



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:02 AM UTC

PDB ID : 8ODQ / pdb_00008odq
Title : SufS-SufU complex from Mycobacterium tuberculosis
Authors : Elchennawi, I.; Carpentier, P.; Caux, C.; Ponge, M.; Ollagnier de Choudens, S.
Deposited on : 2023-03-09
Resolution : 1.65 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

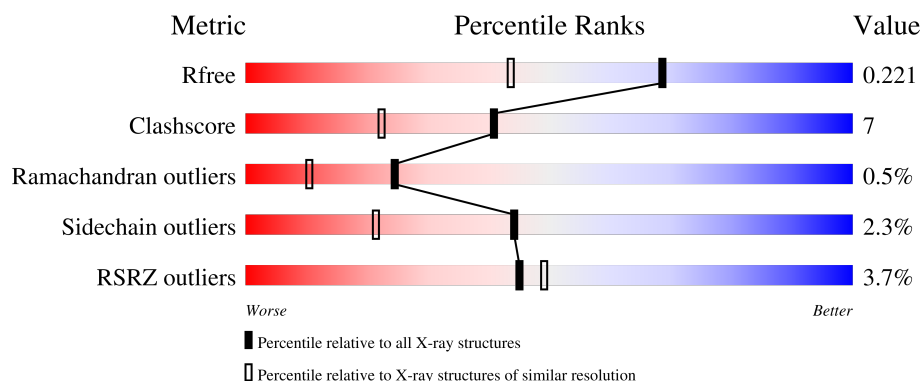
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	B	418	90% 7% .
2	D	418	87% 11% .
3	A	166	9% 73% 15% .. 10%
3	C	166	12% 66% 17% 5% . 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9784 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 Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	408	Total	C	N	O	S	0	7	0
			3121	1958	568	582	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A045IZN1

- Molecule 2 is a protein called Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	410	Total	C	N	O	S	0	16	0
			3193	2008	588	586	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP A0A045IZN1

- Molecule 3 is a protein called Nitrogen fixation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	150	Total	C	N	O	S	0	6	0
			1182	739	203	230	10			
3	C	148	Total	C	N	O	S	0	1	0
			1138	711	200	220	7			

There are 10 discrepancies between the modelled and reference sequences:

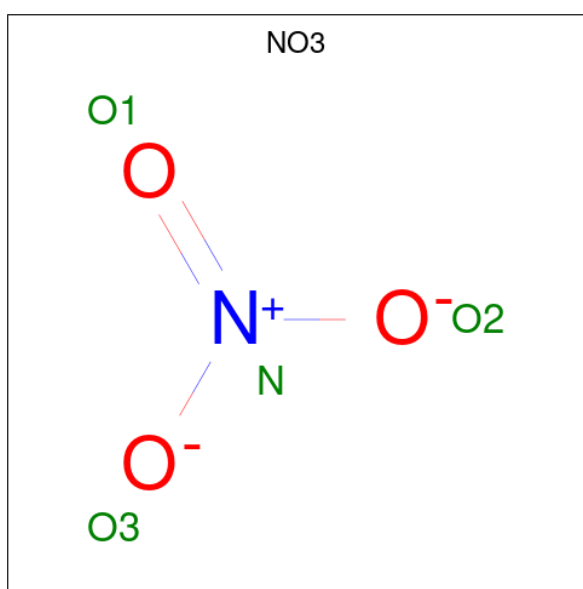
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A045HJY9
A	-2	SER	-	expression tag	UNP A0A045HJY9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP A0A045HJY9
A	0	MET	-	expression tag	UNP A0A045HJY9
A	1	VAL	-	expression tag	UNP A0A045HJY9
C	-3	GLY	-	expression tag	UNP A0A045HJY9
C	-2	SER	-	expression tag	UNP A0A045HJY9
C	-1	HIS	-	expression tag	UNP A0A045HJY9
C	0	MET	-	expression tag	UNP A0A045HJY9
C	1	VAL	-	expression tag	UNP A0A045HJY9

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



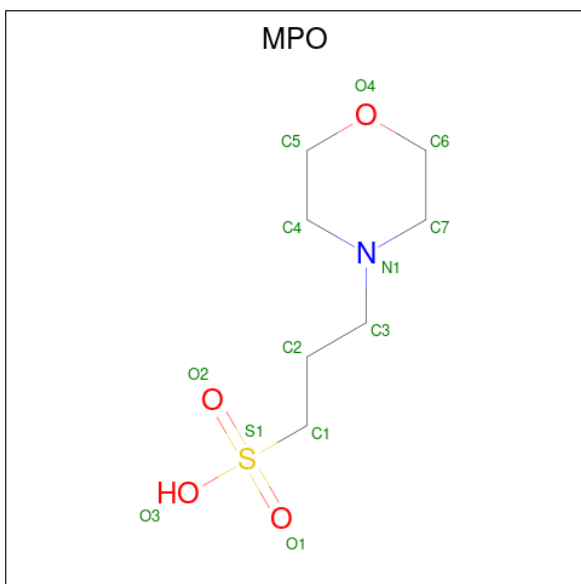
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Zn 1	0	0
7	C	1	Total 1	Zn 1	0	0

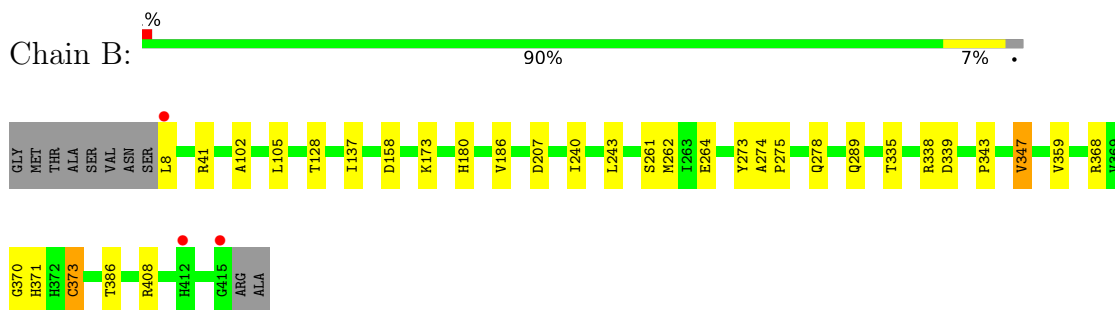
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	479	Total 479	O 479	0	0
8	D	493	Total 493	O 493	0	0
8	A	56	Total 56	O 56	0	0
8	C	53	Total 53	O 53	0	0

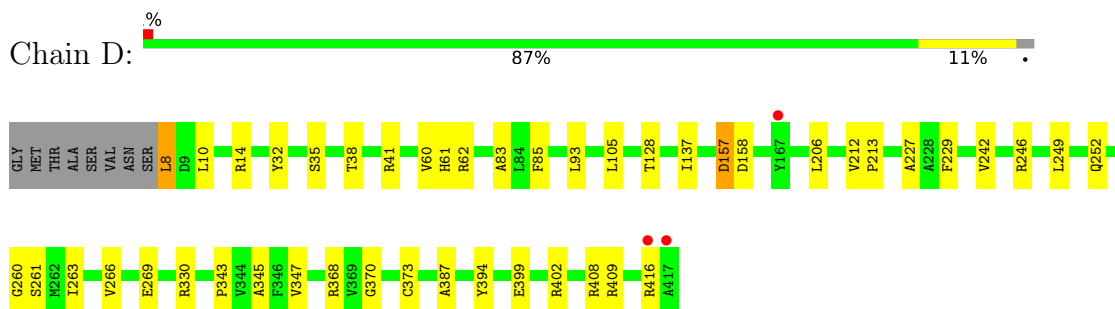
3 Residue-property plots [i](#)

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.

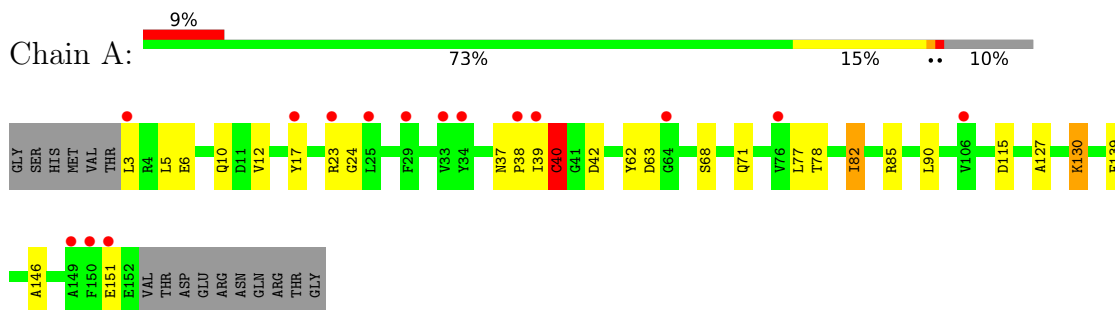
- Molecule 1: Cysteine desulfurase



- Molecule 2: Cysteine desulfurase

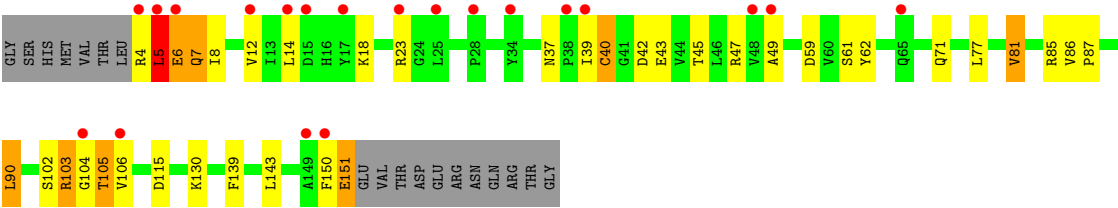


- Molecule 3: Nitrogen fixation protein



- Molecule 3: Nitrogen fixation protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.25Å 75.55Å 75.60Å 92.40° 109.57° 99.71°	Depositor
Resolution (Å)	48.72 – 1.65 48.72 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.72-1.65) 96.1 (48.72-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.179 , 0.214 0.188 , 0.221	Depositor DCC
R_{free} test set	7209 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9784	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: MPO, PLP, ZN, TSY, NO3

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	B	1.11	0/3191	1.25	4/4336 (0.1%)
2	D	1.11	0/3302	1.29	7/4484 (0.2%)
3	A	1.07	0/1201	1.33	0/1630
3	C	1.09	1/1153 (0.1%)	1.45	5/1564 (0.3%)
All	All	1.10	1/8847 (0.0%)	1.30	16/12014 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	3
3	C	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	106	VAL	N-CA	5.32	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	137	ILE	N-CA-CB	9.02	116.18	110.50
2	D	158	ASP	CA-CB-CG	8.14	120.74	112.60
2	D	373	CYS	N-CA-C	-7.11	103.90	112.58
1	B	137	ILE	N-CA-CB	6.36	114.50	110.50
2	D	373	CYS	CB-CA-C	5.89	120.52	111.39
1	B	158	ASP	CA-CB-CG	5.86	118.46	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ILE	CA-C-N	5.54	128.67	122.69
1	B	240	ILE	C-N-CA	5.54	128.67	122.69
3	C	81	VAL	CB-CA-C	5.50	115.90	111.06
2	D	157	ASP	CA-CB-CG	5.34	117.94	112.60
2	D	229	PHE	CA-CB-CG	5.23	119.03	113.80
3	C	85	ARG	CA-C-N	5.05	125.28	120.43
3	C	85	ARG	C-N-CA	5.05	125.28	120.43
3	C	6	GLU	CA-C-N	5.04	130.78	121.70
3	C	6	GLU	C-N-CA	5.04	130.78	121.70
2	D	85	PHE	CA-C-O	-5.03	115.22	120.55

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	39	ILE	Mainchain
3	A	40[A]	TSY	Mainchain
3	A	40[B]	TSY	Mainchain
3	C	39	ILE	Mainchain

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	B	3121	0	3096	29	0
2	D	3193	0	3217	45	0
3	A	1182	0	1153	22	0
3	C	1138	0	1106	25	0
4	B	12	0	0	2	0
4	C	4	0	0	0	0
4	D	8	0	0	0	0
5	B	15	0	6	1	0
5	D	15	0	6	0	0
6	D	13	0	15	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	56	0	0	5	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	479	0	0	15	2
8	C	53	0	0	5	1
8	D	493	0	0	20	2
All	All	9784	0	8599	113	4

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 (113) 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)
2:D:41[A]:ARG:NH2	8:D:602:HOH:O	1.71	1.22
2:D:62:ARG:NH2	8:D:603:HOH:O	1.74	1.19
2:D:330[B]:ARG:HG2	2:D:347[B]:VAL:HG22	1.27	1.14
3:C:49:ALA:O	8:C:301:HOH:O	1.69	1.10
2:D:32:TYR:OH	8:D:601:HOH:O	1.69	1.08
1:B:338:ARG:NH2	8:B:601:HOH:O	1.96	0.98
3:A:85:ARG:NH1	8:A:301:HOH:O	1.97	0.97
2:D:252:GLN:OE1	8:D:604:HOH:O	1.83	0.97
3:A:10[B]:GLN:NE2	8:A:302:HOH:O	1.97	0.95
3:C:7:GLN:N	8:C:302:HOH:O	1.99	0.95
2:D:41[A]:ARG:NE	8:D:607:HOH:O	2.00	0.93
1:B:373:TSY:S2	8:D:930:HOH:O	2.30	0.89
2:D:330[B]:ARG:HG2	2:D:347[B]:VAL:CG2	2.06	0.84
2:D:8:LEU:O	8:D:606:HOH:O	1.95	0.83
2:D:261:SER:HB3	8:D:603:HOH:O	1.78	0.82
2:D:330[B]:ARG:NH1	8:D:605:HOH:O	1.89	0.82
3:A:71:GLN:HG3	8:A:349:HOH:O	1.81	0.81
2:D:261:SER:CB	8:D:603:HOH:O	2.29	0.80
1:B:8:LEU:O	8:B:602:HOH:O	2.01	0.79
2:D:330[A]:ARG:NH2	8:D:610:HOH:O	2.15	0.78
3:A:38:PRO:HA	8:A:352:HOH:O	1.84	0.77
3:C:23:ARG:HH22	3:C:71[A]:GLN:HE21	1.33	0.76
1:B:275:PRO:O	1:B:278:GLN:HG2	1.86	0.75
4:B:503:NO3:O2	8:B:604:HOH:O	2.03	0.75
3:C:59:ASP:N	8:C:301:HOH:O	1.79	0.72
2:D:263:ILE:HD13	2:D:266[A]:VAL:HG23	1.70	0.72
2:D:261:SER:OG	8:D:603:HOH:O	2.09	0.70
1:B:41[A]:ARG:NE	8:B:606:HOH:O	2.24	0.69
2:D:408[A]:ARG:NH2	8:D:611:HOH:O	2.21	0.68
3:A:146:ALA:O	8:A:304:HOH:O	2.11	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:LEU:HD21	3:C:139:PHE:HB2	1.79	0.65
3:A:77:LEU:HD21	3:A:139:PHE:HB2	1.80	0.64
2:D:402:ARG:NH1	8:D:609:HOH:O	2.06	0.64
2:D:14[B]:ARG:NH2	2:D:399:GLU:OE2	2.32	0.64
2:D:246[A]:ARG:NH2	8:D:615:HOH:O	2.31	0.63
1:B:368:ARG:NE	3:A:40[B]:TSY:S2	2.68	0.62
2:D:409:ARG:HH11	3:C:4:ARG:NH1	1.96	0.62
3:C:102:SER:HB2	3:C:105:THR:HG22	1.81	0.62
1:B:173:LYS:NZ	8:B:610:HOH:O	2.33	0.61
3:A:78:THR:O	3:A:82[A]:ILE:HG12	2.01	0.61
2:D:32:TYR:CZ	8:D:601:HOH:O	2.45	0.60
2:D:263:ILE:HD13	2:D:266[A]:VAL:CG2	2.32	0.60
3:A:17:TYR:CD1	3:A:68:SER:HA	2.39	0.57
2:D:157:ASP:HB2	8:D:882:HOH:O	2.06	0.56
1:B:8:LEU:N	8:B:607:HOH:O	2.39	0.55
1:B:262:MET:HE1	1:B:273:TYR:CD1	2.42	0.55
1:B:8:LEU:HA	8:B:974:HOH:O	2.06	0.55
2:D:246[B]:ARG:NH1	2:D:249[B]:LEU:HD22	2.22	0.54
3:C:4:ARG:C	3:C:6:GLU:H	2.15	0.54
2:D:370:GLY:HA3	3:C:40:TSY:S2	2.47	0.54
1:B:8:LEU:N	8:B:617:HOH:O	2.41	0.53
1:B:370:GLY:CA	3:A:40[B]:TSY:HB2	2.39	0.53
1:B:368:ARG:NH1	4:B:502:NO3:O3	2.41	0.52
2:D:41[B]:ARG:HH11	2:D:41[B]:ARG:HG2	1.74	0.52
8:B:904:HOH:O	3:A:3:LEU:HD21	2.09	0.52
3:A:24:GLY:N	3:A:62:TYR:O	2.38	0.52
3:C:6:GLU:HA	3:C:8:ILE:H	1.75	0.52
1:B:371:HIS:CE1	3:A:40[A]:TSY:SG	3.03	0.51
2:D:260:GLY:O	2:D:261:SER:OG	2.27	0.51
3:C:86:VAL:HB	3:C:87:PRO:HD3	1.92	0.51
2:D:32:TYR:CE2	8:D:601:HOH:O	2.63	0.50
3:A:23:ARG:HD2	3:A:62:TYR:CE2	2.47	0.49
3:C:90:LEU:HD13	3:C:143:LEU:HD23	1.95	0.49
3:C:5:LEU:HD11	8:C:337:HOH:O	2.12	0.49
3:C:12:VAL:HG23	8:C:328:HOH:O	2.13	0.48
1:B:370:GLY:HA3	3:A:40[B]:TSY:HB2	1.95	0.48
3:C:102:SER:O	3:C:105:THR:HB	2.14	0.48
1:B:105:LEU:C	1:B:105:LEU:HD23	2.39	0.47
1:B:339:ASP:OD1	8:B:605:HOH:O	2.19	0.47
3:C:102:SER:C	3:C:103:ARG:O	2.53	0.47
2:D:368:ARG:NE	3:C:40:TSY:S2	2.85	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:ARG:HH22	3:C:71[A]:GLN:NE2	2.07	0.47
2:D:14[B]:ARG:NE	2:D:394:TYR:O	2.47	0.46
1:B:274:ALA:HB1	1:B:278:GLN:HG3	1.98	0.46
1:B:289:GLN:NE2	8:B:615:HOH:O	2.40	0.46
3:C:150:PHE:O	3:C:151:GLU:HB2	2.15	0.46
2:D:105:LEU:C	2:D:105:LEU:HD23	2.40	0.45
2:D:60[B]:VAL:HG12	2:D:61:HIS:CD2	2.51	0.45
2:D:260:GLY:C	2:D:261:SER:HG	2.23	0.45
3:C:47:ARG:HB2	3:C:61:SER:OG	2.15	0.45
1:B:359:VAL:HG22	3:A:5:LEU:HD21	1.99	0.45
2:D:252:GLN:CD	8:D:604:HOH:O	2.46	0.45
2:D:83:ALA:HA	2:D:93[B]:LEU:HD11	1.99	0.44
2:D:269:GLU:HA	8:D:873:HOH:O	2.18	0.44
3:C:37:ASN:HB2	3:C:42:ASP:HB2	2.00	0.44
2:D:246[A]:ARG:HB2	2:D:249[A]:LEU:HD12	2.00	0.44
8:B:780:HOH:O	2:D:62:ARG:HD3	2.18	0.43
2:D:330[B]:ARG:CG	2:D:347[B]:VAL:HG22	2.20	0.43
2:D:93[A]:LEU:HG	2:D:242:VAL:CG1	2.49	0.43
3:A:3:LEU:HD23	3:A:6:GLU:HG3	2.00	0.43
1:B:347:VAL:HG12	1:B:386:THR:HG22	2.00	0.43
2:D:212:VAL:N	2:D:213:PRO:CD	2.81	0.42
3:A:37:ASN:HB2	3:A:42:ASP:HB2	2.00	0.42
3:C:45:THR:O	3:C:62:TYR:HA	2.18	0.42
2:D:345:ALA:HA	2:D:387:ALA:O	2.20	0.42
1:B:41[B]:ARG:NE	8:B:603:HOH:O	2.02	0.42
3:A:127:ALA:O	3:A:130:LYS:HG2	2.20	0.42
1:B:102:ALA:HB1	1:B:243:LEU:HB2	2.02	0.42
1:B:373:TSY:S2	2:D:260:GLY:HA2	2.60	0.42
1:B:335:THR:HG23	8:B:870:HOH:O	2.20	0.41
3:C:14:LEU:O	3:C:18:LYS:HG2	2.21	0.41
1:B:408[A]:ARG:NH1	8:B:628:HOH:O	2.54	0.41
3:A:77:LEU:HD21	3:A:139:PHE:CB	2.48	0.41
1:B:371:HIS:HD2	1:B:373:TSY:N	2.19	0.41
1:B:207:ASP:OD2	5:B:504:PLP:N1	2.55	0.40
3:C:12:VAL:HG11	3:C:115:ASP:HB3	2.03	0.40
3:C:90:LEU:HD12	3:C:90:LEU:HA	1.94	0.40
1:B:180:HIS:HA	1:B:186:VAL:O	2.22	0.40
3:A:12:VAL:HG11	3:A:115:ASP:HB3	2.02	0.40
2:D:35[A]:SER:HA	2:D:38:THR:O	2.21	0.40
2:D:41[B]:ARG:HG2	2:D:41[B]:ARG:NH1	2.37	0.40
2:D:206:LEU:O	2:D:227:ALA:HA	2.21	0.40

All (4) 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)
8:B:909:HOH:O	8:A:301:HOH:O[1_545]	1.48	0.72
8:B:819:HOH:O	8:A:305:HOH:O[1_545]	2.04	0.16
8:D:928:HOH:O	8:D:934:HOH:O[1_455]	2.07	0.13
8:D:965:HOH:O	8:C:339:HOH:O[1_565]	2.08	0.12

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	B	412/418 (99%)	402 (98%)	10 (2%)	0	100	100
2	D	425/418 (102%)	415 (98%)	10 (2%)	0	100	100
3	A	152/166 (92%)	148 (97%)	3 (2%)	1 (1%)	18	6
3	C	146/166 (88%)	137 (94%)	5 (3%)	4 (3%)	4	0
All	All	1135/1168 (97%)	1102 (97%)	28 (2%)	5 (0%)	24	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	151	GLU
3	C	5	LEU
3	C	7	GLN
3	C	103	ARG
3	C	104	GLY

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	B	320/320 (100%)	315 (98%)	5 (2%)	55	34
2	D	332/321 (103%)	327 (98%)	5 (2%)	57	37
3	A	125/134 (93%)	121 (97%)	4 (3%)	34	12
3	C	119/134 (89%)	112 (94%)	7 (6%)	18	3
All	All	896/909 (99%)	875 (98%)	21 (2%)	44	21

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	THR
1	B	261	SER
1	B	264	GLU
1	B	343	PRO
1	B	347	VAL
2	D	8	LEU
2	D	10	LEU
2	D	128	THR
2	D	343	PRO
2	D	416	ARG
3	A	82[A]	ILE
3	A	82[B]	ILE
3	A	90	LEU
3	A	130	LYS
3	C	5	LEU
3	C	43	GLU
3	C	81	VAL
3	C	90	LEU
3	C	105	THR
3	C	130	LYS
3	C	151	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	252	GLN
1	B	371	HIS
2	D	28	ASN
3	A	19	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	80	GLN
3	C	22	HIS
3	C	80	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
3	TSY	A	40[B]	-	4,7,8	1.55	1 (25%)	3,7,9	3.74	1 (33%)
1	TSY	B	373	1	4,7,8	1.71	1 (25%)	3,7,9	3.73	1 (33%)
3	TSY	A	40[A]	-	4,7,8	1.54	1 (25%)	3,7,9	0.58	0
3	TSY	C	40	3	4,7,8	1.68	1 (25%)	3,7,9	3.95	1 (33%)

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	TSY	A	40[B]	-	-	1/2/6/8	-
1	TSY	B	373	1	-	1/2/6/8	-
3	TSY	A	40[A]	-	-	1/2/6/8	-
3	TSY	C	40	3	-	2/2/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	40[A]	TSY	O-C	2.89	1.30	1.20
3	A	40[B]	TSY	O-C	2.89	1.30	1.20
3	C	40	TSY	O-C	2.85	1.30	1.20
1	B	373	TSY	O-C	2.06	1.27	1.20

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	40	TSY	CB-SG-S1	6.58	121.10	103.86
3	A	40[B]	TSY	CB-SG-S1	6.42	120.68	103.86
1	B	373	TSY	CB-SG-S1	6.21	120.13	103.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	40[A]	TSY	N-CA-CB-SG
3	C	40	TSY	N-CA-CB-SG
1	B	373	TSY	CA-CB-SG-S1
3	A	40[B]	TSY	CA-CB-SG-S1
3	C	40	TSY	CA-CB-SG-S1

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	40[B]	TSY	3	0
1	B	373	TSY	3	0
3	A	40[A]	TSY	1	0
3	C	40	TSY	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
4	NO3	D	504	-	1,3,3	0.14	0	0,3,3	-	-
4	NO3	B	503	-	1,3,3	0.05	0	0,3,3	-	-
5	PLP	B	504	1	15,15,16	2.54	5 (33%)	21,22,23	1.45	5 (23%)
6	MPO	D	502	-	13,13,13	0.72	1 (7%)	17,17,17	1.24	1 (5%)
4	NO3	C	201	-	1,3,3	0.35	0	0,3,3	-	-
4	NO3	D	503	-	1,3,3	0.43	0	0,3,3	-	-
5	PLP	D	501	2	15,15,16	2.36	5 (33%)	21,22,23	1.78	5 (23%)
4	NO3	B	501	-	1,3,3	0.66	0	0,3,3	-	-
4	NO3	B	502	-	1,3,3	0.28	0	0,3,3	-	-

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
6	MPO	D	502	-	-	1/7/15/15	0/1/1/1
5	PLP	D	501	2	-	0/6/6/8	0/1/1/1
5	PLP	B	504	1	-	0/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	PLP	C5-C4	6.14	1.47	1.40
5	B	504	PLP	C3-C2	5.57	1.46	1.41
5	B	504	PLP	C3-C4	4.73	1.49	1.40
5	B	504	PLP	C5-C4	4.73	1.45	1.40
5	D	501	PLP	C3-C2	3.49	1.44	1.41
5	D	501	PLP	C4A-C4	-3.34	1.44	1.51
5	B	504	PLP	C4A-C4	-2.84	1.45	1.51
5	D	501	PLP	C3-C4	2.45	1.44	1.40
5	B	504	PLP	P-O1P	-2.35	1.43	1.50
6	D	502	MPO	O3-S1	2.10	1.55	1.47
5	D	501	PLP	P-O1P	2.05	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	502	MPO	O3-S1-C1	-4.30	97.60	106.00
5	D	501	PLP	C6-N1-C2	3.43	125.42	119.20
5	D	501	PLP	O3P-P-O1P	3.22	123.36	110.83
5	D	501	PLP	O4P-C5A-C5	2.73	114.47	109.36
5	B	504	PLP	C5A-C5-C6	2.53	123.48	119.36
5	B	504	PLP	O3-C3-C2	2.42	122.60	117.58
5	D	501	PLP	C3-C2-N1	-2.42	117.91	120.96
5	D	501	PLP	O2P-P-O1P	-2.40	101.49	110.83
5	B	504	PLP	O4P-C5A-C5	2.16	113.40	109.36
5	B	504	PLP	O3P-P-O1P	2.10	119.03	110.83
5	B	504	PLP	C5A-C5-C4	-2.06	118.58	122.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

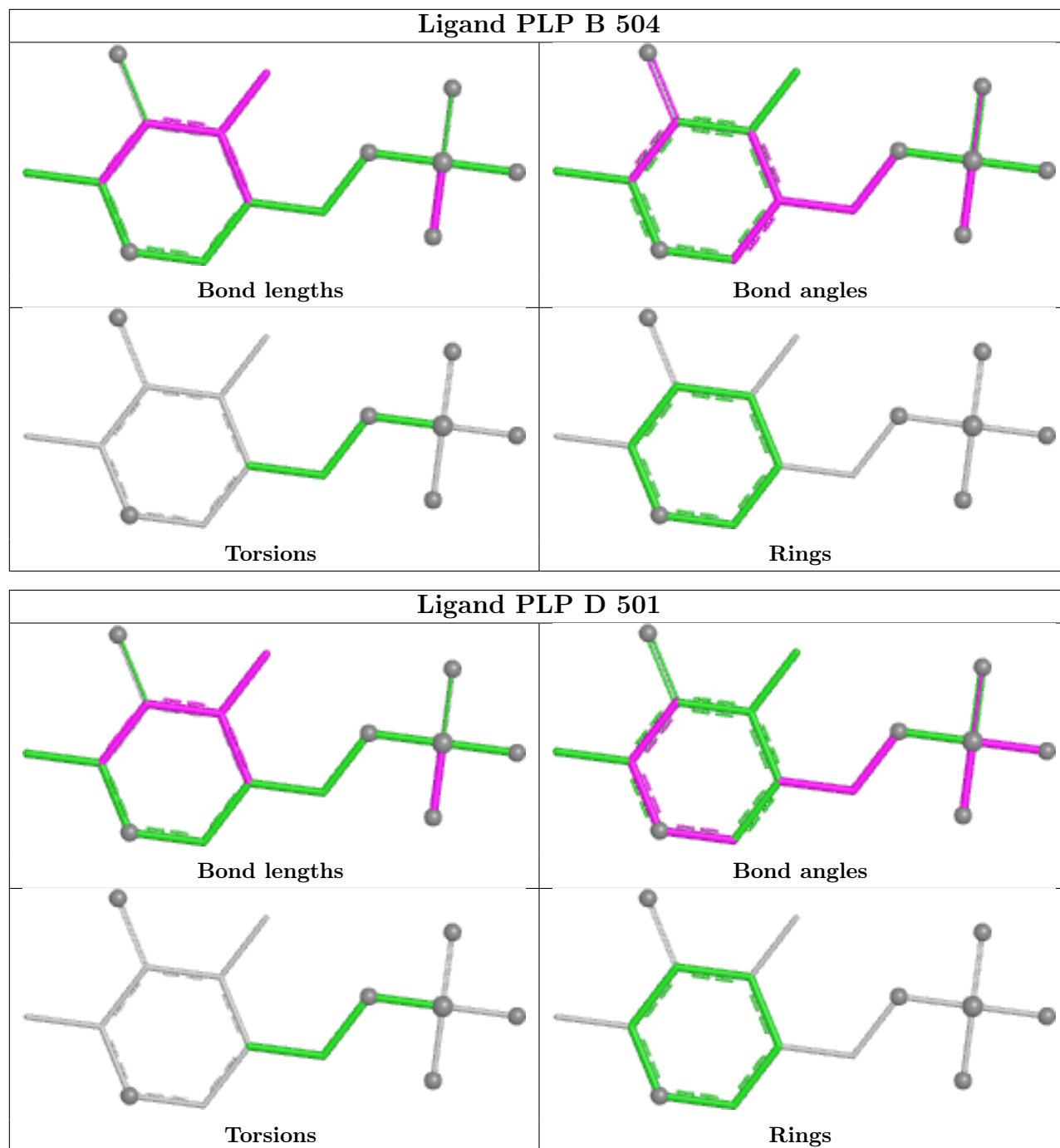
Mol	Chain	Res	Type	Atoms
6	D	502	MPO	C2-C1-S1-O1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	NO3	1	0
5	B	504	PLP	1	0
4	B	502	NO3	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	B	407/418 (97%)	-0.06	3 (0%)	84 89	9, 22, 33, 61	7 (1%)
2	D	410/418 (98%)	-0.04	3 (0%)	84 89	9, 21, 34, 69	16 (3%)
3	A	149/166 (89%)	1.03	15 (10%)	12 13	16, 40, 55, 90	5 (3%)
3	C	147/166 (88%)	1.21	20 (13%)	7 7	22, 41, 61, 78	1 (0%)
All	All	1113/1168 (95%)	0.26	41 (3%)	45 49	9, 23, 51, 90	29 (2%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	5.4
3	C	5	LEU	4.9
2	D	417	ALA	4.5
3	A	39	ILE	4.2
3	C	39	ILE	4.1
3	A	3	LEU	3.8
3	C	149	ALA	3.6
1	B	415	GLY	3.6
3	A	34	TYR	3.2
3	A	17	TYR	3.1
3	C	12	VAL	3.0
3	C	38	PRO	2.9
3	C	104	GLY	2.8
3	C	17	TYR	2.8
3	C	6	GLU	2.7
3	A	25	LEU	2.7
3	C	25	LEU	2.6
3	A	151	GLU	2.6
3	C	4	ARG	2.5
3	C	28	PRO	2.5
3	C	106	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	150	PHE	2.4
3	A	38	PRO	2.4
3	A	33	VAL	2.4
3	A	29	PHE	2.4
3	C	23	ARG	2.4
3	A	106	VAL	2.3
3	A	149	ALA	2.3
2	D	416	ARG	2.2
3	C	14	LEU	2.2
2	D	167	TYR	2.2
3	C	34	TYR	2.2
3	C	49	ALA	2.2
3	C	65	GLN	2.2
3	A	64	GLY	2.2
3	C	150	PHE	2.2
3	C	15	ASP	2.1
3	C	48	VAL	2.1
3	A	23	ARG	2.1
1	B	412	HIS	2.0
3	A	76	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	TSY	A	40[A]	8/9	0.83	0.20	29,32,50,54	5
3	TSY	A	40[B]	8/9	0.83	0.20	28,33,48,56	5
3	TSY	C	40	8/9	0.85	0.16	34,41,66,69	0
1	TSY	B	373	8/9	0.94	0.08	16,17,45,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

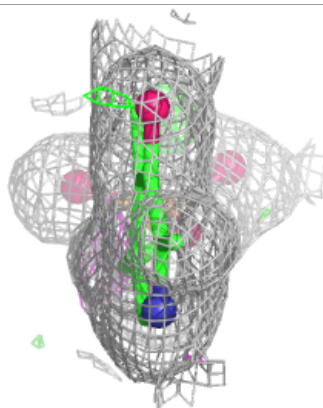
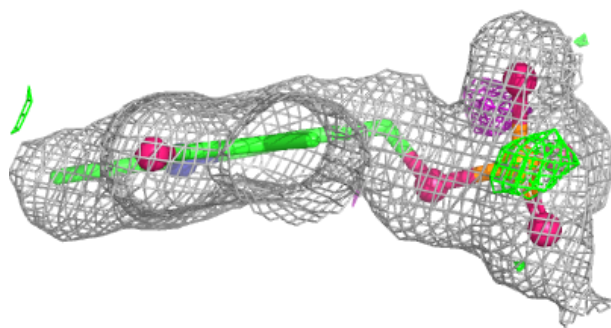
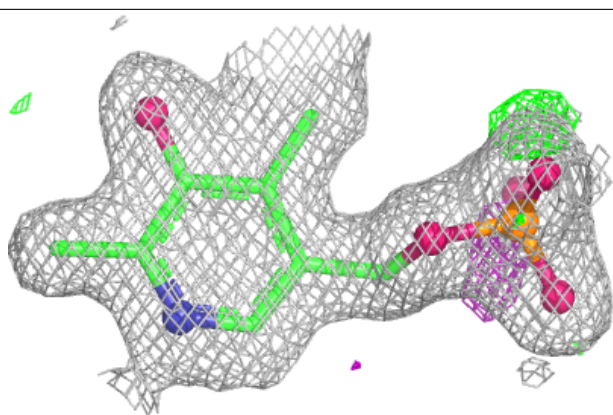
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NO3	C	201	4/4	0.88	0.11	39,42,45,50	0
4	NO3	B	503	4/4	0.89	0.10	49,54,59,64	0
4	NO3	D	504	4/4	0.90	0.11	33,36,39,40	0
4	NO3	D	503	4/4	0.94	0.09	30,32,39,46	0
6	MPO	D	502	13/13	0.94	0.09	23,26,38,38	0
4	NO3	B	501	4/4	0.95	0.10	26,30,30,35	0
4	NO3	B	502	4/4	0.96	0.08	32,37,42,47	0
5	PLP	D	501	15/16	0.98	0.05	16,18,21,23	0
5	PLP	B	504	15/16	0.98	0.06	16,19,22,23	0
7	ZN	A	201	1/1	0.99	0.03	28,28,28,28	0
7	ZN	C	202	1/1	0.99	0.03	26,26,26,26	0

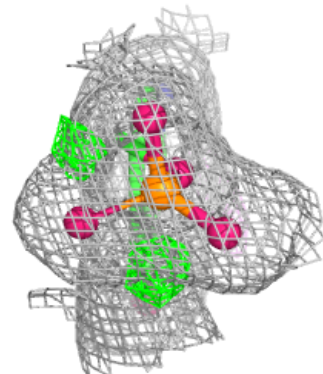
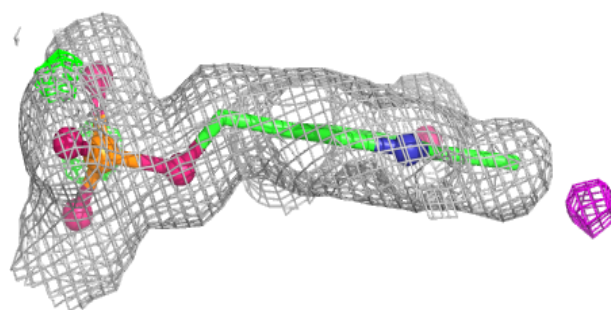
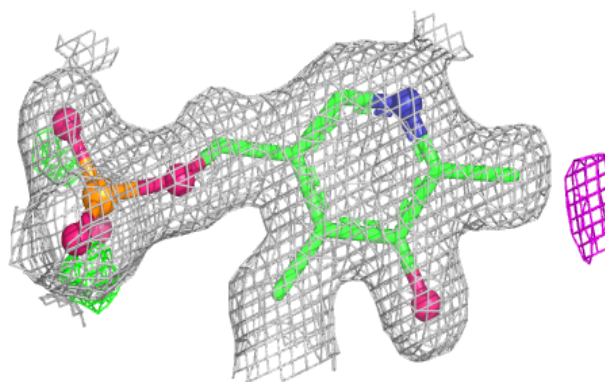
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLP D 501:

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

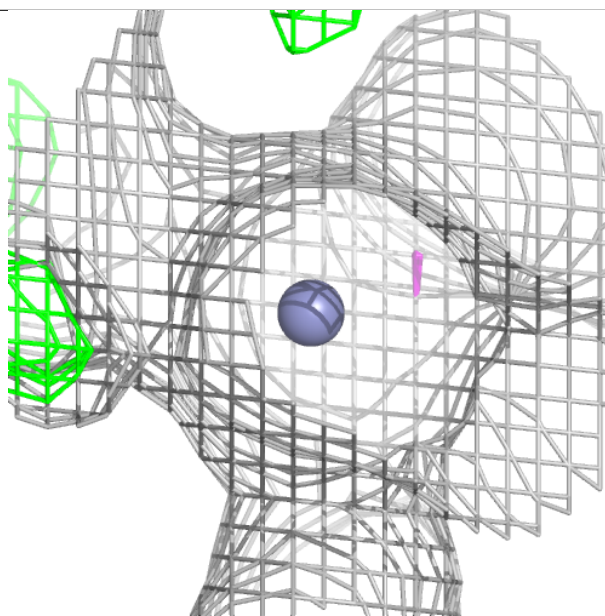
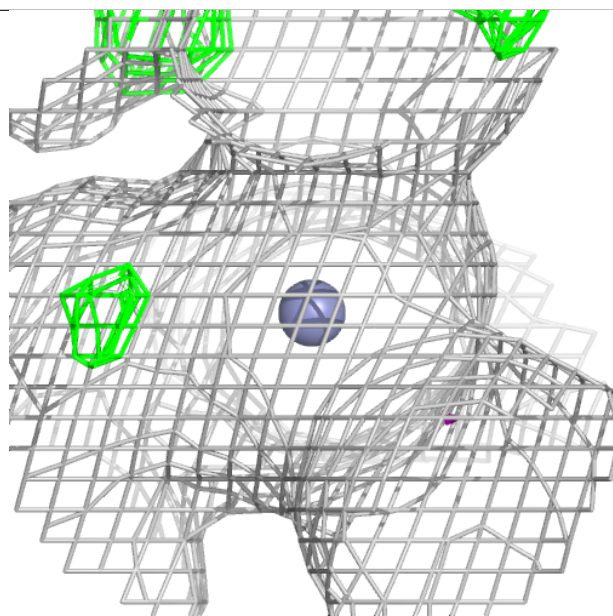
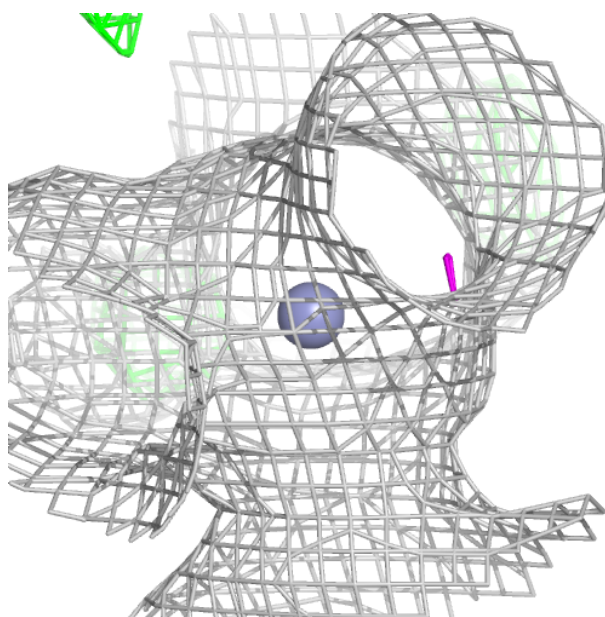
**Electron density around PLP B 504:**

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



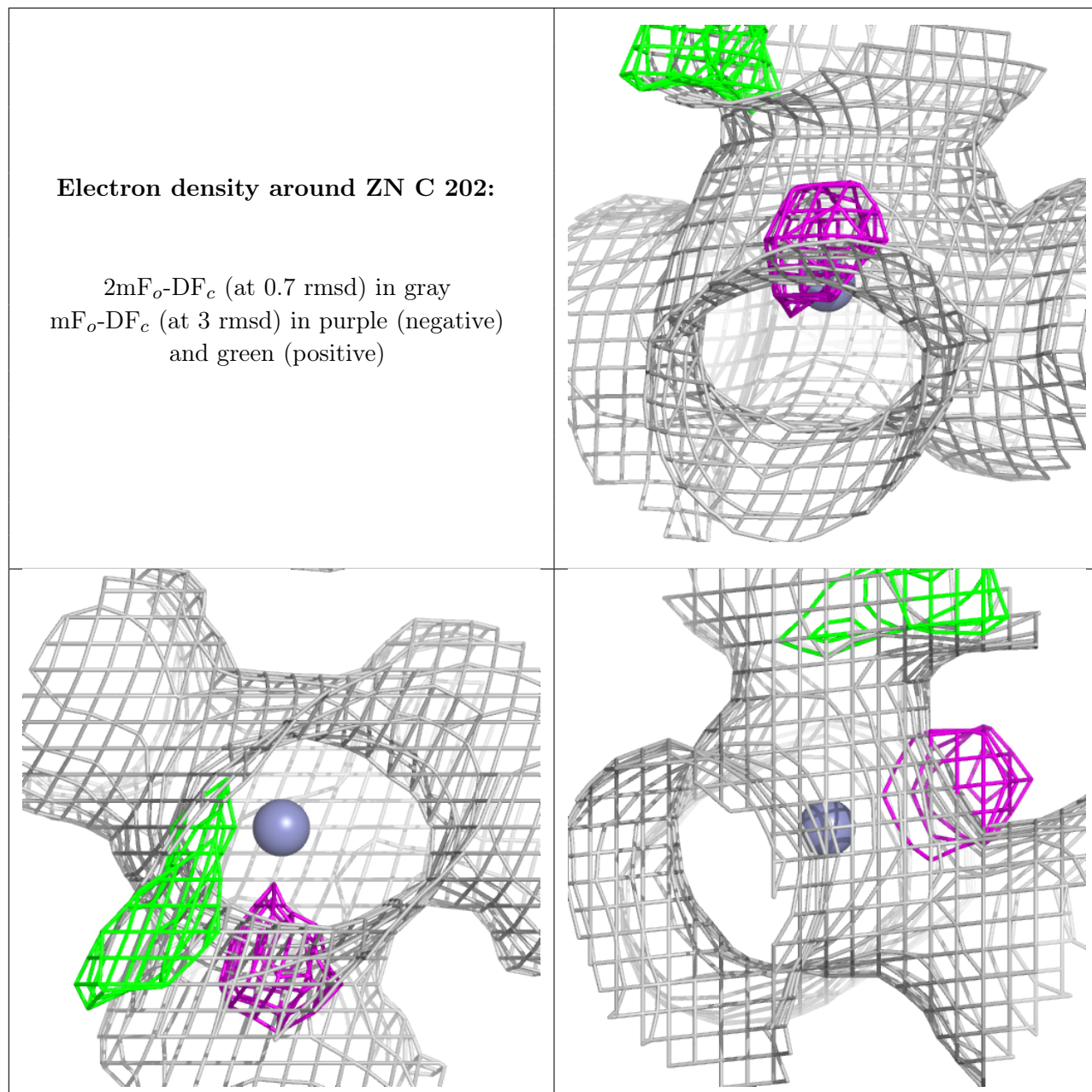
Electron density around ZN A 201:

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



Electron density around ZN C 202:

$2mF_o-DF_c$ (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.