



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:33 PM UTC

PDB ID : 9KGM / pdb_00009kgm
Title : Complex structure of OsHPPD with MBQ
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Deposited on : 2024-11-08
Resolution : 2.89 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

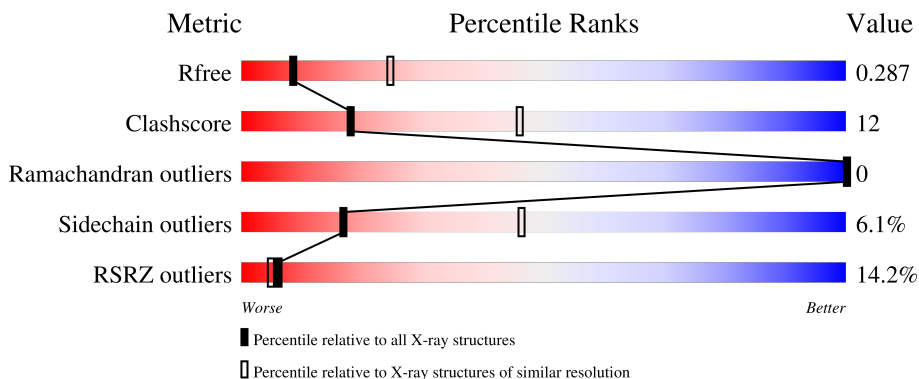
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	446	<div> <div>13%</div> <div>60%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
1	B	446	<div> <div>11%</div> <div>63%</div> <div>22%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5571 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.

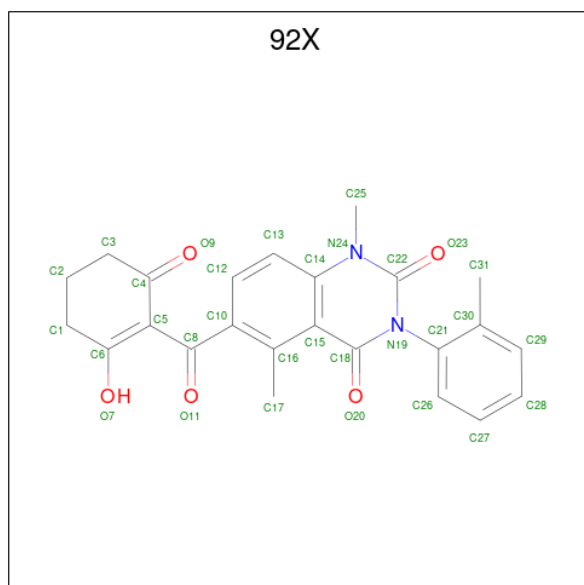
- Molecule 1 is a protein called 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2759	1748	495	509	7			
1	B	380	Total	C	N	O	S	0	0	0
			2748	1743	488	510	7			

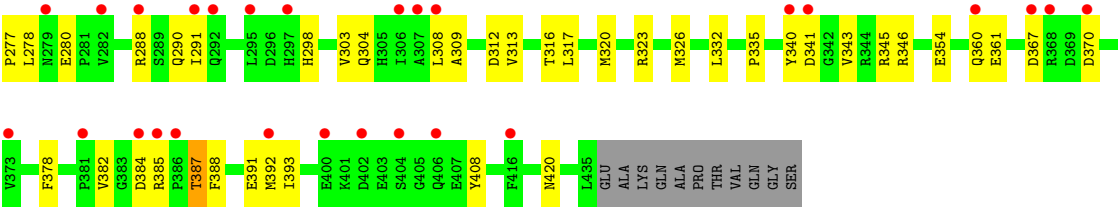
- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

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 1,5-dimethyl-3-(2-methylphenyl)-6-(2-oxidanyl-6-oxidanylidene-cyclohexen-1-yl)carbonyl-quinazoline-2,4-dione (CCD ID: 92X) (formula: C₂₄H₂₂N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	24	2	5		
3	B	1	Total	C	N	O	0	0
			31	24	2	5		



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.68Å 153.68Å 81.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.79 – 2.89 40.79 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.79-2.89) 99.9 (40.79-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.276 , 0.292 0.275 , 0.287	Depositor DCC
R_{free} test set	1108 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.1	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	0.89	EDS
Total number of atoms	5571	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: CO, 92X

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	0.20	0/2825	0.36	2/3845 (0.1%)
1	B	0.21	0/2813	0.40	1/3831 (0.0%)
All	All	0.21	0/5638	0.38	3/7676 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	PRO	N-CA-C	-5.48	104.91	113.78
1	A	389	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	263	ASN	CB-CA-C	5.30	118.50	109.75

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	2759	0	2566	75	0
1	B	2748	0	2562	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	0	0	0
3	B	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5571	0	5128	130	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 12.

All (130) 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:228:VAL:HG21	1:B:234:VAL:HG21	1.69	0.74
1:B:136:HIS:NE2	1:B:185:ASP:OD2	2.23	0.71
1:B:53:GLU:HB3	1:B:142:ALA:HB3	1.73	0.71
1:A:195:ASP:OD1	1:A:195:ASP:N	2.24	0.70
1:A:228:VAL:HG11	1:A:234:VAL:HG21	1.75	0.68
1:A:242:THR:HG23	1:A:244:PHE:H	1.58	0.67
1:A:53:GLU:OE1	1:A:189:ARG:NH1	2.28	0.66
1:A:147:VAL:HG11	1:A:153:ALA:HB2	1.79	0.64
1:A:376:GLN:NE2	1:A:391:GLU:OE2	2.33	0.62
1:B:216:TYR:OH	1:B:323:ARG:NH1	2.31	0.62
1:A:238:ILE:HD12	1:A:278:LEU:HD11	1.82	0.60
1:B:343:VAL:HG12	1:B:346:ARG:HH21	1.66	0.60
1:A:368:ARG:HG2	1:A:373:VAL:HG22	1.83	0.60
1:B:238:ILE:HD12	1:B:278:LEU:HD21	1.84	0.59
1:A:351:LEU:HD21	1:A:375:LEU:HD21	1.84	0.59
1:A:54:LEU:HA	1:A:140:VAL:HA	1.85	0.58
1:A:228:VAL:HG12	1:A:229:PRO:HD2	1.84	0.58
1:A:326:MET:HB3	1:B:214:VAL:HG21	1.85	0.58
1:A:384:ASP:OD2	1:B:59:ALA:N	2.36	0.58
1:A:216:TYR:OH	1:A:323:ARG:NH1	2.37	0.57
1:B:290:GLN:HG2	1:B:291:ILE:HD12	1.86	0.57
1:A:61:SER:HA	1:B:65:ARG:HD2	1.86	0.57
1:A:178:ALA:HB3	1:A:190:PHE:HB2	1.87	0.57
1:A:73:PRO:HG3	1:B:326:MET:HE1	1.87	0.56
1:B:220:ARG:HG2	1:B:309:ALA:HB3	1.88	0.55
1:A:352:SER:HB3	1:A:355:GLN:HG3	1.88	0.55
1:B:266:VAL:HA	1:B:277:PRO:HA	1.87	0.55
1:B:136:HIS:ND1	1:B:298:HIS:O	2.32	0.54
1:B:53:GLU:OE2	1:B:55:TRP:NE1	2.41	0.53
1:A:182:LEU:HG	1:A:188:LEU:HB2	1.91	0.53
1:A:326:MET:HB3	1:B:214:VAL:HG11	1.91	0.53
1:B:91:LEU:HD11	1:B:98:ALA:HB1	1.90	0.53
1:B:96:SER:OG	1:B:219:ARG:O	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:O	1:A:242:THR:HG22	2.10	0.52
1:A:76:ALA:HB3	1:A:91:LEU:HB3	1.90	0.52
1:B:239:SER:HB3	1:B:267:LEU:HD11	1.90	0.52
1:A:171:LEU:HD21	1:A:177:LEU:HB2	1.92	0.52
1:B:182:LEU:HD13	1:B:188:LEU:HB2	1.90	0.52
1:B:313:VAL:HG22	1:B:317:LEU:HD23	1.92	0.52
1:A:145:LEU:HD22	1:A:274:VAL:HG11	1.92	0.51
1:B:177:LEU:HD11	1:B:189:ARG:HD3	1.92	0.51
1:A:223:HIS:HB3	1:A:275:LEU:HB2	1.93	0.51
1:B:42:ASP:OD2	1:B:270:ASN:N	2.43	0.51
1:A:43:ARG:NH1	1:A:240:GLY:O	2.44	0.51
1:A:160:ALA:HB3	1:A:241:PHE:HA	1.93	0.50
1:A:238:ILE:HA	1:A:241:PHE:CE2	2.45	0.50
1:B:332:LEU:HD12	1:B:378:PHE:HB2	1.93	0.50
1:B:71:GLY:HA3	1:B:216:TYR:CG	2.47	0.50
1:A:83:GLY:O	1:A:118:THR:OG1	2.27	0.50
1:A:91:LEU:HD11	1:A:98:ALA:HB1	1.93	0.50
1:A:266:VAL:HG22	1:A:277:PRO:HB3	1.94	0.50
1:B:308:LEU:HD12	1:B:392:MET:HE1	1.93	0.50
1:A:369:ASP:OD1	1:A:370:ASP:N	2.44	0.49
1:A:385:ARG:O	1:A:387:THR:N	2.42	0.49
1:B:65:ARG:HA	1:B:68:PHE:CE2	2.46	0.49
1:A:85:SER:HB3	1:A:118:THR:HG21	1.95	0.49
1:A:343:VAL:HG12	1:A:346:ARG:NH2	2.28	0.48
1:B:367:ASP:HB2	1:B:420:ASN:HD21	1.78	0.48
1:B:74:LEU:HG	1:B:208:VAL:HG21	1.96	0.48
1:B:186:VAL:HG11	1:B:303:VAL:HG23	1.95	0.48
1:A:332:LEU:HD23	1:A:380:LYS:HG2	1.95	0.48
1:A:231:LEU:HD21	1:A:265:VAL:HG12	1.95	0.48
1:B:326:MET:HA	1:B:326:MET:HE2	1.95	0.48
1:B:354:GLU:H	1:B:354:GLU:CD	2.22	0.47
1:B:391:GLU:HG2	1:B:393:ILE:HG23	1.97	0.47
1:B:370:ASP:OD1	1:B:370:ASP:N	2.42	0.47
1:A:65:ARG:HD2	1:B:61:SER:HA	1.97	0.47
1:A:398:CYS:CB	1:A:413:CYS:SG	3.03	0.47
1:A:424:LEU:O	1:A:428:ILE:HG12	2.15	0.47
1:A:323:ARG:HD3	1:A:326:MET:HE3	1.97	0.46
1:A:338:ASN:OD1	1:A:338:ASN:N	2.47	0.46
3:B:502:92X:O11	3:B:502:92X:O7	2.30	0.46
1:B:267:LEU:HD23	1:B:278:LEU:HD13	1.98	0.46
1:A:59:ALA:N	1:B:384:ASP:OD2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASP:N	1:A:311:ASP:OD1	2.49	0.46
1:A:96:SER:HB2	1:A:220:ARG:HD2	1.96	0.46
1:A:374:LEU:HD11	1:A:393:ILE:HB	1.96	0.46
1:A:54:LEU:HG	1:A:140:VAL:HG12	1.98	0.45
1:A:228:VAL:HG23	1:A:279:ASN:O	2.16	0.45
1:B:262:LEU:HD22	1:B:263:ASN:N	2.32	0.45
1:B:238:ILE:HA	1:B:241:PHE:CE2	2.51	0.45
1:B:312:ASP:O	1:B:316:THR:HG23	2.17	0.45
1:A:343:VAL:HG12	1:A:346:ARG:HH21	1.82	0.45
1:B:53:GLU:HA	1:B:100:LEU:HB3	1.98	0.45
1:B:113:ALA:H	1:B:116:ALA:HB2	1.81	0.45
1:B:266:VAL:HG22	1:B:277:PRO:HB3	1.97	0.45
1:A:104:PRO:HB3	1:A:124:PHE:HZ	1.81	0.44
1:A:339:TYR:O	1:A:343:VAL:HG13	2.17	0.44
1:A:226:GLY:C	1:A:227:ASN:HD22	2.26	0.44
1:B:367:ASP:HB2	1:B:420:ASN:ND2	2.33	0.44
1:A:182:LEU:HB2	1:A:183:TYR:CD1	2.52	0.44
1:B:288:ARG:HD2	1:B:288:ARG:HA	1.72	0.44
1:A:266:VAL:HA	1:A:277:PRO:HA	1.98	0.44
1:B:335:PRO:HG2	1:B:340:TYR:CE2	2.52	0.44
1:A:92:LEU:HD22	1:A:101:PHE:CE1	2.52	0.44
1:A:150:ALA:N	1:A:192:SER:OG	2.51	0.43
1:A:349:ASP:OD1	1:A:349:ASP:N	2.51	0.43
1:A:397:GLY:O	1:A:409:GLN:NE2	2.48	0.43
1:B:231:LEU:HB2	1:B:280:GLU:HB3	1.99	0.43
1:A:50:HIS:ND1	1:A:191:VAL:HG21	2.32	0.43
1:B:70:LEU:HA	1:B:320:MET:HE2	2.00	0.43
1:B:246:GLU:HG2	1:B:247:PHE:H	1.83	0.43
1:A:98:ALA:H	1:A:221:PHE:HE2	1.65	0.43
1:A:229:PRO:HD3	1:A:301:PRO:HB3	2.01	0.43
1:B:65:ARG:NH1	1:B:382:VAL:O	2.50	0.43
1:A:50:HIS:HD1	1:A:191:VAL:HG21	1.84	0.43
1:A:266:VAL:HG11	1:A:416:PHE:CZ	2.53	0.43
1:B:87:HIS:HB3	1:B:124:PHE:CE2	2.54	0.43
1:B:304:GLN:O	1:B:388:PHE:HA	2.19	0.42
1:B:127:GLY:O	1:B:131:ARG:HB2	2.18	0.42
1:A:43:ARG:HB3	1:A:156:ALA:HB1	2.02	0.42
1:B:163:ARG:HG3	1:B:181:GLU:HB2	2.01	0.42
1:B:97:VAL:HG23	1:B:221:PHE:CZ	2.54	0.42
1:B:115:ALA:C	1:B:117:THR:H	2.26	0.42
1:A:177:LEU:HD11	1:A:189:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:HG22	1:A:277:PRO:HB2	2.02	0.42
1:B:341:ASP:O	1:B:345:ARG:HG3	2.19	0.42
1:A:336:PRO:HG2	1:A:427:SER:OG	2.19	0.41
1:A:401:LYS:HA	1:A:406:GLN:O	2.19	0.41
1:B:385:ARG:O	1:B:387:THR:N	2.53	0.41
1:B:154:PHE:CD2	1:B:168:PRO:HD3	2.55	0.41
1:A:48:ALA:HB1	1:A:220:ARG:HH22	1.85	0.41
1:A:314:LEU:HD13	1:A:314:LEU:HA	1.95	0.41
1:A:247:PHE:CE1	1:A:272:GLU:HG2	2.55	0.41
1:B:245:HIS:NE2	1:B:269:ASN:O	2.51	0.41
1:A:222:ASP:CG	1:A:393:ILE:HD11	2.45	0.41
1:A:228:VAL:O	1:A:229:PRO:C	2.64	0.41
1:A:317:LEU:HB3	1:A:362:LEU:HD13	2.03	0.41
1:A:381:PRO:HG2	1:A:386:PRO:HA	2.02	0.40
1:B:238:ILE:HA	1:B:241:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	377/446 (84%)	354 (94%)	23 (6%)	0	100	100
1	B	372/446 (83%)	346 (93%)	26 (7%)	0	100	100
All	All	749/892 (84%)	700 (94%)	49 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	254/329 (77%)	234 (92%)	20 (8%)	11	34
1	B	257/329 (78%)	246 (96%)	11 (4%)	26	60
All	All	511/658 (78%)	480 (94%)	31 (6%)	17	46

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	VAL
1	A	147	VAL
1	A	167	GLN
1	A	171	LEU
1	A	182	LEU
1	A	183	TYR
1	A	193	HIS
1	A	195	ASP
1	A	202	LEU
1	A	228	VAL
1	A	257	THR
1	A	295	LEU
1	A	317	LEU
1	A	319	GLU
1	A	338	ASN
1	A	350	VAL
1	A	351	LEU
1	A	361	GLU
1	A	399	MET
1	A	409	GLN
1	B	42	ASP
1	B	56	CYS
1	B	81	SER
1	B	186	VAL
1	B	259	GLU
1	B	262	LEU
1	B	264	SER
1	B	360	GLN
1	B	361	GLU
1	B	387	THR
1	B	408	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	263	ASN
1	A	355	GLN
1	B	279	ASN

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 [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	92X	A	502	2	34,34,34	1.98	13 (38%)	45,51,51	1.93	11 (24%)
3	92X	B	502	2	34,34,34	1.97	12 (35%)	45,51,51	2.06	14 (31%)

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	92X	A	502	2	-	0/12/26/26	0/4/4/4
3	92X	B	502	2	-	2/12/26/26	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	92X	C14-N24	-4.21	1.32	1.40
3	B	502	92X	C14-N24	-4.21	1.32	1.40
3	A	502	92X	C15-C18	-4.12	1.38	1.47
3	B	502	92X	C15-C18	-4.10	1.38	1.47
3	A	502	92X	C18-N19	-3.94	1.33	1.40
3	B	502	92X	C18-N19	-3.80	1.33	1.40
3	B	502	92X	C5-C4	3.32	1.53	1.45
3	A	502	92X	C5-C4	3.11	1.53	1.45
3	A	502	92X	O7-C6	2.98	1.40	1.32
3	B	502	92X	O7-C6	2.97	1.40	1.32
3	A	502	92X	C1-C6	2.93	1.54	1.49
3	A	502	92X	C10-C8	2.67	1.54	1.49
3	B	502	92X	C10-C8	2.65	1.54	1.49
3	A	502	92X	C22-N24	-2.48	1.35	1.38
3	A	502	92X	C22-N19	-2.44	1.35	1.40
3	B	502	92X	C22-N24	-2.38	1.35	1.38
3	B	502	92X	C1-C6	2.34	1.53	1.49
3	B	502	92X	C22-N19	-2.25	1.35	1.40
3	B	502	92X	O11-C8	-2.17	1.18	1.23
3	B	502	92X	O9-C4	-2.16	1.18	1.23
3	B	502	92X	C5-C6	-2.16	1.32	1.39
3	A	502	92X	O9-C4	-2.11	1.18	1.23
3	A	502	92X	O11-C8	-2.10	1.18	1.23
3	A	502	92X	C5-C6	-2.03	1.33	1.39
3	A	502	92X	C15-C14	-2.01	1.38	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	92X	C18-N19-C22	-5.17	120.18	125.45
3	B	502	92X	C15-C18-N19	5.15	120.87	115.14
3	B	502	92X	C17-C16-C10	-5.14	114.62	122.29
3	A	502	92X	C15-C18-N19	4.95	120.65	115.14
3	A	502	92X	C18-N19-C22	-4.70	120.66	125.45
3	A	502	92X	C17-C16-C10	-4.60	115.43	122.29
3	A	502	92X	O20-C18-N19	-4.03	115.02	120.38
3	A	502	92X	C2-C3-C4	-3.75	106.37	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	92X	O20-C18-N19	-3.48	115.75	120.38
3	A	502	92X	C21-N19-C18	3.29	120.51	117.21
3	B	502	92X	C30-C21-N19	2.88	122.32	118.69
3	B	502	92X	C21-N19-C18	2.86	120.08	117.21
3	A	502	92X	C13-C14-N24	-2.66	117.50	121.04
3	B	502	92X	O23-C22-N24	-2.61	119.89	122.10
3	B	502	92X	C13-C14-N24	-2.58	117.61	121.04
3	A	502	92X	C2-C1-C6	2.52	115.09	112.49
3	B	502	92X	C2-C1-C6	-2.51	109.91	112.49
3	B	502	92X	C21-N19-C22	2.45	119.73	116.72
3	B	502	92X	C1-C6-C5	-2.41	120.31	122.90
3	A	502	92X	O7-C6-C5	-2.38	117.29	121.95
3	A	502	92X	O23-C22-N24	-2.35	120.10	122.10
3	B	502	92X	C17-C16-C15	2.28	124.95	121.39
3	B	502	92X	C10-C8-C5	2.16	124.92	120.83
3	A	502	92X	C30-C21-N19	2.04	121.27	118.69
3	B	502	92X	C29-C30-C21	2.04	119.95	117.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	92X	C16-C10-C8-C5
3	B	502	92X	C16-C10-C8-O11

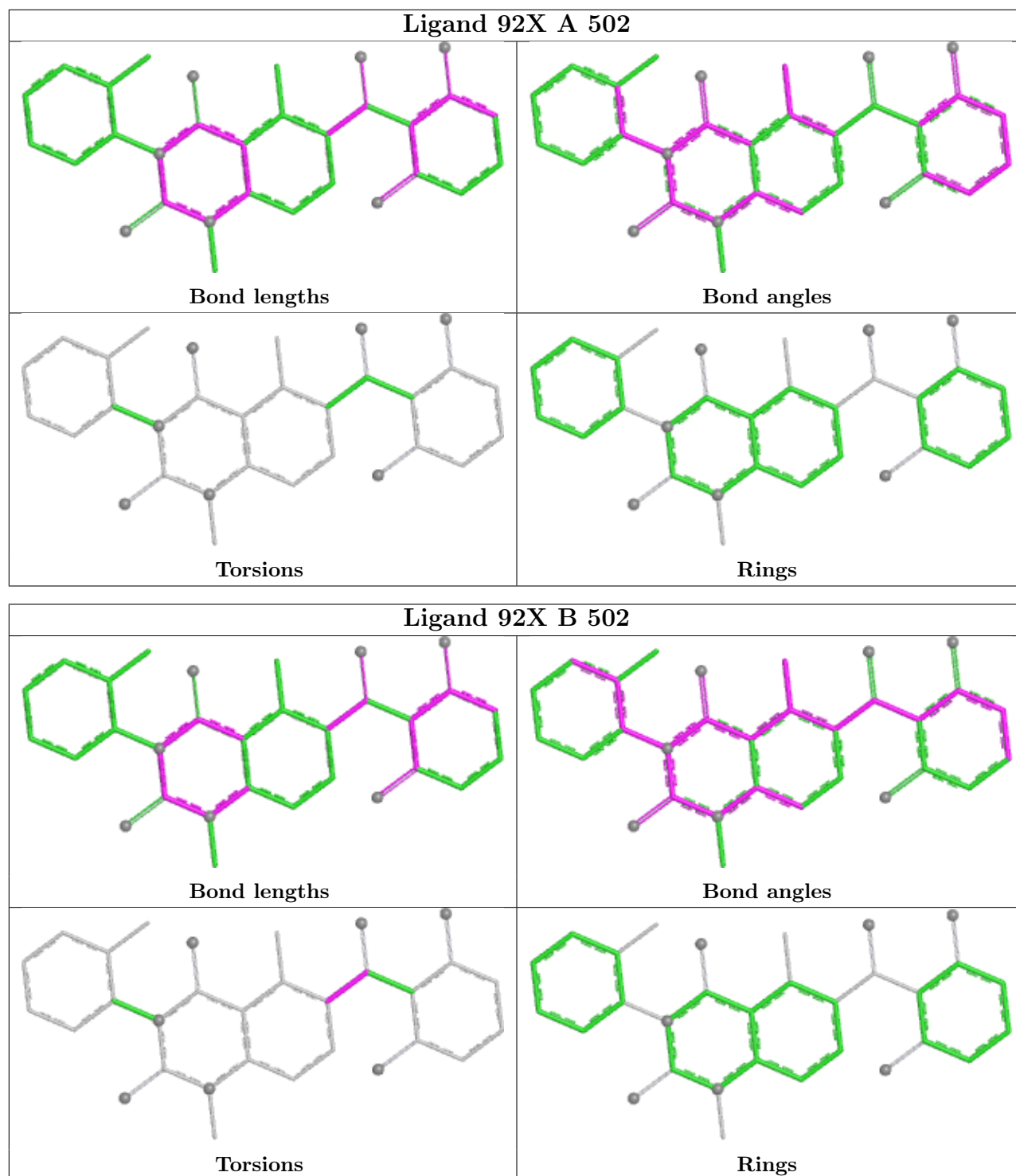
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	92X	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	385/446 (86%)	1.10	59 (15%) 5 4	48, 73, 104, 120	0
1	B	380/446 (85%)	1.07	50 (13%) 7 6	49, 73, 106, 123	0
All	All	765/892 (85%)	1.08	109 (14%) 6 5	48, 73, 106, 123	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	VAL	5.3
1	B	70	LEU	5.2
1	B	279	ASN	4.6
1	A	264	SER	4.2
1	B	37	ALA	4.0
1	A	241	PHE	3.9
1	A	171	LEU	3.8
1	B	292	GLN	3.7
1	B	360	GLN	3.6
1	B	307	ALA	3.6
1	A	292	GLN	3.4
1	B	386	PRO	3.4
1	B	367	ASP	3.4
1	B	370	ASP	3.3
1	A	293	THR	3.2
1	A	370	ASP	3.2
1	B	291	ILE	3.2
1	A	408	TYR	3.1
1	B	274	VAL	3.1
1	B	297	HIS	3.1
1	B	340	TYR	3.0
1	A	165	ALA	3.0
1	A	373	VAL	2.9
1	B	154	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	384	ASP	2.9
1	B	260	SER	2.9
1	A	372	GLY	2.8
1	B	71	GLY	2.8
1	A	384	ASP	2.8
1	B	182	LEU	2.8
1	A	281	PRO	2.8
1	A	274	VAL	2.8
1	B	191	VAL	2.8
1	A	145	LEU	2.8
1	B	272	GLU	2.7
1	A	398	CYS	2.7
1	A	210	ASN	2.7
1	A	361	GLU	2.6
1	A	115	ALA	2.6
1	A	291	ILE	2.6
1	B	288	ARG	2.6
1	A	256	GLY	2.6
1	A	311	ASP	2.6
1	B	156	ALA	2.6
1	B	261	GLY	2.6
1	A	416	PHE	2.6
1	B	49	PHE	2.6
1	A	177	LEU	2.5
1	A	183	TYR	2.5
1	A	175	PHE	2.5
1	A	273	THR	2.5
1	A	57	ALA	2.5
1	B	38	ASN	2.5
1	B	217	GLY	2.5
1	B	404	SER	2.5
1	A	272	GLU	2.5
1	A	43	ARG	2.5
1	B	193	HIS	2.5
1	A	185	ASP	2.4
1	A	392	MET	2.4
1	A	306	ILE	2.4
1	A	112	GLY	2.4
1	B	115	ALA	2.4
1	A	135	ASP	2.4
1	A	358	GLU	2.4
1	B	341	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	307	ALA	2.4
1	A	70	LEU	2.4
1	A	109	HIS	2.4
1	B	381	PRO	2.4
1	B	402	ASP	2.3
1	B	264	SER	2.3
1	A	216	TYR	2.3
1	A	259	GLU	2.3
1	B	373	VAL	2.3
1	A	267	LEU	2.2
1	B	188	LEU	2.2
1	B	406	GLN	2.2
1	B	189	ARG	2.2
1	A	199	ALA	2.2
1	B	306	ILE	2.2
1	A	400	GLU	2.2
1	B	400	GLU	2.2
1	B	368	ARG	2.2
1	A	140	VAL	2.2
1	A	431	TYR	2.2
1	A	44	PHE	2.2
1	B	262	LEU	2.2
1	B	416	PHE	2.2
1	A	316	THR	2.1
1	A	231	LEU	2.1
1	A	56	CYS	2.1
1	A	263	ASN	2.1
1	A	242	THR	2.1
1	A	138	LEU	2.1
1	A	260	SER	2.1
1	A	54	LEU	2.1
1	A	137	GLY	2.1
1	B	385	ARG	2.1
1	A	144	ALA	2.1
1	B	223	HIS	2.1
1	B	295	LEU	2.1
1	B	308	LEU	2.1
1	A	378	PHE	2.1
1	B	282	VAL	2.0
1	A	386	PRO	2.0
1	A	280	GLU	2.0
1	B	392	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	105	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](#)

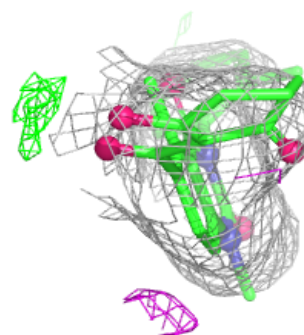
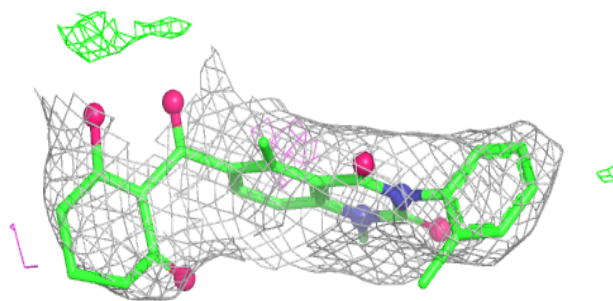
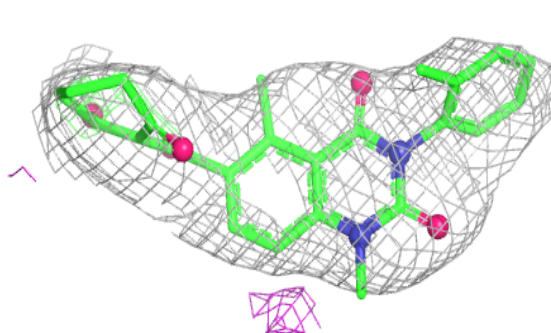
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	92X	A	502	31/31	0.91	0.13	55,71,88,92	0
3	92X	B	502	31/31	0.91	0.14	63,74,81,88	0
2	CO	B	501	1/1	0.98	0.07	67,67,67,67	0
2	CO	A	501	1/1	0.99	0.06	63,63,63,63	0

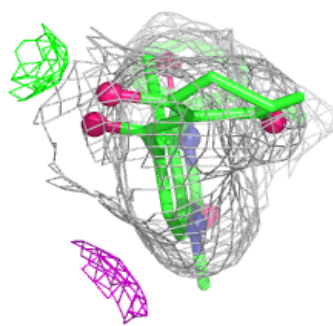
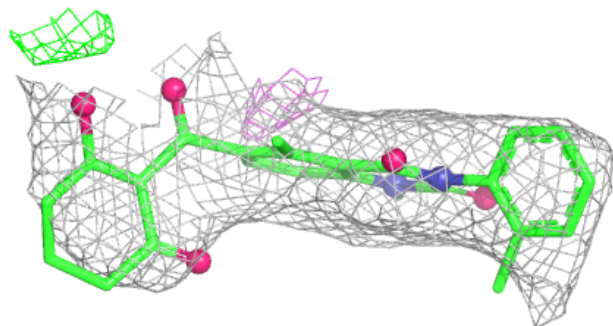
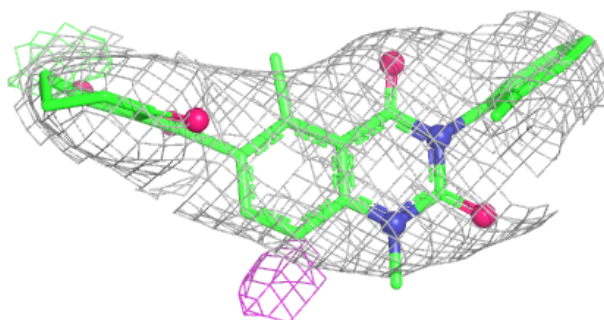
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 92X 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 92X 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.