



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:56 PM UTC

PDB ID : 8CYZ / pdb_00008cyz
Title : Crystal structure of SARS-CoV-2 Mpro with compound C4
Authors : Worrall, L.J.; Lee, J.; Strynadka, N.C.J.
Deposited on : 2022-05-24
Resolution : 1.90 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

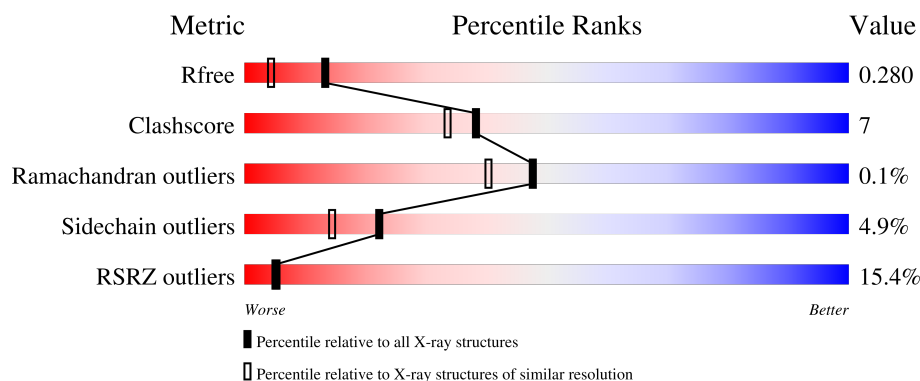
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	306	10% 84% 13% .
1	B	306	10% 88% 11% .
1	C	306	15% 82% 15% .
1	D	306	26% 81% 17% .

2 Entry composition [i](#)

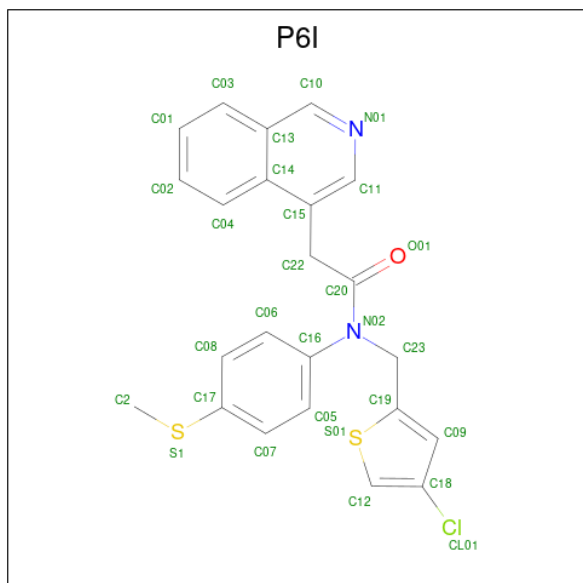
There are 3 unique types of molecules in this entry. The entry contains 10304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	5	0
			2394	1515	405	451	23			
1	B	305	Total	C	N	O	S	0	5	0
			2394	1515	405	451	23			
1	C	305	Total	C	N	O	S	0	5	0
			2394	1515	405	451	23			
1	D	305	Total	C	N	O	S	0	5	0
			2394	1515	405	451	23			

- Molecule 2 is N-[(4-chlorothiophen-2-yl)methyl]-2-(isoquinolin-4-yl)-N-[4-(methylsulfonyl)phenyl]acetamide (CCD ID: P6I) (formula: $C_{23}H_{19}ClN_2OS_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			29	23	1	2	1	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 29	C 23	Cl 1	N 2	O 1	S 2	0	0
2	C	1	Total 29	C 23	Cl 1	N 2	O 1	S 2	0	0
2	D	1	Total 29	C 23	Cl 1	N 2	O 1	S 2	0	0

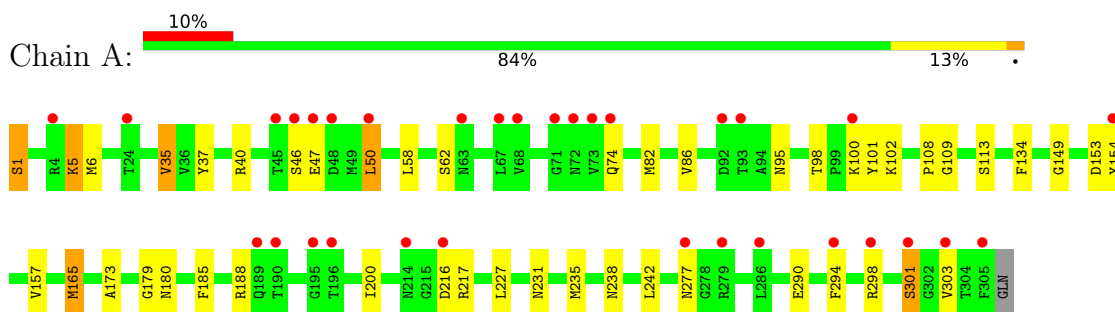
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total 198	O 198	0	0
3	B	141	Total 141	O 141	0	0
3	C	146	Total 146	O 146	0	0
3	D	127	Total 127	O 127	0	0

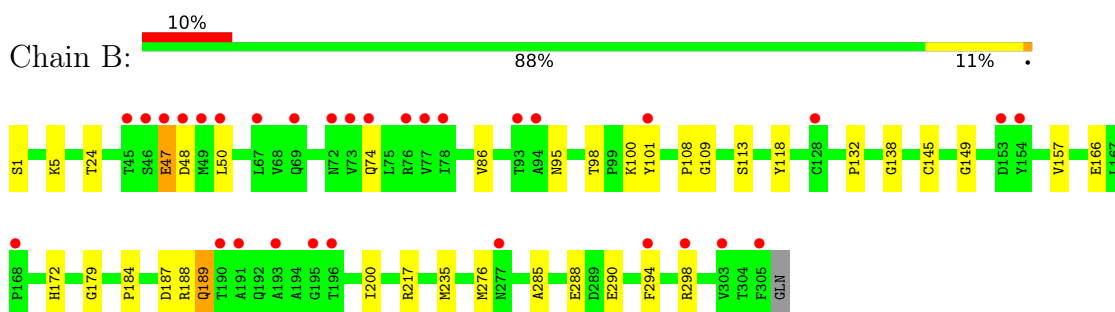
3 Residue-property plots [i](#)

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

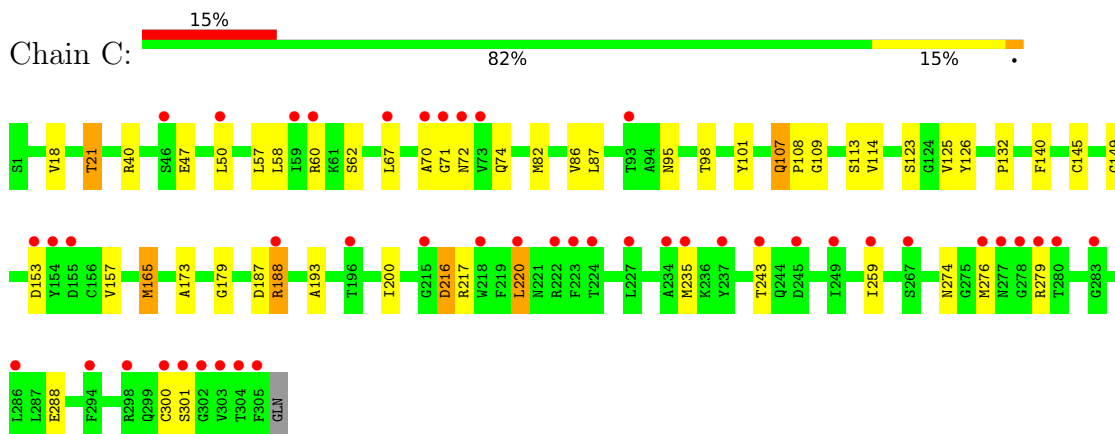
- Molecule 1: 3C-like proteinase



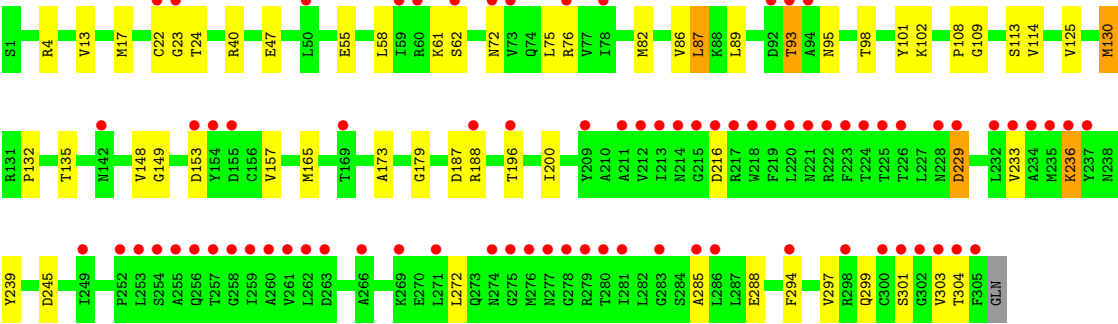
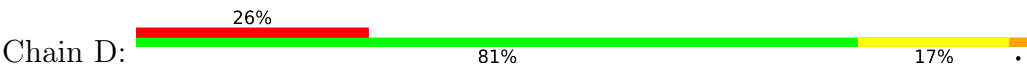
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.43Å 102.62Å 102.22Å 90.00° 100.19° 90.00°	Depositor
Resolution (Å)	45.75 – 1.90 45.75 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.75-1.90) 99.8 (45.75-1.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.245 , 0.278 0.253 , 0.280	Depositor DCC
R_{free} test set	5470 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10304	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8177e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P6I

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	1.00	0/2448	1.28	0/3327
1	B	0.99	1/2448 (0.0%)	1.27	0/3327
1	C	1.01	0/2448	1.29	2/3327 (0.1%)
1	D	0.98	0/2448	1.29	2/3327 (0.1%)
All	All	1.00	1/9792 (0.0%)	1.28	4/13308 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	PRO	C-O	-5.10	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	GLU	CB-CA-C	5.18	119.39	110.79
1	C	216[A]	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	216[B]	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	229	ASP	CA-CB-CG	5.08	117.68	112.60

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	2394	0	2333	33	0
1	B	2394	0	2333	21	0
1	C	2394	0	2333	32	0
1	D	2394	0	2333	56	0
2	A	29	0	0	1	0
2	B	29	0	0	2	0
2	C	29	0	0	1	0
2	D	29	0	0	1	0
3	A	198	0	0	11	1
3	B	141	0	0	6	0
3	C	146	0	0	12	1
3	D	127	0	0	9	0
All	All	10304	0	9332	132	1

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

All (132) 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:301:SER:HB3	3:A:562:HOH:O	1.41	1.17
1:D:130:MET:HA	1:D:130:MET:HE3	1.31	1.05
1:D:4:ARG:H	1:D:299:GLN:HE22	1.16	0.94
1:A:277:ASN:HB2	3:A:684:HOH:O	1.68	0.93
1:A:46:SER:HB3	3:A:675:HOH:O	1.73	0.88
1:A:294:PHE:HB2	3:A:673:HOH:O	1.78	0.82
1:B:288:GLU:HG2	3:B:538:HOH:O	1.78	0.81
1:A:231:ASN:HD21	1:A:242:LEU:H	1.28	0.81
1:D:245:ASP:HB3	3:D:550:HOH:O	1.81	0.81
1:D:102:LYS:HE3	3:D:618:HOH:O	1.82	0.79
1:C:288:GLU:HG2	3:C:507:HOH:O	1.81	0.79
1:A:154:TYR:HB2	1:D:23:GLY:HA2	1.63	0.79
1:C:243:THR:HG22	3:C:619:HOH:O	1.87	0.75
1:D:130:MET:HA	1:D:130:MET:CE	2.16	0.73
1:C:300:CYS:SG	3:C:635:HOH:O	2.47	0.71
1:D:303:VAL:HG23	3:D:598:HOH:O	1.89	0.71
1:D:130:MET:HE3	1:D:130:MET:CA	2.16	0.70
1:A:62:SER:HB3	3:A:592:HOH:O	1.92	0.68
1:D:87:LEU:CD1	1:D:89:LEU:HD21	2.24	0.68
1:D:288:GLU:HG2	3:D:506:HOH:O	1.94	0.68
1:A:301:SER:CB	3:A:562:HOH:O	2.18	0.67
1:D:13:VAL:CG1	1:D:17:MET:CE	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LYS:HB3	3:D:503:HOH:O	1.96	0.66
1:C:21:THR:CG2	3:C:567:HOH:O	2.43	0.65
1:D:13:VAL:HG12	1:D:17:MET:CE	2.26	0.65
1:D:58:LEU:HD22	1:D:82:MET:HE3	1.79	0.65
1:A:58:LEU:HD22	1:A:82:MET:HE3	1.79	0.64
1:C:243:THR:CG2	3:C:619:HOH:O	2.45	0.63
1:C:58:LEU:HD22	1:C:82:MET:HE3	1.80	0.62
1:B:294:PHE:HB2	3:B:624:HOH:O	1.98	0.62
1:D:153:ASP:HB2	3:D:608:HOH:O	1.98	0.62
1:D:4:ARG:H	1:D:299:GLN:NE2	1.93	0.61
1:C:18:VAL:HG12	1:C:70:ALA:HA	1.82	0.60
1:C:188:ARG:HD3	3:C:611:HOH:O	2.01	0.59
1:A:216[A]:ASP:OD2	3:A:501:HOH:O	2.17	0.59
1:B:138:GLY:H	1:B:172:HIS:HD2	1.51	0.59
1:D:245:ASP:CB	3:D:550:HOH:O	2.47	0.59
1:D:75:LEU:HD22	1:D:93:THR:CG2	2.32	0.59
1:D:130:MET:CE	1:D:135:THR:O	2.51	0.58
1:D:87:LEU:HD11	1:D:89:LEU:HD21	1.86	0.56
1:D:165:MET:HG2	1:D:173:ALA:HB3	1.87	0.56
1:B:288:GLU:CG	3:B:538:HOH:O	2.45	0.56
1:A:231:ASN:ND2	1:A:242:LEU:H	1.99	0.55
1:D:13:VAL:HG12	1:D:17:MET:HE3	1.87	0.55
1:C:165:MET:HG2	1:C:173:ALA:HB3	1.89	0.55
1:D:87:LEU:HD13	1:D:89:LEU:HD21	1.88	0.54
1:A:165:MET:HG2	1:A:173:ALA:HB3	1.91	0.53
1:C:21:THR:HG22	3:C:567:HOH:O	2.04	0.53
1:B:118:TYR:HB2	1:D:304:THR:HG21	1.90	0.52
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.91	0.52
1:B:118:TYR:HB2	1:D:304:THR:CG2	2.39	0.52
1:C:86:VAL:HG13	1:C:179:GLY:HA2	1.92	0.52
1:D:13:VAL:CG1	1:D:17:MET:HE2	2.39	0.52
1:B:285:ALA:HB3	1:D:285:ALA:HB3	1.91	0.52
1:A:154:TYR:CB	1:D:23:GLY:HA2	2.37	0.52
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.10	0.52
1:C:95:ASN:HB3	1:C:98:THR:OG1	2.10	0.51
1:D:75:LEU:HD22	1:D:93:THR:HG23	1.90	0.51
1:C:145:CYS:SG	3:C:598:HOH:O	2.41	0.51
1:D:22:CYS:SG	1:D:61:LYS:HD2	2.50	0.51
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.11	0.51
1:D:95:ASN:HB3	1:D:98:THR:OG1	2.11	0.51
1:A:165:MET:HE2	2:A:401:P6I:CL01	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:VAL:HG13	1:D:179:GLY:HA2	1.93	0.50
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.93	0.50
1:B:47:GLU:HG3	1:B:48:ASP:N	2.25	0.50
1:D:17:MET:HE1	1:D:148:VAL:HG22	1.94	0.50
1:A:298:ARG:HD3	3:A:517:HOH:O	2.11	0.49
1:D:187:ASP:HA	2:D:401:P6I:CL01	2.50	0.49
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.93	0.49
1:A:113:SER:O	1:A:149:GLY:HA2	2.12	0.48
1:D:113:SER:O	1:D:149:GLY:HA2	2.14	0.48
1:C:113:SER:O	1:C:149:GLY:HA2	2.13	0.48
1:B:113:SER:O	1:B:149:GLY:HA2	2.13	0.48
1:A:6:MET:HE2	1:C:126:TYR:CD2	2.49	0.47
1:C:274:ASN:O	3:C:501:HOH:O	2.20	0.47
1:D:13:VAL:HG12	1:D:17:MET:HE2	1.95	0.47
1:D:239:TYR:CZ	1:D:272:LEU:HD21	2.50	0.47
1:C:40:ARG:HB2	1:C:82:MET:HE2	1.97	0.47
1:B:101:TYR:HA	1:B:157:VAL:O	2.15	0.47
1:C:101:TYR:HA	1:C:157:VAL:O	2.15	0.47
1:C:187:ASP:HA	2:C:401:P6I:CL01	2.52	0.47
1:A:101:TYR:HA	1:A:157:VAL:O	2.15	0.47
1:D:109:GLY:HA2	1:D:200:ILE:HD13	1.97	0.47
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.97	0.46
1:D:87:LEU:HD13	1:D:89:LEU:CD2	2.45	0.46
1:D:188:ARG:HG2	3:D:577:HOH:O	2.16	0.46
1:D:13:VAL:HG13	1:D:17:MET:CE	2.46	0.46
1:A:5:LYS:NZ	1:A:290:GLU:HB2	2.32	0.46
1:D:101:TYR:HA	1:D:157:VAL:O	2.16	0.45
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.98	0.45
1:A:180:ASN:ND2	3:A:505:HOH:O	2.36	0.45
1:A:153:ASP:OD1	1:D:24:THR:HG22	2.16	0.45
1:B:5:LYS:HD3	3:B:517:HOH:O	2.16	0.45
1:A:185:PHE:O	3:A:502:HOH:O	2.21	0.45
1:B:166:GLU:OE2	1:B:172:HIS:HE1	1.99	0.45
1:A:100:LYS:HE2	1:A:100:LYS:HB3	1.74	0.44
1:B:189:GLN:HG3	2:B:401:P6I:S01	2.56	0.44
1:A:6:MET:HE2	1:C:126:TYR:CE2	2.52	0.44
1:D:130:MET:CE	1:D:130:MET:CA	2.87	0.44
1:D:40:ARG:HB2	1:D:82:MET:HE2	2.00	0.44
1:B:145:CYS:SG	3:B:612:HOH:O	2.15	0.44
1:B:187:ASP:HA	2:B:401:P6I:CL01	2.55	0.44
1:D:165:MET:HE3	1:D:165:MET:HB2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:MET:HE1	1:D:148:VAL:CG2	2.47	0.43
1:B:298:ARG:HD3	3:B:511:HOH:O	2.18	0.43
3:A:571:HOH:O	1:D:72:ASN:HA	2.18	0.43
1:C:193:ALA:O	3:C:502:HOH:O	2.21	0.42
1:D:301:SER:CB	3:D:598:HOH:O	2.67	0.42
1:A:1:SER:N	1:C:140:PHE:O	2.51	0.42
1:B:5:LYS:NZ	1:B:290:GLU:HB2	2.35	0.42
1:A:35:VAL:HG22	1:A:37:TYR:CE1	2.55	0.41
1:C:108[B]:PRO:HB3	1:C:132:PRO:HA	2.02	0.41
1:C:301:SER:CB	3:C:638:HOH:O	2.68	0.41
1:C:279:ARG:HA	3:C:538:HOH:O	2.19	0.41
1:A:50:LEU:HD13	1:A:50:LEU:HA	1.95	0.41
1:C:21:THR:HG23	1:C:67:LEU:HB2	2.03	0.41
1:D:22:CYS:SG	1:D:61:LYS:CD	3.08	0.41
1:C:114:VAL:O	1:C:125:VAL:HA	2.21	0.41
1:D:294:PHE:HA	1:D:297:VAL:HG22	2.03	0.41
1:C:108[A]:PRO:HB3	1:C:132:PRO:HA	2.02	0.41
1:C:220:LEU:HD11	1:C:259:ILE:HD12	2.02	0.41
1:D:108[A]:PRO:HB3	1:D:132:PRO:HA	2.02	0.41
1:D:4:ARG:N	1:D:299:GLN:HE22	1.99	0.41
1:D:114:VAL:O	1:D:125:VAL:HA	2.21	0.41
1:A:303:VAL:O	1:C:123:SER:CB	2.69	0.41
1:D:196:THR:HG23	1:D:196:THR:O	2.21	0.41
1:A:108[B]:PRO:HG3	1:A:134:PHE:CE1	2.56	0.40
1:B:108[B]:PRO:HB3	1:B:132:PRO:HA	2.03	0.40
1:C:107:GLN:HG3	1:C:108[B]:PRO:HD2	2.03	0.40
1:A:40:ARG:HB2	1:A:82:MET:HE2	2.03	0.40
1:D:229:ASP:O	1:D:233:VAL:HG23	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:593:HOH:O	3:C:604:HOH:O[2_444]	2.17	0.03

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	308/306 (101%)	300 (97%)	8 (3%)	0	100	100
1	B	308/306 (101%)	298 (97%)	10 (3%)	0	100	100
1	C	308/306 (101%)	299 (97%)	8 (3%)	1 (0%)	36	29
1	D	308/306 (101%)	301 (98%)	7 (2%)	0	100	100
All	All	1232/1224 (101%)	1198 (97%)	33 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	GLY

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	267/263 (102%)	253 (95%)	14 (5%)	21	13
1	B	267/263 (102%)	255 (96%)	12 (4%)	24	17
1	C	267/263 (102%)	247 (92%)	20 (8%)	12	6
1	D	267/263 (102%)	258 (97%)	9 (3%)	32	25
All	All	1068/1052 (102%)	1013 (95%)	55 (5%)	22	13

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS
1	A	35	VAL
1	A	47	GLU
1	A	50	LEU
1	A	74	GLN
1	A	102	LYS
1	A	165	MET
1	A	188	ARG
1	A	217	ARG
1	A	227	LEU
1	A	235	MET
1	A	238	ASN
1	A	301	SER
1	B	1	SER
1	B	24	THR
1	B	47	GLU
1	B	50	LEU
1	B	74	GLN
1	B	100	LYS
1	B	188	ARG
1	B	189	GLN
1	B	217	ARG
1	B	235	MET
1	B	276[A]	MET
1	B	276[B]	MET
1	C	21	THR
1	C	47	GLU
1	C	50	LEU
1	C	57	LEU
1	C	60	ARG
1	C	62	SER
1	C	72	ASN
1	C	74	GLN
1	C	87	LEU
1	C	107	GLN
1	C	153	ASP
1	C	165	MET
1	C	188	ARG
1	C	216[A]	ASP
1	C	216[B]	ASP
1	C	217	ARG
1	C	220	LEU

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Mol	Chain	Res	Type
1	C	235	MET
1	C	276[A]	MET
1	C	276[B]	MET
1	D	47	GLU
1	D	62	SER
1	D	76	ARG
1	D	87	LEU
1	D	93	THR
1	D	130	MET
1	D	216[A]	ASP
1	D	216[B]	ASP
1	D	236	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	80	HIS
1	A	119	ASN
1	A	164	HIS
1	A	189	GLN
1	A	231	ASN
1	A	244	GLN
1	A	274	ASN
1	B	63	ASN
1	B	151	ASN
1	B	172	HIS
1	B	203	ASN
1	B	244	GLN
1	B	274	ASN
1	C	51	ASN
1	C	64	HIS
1	C	72	ASN
1	C	164	HIS
1	D	64	HIS
1	D	164	HIS
1	D	274	ASN
1	D	299	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	P6I	C	401	-	32,32,32	1.32	2 (6%)	41,44,44	2.67	10 (24%)
2	P6I	B	401	-	32,32,32	1.57	2 (6%)	41,44,44	2.32	10 (24%)
2	P6I	D	401	-	32,32,32	1.36	5 (15%)	41,44,44	2.96	13 (31%)
2	P6I	A	401	-	32,32,32	1.65	3 (9%)	41,44,44	2.66	11 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P6I	C	401	-	-	2/18/18/18	0/4/4/4
2	P6I	B	401	-	-	2/18/18/18	0/4/4/4
2	P6I	D	401	-	-	2/18/18/18	0/4/4/4
2	P6I	A	401	-	-	2/18/18/18	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	P6I	C18-CL01	6.52	1.85	1.73
2	A	401	P6I	C18-CL01	6.24	1.85	1.73
2	D	401	P6I	C18-CL01	4.94	1.82	1.73
2	C	401	P6I	C18-CL01	4.52	1.81	1.73
2	B	401	P6I	C22-C20	2.68	1.55	1.52
2	A	401	P6I	C22-C20	2.50	1.54	1.52
2	C	401	P6I	C02-C04	2.33	1.41	1.36
2	D	401	P6I	C16-N02	-2.17	1.39	1.43
2	A	401	P6I	C01-C02	2.16	1.43	1.38
2	D	401	P6I	C02-C04	2.12	1.41	1.36
2	D	401	P6I	C01-C03	2.06	1.41	1.36
2	D	401	P6I	C20-N02	-2.01	1.33	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	P6I	C18-C12-S01	-10.02	104.28	110.87
2	D	401	P6I	C09-C18-C12	8.58	120.97	107.54
2	A	401	P6I	C18-C12-S01	-8.33	105.39	110.87
2	C	401	P6I	C09-C18-C12	8.33	120.58	107.54
2	A	401	P6I	C09-C18-C12	7.56	119.39	107.54
2	B	401	P6I	C09-C18-C12	7.08	118.62	107.54
2	C	401	P6I	C18-C12-S01	-6.90	106.33	110.87
2	D	401	P6I	C12-C18-CL01	-6.55	118.83	126.58
2	D	401	P6I	C19-C23-N02	-6.41	105.82	112.92
2	B	401	P6I	C18-C12-S01	-6.25	106.76	110.87
2	A	401	P6I	C19-C23-N02	-5.86	106.43	112.92
2	B	401	P6I	C12-C18-CL01	-5.64	119.90	126.58
2	C	401	P6I	C19-C23-N02	-5.53	106.80	112.92
2	C	401	P6I	C10-N01-C11	5.40	122.15	117.03
2	B	401	P6I	C19-C23-N02	-5.35	106.99	112.92
2	D	401	P6I	C10-N01-C11	4.71	121.50	117.03
2	A	401	P6I	C10-N01-C11	4.62	121.42	117.03
2	C	401	P6I	C23-N02-C16	-4.43	110.15	118.38
2	C	401	P6I	C12-C18-CL01	-4.38	121.40	126.58
2	C	401	P6I	C23-N02-C20	4.23	123.21	117.14
2	A	401	P6I	C23-N02-C20	4.11	123.04	117.14
2	A	401	P6I	C12-C18-CL01	-3.85	122.02	126.58
2	A	401	P6I	C15-C11-N01	-3.57	119.88	124.57
2	B	401	P6I	C10-C13-C14	3.22	120.96	117.84
2	D	401	P6I	C12-S01-C19	3.20	95.26	92.56
2	C	401	P6I	C22-C15-C11	-3.19	117.09	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	P6I	C12-S01-C19	3.19	95.25	92.56
2	C	401	P6I	C09-C18-CL01	-3.09	118.02	125.45
2	A	401	P6I	C22-C15-C11	-2.91	117.54	122.20
2	D	401	P6I	C15-C11-N01	-2.86	120.81	124.57
2	A	401	P6I	C09-C18-CL01	-2.86	118.58	125.45
2	D	401	P6I	C23-N02-C20	2.80	121.15	117.14
2	C	401	P6I	C15-C11-N01	-2.79	120.91	124.57
2	B	401	P6I	C23-N02-C20	2.67	120.97	117.14
2	D	401	P6I	O01-C20-N02	-2.66	118.00	121.70
2	D	401	P6I	C23-N02-C16	-2.60	113.55	118.38
2	D	401	P6I	C22-C15-C11	-2.60	118.05	122.20
2	A	401	P6I	C23-N02-C16	-2.40	113.93	118.38
2	B	401	P6I	O01-C20-N02	-2.29	118.51	121.70
2	B	401	P6I	C10-N01-C11	2.23	119.15	117.03
2	B	401	P6I	C12-S01-C19	2.23	94.44	92.56
2	D	401	P6I	C09-C18-CL01	-2.20	120.16	125.45
2	B	401	P6I	C22-C15-C11	-2.05	118.92	122.20
2	D	401	P6I	C2-S1-C17	2.03	107.92	103.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

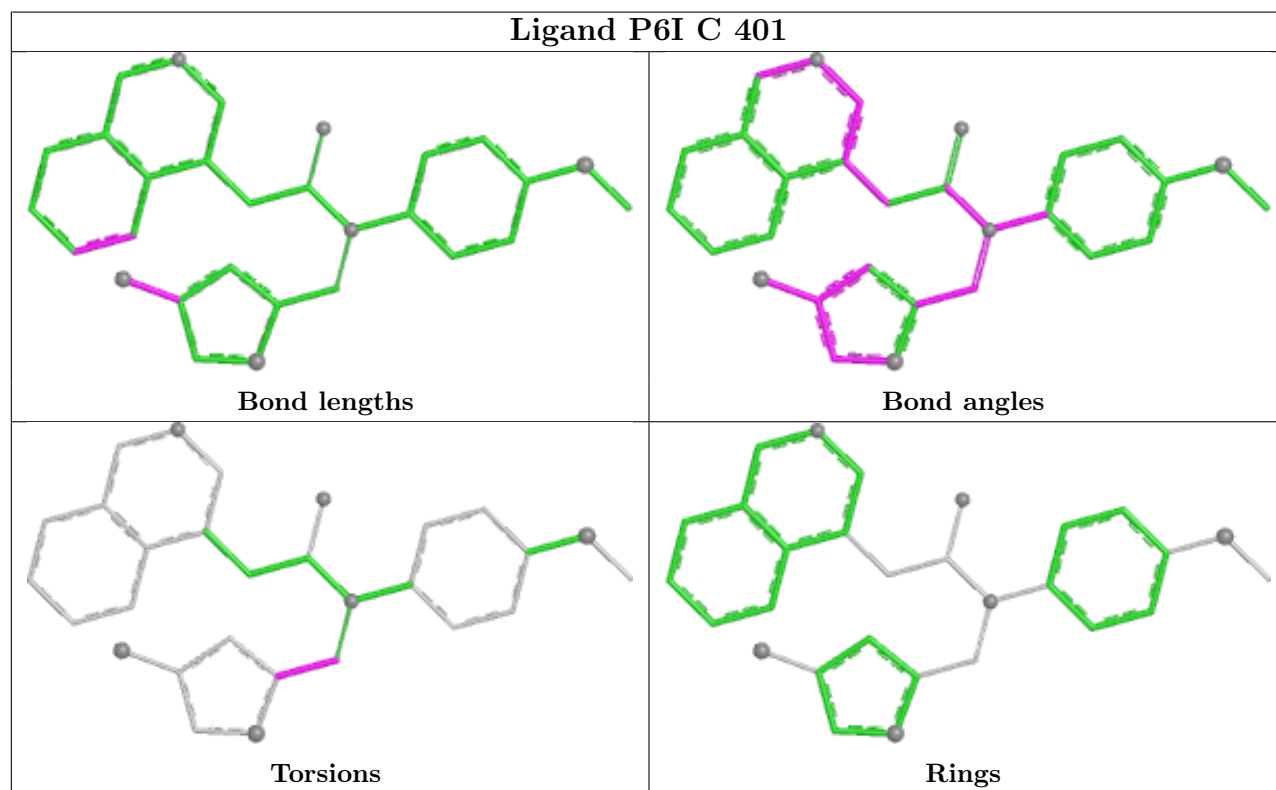
Mol	Chain	Res	Type	Atoms
2	D	401	P6I	S01-C19-C23-N02
2	C	401	P6I	S01-C19-C23-N02
2	B	401	P6I	C09-C19-C23-N02
2	C	401	P6I	C09-C19-C23-N02
2	A	401	P6I	C09-C19-C23-N02
2	D	401	P6I	C09-C19-C23-N02
2	A	401	P6I	S01-C19-C23-N02
2	B	401	P6I	S01-C19-C23-N02

There are no ring outliers.

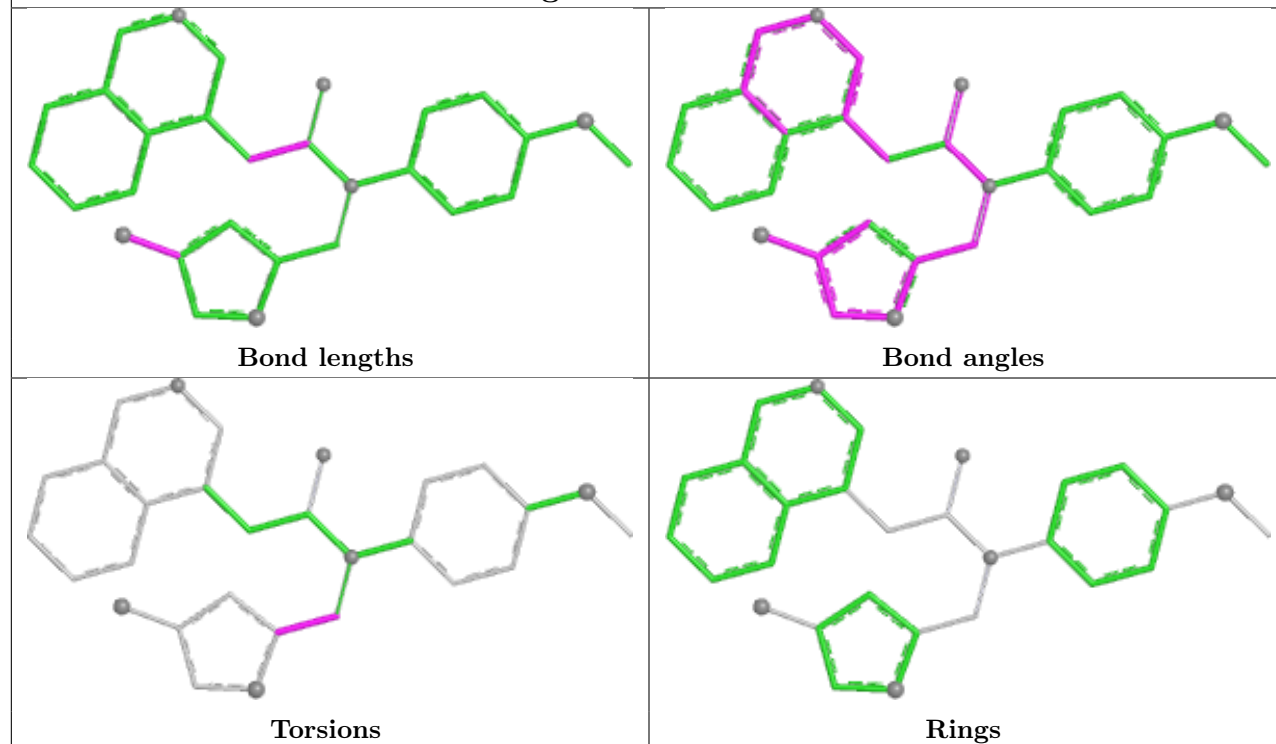
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	P6I	1	0
2	B	401	P6I	2	0
2	D	401	P6I	1	0
2	A	401	P6I	1	0

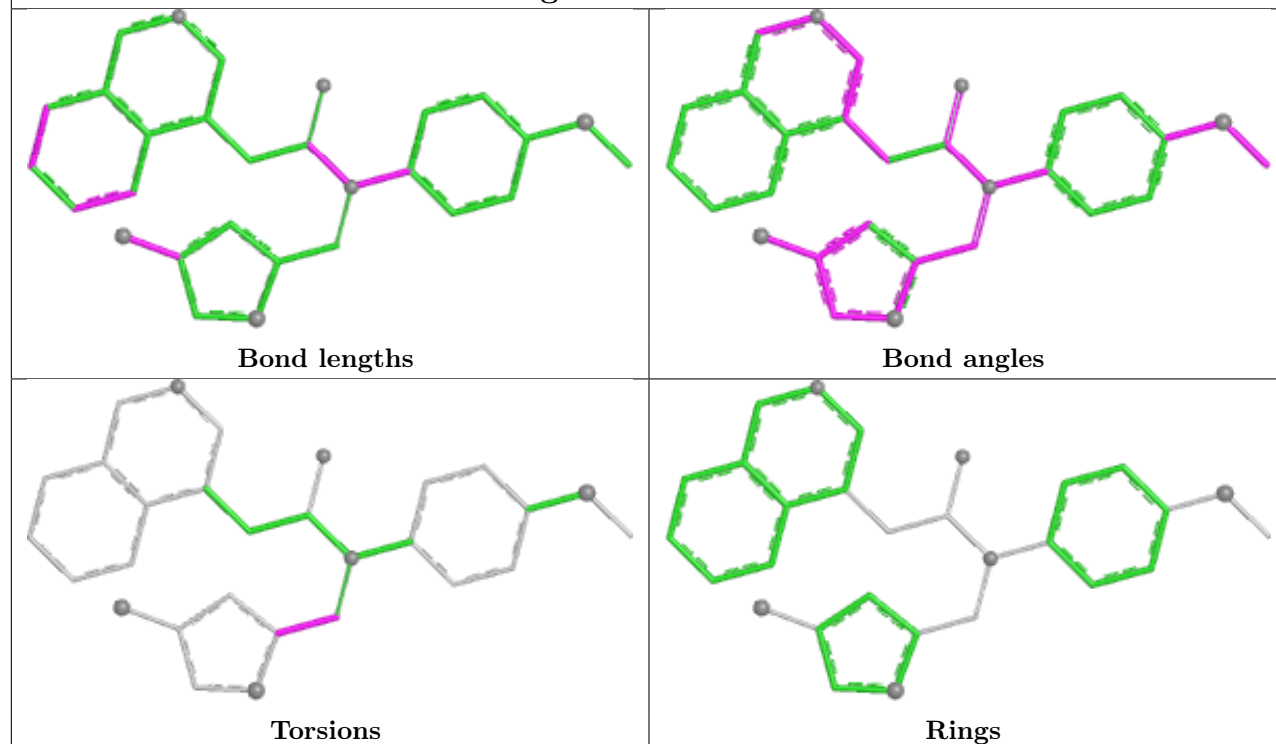
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

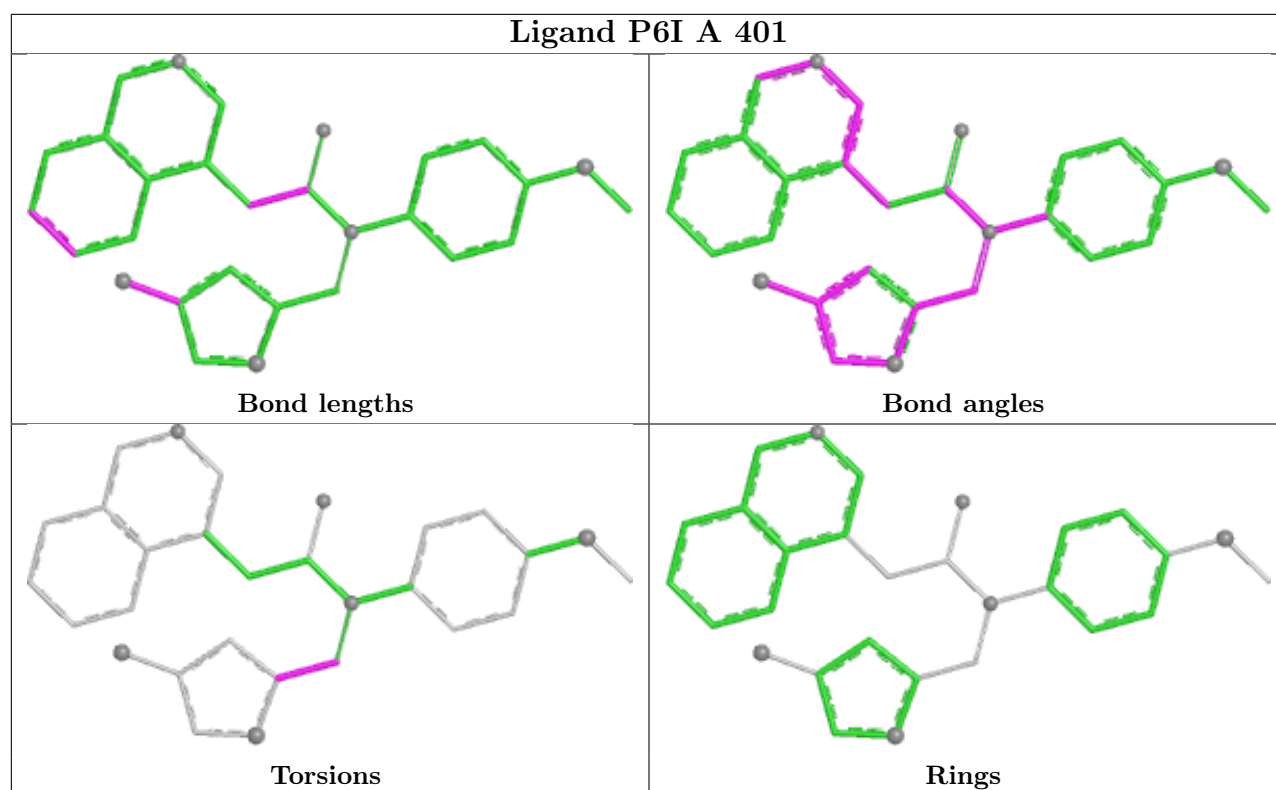


Ligand P6I B 401



Ligand P6I D 401





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	305/306 (99%)	0.61	32 (10%)	11 12	13, 27, 47, 80	6 (1%)
1	B	305/306 (99%)	0.68	31 (10%)	12 12	14, 28, 51, 70	5 (1%)
1	C	305/306 (99%)	0.89	45 (14%)	5 6	13, 31, 57, 78	5 (1%)
1	D	305/306 (99%)	1.29	80 (26%)	1 1	13, 35, 67, 98	5 (1%)
All	All	1220/1224 (99%)	0.87	188 (15%)	5 5	13, 30, 57, 98	21 (1%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	276[A]	MET	7.1
1	C	276[A]	MET	7.1
1	D	223	PHE	6.6
1	D	278	GLY	6.6
1	D	305	PHE	6.4
1	D	218	TRP	6.1
1	D	303	VAL	6.1
1	C	303	VAL	5.3
1	D	302	GLY	5.2
1	D	220	LEU	5.1
1	D	216[A]	ASP	5.1
1	D	232	LEU	5.0
1	C	70	ALA	4.9
1	D	62	SER	4.6
1	A	294	PHE	4.6
1	C	301	SER	4.4
1	C	305	PHE	4.4
1	C	72	ASN	4.4
1	D	257	THR	4.3
1	D	304	THR	4.3
1	D	279	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	154	TYR	4.3
1	D	255	ALA	4.2
1	D	259	ILE	4.1
1	D	233	VAL	4.0
1	D	275	GLY	3.9
1	C	71	GLY	3.9
1	B	294	PHE	3.8
1	B	154	TYR	3.8
1	D	219	PHE	3.8
1	A	73	VAL	3.8
1	D	23	GLY	3.7
1	B	47	GLU	3.7
1	C	294	PHE	3.6
1	D	224	THR	3.5
1	D	225	THR	3.5
1	B	305	PHE	3.5
1	C	50	LEU	3.5
1	C	188	ARG	3.4
1	C	280	THR	3.4
1	D	226	THR	3.4
1	D	154	TYR	3.4
1	B	46	SER	3.4
1	C	302	GLY	3.3
1	C	73	VAL	3.3
1	B	191	ALA	3.3
1	A	72	ASN	3.3
1	D	300	CYS	3.3
1	D	72	ASN	3.3
1	A	216[A]	ASP	3.2
1	A	305	PHE	3.2
1	A	154	TYR	3.2
1	D	209	TYR	3.2
1	D	73	VAL	3.2
1	C	59	ILE	3.2
1	B	195	GLY	3.2
1	D	236	LYS	3.1
1	A	71	GLY	3.1
1	C	227	LEU	3.1
1	A	298	ARG	3.1
1	A	46	SER	3.1
1	D	253	LEU	3.1
1	C	220	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	223	PHE	3.0
1	D	294	PHE	3.0
1	D	285	ALA	3.0
1	D	249	ILE	3.0
1	A	67	LEU	3.0
1	D	155	ASP	3.0
1	C	300	CYS	3.0
1	D	228	ASN	3.0
1	D	277	ASN	3.0
1	A	301	SER	3.0
1	C	267	SER	3.0
1	B	72	ASN	3.0
1	C	67	LEU	2.9
1	D	301	SER	2.9
1	D	222	ARG	2.9
1	D	221	ASN	2.9
1	D	153	ASP	2.9
1	D	258	GLY	2.9
1	D	59	ILE	2.9
1	C	93	THR	2.9
1	B	78	ILE	2.9
1	D	271	LEU	2.9
1	C	243	THR	2.8
1	B	298	ARG	2.8
1	D	213	ILE	2.8
1	D	188	ARG	2.8
1	C	153	ASP	2.8
1	B	50	LEU	2.8
1	B	190	THR	2.8
1	B	196	THR	2.8
1	C	222	ARG	2.7
1	A	45	THR	2.7
1	D	196	THR	2.7
1	D	281	ILE	2.7
1	D	269	LYS	2.7
1	C	224	THR	2.7
1	C	277	ASN	2.7
1	A	303	VAL	2.7
1	B	48	ASP	2.7
1	C	235	MET	2.7
1	D	22	CYS	2.7
1	C	304	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	67	LEU	2.7
1	D	254[A]	SER	2.7
1	A	100	LYS	2.6
1	D	298	ARG	2.6
1	D	263	ASP	2.6
1	D	217	ARG	2.6
1	D	280	THR	2.6
1	A	92	ASP	2.5
1	D	260	ALA	2.5
1	C	60	ARG	2.5
1	D	50	LEU	2.5
1	C	283	GLY	2.5
1	D	211	ALA	2.5
1	A	195	GLY	2.5
1	C	279	ARG	2.5
1	D	76	ARG	2.5
1	B	45	THR	2.5
1	D	60	ARG	2.4
1	D	215	GLY	2.4
1	D	274	ASN	2.4
1	B	69	GLN	2.4
1	B	153	ASP	2.4
1	C	259	ILE	2.4
1	C	245	ASP	2.4
1	D	78	ILE	2.4
1	B	74	GLN	2.4
1	B	168	PRO	2.4
1	D	283	GLY	2.3
1	A	48	ASP	2.3
1	D	262	LEU	2.3
1	C	155	ASP	2.3
1	C	286	LEU	2.3
1	A	93	THR	2.3
1	D	266	ALA	2.3
1	C	46	SER	2.3
1	B	73	VAL	2.3
1	B	303	VAL	2.3
1	A	277	ASN	2.3
1	A	190	THR	2.3
1	B	93	THR	2.3
1	D	94	ALA	2.2
1	D	142	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	235	MET	2.2
1	D	93	THR	2.2
1	A	47	GLU	2.2
1	A	286	LEU	2.2
1	B	277	ASN	2.2
1	A	50	LEU	2.2
1	D	92	ASP	2.2
1	B	193	ALA	2.2
1	D	237	TYR	2.2
1	D	261	VAL	2.2
1	A	196	THR	2.2
1	A	4	ARG	2.2
1	C	298	ARG	2.2
1	C	218	TRP	2.1
1	C	196	THR	2.1
1	D	169	THR	2.1
1	D	229	ASP	2.1
1	C	215	GLY	2.1
1	C	278	GLY	2.1
1	D	286	LEU	2.1
1	B	49	MET	2.1
1	D	234	ALA	2.1
1	C	249	ILE	2.1
1	A	74	GLN	2.1
1	B	101	TYR	2.1
1	C	237	TYR	2.1
1	B	76	ARG	2.1
1	D	212	VAL	2.1
1	A	189	GLN	2.1
1	A	214	ASN	2.0
1	D	256	GLN	2.0
1	A	68	VAL	2.0
1	B	77	VAL	2.0
1	D	252	PRO	2.0
1	B	128	CYS	2.0
1	A	279	ARG	2.0
1	B	94	ALA	2.0
1	C	234	ALA	2.0
1	A	24	THR	2.0
1	A	63	ASN	2.0
1	D	214	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

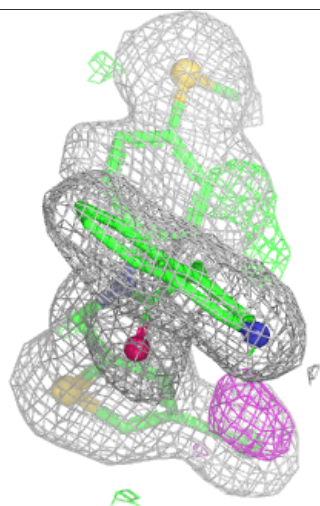
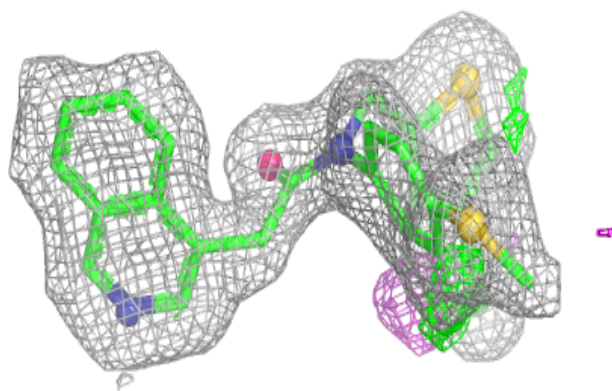
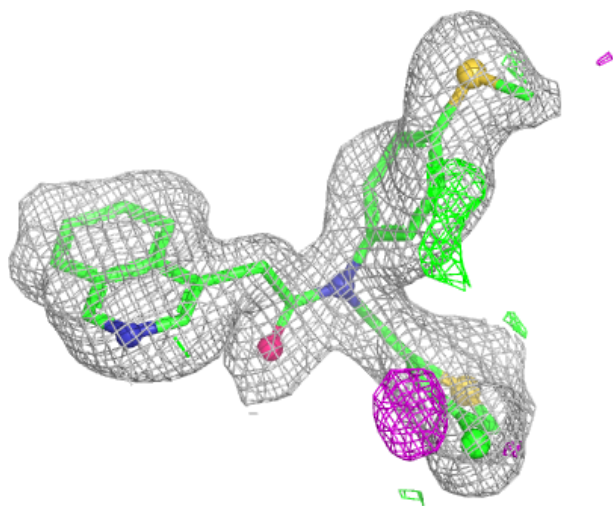
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P6I	A	401	29/29	0.91	0.10	20,27,36,37	0
2	P6I	B	401	29/29	0.91	0.10	24,32,39,42	0
2	P6I	D	401	29/29	0.94	0.10	28,33,39,40	0
2	P6I	C	401	29/29	0.95	0.08	23,31,41,48	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.

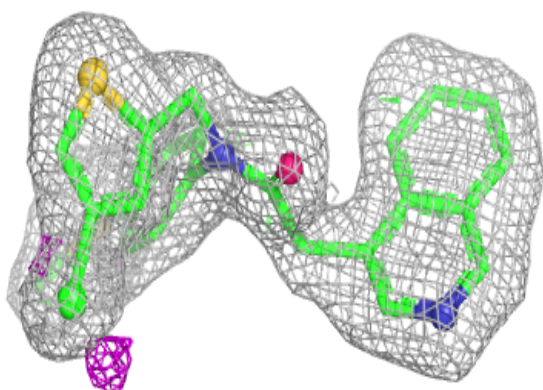
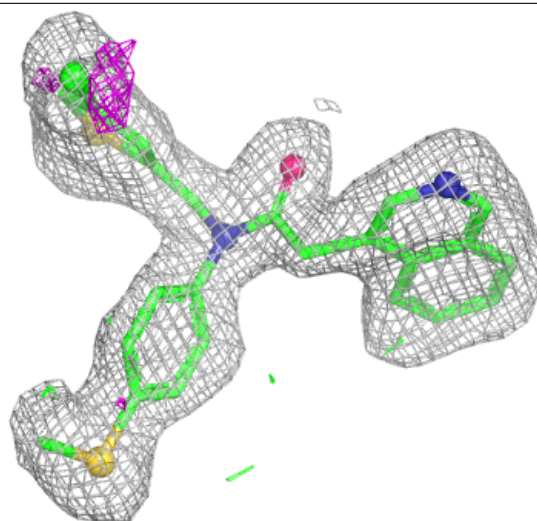
Electron density around P6I A 401:

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



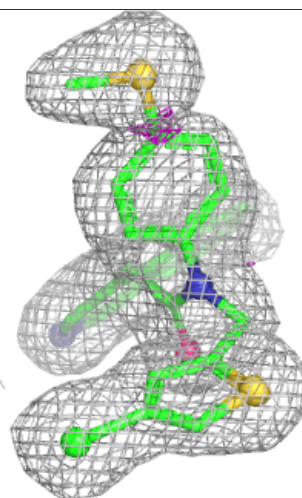
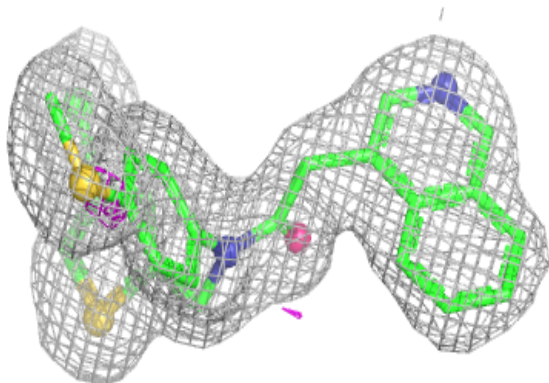
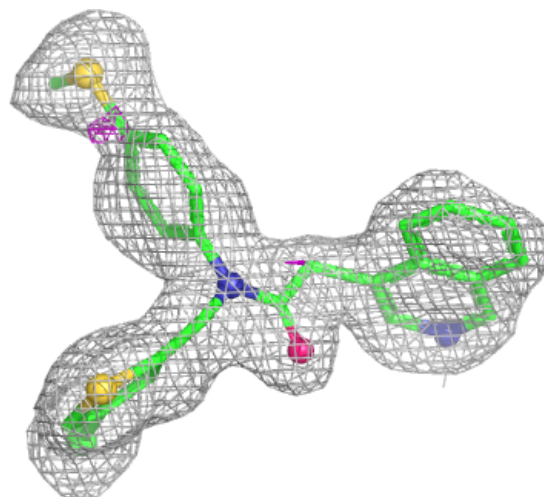
Electron density around P6I B 401:

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



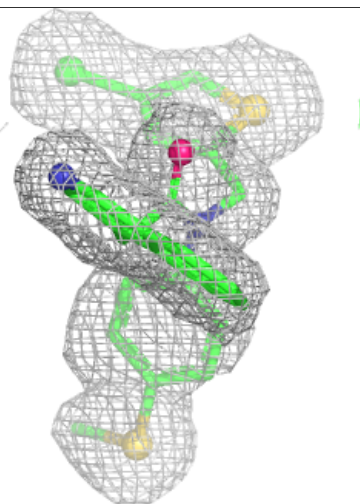
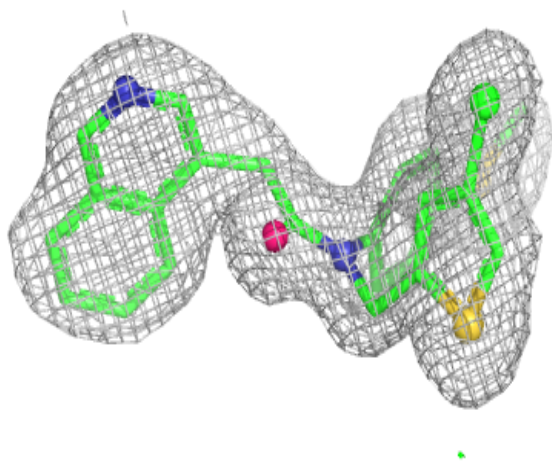
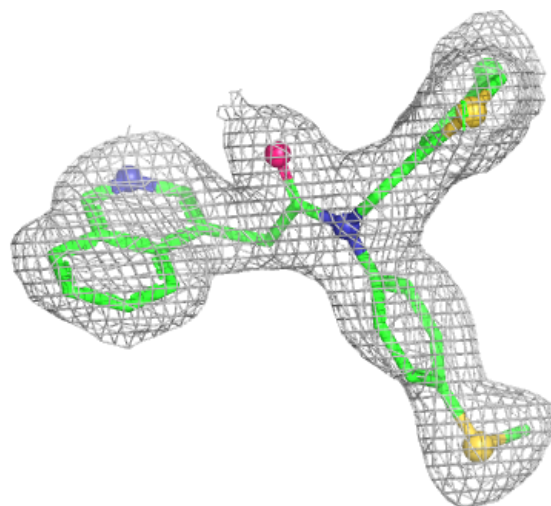
Electron density around P6I D 401:

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



Electron density around P6I C 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.