



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:27 PM UTC

PDB ID : 3NMN / pdb_00003nmn
Title : Crystal structure of pyrabactin-bound abscisic acid receptor PYL1 in complex with type 2C protein phosphatase ABI1
Authors : Zhou, X.E.; Melcher, K.; Ng, L.-M.; Soon, F.-F.; Xu, Y.; Suino-Powell, K.M.; Kovach, A.; Li, J.; Yong, E.-L.; Xu, H.E.
Deposited on : 2010-06-22
Resolution : 2.15 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

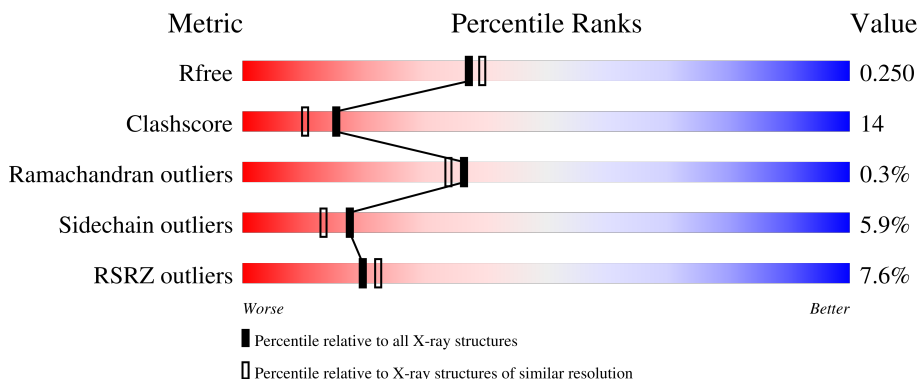
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	178	 7% 61% 28% 5% 6%
1	C	178	 6% 70% 21% 5% .
2	B	319	 6% 59% 23% . 15%
2	D	319	 8% 66% 20% . 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7184 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 Abscisic acid receptor PYL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	168	1354	843	246	260	5	0	0	0
1	C	171	1384	859	256	264	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q8VZS8
A	35	SER	-	expression tag	UNP Q8VZS8
C	34	GLY	-	expression tag	UNP Q8VZS8
C	35	SER	-	expression tag	UNP Q8VZS8

- Molecule 2 is a protein called Protein phosphatase 2C 56.

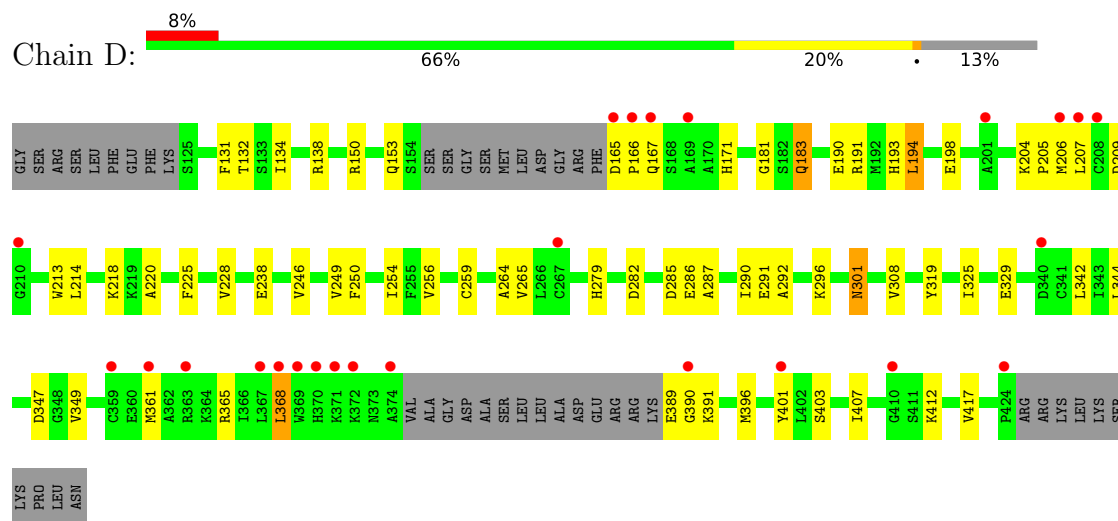
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	271	2092	1318	366	395	13	0	0	0
2	D	276	2126	1337	373	402	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	116	GLY	-	expression tag	UNP P49597
D	116	GLY	-	expression tag	UNP P49597

- Molecule 3 is 4-bromo-N-(pyridin-2-ylmethyl)naphthalene-1-sulfonamide (CCD ID: PYV) (formula: C₁₆H₁₃BrN₂O₂S).

- Molecule 2: Protein phosphatase 2C 56



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.98Å 66.71Å 72.60Å 115.78° 95.43° 105.60°	Depositor
Resolution (Å)	29.62 – 2.15 29.62 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.62-2.15) 96.9 (29.62-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.210 , 0.248 0.217 , 0.250	Depositor DCC
R_{free} test set	3617 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtrriage
Anisotropy	0.282	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	1.12	1/1378 (0.1%)	1.03	4/1865 (0.2%)
1	C	1.27	3/1408 (0.2%)	1.00	0/1904
2	B	1.21	7/2132 (0.3%)	1.00	1/2881 (0.0%)
2	D	1.22	3/2167 (0.1%)	1.02	3/2929 (0.1%)
All	All	1.21	14/7085 (0.2%)	1.01	8/9579 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	254	ILE	CA-CB	-6.37	1.46	1.54
2	B	237	PRO	C-O	-6.25	1.16	1.23
1	C	142	HIS	C-O	-6.07	1.17	1.24
2	B	325	ILE	CA-CB	-5.72	1.48	1.55
1	C	202	ALA	CA-CB	5.68	1.62	1.53
2	B	184	VAL	CA-C	-5.55	1.45	1.52
2	D	220	ALA	CA-CB	-5.53	1.44	1.53
2	D	228	VAL	CA-CB	-5.36	1.48	1.54
1	C	132	VAL	CA-CB	-5.34	1.47	1.54
1	A	170	LEU	C-O	-5.32	1.17	1.24
2	B	273	LEU	C-O	-5.31	1.19	1.24
2	D	325	ILE	CA-CB	-5.26	1.49	1.55
2	B	243	THR	CA-CB	-5.15	1.44	1.53
2	B	242	SER	N-CA	-5.03	1.40	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	235	VAL	CB-CA-C	-8.54	103.10	111.30
1	A	110	VAL	N-CA-C	-5.77	103.76	110.05
2	D	181	GLY	N-CA-C	-5.42	104.50	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	390	GLY	N-CA-C	-5.41	100.36	113.18
1	A	114	LEU	CA-C-N	5.31	125.12	119.28
1	A	114	LEU	C-N-CA	5.31	125.12	119.28
2	D	301	ASN	N-CA-C	-5.04	104.35	111.56
1	A	112	SER	N-CA-C	5.03	117.17	110.53

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	1354	0	1325	54	0
1	C	1384	0	1357	44	1
2	B	2092	0	2080	53	0
2	D	2126	0	2113	47	1
3	A	22	0	13	0	0
3	C	22	0	13	1	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	A	31	0	0	6	0
5	B	45	0	0	3	0
5	C	40	0	0	11	0
5	D	64	0	0	8	0
All	All	7184	0	6901	188	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 14.

All (188) 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:151:THR:HG23	5:A:215:HOH:O	1.52	1.10
1:C:118:THR:HB	5:C:20:HOH:O	1.54	1.05
2:D:249:VAL:HG22	5:D:51:HOH:O	1.59	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLN:HE21	1:C:83:GLN:H	1.12	0.98
2:D:361:MET:HE3	2:D:401:TYR:HB3	1.46	0.93
2:B:333:VAL:HG12	2:D:292:ALA:HB1	1.51	0.91
2:B:209:ASP:HB2	2:B:213:TRP:HB2	1.52	0.90
1:C:77:ARG:HG2	5:C:215:HOH:O	1.74	0.87
2:D:132:THR:HB	5:D:59:HOH:O	1.76	0.85
2:D:361:MET:CE	2:D:401:TYR:HB3	2.05	0.85
1:C:81:ARG:HA	1:C:83:GLN:HE22	1.42	0.83
2:D:254:ILE:HG23	5:D:51:HOH:O	1.77	0.83
2:B:391:LYS:NZ	2:B:396:MET:HE1	1.93	0.82
1:C:182:SER:O	1:C:186:THR:HG23	1.80	0.82
2:B:391:LYS:HZ2	2:B:396:MET:HE1	1.44	0.80
1:C:72:VAL:HG22	1:C:205:THR:HG21	1.66	0.78
1:A:188:LEU:HD13	2:B:296:LYS:HD2	1.66	0.77
1:C:132:VAL:HG22	1:C:152:THR:HG22	1.67	0.76
1:A:111:ILE:HG23	2:B:180:GLY:HA2	1.68	0.75
1:C:83:GLN:H	1:C:83:GLN:NE2	1.85	0.74
1:A:60:LEU:C	1:A:60:LEU:HD23	2.12	0.73
1:A:72:VAL:HG22	1:A:205:THR:HG21	1.70	0.73
2:D:134:ILE:CD1	2:D:407:ILE:HD11	2.19	0.73
1:A:99:GLU:HB3	5:A:232:HOH:O	1.91	0.71
2:D:391:LYS:HD3	2:D:396:MET:HE3	1.74	0.69
2:B:204:LYS:HG2	2:B:206:MET:HE1	1.74	0.69
1:A:201:LEU:O	1:A:205:THR:HB	1.93	0.68
1:A:60:LEU:HD23	1:A:61:LEU:N	2.09	0.68
2:D:183:GLN:HE21	2:D:183:GLN:H	1.42	0.67
2:B:209:ASP:HB3	2:B:212:THR:HB	1.76	0.67
1:C:78:ARG:N	5:C:215:HOH:O	2.26	0.67
1:A:125:LEU:HD23	1:A:125:LEU:N	2.10	0.67
1:A:110:VAL:HG21	1:A:116:ALA:O	1.96	0.66
2:D:403:SER:HB3	5:D:59:HOH:O	1.95	0.66
1:A:72:VAL:HG21	1:A:167:THR:HG21	1.79	0.65
1:C:78:ARG:HG2	5:C:215:HOH:O	1.96	0.64
1:C:81:ARG:CZ	1:C:84:ILE:HD11	2.28	0.64
1:C:114:LEU:HB3	1:C:115:PRO:HD2	1.80	0.64
2:B:203:GLU:HB3	2:B:216:LYS:HG3	1.79	0.63
1:C:52:LEU:HB2	5:C:235:HOH:O	1.98	0.63
2:B:207:LEU:HD13	2:B:207:LEU:C	2.23	0.63
2:D:206:MET:HB2	2:D:209:ASP:OD1	2.00	0.62
2:B:343:ILE:HD12	2:B:419:VAL:HG22	1.82	0.62
1:A:81:ARG:HA	1:A:83:GLN:HE22	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:NH1	1:C:81:ARG:HD3	2.15	0.61
1:A:47:PHE:HB3	1:A:150:VAL:HG11	1.83	0.61
2:B:258:ASN:ND2	5:B:438:HOH:O	2.33	0.60
2:B:193:HIS:CE1	2:B:194:LEU:HD13	2.37	0.60
1:A:60:LEU:HD21	1:A:170:LEU:HD22	1.83	0.60
1:A:188:LEU:CD1	2:B:296:LYS:HD2	2.32	0.60
2:B:277:VAL:HG21	2:D:285:ASP:HA	1.82	0.59
2:B:315:ILE:N	2:B:315:ILE:HD12	2.18	0.59
1:C:88:PHE:CD2	1:C:114:LEU:HD11	2.37	0.58
2:D:134:ILE:HD11	2:D:407:ILE:HD11	1.85	0.58
2:B:352:VAL:HB	2:B:409:ARG:HB3	1.85	0.58
2:D:193:HIS:CE1	2:D:194:LEU:HD13	2.39	0.58
1:C:47:PHE:HB3	1:C:150:VAL:HG11	1.86	0.57
2:D:209:ASP:HB2	2:D:213:TRP:HB2	1.86	0.57
2:D:249:VAL:HA	5:D:51:HOH:O	2.05	0.57
1:A:65:ILE:HB	1:A:167:THR:HG23	1.85	0.57
1:C:96:GLU:H	1:C:96:GLU:CD	2.13	0.57
2:B:204:LYS:CG	2:B:206:MET:HE1	2.34	0.56
1:A:111:ILE:CG2	2:B:180:GLY:HA2	2.36	0.56
2:B:264:ALA:HB2	2:B:344:LEU:HD22	1.87	0.55
1:C:72:VAL:CG2	1:C:205:THR:HG21	2.35	0.55
1:A:122:ARG:NH1	1:A:124:ASP:OD1	2.39	0.55
2:B:391:LYS:HD3	2:B:396:MET:HE2	1.88	0.55
2:B:270:LYS:HA	2:B:363:ARG:NH2	2.22	0.55
1:A:83:GLN:HE21	1:A:83:GLN:H	1.54	0.54
1:A:171:GLU:HB2	5:A:215:HOH:O	2.07	0.54
2:D:287:ALA:O	2:D:291:GLU:HG2	2.07	0.54
1:A:125:LEU:HD21	1:A:134:GLY:HA3	1.91	0.53
2:D:150:ARG:H	2:D:171:HIS:HD2	1.56	0.53
1:A:59:SER:HB2	1:A:187:ARG:HD3	1.91	0.53
2:D:167:GLN:HA	2:D:250:PHE:HE1	1.72	0.53
2:B:337:LYS:HG3	2:B:338:GLU:OE2	2.08	0.53
1:A:122:ARG:NH1	5:A:216:HOH:O	2.31	0.53
1:C:188:LEU:HD13	2:D:296:LYS:HD2	1.90	0.52
2:D:132:THR:HG22	2:D:134:ILE:HG23	1.90	0.52
1:A:200:LYS:HG2	1:A:204:ILE:HD13	1.91	0.52
2:B:368:LEU:C	2:B:368:LEU:HD12	2.35	0.52
1:C:114:LEU:HB3	1:C:115:PRO:CD	2.38	0.52
2:B:333:VAL:CG1	2:D:292:ALA:HB1	2.33	0.52
1:C:59:SER:HB3	1:C:173:TYR:CE2	2.45	0.52
2:D:365:ARG:HA	2:D:368:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:HB2	1:A:101:ARG:HD2	1.92	0.51
1:A:178:PRO:HG2	2:B:300:TRP:CH2	2.46	0.51
1:C:78:ARG:HH12	1:C:81:ARG:HD3	1.76	0.51
1:C:61:LEU:HD12	1:C:61:LEU:N	2.26	0.51
2:D:365:ARG:HD3	5:D:437:HOH:O	2.11	0.51
1:A:110:VAL:CG2	1:A:116:ALA:O	2.59	0.50
2:D:138:ARG:HG2	2:D:412:LYS:O	2.11	0.50
2:B:222:PHE:CD1	2:B:328:PRO:HD2	2.46	0.50
2:D:391:LYS:CD	2:D:396:MET:HE3	2.41	0.50
2:D:225:PHE:HE2	2:D:259:CYS:HB3	1.77	0.50
1:A:83:GLN:HG3	1:A:89:ILE:HG21	1.94	0.49
1:C:81:ARG:CA	1:C:83:GLN:HE22	2.20	0.49
2:D:254:ILE:HG12	5:D:51:HOH:O	2.12	0.49
2:B:274:PRO:HD2	5:B:17:HOH:O	2.12	0.49
1:C:77:ARG:CG	5:C:215:HOH:O	2.45	0.48
2:D:191:ARG:HH22	2:D:198:GLU:CD	2.21	0.48
1:A:88:PHE:C	1:A:111:ILE:HD12	2.39	0.48
1:A:83:GLN:H	1:A:83:GLN:NE2	2.10	0.48
1:A:114:LEU:HB3	1:A:115:PRO:HD2	1.95	0.48
2:B:305:VAL:HG21	2:B:324:ILE:HD11	1.96	0.48
1:A:40:LEU:C	1:A:40:LEU:HD23	2.38	0.48
1:C:80:ASP:OD2	1:C:94:VAL:HG11	2.14	0.47
1:C:51:GLN:HB3	5:C:233:HOH:O	2.14	0.47
1:C:52:LEU:HD13	1:C:54:ASN:O	2.14	0.47
1:C:114:LEU:HD22	2:D:308:VAL:HG13	1.96	0.47
1:A:64:ARG:HG3	1:A:168:VAL:HG22	1.95	0.47
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.80	0.47
2:B:127:PRO:HB3	2:B:171:HIS:CD2	2.49	0.47
2:D:368:LEU:C	2:D:368:LEU:HD23	2.40	0.47
2:B:203:GLU:OE2	2:B:219:LYS:HD3	2.14	0.47
1:A:97:ASP:O	5:A:224:HOH:O	2.20	0.47
1:A:114:LEU:HB3	1:A:115:PRO:CD	2.45	0.47
1:A:101:ARG:HD3	1:A:101:ARG:O	2.15	0.46
1:C:101:ARG:O	1:C:102:VAL:C	2.57	0.46
2:B:313:ARG:O	2:B:314:SER:HB3	2.15	0.46
2:B:273:LEU:HD23	5:B:17:HOH:O	2.16	0.46
2:D:403:SER:O	2:D:407:ILE:HG13	2.16	0.46
1:C:56:ARG:NE	5:C:227:HOH:O	2.49	0.46
1:C:60:LEU:C	1:C:61:LEU:HD12	2.40	0.46
2:D:131:PHE:H	2:D:396:MET:HE1	1.81	0.46
2:B:251:PRO:O	2:B:335:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:VAL:O	2:D:342:LEU:HD12	2.16	0.46
1:A:169:VAL:HG12	5:A:215:HOH:O	2.16	0.45
1:C:107:ASP:OD1	1:C:120:ARG:HG3	2.16	0.45
1:A:40:LEU:HD23	1:A:40:LEU:O	2.16	0.45
1:C:118:THR:HG22	1:C:119:SER:N	2.31	0.45
2:B:268:ARG:HH11	2:B:336:VAL:HG22	1.81	0.45
1:A:190:ALA:O	1:A:193:VAL:HG22	2.16	0.45
2:B:245:VAL:O	2:B:245:VAL:HG13	2.16	0.45
2:B:244:SER:HB3	2:B:315:ILE:HD11	1.99	0.44
2:B:184:VAL:HG23	2:B:240:VAL:HG12	1.99	0.44
2:B:252:SER:OG	2:B:253:HIS:HD2	2.00	0.44
1:A:81:ARG:HA	1:A:83:GLN:NE2	2.30	0.44
2:B:268:ARG:HD3	2:B:339:ASP:OD1	2.17	0.44
2:D:286:GLU:O	2:D:290:ILE:HG12	2.16	0.44
1:C:56:ARG:CZ	5:C:227:HOH:O	2.65	0.44
1:C:139:GLY:O	1:C:142:HIS:HE1	2.00	0.44
1:C:81:ARG:NH2	1:C:84:ILE:HD11	2.33	0.44
1:A:60:LEU:C	1:A:60:LEU:CD2	2.83	0.43
2:D:207:LEU:HD13	2:D:213:TRP:CZ2	2.53	0.43
1:C:52:LEU:HD23	5:C:235:HOH:O	2.18	0.43
2:D:264:ALA:HB2	2:D:344:LEU:CD2	2.47	0.43
2:D:347:ASP:OD2	2:D:347:ASP:C	2.61	0.43
2:D:238:GLU:O	2:D:319:TYR:HD2	2.01	0.43
2:B:342:LEU:C	2:B:343:ILE:HD13	2.44	0.43
2:D:166:PRO:O	2:D:207:LEU:HD22	2.18	0.43
1:A:166:TRP:HA	1:A:166:TRP:CE3	2.54	0.43
2:B:207:LEU:HD22	2:B:207:LEU:O	2.18	0.43
2:D:349:VAL:HG21	2:D:417:VAL:HG22	2.00	0.43
2:D:204:LYS:N	2:D:205:PRO:HD3	2.35	0.42
1:C:57:CYS:HB3	1:C:183:GLU:HG2	2.01	0.42
1:A:68:PRO:HG2	1:A:71:THR:OG1	2.19	0.42
2:B:170:ALA:HB2	2:B:250:PHE:CZ	2.55	0.42
1:C:177:VAL:HG13	1:C:186:THR:HG21	2.00	0.42
1:A:65:ILE:HG21	1:A:205:THR:CG2	2.49	0.42
1:C:114:LEU:HD13	3:C:900:PYV:BR	2.75	0.42
1:C:120:ARG:N	1:C:120:ARG:HD3	2.34	0.42
1:A:193:VAL:HG23	1:A:194:ILE:N	2.33	0.42
2:B:191:ARG:O	2:B:192:MET:C	2.62	0.42
1:A:99:GLU:HB2	1:A:101:ARG:CD	2.49	0.42
2:B:200:ILE:HD12	2:B:220:ALA:HB1	2.02	0.42
1:A:65:ILE:HG21	1:A:205:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ALA:CB	2:B:344:LEU:HD22	2.50	0.41
1:A:66:HIS:HB3	1:A:166:TRP:CH2	2.56	0.41
1:A:99:GLU:HG3	1:A:104:CYS:SG	2.61	0.41
2:B:179:HIS:HE2	2:B:317:ASP:CG	2.29	0.41
1:C:118:THR:CB	5:C:20:HOH:O	2.35	0.41
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.90	0.41
2:B:147:THR:C	2:B:148:ILE:HG13	2.46	0.41
2:B:149:PRO:O	2:B:150:ARG:C	2.63	0.41
2:B:247:ALA:HA	2:B:255:PHE:O	2.21	0.41
2:D:165:ASP:HB3	2:D:166:PRO:HD3	2.02	0.41
2:D:214:LEU:O	2:D:214:LEU:HD23	2.21	0.41
1:A:110:VAL:HG22	1:A:117:ASN:C	2.46	0.41
2:B:342:LEU:O	2:B:343:ILE:HD13	2.21	0.41
1:C:81:ARG:HA	1:C:83:GLN:NE2	2.23	0.41
2:B:145:VAL:HG12	2:B:146:SER:N	2.36	0.40
2:D:246:VAL:O	2:D:256:VAL:HA	2.20	0.40
2:B:340:ASP:CG	2:B:363:ARG:HD3	2.45	0.40
2:D:218:LYS:NZ	5:D:44:HOH:O	2.55	0.40
1:A:118:THR:HG22	1:A:119:SER:N	2.35	0.40
1:A:166:TRP:HA	1:A:166:TRP:HE3	1.86	0.40
2:D:279:HIS:HE2	2:D:329:GLU:CG	2.35	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)
1:C:54:ASN:ND2	2:D:389:GLU:O[1_455]	2.16	0.04

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	164/178 (92%)	156 (95%)	8 (5%)	0	100	100
1	C	167/178 (94%)	159 (95%)	8 (5%)	0	100	100
2	B	263/319 (82%)	245 (93%)	15 (6%)	3 (1%)	11	7
2	D	270/319 (85%)	257 (95%)	13 (5%)	0	100	100
All	All	864/994 (87%)	817 (95%)	44 (5%)	3 (0%)	36	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	153	GLN
2	B	269	GLY
2	B	166	PRO

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	153/162 (94%)	140 (92%)	13 (8%)	10	6
1	C	156/162 (96%)	143 (92%)	13 (8%)	10	6
2	B	225/265 (85%)	213 (95%)	12 (5%)	20	17
2	D	229/265 (86%)	222 (97%)	7 (3%)	35	37
All	All	763/854 (89%)	718 (94%)	45 (6%)	18	13

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	49	THR
1	A	51	GLN
1	A	60	LEU
1	A	83	GLN
1	A	101	ARG
1	A	111	ILE
1	A	123	LEU

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Mol	Chain	Res	Type
1	A	148	LYS
1	A	166	TRP
1	A	179	GLU
1	A	186	THR
1	A	205	THR
2	B	140	GLU
2	B	150	ARG
2	B	183	GLN
2	B	194	LEU
2	B	202	LYS
2	B	204	LYS
2	B	206	MET
2	B	207	LEU
2	B	216	LYS
2	B	235	VAL
2	B	284	GLU
2	B	337	LYS
1	C	51	GLN
1	C	52	LEU
1	C	60	LEU
1	C	83	GLN
1	C	96	GLU
1	C	97	ASP
1	C	99	GLU
1	C	120	ARG
1	C	121	GLU
1	C	123	LEU
1	C	156	PHE
1	C	186	THR
1	C	206	GLU
2	D	153	GLN
2	D	183	GLN
2	D	190	GLU
2	D	194	LEU
2	D	282	ASP
2	D	301	ASN
2	D	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN

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Mol	Chain	Res	Type
1	A	83	GLN
1	A	93	ASN
1	A	146	ASN
2	B	167	GLN
2	B	183	GLN
2	B	193	HIS
2	B	253	HIS
2	B	258	ASN
2	B	299	GLN
2	B	408	GLN
1	C	42	GLN
1	C	51	GLN
1	C	66	HIS
1	C	83	GLN
1	C	117	ASN
1	C	142	HIS
1	C	154	HIS
1	C	199	GLN
2	D	171	HIS
2	D	183	GLN
2	D	193	HIS
2	D	223	ASN
2	D	253	HIS
2	D	299	GLN
2	D	408	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	PYV	C	900	-	24,24,24	4.23	8 (33%)	33,34,34	3.18	12 (36%)
3	PYV	A	900	-	24,24,24	4.29	8 (33%)	33,34,34	2.97	14 (42%)

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	PYV	C	900	-	-	1/12/12/12	0/3/3/3
3	PYV	A	900	-	-	0/12/12/12	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	PYV	BR-C1	-13.88	1.52	1.90
3	C	900	PYV	C4-S	-13.59	1.63	1.77
3	C	900	PYV	BR-C1	-13.17	1.54	1.90
3	A	900	PYV	C4-S	-12.81	1.64	1.77
3	A	900	PYV	C3-C2	5.63	1.54	1.43
3	C	900	PYV	C3-C2	5.08	1.53	1.43
3	A	900	PYV	C5-C4	3.23	1.41	1.37
3	C	900	PYV	C11-N1	-3.21	1.42	1.47
3	C	900	PYV	C5-C4	3.01	1.41	1.37
3	A	900	PYV	C11-N1	-3.00	1.42	1.47
3	A	900	PYV	O2-S	2.55	1.46	1.43
3	C	900	PYV	C6-C5	2.39	1.42	1.38
3	A	900	PYV	C9-C10	2.37	1.41	1.36
3	A	900	PYV	C6-C1	2.21	1.41	1.36
3	C	900	PYV	C15-C16	2.08	1.42	1.38
3	C	900	PYV	O2-S	2.03	1.45	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	900	PYV	O2-S-O1	-10.62	106.62	119.52
3	A	900	PYV	O2-S-O1	-8.28	109.47	119.52
3	C	900	PYV	C6-C1-C2	-6.30	112.31	121.87
3	C	900	PYV	C1-C2-C3	6.21	123.99	117.56
3	A	900	PYV	C6-C1-C2	-5.99	112.79	121.87
3	A	900	PYV	C1-C2-C3	5.66	123.42	117.56
3	C	900	PYV	C5-C4-C3	-5.11	115.25	120.95
3	A	900	PYV	C13-N2-C12	4.95	124.36	117.41
3	A	900	PYV	C5-C4-C3	-4.88	115.50	120.95
3	C	900	PYV	O2-S-N1	4.51	114.06	107.03
3	C	900	PYV	C3-C4-S	4.45	126.89	121.66
3	A	900	PYV	BR-C1-C2	4.05	127.49	119.75
3	C	900	PYV	BR-C1-C2	4.01	127.42	119.75
3	C	900	PYV	C4-S-N1	3.59	113.42	106.78
3	A	900	PYV	C4-S-N1	3.33	112.94	106.78
3	C	900	PYV	O1-S-N1	-3.29	101.91	107.03
3	A	900	PYV	C3-C4-S	3.17	125.38	121.66
3	A	900	PYV	C6-C5-C4	3.10	125.43	121.66
3	A	900	PYV	C16-C12-N2	-3.07	117.80	122.22
3	A	900	PYV	O1-S-C4	3.03	113.37	108.09
3	A	900	PYV	O2-S-N1	-2.98	102.39	107.03
3	C	900	PYV	C5-C6-C1	2.71	125.50	120.69
3	C	900	PYV	C10-C2-C1	-2.56	119.15	124.93
3	A	900	PYV	C14-C13-N2	-2.30	119.78	123.42
3	A	900	PYV	C10-C2-C1	-2.19	119.97	124.93
3	C	900	PYV	O2-S-C4	2.01	111.59	108.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	900	PYV	C11-N1-S-O2

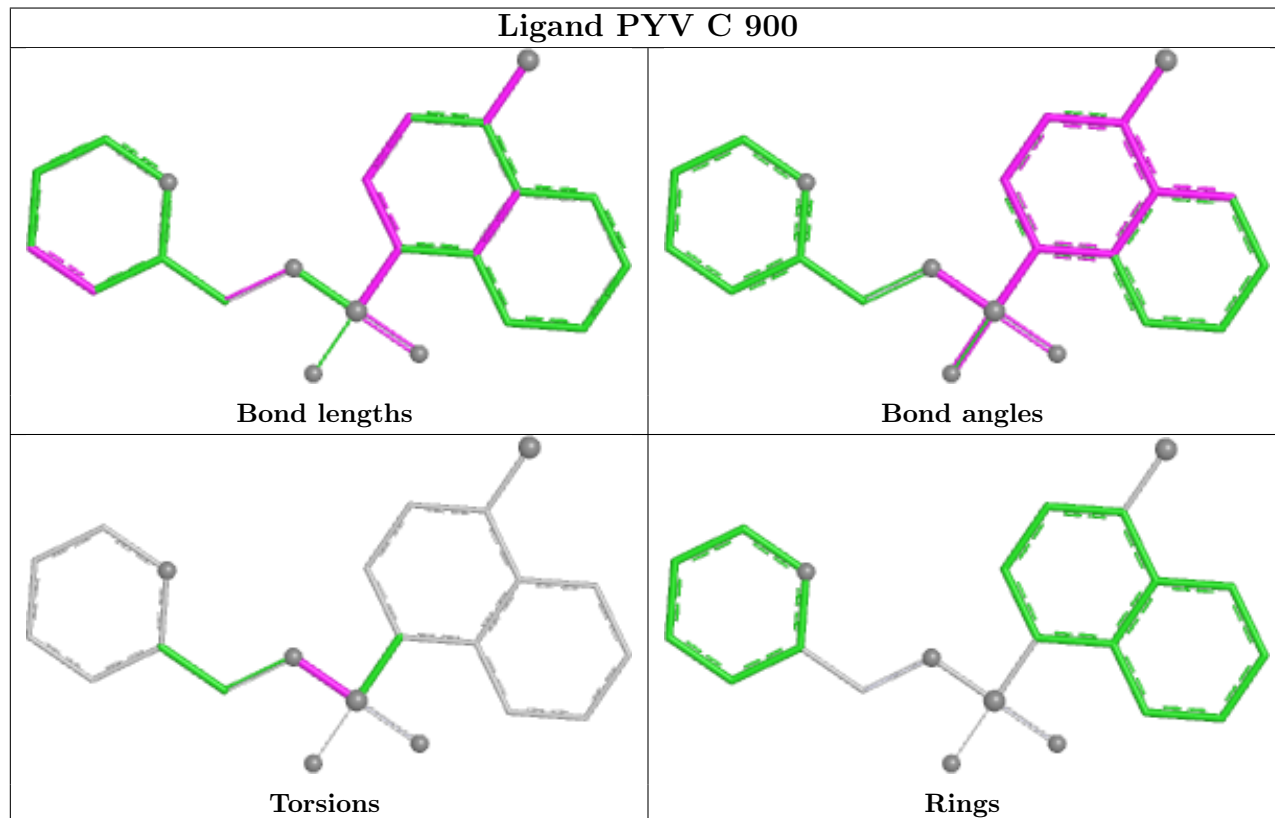
There are no ring outliers.

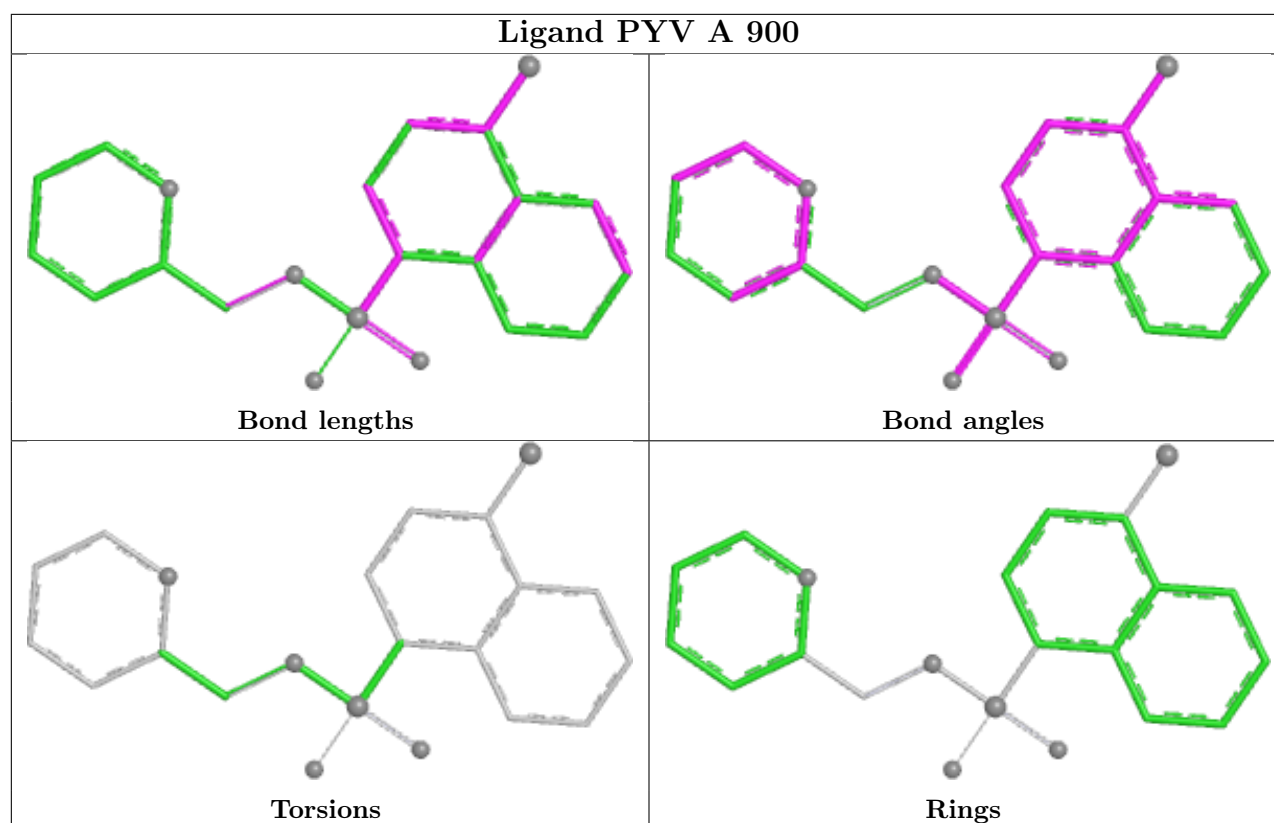
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	900	PYV	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.





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	168/178 (94%)	0.60	13 (7%) 19 22	28, 47, 90, 107	0
1	C	171/178 (96%)	0.29	11 (6%) 25 28	21, 38, 74, 105	0
2	B	271/319 (84%)	0.37	18 (6%) 24 27	17, 42, 86, 123	0
2	D	276/319 (86%)	0.49	25 (9%) 15 16	24, 43, 92, 111	0
All	All	886/994 (89%)	0.43	67 (7%) 20 22	17, 43, 87, 123	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	207	LEU	5.2
1	A	98	PHE	5.1
1	A	97	ASP	4.6
2	B	369	TRP	4.5
2	B	368	LEU	4.5
1	C	52	LEU	4.3
2	B	207	LEU	4.2
2	D	167	GLN	4.2
2	D	401	TYR	4.0
2	D	371	LYS	3.9
1	A	156	PHE	3.8
1	A	165	ILE	3.8
2	D	368	LEU	3.8
1	C	35	SER	3.6
2	D	267	CYS	3.3
1	C	165	ILE	3.3
1	C	166	TRP	3.3
2	D	390	GLY	3.2
2	B	209	ASP	3.1
1	A	166	TRP	3.1
2	B	401	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	390	GLY	3.1
1	A	96	GLU	3.1
2	D	169	ALA	3.1
2	D	374	ALA	3.0
2	B	205	PRO	3.0
2	B	166	PRO	2.9
1	C	54	ASN	2.9
2	D	166	PRO	2.8
2	B	206	MET	2.7
1	C	37	PHE	2.6
2	D	367	LEU	2.6
2	D	369	TRP	2.6
2	D	424	PRO	2.6
1	C	164	ARG	2.6
2	D	340	ASP	2.6
1	A	35	SER	2.6
1	A	207	ALA	2.5
2	B	394	ALA	2.5
2	D	361	MET	2.5
2	B	126	VAL	2.5
2	D	208	CYS	2.5
2	D	201	ALA	2.5
2	D	210	GLY	2.4
2	B	154	SER	2.4
2	D	372	LYS	2.4
2	B	412	LYS	2.4
2	D	410	GLY	2.3
1	C	211	ASN	2.3
1	A	102	VAL	2.3
2	B	365	ARG	2.3
2	B	366	ILE	2.2
2	D	206	MET	2.2
1	C	80	ASP	2.2
2	D	359	CYS	2.2
2	B	393	PRO	2.1
1	A	66	HIS	2.1
1	A	205	THR	2.1
2	B	370	HIS	2.1
2	D	363	ARG	2.1
2	D	165	ASP	2.1
1	A	53	GLY	2.1
1	C	53	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	94	VAL	2.1
1	C	156	PHE	2.1
2	B	167	GLN	2.0
2	D	370	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

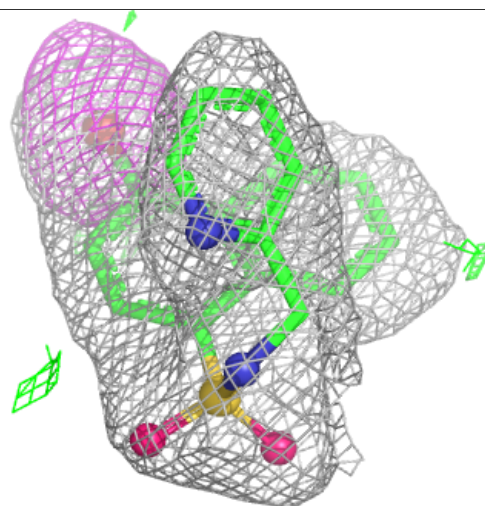
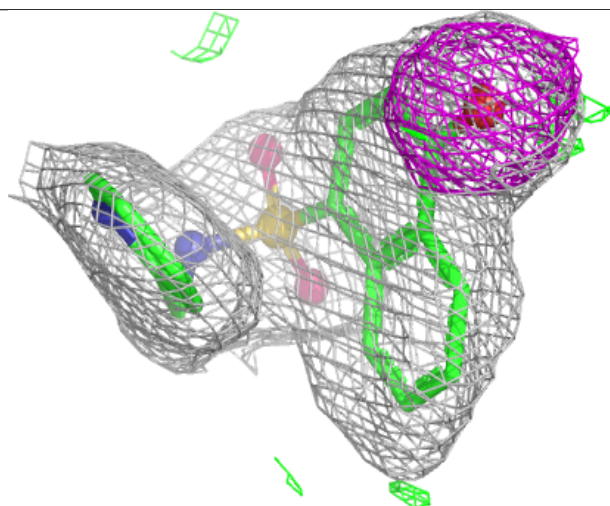
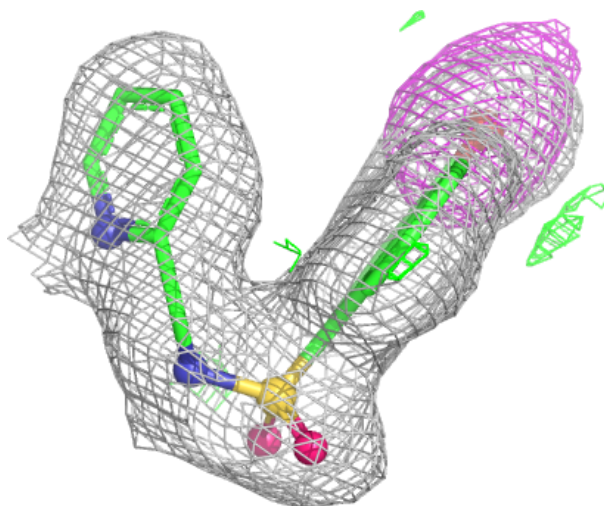
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

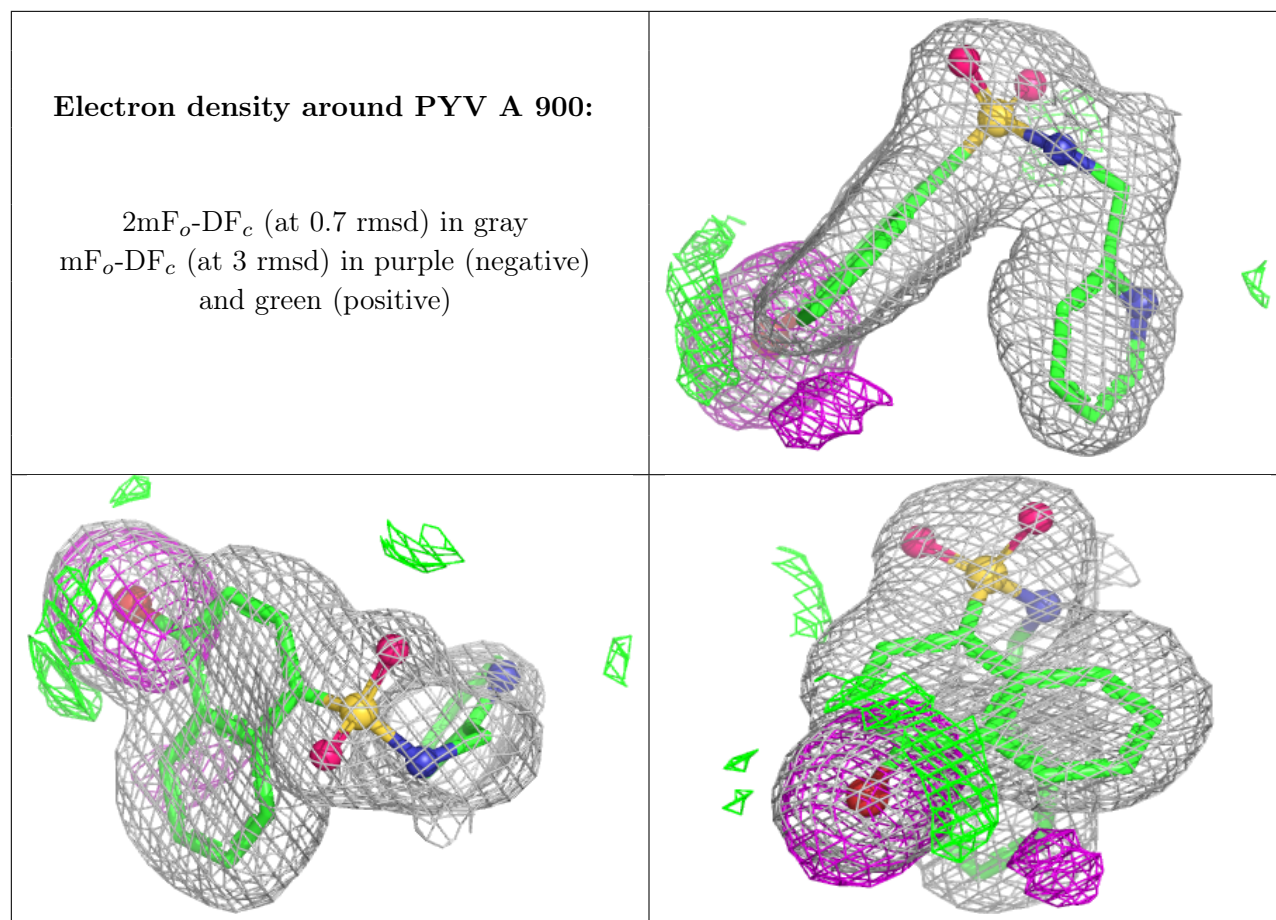
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	D	999	1/1	0.76	0.20	64,64,64,64	0
3	PYV	C	900	22/22	0.90	0.14	31,43,44,44	0
3	PYV	A	900	22/22	0.91	0.14	25,43,46,49	0
4	MG	B	998	1/1	0.96	0.10	52,52,52,52	0
4	MG	D	998	1/1	0.98	0.10	34,34,34,34	0
4	MG	B	999	1/1	0.98	0.12	43,43,43,43	0

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 PYV C 900:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.