



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:41 AM UTC

PDB ID : 5YWG / pdb_00005ywg
Title : Crystal structure of Arabidopsis thaliana HPPD complexed with Mesotrione
Authors : Lin, H.Y.; Yang, W.C.
Deposited on : 2017-11-29
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

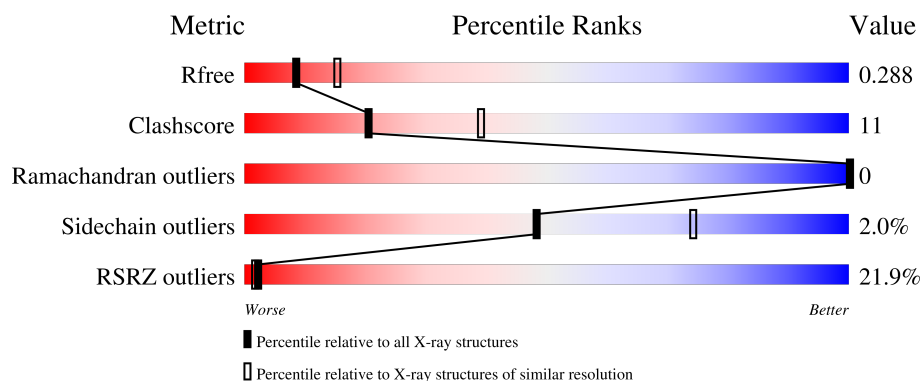
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	445	17% 62% 19% • 18%
1	B	445	20% 62% 21% 17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5743 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.

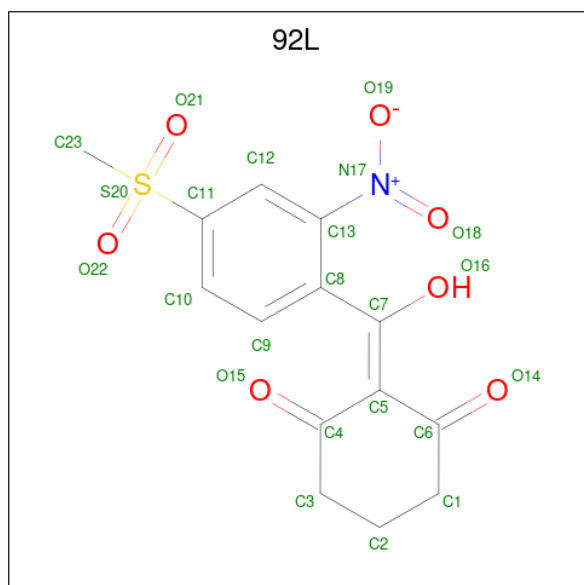
- Molecule 1 is a protein called 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	3	0
			2830	1807	484	525	14			
1	B	369	Total	C	N	O	S	0	2	0
			2855	1829	485	527	14			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		

- Molecule 3 is 2-[(4-methylsulfonyl-2-nitro-phenyl)-oxidanyl-methylidene]cyclohexane-1,3-dione (CCD ID: 92L) (formula: C₁₄H₁₃NO₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	14	1	7	1		
3	B	1	Total	C	N	O	S	0	0
			23	14	1	7	1		

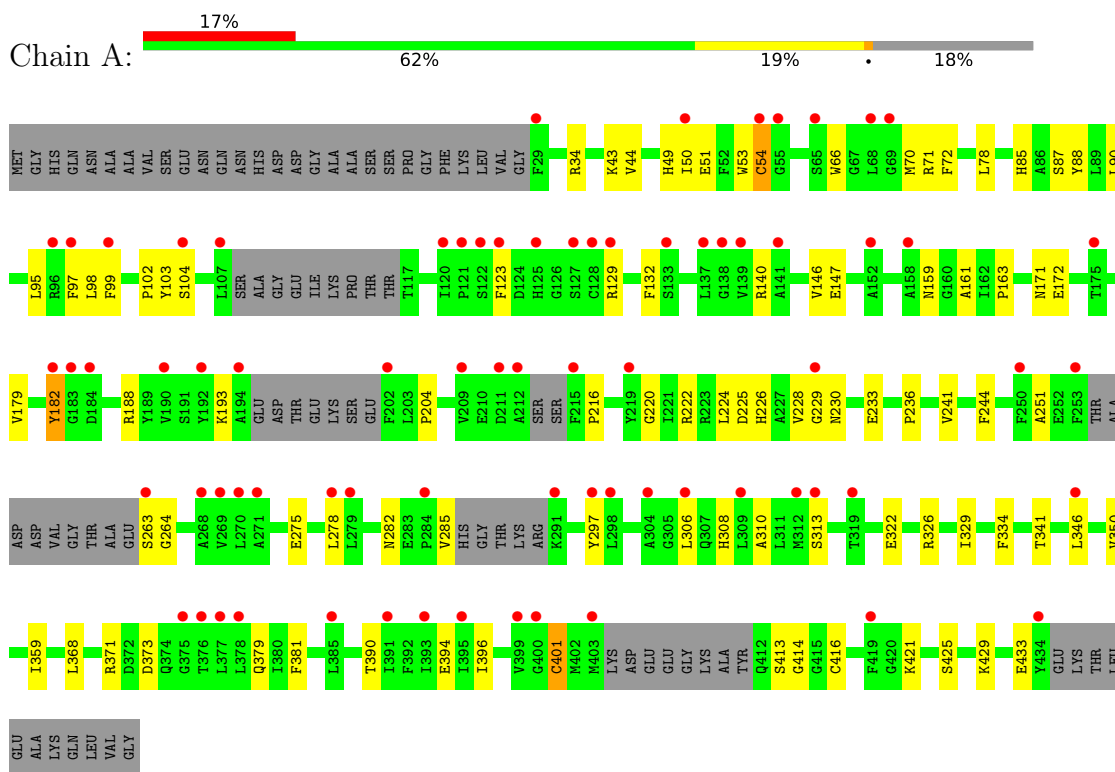
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	4	Total	O	0	0
			4	4		

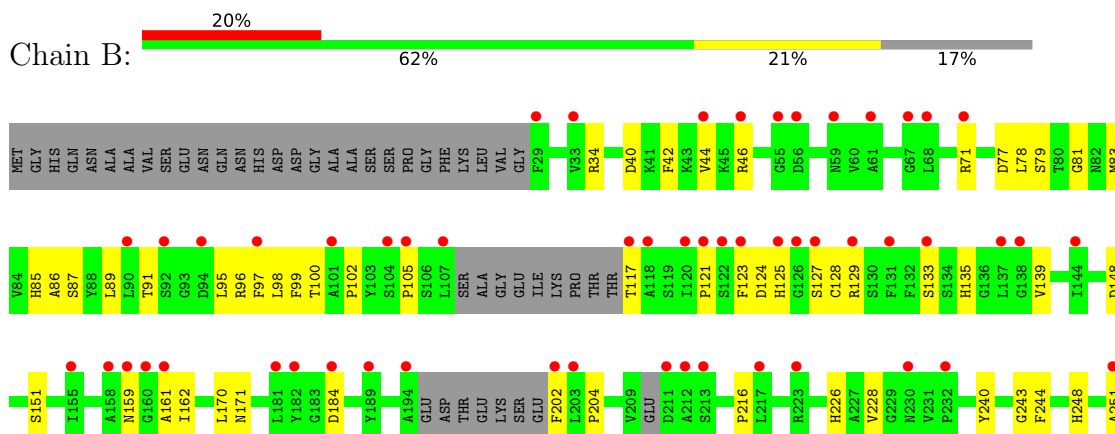
3 Residue-property plots [i](#)

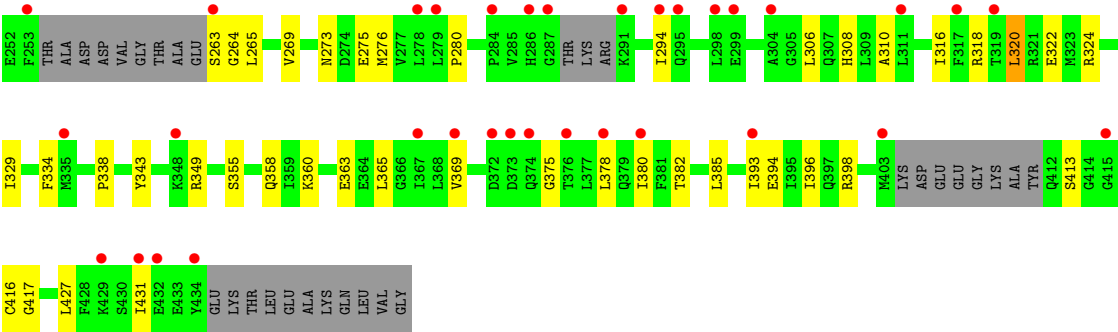
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-hydroxyphenylpyruvate dioxygenase



- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.72Å 95.72Å 195.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.76 – 2.60 35.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (35.76-2.60) 98.9 (35.76-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.262 , 0.307 (Not available) , 0.288	Depositor DCC
R_{free} test set	1442 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5743	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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 24.27 % 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 3.9626e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 92L, CO

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	0.44	0/2910	0.65	2/3926 (0.1%)
1	B	0.43	0/2931	0.64	0/3955
All	All	0.43	0/5841	0.65	2/7881 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	PHE	CA-C-N	5.17	128.01	120.51
1	A	334	PHE	C-N-CA	5.17	128.01	120.51

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	2830	0	2754	62	0
1	B	2855	0	2780	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	23	0	0	2	0
3	B	23	0	0	0	0
4	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
All	All	5743	0	5534	126	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 11.

All (126) 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:B:161:ALA:HB2	1:B:244:PHE:CG	2.26	0.70
1:B:91:THR:HG22	1:B:96:ARG:HG2	1.76	0.67
1:B:161:ALA:HB2	1:B:244:PHE:CD2	2.30	0.67
1:B:139:VAL:HG11	1:B:306:LEU:HD13	1.77	0.66
1:A:171:ASN:ND2	1:A:204:PRO:HB3	2.11	0.66
1:B:135:HIS:NE2	1:B:184:ASP:OD2	2.28	0.63
1:A:129:ARG:HH22	1:B:129:ARG:HH22	1.45	0.63
1:B:102:PRO:HD3	1:B:128:CYS:SG	2.39	0.62
1:A:229:GLY:HA2	1:A:306:LEU:HA	1.82	0.62
1:A:421:LYS:HB2	4:A:601:HOH:O	2.00	0.62
1:A:34:ARG:NH2	1:A:373:ASP:OD1	2.33	0.62
1:A:70:MET:HE1	1:A:97:PHE:HB2	1.81	0.60
1:B:87:SER:HA	1:B:99:PHE:O	2.00	0.60
1:A:225:ASP:OD2	1:A:226:HIS:ND1	2.31	0.59
1:B:248:HIS:NE2	1:B:275:GLU:OE1	2.32	0.59
1:B:87:SER:HB3	1:B:98:LEU:HD11	1.84	0.58
1:A:322:GLU:OE1	1:A:326:ARG:NH1	2.34	0.58
1:A:228:VAL:HG21	1:A:308:HIS:CE1	2.39	0.58
1:A:230:ASN:ND2	1:A:282:ASN:HB2	2.18	0.58
1:B:427:LEU:O	1:B:431:ILE:HG12	2.03	0.58
1:A:71:ARG:HD3	1:A:216:PRO:HB2	1.86	0.58
1:B:95:LEU:HD12	1:B:96:ARG:N	2.20	0.57
1:B:398:ARG:NH1	1:B:416:CYS:O	2.32	0.57
1:A:34:ARG:NH1	1:A:251:ALA:O	2.37	0.57
1:B:77:ASP:OD1	1:B:79:SER:OG	2.21	0.57
1:A:95:LEU:HD13	1:A:224:LEU:HB2	1.86	0.57
1:A:233:GLU:O	1:A:236:PRO:HD2	2.05	0.57
1:A:350:VAL:HG12	1:A:371:ARG:HD2	1.87	0.57
1:B:71:ARG:HD3	1:B:216:PRO:HB2	1.86	0.57
1:A:401:CYS:N	1:A:416:CYS:SG	2.74	0.56
1:A:72:PHE:HE1	1:A:88:TYR:HB3	1.70	0.55
1:A:263:SER:OG	1:A:264:GLY:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ARG:NH2	1:B:369:VAL:O	2.40	0.54
1:B:121:PRO:HG3	1:B:170:LEU:HD21	1.88	0.54
1:B:320:LEU:HD21	1:B:380:ILE:HG21	1.90	0.54
1:A:53:TRP:CE2	1:A:140:ARG:HG2	2.43	0.54
1:B:124:ASP:HB3	1:B:127:SER:HB2	1.89	0.54
1:A:163:PRO:HA	1:A:179:VAL:HG12	1.89	0.53
1:B:263:SER:OG	1:B:264:GLY:N	2.41	0.53
1:A:43:LYS:HG2	1:A:147:GLU:HG3	1.89	0.53
1:B:40:ASP:HB2	1:B:273:ASN:ND2	2.24	0.53
1:A:71:ARG:HH11	1:A:216:PRO:HB2	1.74	0.53
1:B:394:GLU:HG2	1:B:396:ILE:HG23	1.91	0.53
1:B:226:HIS:CE1	1:B:310:ALA:HB2	2.45	0.52
1:B:171:ASN:ND2	1:B:204:PRO:HB3	2.25	0.52
1:A:230:ASN:HD22	1:A:282:ASN:HB2	1.75	0.52
1:A:228:VAL:O	1:A:306:LEU:HG	2.10	0.51
1:B:385:LEU:HD11	1:B:393:ILE:HG13	1.94	0.50
1:A:226:HIS:HB3	1:A:278:LEU:HB2	1.93	0.50
1:B:338:PRO:HD2	1:B:343:TYR:OH	2.11	0.50
1:A:381:PHE:CE2	3:A:502:92L:O19	2.65	0.49
1:A:379:GLN:HB3	1:A:396:ILE:HG22	1.93	0.49
1:A:102:PRO:HB3	1:A:123:PHE:HZ	1.77	0.49
3:A:502:92L:O19	3:A:502:92L:O16	2.29	0.49
1:A:44:VAL:HG12	1:A:146:VAL:HG12	1.95	0.49
1:A:66:TRP:CE3	1:B:329:ILE:HB	2.48	0.49
1:A:159:ASN:HB3	1:A:244:PHE:HA	1.95	0.49
1:A:161:ALA:HB2	1:A:244:PHE:CG	2.49	0.48
1:A:220:GLY:O	1:A:222:ARG:HG2	2.13	0.48
1:A:310:ALA:HA	1:A:394:GLU:O	2.13	0.48
1:B:369:VAL:HG22	1:B:378:LEU:HD13	1.96	0.48
1:B:46:ARG:CZ	1:B:276:MET:HG3	2.44	0.48
1:A:72:PHE:CE1	1:A:88:TYR:HB3	2.49	0.47
1:B:162:ILE:HD12	1:B:240:TYR:CE1	2.49	0.47
1:A:275:GLU:O	1:A:414:GLY:HA3	2.14	0.47
1:A:182:TYR:O	1:A:182:TYR:HD1	1.98	0.47
1:A:264:GLY:HA2	1:A:285:VAL:HB	1.97	0.47
1:B:161:ALA:HA	1:B:240:TYR:CE1	2.49	0.47
1:A:346:LEU:HD12	1:A:359:ILE:HG23	1.96	0.47
1:A:241:VAL:HA	1:A:244:PHE:CE2	2.50	0.47
1:B:89:LEU:HD22	1:B:202:PHE:CG	2.50	0.47
1:B:228:VAL:HG13	1:B:280:PRO:HB2	1.97	0.46
1:B:363:GLU:C	1:B:365:LEU:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:CZ	1:B:129:ARG:HH12	2.28	0.46
1:B:34:ARG:NH1	1:B:251:ALA:O	2.40	0.46
1:A:225:ASP:CG	1:A:396:ILE:HD11	2.40	0.46
1:B:269:VAL:HA	1:B:280:PRO:HA	1.96	0.46
1:B:310:ALA:HA	1:B:394:GLU:HB3	1.98	0.46
1:A:87:SER:HA	1:A:99:PHE:O	2.15	0.46
1:A:97:PHE:HB3	1:A:99:PHE:CE1	2.51	0.45
1:A:429:LYS:O	1:A:433:GLU:HG2	2.15	0.45
1:B:139:VAL:HG21	1:B:306:LEU:HD22	1.99	0.45
1:A:225:ASP:CB	1:A:396:ILE:HD11	2.47	0.45
1:A:373:ASP:OD1	1:A:373:ASP:N	2.44	0.45
1:B:85:HIS:HB3	1:B:123:PHE:CE2	2.51	0.45
1:B:269:VAL:HG22	1:B:280:PRO:HG3	1.98	0.44
1:A:172:GLU:O	1:A:193:LYS:HE2	2.17	0.44
1:B:334:PHE:CE2	1:B:382:THR:HG22	2.53	0.44
1:B:324:ARG:HH21	1:B:380:ILE:HD11	1.82	0.44
1:A:78:LEU:HG	1:A:103:TYR:CE2	2.53	0.44
1:B:228:VAL:HG21	1:B:308:HIS:CE1	2.53	0.43
1:B:427:LEU:HA	1:B:427:LEU:HD12	1.76	0.43
1:B:85:HIS:HB3	1:B:123:PHE:CZ	2.53	0.43
1:A:85:HIS:HB3	1:A:123:PHE:CZ	2.54	0.43
1:B:78:LEU:HD23	1:B:83:MET:HG2	2.00	0.43
1:B:375:GLY:O	1:B:417:GLY:HA2	2.18	0.43
1:A:70:MET:HB3	1:A:90:LEU:HB3	2.01	0.43
1:A:85:HIS:HB3	1:A:123:PHE:CE2	2.54	0.43
1:A:297:TYR:HD1	1:A:390:THR:HA	1.84	0.43
1:B:360:LYS:HE3	1:B:360:LYS:HB3	1.86	0.43
1:B:105:PRO:HD3	1:B:125:HIS:NE2	2.33	0.43
1:A:51:GLU:OE1	1:A:188:ARG:NH2	2.46	0.43
1:B:148:ASP:HB3	1:B:151:SER:OG	2.18	0.43
1:A:49:HIS:O	1:A:50:ILE:HD13	2.19	0.42
1:B:265[A]:LEU:HB3	1:B:294:ILE:HG13	2.01	0.42
1:B:320:LEU:HD21	1:B:380:ILE:CG2	2.49	0.42
1:B:86:ALA:O	1:B:100:THR:HA	2.19	0.42
1:B:343:TYR:CD2	1:B:363:GLU:HG3	2.55	0.42
1:B:91:THR:HA	1:B:95:LEU:O	2.20	0.42
1:B:318:ARG:O	1:B:322:GLU:HG2	2.20	0.42
1:B:228:VAL:HG21	1:B:308:HIS:NE2	2.35	0.42
1:A:43:LYS:HG2	1:A:147:GLU:CG	2.50	0.42
1:A:51:GLU:HG3	1:A:98:LEU:HD23	2.01	0.42
1:B:159:ASN:HB3	1:B:243:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265[B]:LEU:HB3	1:B:294:ILE:HG13	2.02	0.42
1:B:355:SER:OG	1:B:358:GLN:HG3	2.19	0.42
1:B:226:HIS:CE1	1:B:310:ALA:CB	3.03	0.41
1:A:401:CYS:HB2	1:A:413:SER:HB2	2.02	0.41
1:A:341:THR:HG21	1:A:433:GLU:O	2.21	0.41
1:B:320:LEU:HD13	1:B:320:LEU:HA	1.90	0.41
1:A:368:LEU:HB2	1:A:379:GLN:HG3	2.03	0.41
1:B:78:LEU:CD2	1:B:83:MET:HG2	2.50	0.41
1:B:81:GLY:O	1:B:117:THR:HB	2.21	0.41
1:A:326:ARG:HA	1:A:329:ILE:CG1	2.51	0.40
1:B:40:ASP:HB3	1:B:42:PHE:O	2.21	0.40
1:A:54:CYS:HA	1:A:132:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	355/445 (80%)	335 (94%)	20 (6%)	0	100	100
1	B	357/445 (80%)	331 (93%)	26 (7%)	0	100	100
All	All	712/890 (80%)	666 (94%)	46 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	304/371 (82%)	298 (98%)	6 (2%)	48	74
1	B	306/371 (82%)	300 (98%)	6 (2%)	48	74
All	All	610/742 (82%)	598 (98%)	12 (2%)	48	74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	104	SER
1	A	182	TYR
1	A	313	SER
1	A	401	CYS
1	A	425	SER
1	B	44	VAL
1	B	97	PHE
1	B	133	SER
1	B	316	ILE
1	B	320	LEU
1	B	413	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	230	ASN
1	A	266	ASN
1	A	282	ASN
1	A	307	GLN
1	A	374	GLN
1	A	412	GLN
1	B	301	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	92L	A	502	2	23,24,24	3.83	10 (43%)	27,36,36	4.19	12 (44%)
3	92L	B	502	2	23,24,24	3.82	8 (34%)	27,36,36	3.61	11 (40%)

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	92L	A	502	2	-	5/16/32/32	0/2/2/2
3	92L	B	502	2	-	6/16/32/32	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	92L	O15-C4	10.58	1.44	1.23
3	B	502	92L	O15-C4	9.98	1.43	1.23
3	B	502	92L	C13-N17	-7.97	1.31	1.45
3	A	502	92L	O18-N17	7.78	1.36	1.22
3	B	502	92L	O18-N17	7.75	1.36	1.22
3	A	502	92L	C13-N17	-7.15	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	92L	C1-C6	5.65	1.58	1.50
3	B	502	92L	C5-C7	5.08	1.51	1.39
3	A	502	92L	C5-C7	5.05	1.51	1.39
3	B	502	92L	C5-C6	5.01	1.57	1.45
3	A	502	92L	C1-C6	4.73	1.57	1.50
3	A	502	92L	C5-C6	4.19	1.55	1.45
3	A	502	92L	C5-C4	3.72	1.54	1.45
3	A	502	92L	O16-C7	3.02	1.41	1.33
3	B	502	92L	C5-C4	2.93	1.52	1.45
3	B	502	92L	O16-C7	2.87	1.40	1.33
3	A	502	92L	C11-S20	2.79	1.79	1.77
3	A	502	92L	O14-C6	-2.70	1.17	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	92L	C23-S20-C11	9.37	114.86	104.55
3	A	502	92L	O22-S20-O21	-8.93	102.85	117.99
3	B	502	92L	C23-S20-C11	8.60	114.02	104.55
3	A	502	92L	O15-C4-C5	-8.51	108.91	122.77
3	B	502	92L	O15-C4-C5	-8.23	109.37	122.77
3	A	502	92L	O16-C7-C5	-8.13	106.54	120.11
3	B	502	92L	O22-S20-O21	-8.09	104.27	117.99
3	A	502	92L	O22-S20-C11	-7.19	102.64	108.23
3	B	502	92L	O16-C7-C5	-6.72	108.89	120.11
3	A	502	92L	O15-C4-C3	-6.71	109.87	120.87
3	B	502	92L	O15-C4-C3	-5.58	111.72	120.87
3	A	502	92L	O21-S20-C11	4.36	111.61	108.23
3	B	502	92L	C6-C5-C4	-3.48	112.09	118.97
3	B	502	92L	C1-C6-C5	-3.23	110.97	116.94
3	A	502	92L	O21-S20-C23	3.16	113.11	108.47
3	A	502	92L	C6-C5-C4	-2.98	113.07	118.97
3	A	502	92L	C1-C6-C5	-2.85	111.67	116.94
3	B	502	92L	C8-C7-C5	-2.78	120.75	126.41
3	B	502	92L	O18-N17-C13	2.20	122.80	119.03
3	B	502	92L	C9-C10-C11	-2.20	117.30	119.44
3	B	502	92L	O22-S20-C23	2.16	111.64	108.47
3	A	502	92L	C9-C8-C13	2.12	121.38	118.37
3	A	502	92L	C10-C9-C8	-2.11	117.38	120.86

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	92L	C8-C13-N17-O18
3	A	502	92L	C12-C13-N17-O18
3	A	502	92L	C4-C5-C7-C8
3	A	502	92L	C4-C5-C7-O16
3	B	502	92L	C8-C13-N17-O18
3	B	502	92L	C12-C13-N17-O18
3	B	502	92L	C4-C5-C7-C8
3	B	502	92L	C4-C5-C7-O16
3	B	502	92L	O16-C7-C8-C9
3	A	502	92L	C10-C11-S20-O21
3	B	502	92L	C12-C11-S20-O22

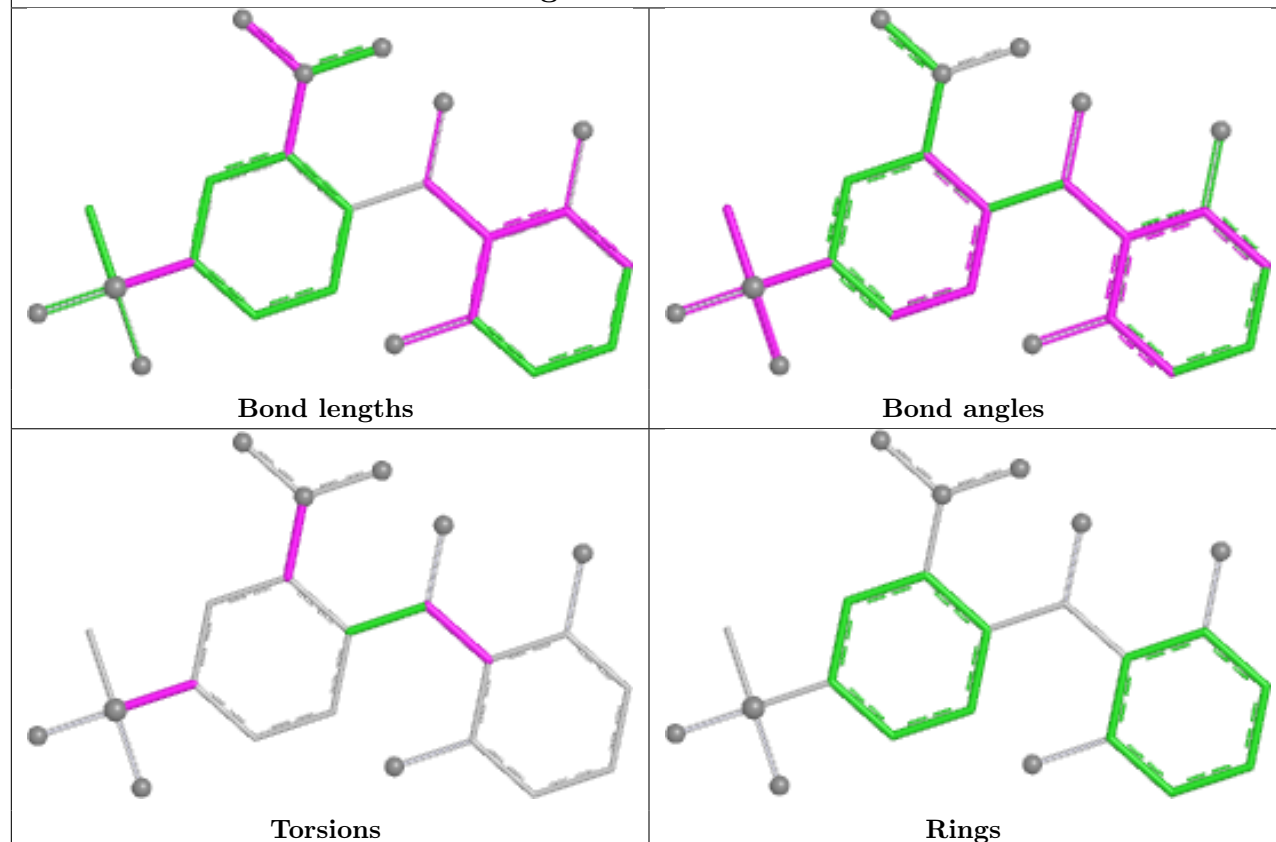
There are no ring outliers.

1 monomer is involved in 2 short contacts:

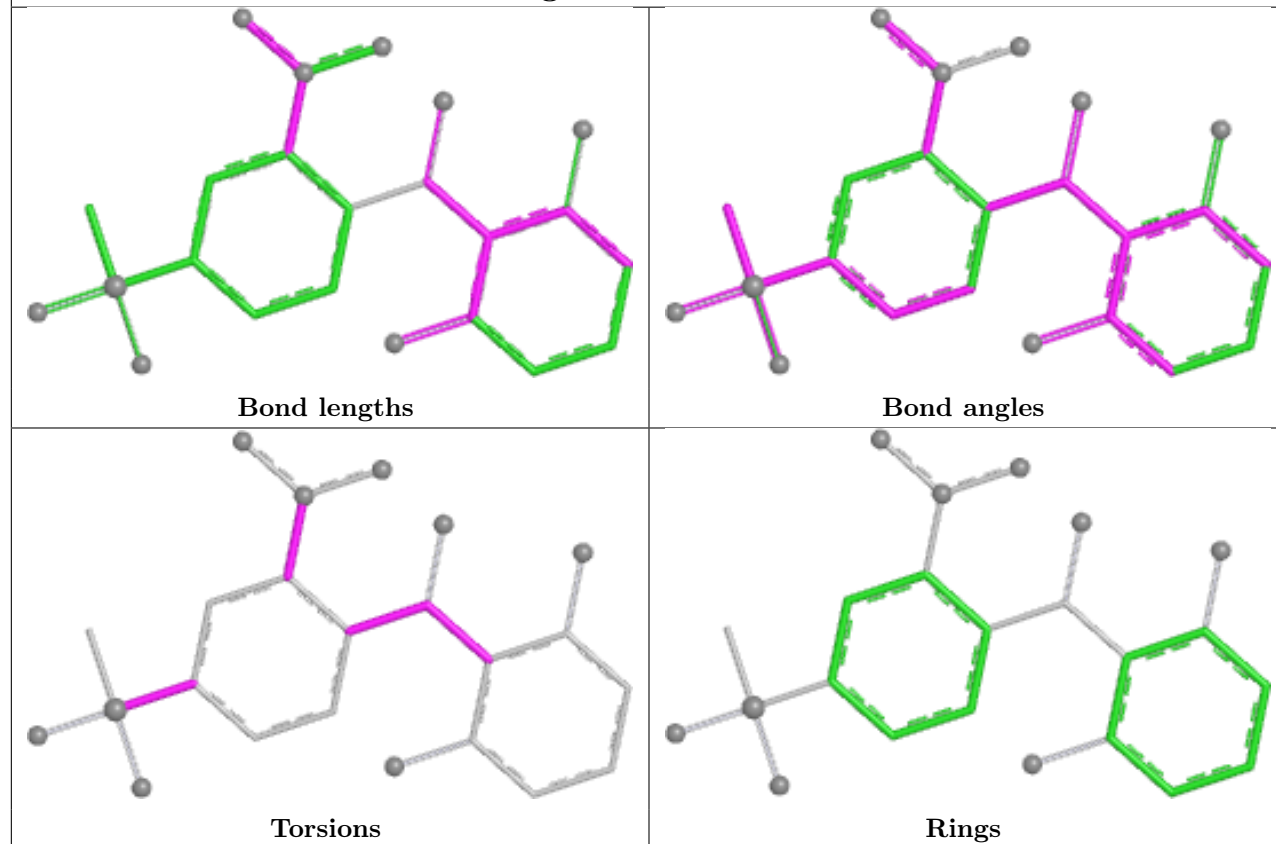
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	92L	2	0

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 92L A 502



Ligand 92L B 502



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	366/445 (82%)	1.33	74 (20%) 3 2	29, 49, 75, 93	3 (0%)
1	B	369/445 (82%)	1.48	87 (23%) 2 1	30, 51, 79, 103	2 (0%)
All	All	735/890 (82%)	1.41	161 (21%) 2 2	29, 50, 78, 103	5 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	SER	9.6
1	A	253	PHE	6.7
1	A	122	SER	6.2
1	B	121	PRO	5.7
1	A	129	ARG	5.3
1	B	434	TYR	5.1
1	B	67	GLY	4.6
1	A	212	ALA	4.4
1	A	393	ILE	4.4
1	A	128	CYS	4.4
1	B	202	PHE	4.3
1	B	348	LYS	4.3
1	B	68	LEU	4.2
1	A	434	TYR	4.2
1	B	127	SER	4.2
1	B	158	ALA	4.1
1	B	159	ASN	4.0
1	B	253	PHE	3.9
1	A	215	PHE	3.7
1	B	137	LEU	3.6
1	A	209	VAL	3.6
1	A	194	ALA	3.6
1	A	263	SER	3.6
1	B	263	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	125	HIS	3.5
1	A	400	GLY	3.5
1	B	120	ILE	3.5
1	B	367	ILE	3.5
1	B	211	ASP	3.4
1	B	123	PHE	3.4
1	A	121	PRO	3.4
1	A	123	PHE	3.4
1	B	291	LYS	3.3
1	B	125	HIS	3.3
1	A	141	ALA	3.3
1	B	29	PHE	3.2
1	A	291	LYS	3.2
1	B	376	THR	3.2
1	B	138	GLY	3.2
1	B	129	ARG	3.1
1	A	385	LEU	3.0
1	A	229	GLY	3.0
1	B	105	PRO	2.9
1	B	213	SER	2.9
1	B	374	GLN	2.9
1	A	120	ILE	2.9
1	B	107	LEU	2.9
1	A	65	SER	2.9
1	B	61	ALA	2.9
1	B	56	ASP	2.8
1	A	309	LEU	2.8
1	A	271	ALA	2.8
1	B	104	SER	2.8
1	B	184	ASP	2.8
1	B	118	ALA	2.8
1	A	376	THR	2.7
1	B	415	GLY	2.7
1	B	369	VAL	2.7
1	B	403	MET	2.7
1	B	286	HIS	2.7
1	A	139	VAL	2.7
1	A	250	PHE	2.7
1	B	311	LEU	2.7
1	B	46	ARG	2.7
1	A	190	VAL	2.6
1	A	313	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	175	THR	2.6
1	B	380	ILE	2.6
1	B	194	ALA	2.6
1	A	133	SER	2.6
1	B	92	SER	2.6
1	B	133	SER	2.6
1	B	203	LEU	2.6
1	A	96	ARG	2.6
1	B	429	LYS	2.6
1	B	126	GLY	2.6
1	B	230	ASN	2.6
1	A	69	GLY	2.5
1	B	161	ALA	2.5
1	A	107	LEU	2.5
1	B	278	LEU	2.5
1	A	182	TYR	2.5
1	B	431	ILE	2.5
1	B	97	PHE	2.5
1	A	127	SER	2.5
1	B	189	TYR	2.5
1	A	306	LEU	2.4
1	B	372	ASP	2.4
1	A	419	PHE	2.4
1	A	104	SER	2.4
1	A	312[A]	MET	2.4
1	B	284	PRO	2.4
1	B	44	VAL	2.4
1	B	144	ILE	2.4
1	B	279	LEU	2.4
1	B	298	LEU	2.4
1	B	432	GLU	2.4
1	A	158	ALA	2.4
1	A	270	LEU	2.4
1	A	184	ASP	2.4
1	B	232	PRO	2.4
1	B	295	GLN	2.4
1	B	304	ALA	2.4
1	A	137	LEU	2.3
1	B	155	ILE	2.3
1	B	287	GLY	2.3
1	A	268	ALA	2.3
1	B	212	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	71	ARG	2.3
1	A	269	VAL	2.3
1	A	391	ILE	2.3
1	B	393	ILE	2.3
1	B	94	ASP	2.3
1	A	183	GLY	2.3
1	B	160	GLY	2.3
1	A	99	PHE	2.3
1	B	378	LEU	2.3
1	A	395	ILE	2.3
1	A	297	TYR	2.3
1	A	97	PHE	2.3
1	B	294	ILE	2.2
1	B	335	MET	2.2
1	A	202	PHE	2.2
1	A	152	ALA	2.2
1	B	319	THR	2.2
1	A	279	LEU	2.2
1	B	251	ALA	2.2
1	A	346	LEU	2.2
1	B	90	LEU	2.2
1	B	223	ARG	2.2
1	B	182	TYR	2.2
1	A	55	GLY	2.2
1	A	298	LEU	2.2
1	A	378	LEU	2.2
1	B	373	ASP	2.2
1	A	50	ILE	2.2
1	B	101	ALA	2.1
1	A	68	LEU	2.1
1	A	278	LEU	2.1
1	A	377	LEU	2.1
1	A	399	VAL	2.1
1	A	219	TYR	2.1
1	B	55	GLY	2.1
1	A	211	ASP	2.1
1	B	299	GLU	2.1
1	A	284	PRO	2.1
1	A	54	CYS	2.1
1	A	138	GLY	2.1
1	A	29	PHE	2.1
1	B	131	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	317	PHE	2.1
1	A	304	ALA	2.1
1	B	117	THR	2.1
1	B	181	LEU	2.1
1	B	217	LEU	2.0
1	B	59	ASN	2.0
1	A	375	GLY	2.0
1	B	33	VAL	2.0
1	A	319	THR	2.0
1	A	403	MET	2.0
1	A	192	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

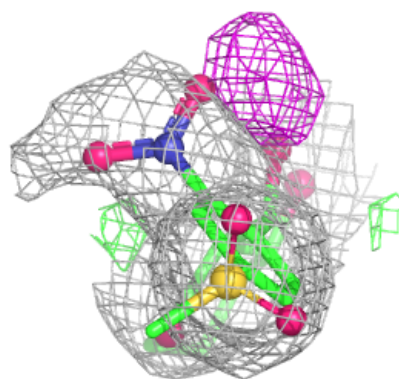
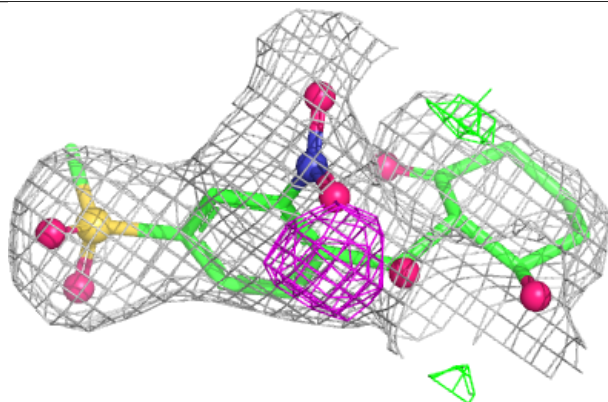
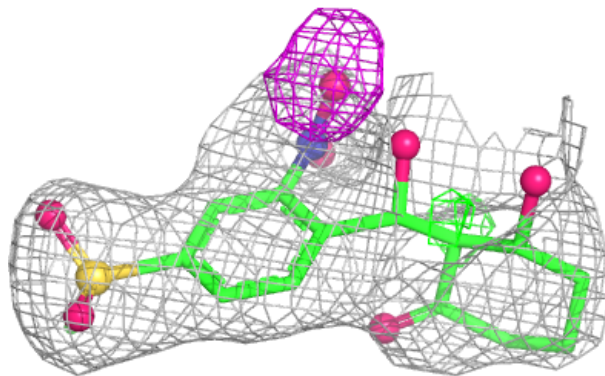
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	92L	A	502	23/23	0.85	0.14	50,50,50,50	0
3	92L	B	502	23/23	0.88	0.11	47,47,47,47	0
2	CO	B	501	1/1	0.96	0.07	48,48,48,48	0
2	CO	A	501	1/1	0.97	0.04	41,41,41,41	0

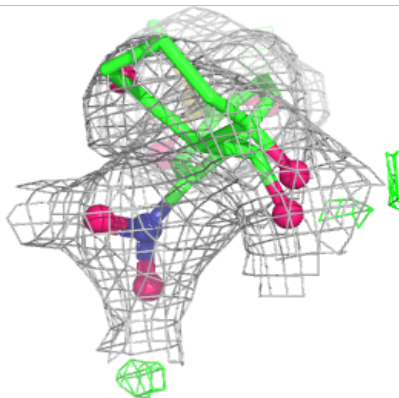
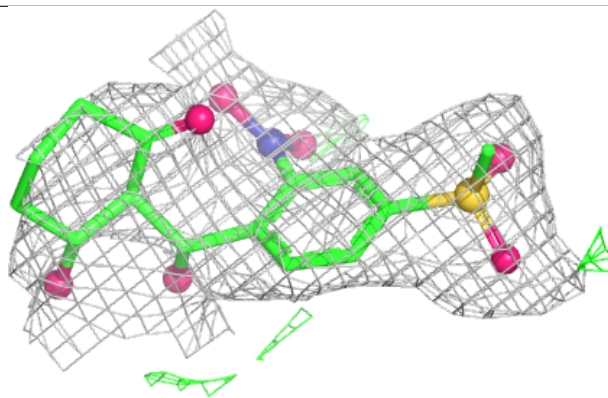
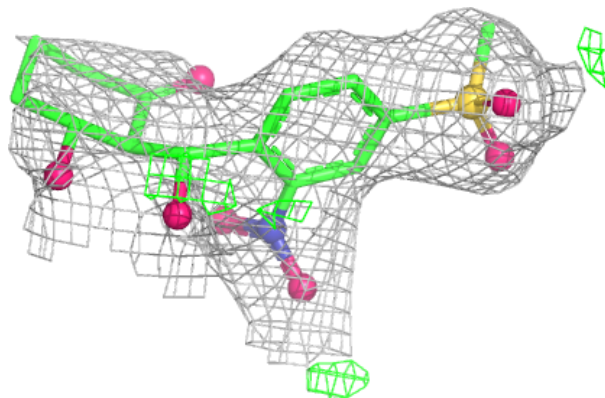
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 92L A 502:

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

**Electron density around 92L B 502:**

$2mF_o-DF_c$ (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.