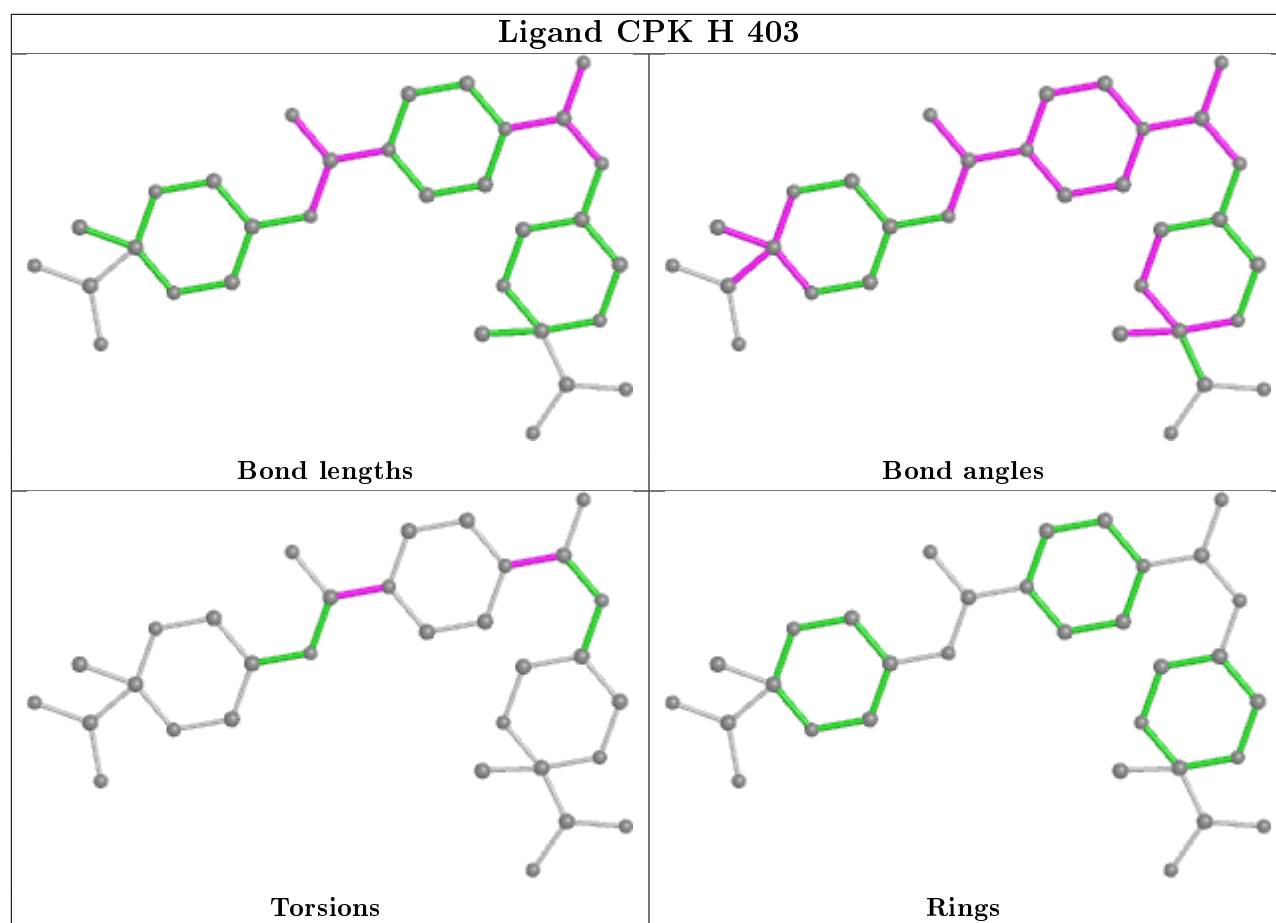
Mol	Chain	Res	Type	Atoms
3	I	401	CPK	O21-C20-N17-C16
3	I	401	CPK	O21-C20-N17-C18
3	I	401	CPK	O13-C12-N14-C15
3	I	401	CPK	O11-C12-N14-C15
3	I	401	CPK	O13-C12-N14-C19
3	I	401	CPK	O11-C12-N14-C19
3	H	403	CPK	O22-C20-N17-C16
3	H	403	CPK	O22-C20-N17-C18
3	H	403	CPK	O21-C20-N17-C16
3	H	403	CPK	O21-C20-N17-C18
3	H	403	CPK	O13-C12-N14-C15
3	H	403	CPK	O11-C12-N14-C15
3	H	403	CPK	O13-C12-N14-C19
3	H	403	CPK	O11-C12-N14-C19
3	C	402	CPK	O22-C20-N17-C16
3	C	402	CPK	O22-C20-N17-C18
3	C	402	CPK	O21-C20-N17-C18
3	C	402	CPK	O13-C12-N14-C19
3	C	402	CPK	O11-C12-N14-C19
3	C	402	CPK	O21-C20-N17-C16

There are no ring outliers.

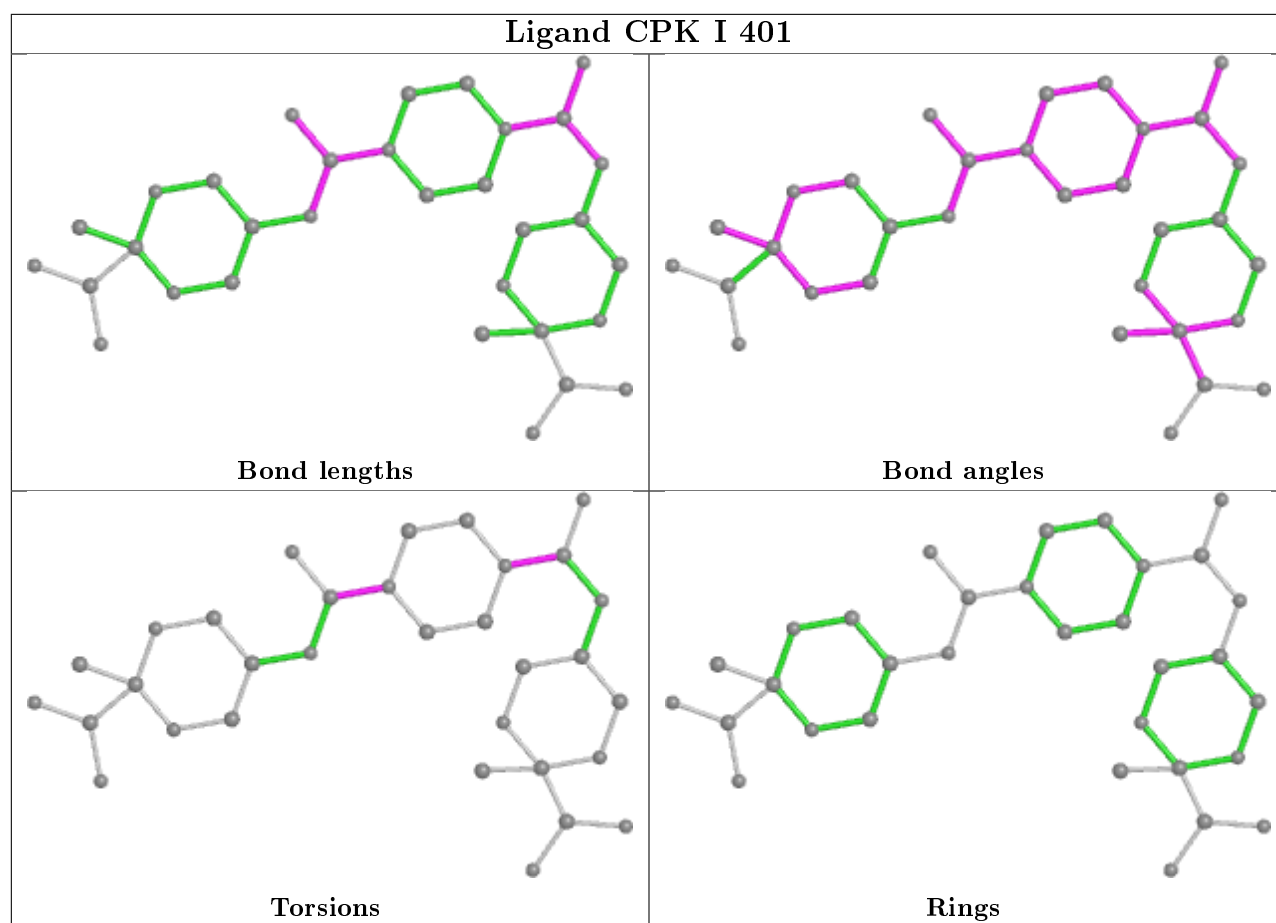
No monomer is involved in short contacts.

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.









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	204/204 (100%)	0.37	10 (4%) 29 11	9, 11, 13, 14	0
1	B	204/204 (100%)	0.50	16 (7%) 13 4	9, 11, 13, 15	0
1	C	204/204 (100%)	-0.27	1 (0%) 91 75	7, 11, 14, 16	0
1	D	204/204 (100%)	-0.48	0 100 100	7, 11, 15, 20	0
1	E	204/204 (100%)	-0.24	1 (0%) 91 75	6, 11, 14, 20	0
1	F	204/204 (100%)	0.42	10 (4%) 29 11	9, 12, 14, 17	0
1	G	204/204 (100%)	0.41	17 (8%) 11 3	9, 12, 14, 17	0
1	H	204/204 (100%)	-0.34	0 100 100	7, 11, 14, 17	0
1	I	204/204 (100%)	-0.40	0 100 100	7, 11, 15, 19	0
1	J	204/204 (100%)	-0.14	2 (0%) 82 59	7, 11, 14, 18	0
All	All	2040/2040 (100%)	-0.02	57 (2%) 53 25	6, 11, 14, 20	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	HIS	6.2
1	F	128	GLN	4.2
1	G	157	LEU	4.0
1	B	105	ALA	3.9
1	G	1	HIS	3.8
1	A	26	LEU	3.8
1	F	159	MET	3.5
1	F	5	SER	3.4
1	G	25	PRO	3.3
1	B	118	GLY	3.2
1	B	22	LEU	3.2
1	G	116	LYS	3.1
1	A	56	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	31	GLN	2.9
1	B	204	VAL	2.9
1	B	52	TYR	2.9
1	F	4	LEU	2.8
1	B	104	ILE	2.8
1	F	105	ALA	2.7
1	B	61	LEU	2.5
1	G	132	VAL	2.5
1	A	61	LEU	2.5
1	F	55	GLN	2.5
1	B	62	LEU	2.4
1	G	159	MET	2.4
1	A	52	TYR	2.4
1	B	94	ILE	2.4
1	G	21	ASN	2.3
1	G	37	PHE	2.3
1	G	23	ILE	2.3
1	A	24	THR	2.3
1	A	50	PHE	2.3
1	A	4	LEU	2.3
1	G	26	LEU	2.2
1	B	106	GLU	2.2
1	G	160	TRP	2.2
1	A	182	ILE	2.2
1	G	30	LEU	2.2
1	B	26	LEU	2.2
1	G	177	PRO	2.2
1	A	25	PRO	2.2
1	B	179	PRO	2.2
1	F	181	ASN	2.2
1	G	24	THR	2.1
1	B	58	ASP	2.1
1	F	147	SER	2.1
1	C	55	GLN	2.1
1	G	121	GLN	2.1
1	B	141	GLY	2.1
1	J	204	VAL	2.1
1	F	19	HIS	2.1
1	B	157	LEU	2.1
1	B	23	ILE	2.1
1	G	158	TYR	2.0
1	A	3	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	50	PHE	2.0
1	J	26	LEU	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 carbohydrates 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, 95<sup>th</sup> 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.

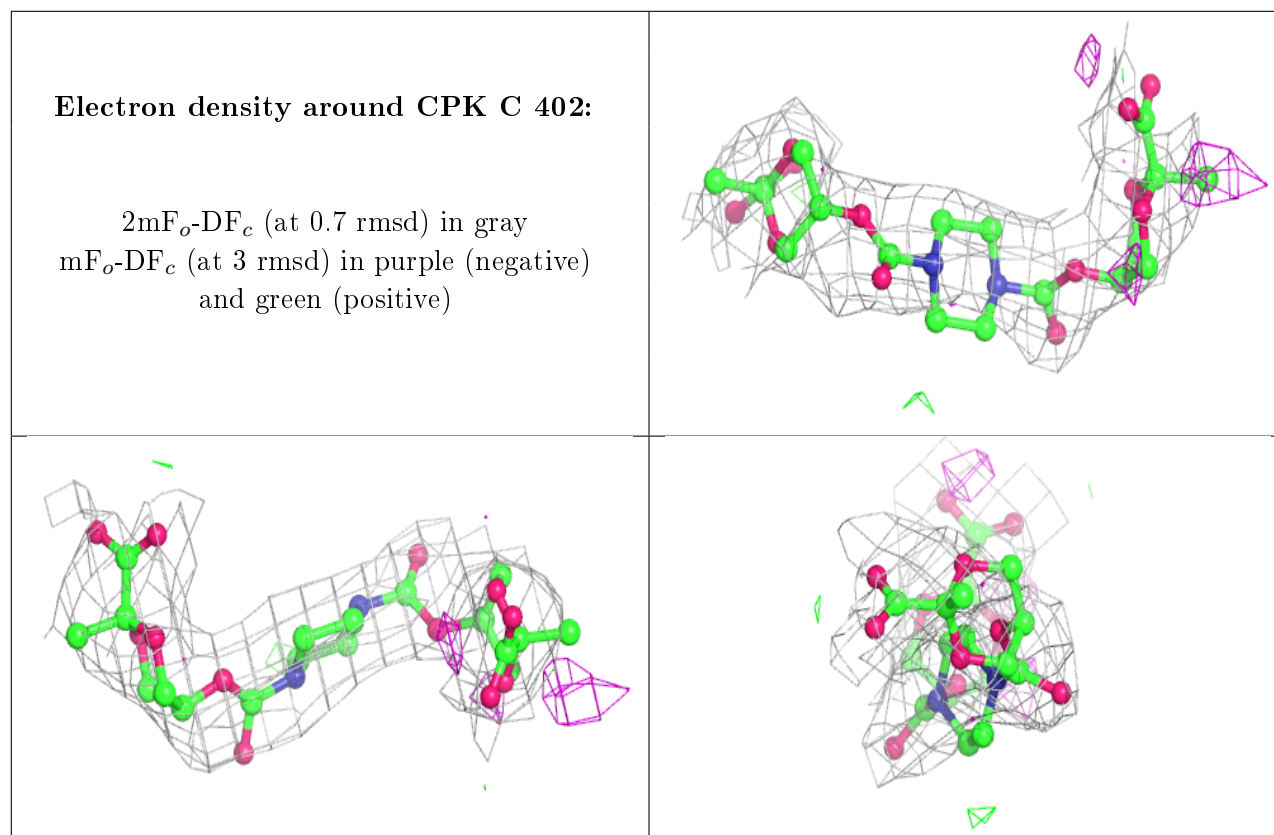
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	304	1/1	0.59	0.16	102,102,102,102	0
2	CA	A	301	1/1	0.65	0.09	106,106,106,106	0
2	CA	G	313	1/1	0.65	0.13	106,106,106,106	0
2	CA	B	303	1/1	0.66	0.13	102,102,102,102	0
2	CA	F	311	1/1	0.79	0.13	116,116,116,116	0
2	CA	G	314	1/1	0.80	0.14	103,103,103,103	0
3	CPK	C	402	32/32	0.87	0.27	75,87,92,95	0
2	CA	F	312	1/1	0.89	0.10	110,110,110,110	0
2	CA	J	320	1/1	0.90	0.13	93,93,93,93	0
2	CA	I	318	1/1	0.92	0.20	59,59,59,59	0
2	CA	A	302	1/1	0.93	0.17	105,105,105,105	0
2	CA	C	305	1/1	0.93	0.15	84,84,84,84	0
3	CPK	H	403	32/32	0.94	0.21	63,82,89,95	0
3	CPK	I	401	32/32	0.94	0.21	72,79,88,92	0
2	CA	C	306	1/1	0.94	0.19	80,80,80,80	0
2	CA	H	315	1/1	0.96	0.13	59,59,59,59	0
2	CA	J	319	1/1	0.97	0.12	100,100,100,100	0
2	CA	E	310	1/1	0.97	0.14	74,74,74,74	0
2	CA	I	317	1/1	0.97	0.13	60,60,60,60	0
2	CA	H	316	1/1	0.97	0.14	69,69,69,69	0
2	CA	D	307	1/1	0.98	0.19	44,44,44,44	0

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*Continued from previous page...*

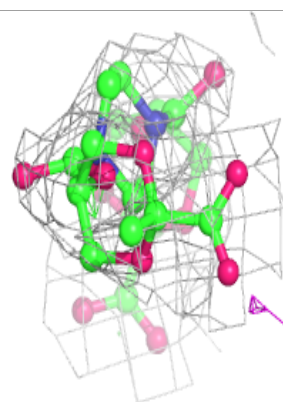
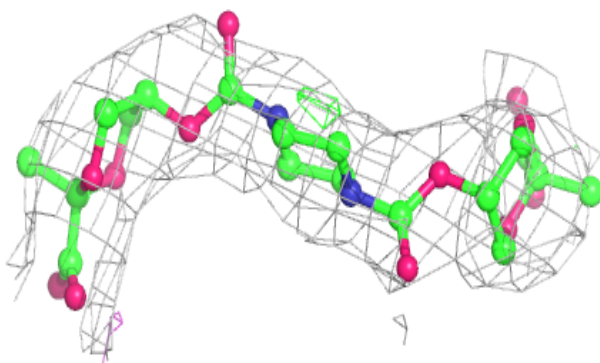
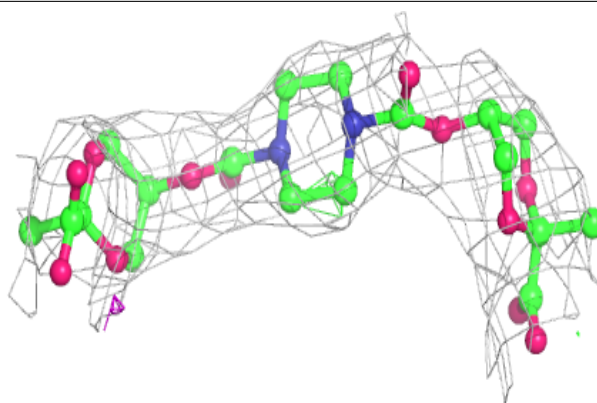
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	E	309	1/1	0.98	0.14	76,76,76,76	0
2	CA	D	308	1/1	0.98	0.21	65,65,65,65	0

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.

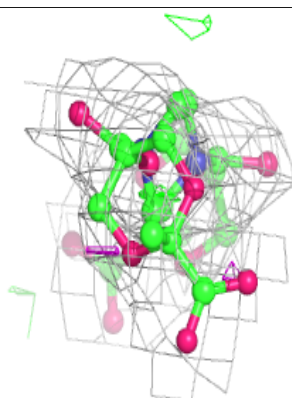
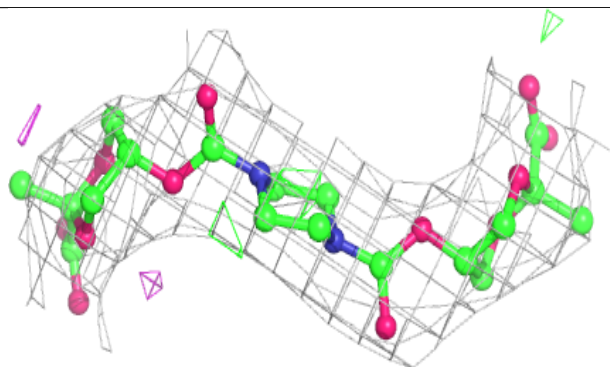
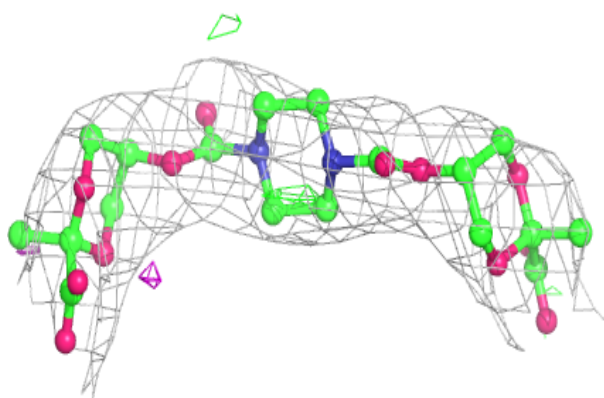


**Electron density around CPK H 403:**

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

**Electron density around CPK I 401:**

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



## 6.5 Other polymers

There are no such residues in this entry.