



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:18 AM UTC

PDB ID : 7AYQ / pdb_00007ayq
Title : Crystal structure of DPP8 in complex with a 4-oxo-b-lactam based inhibitor, B114
Authors : Ross, B.; Huber, R.
Deposited on : 2020-11-13
Resolution : 2.45 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

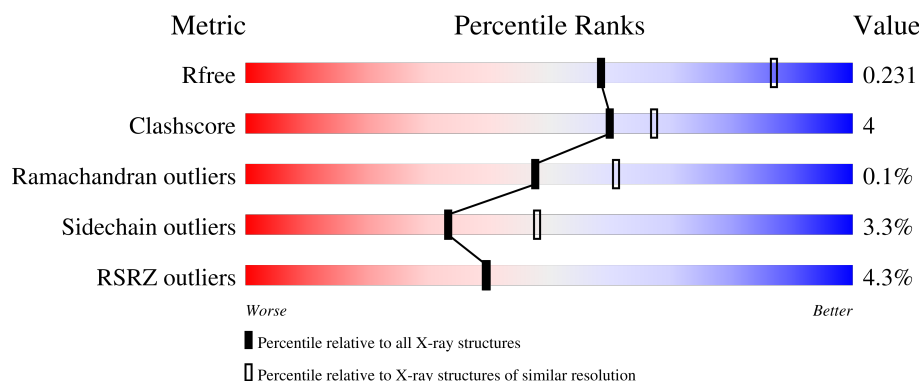
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	898	4% 78% 11% 10%
1	B	898	4% 77% 12% 10%

2 Entry composition [i](#)

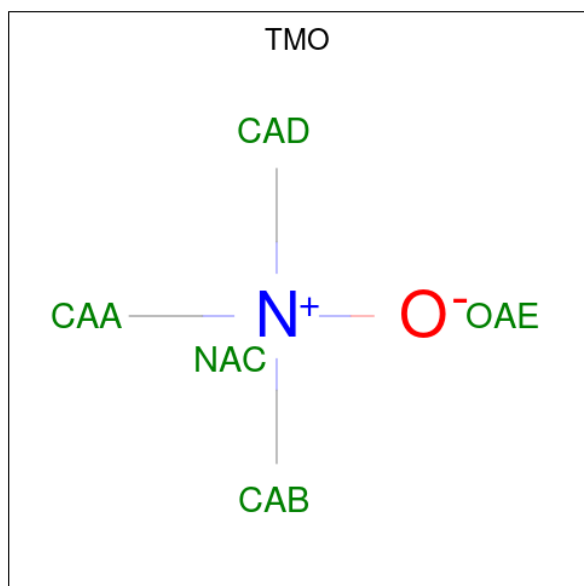
There are 6 unique types of molecules in this entry. The entry contains 13428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 8.

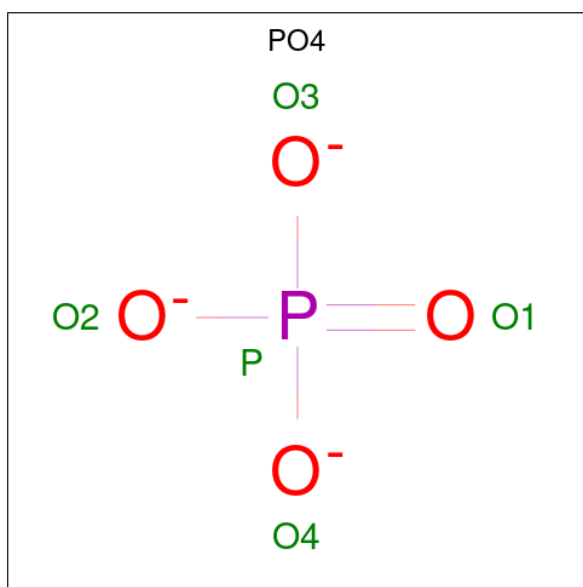
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	3	0
			6584	4238	1098	1222	26			
1	B	811	Total	C	N	O	S	9	1	0
			6583	4238	1094	1224	27			

- Molecule 2 is trimethylamine oxide (CCD ID: TMO) (formula: C₃H₉NO).



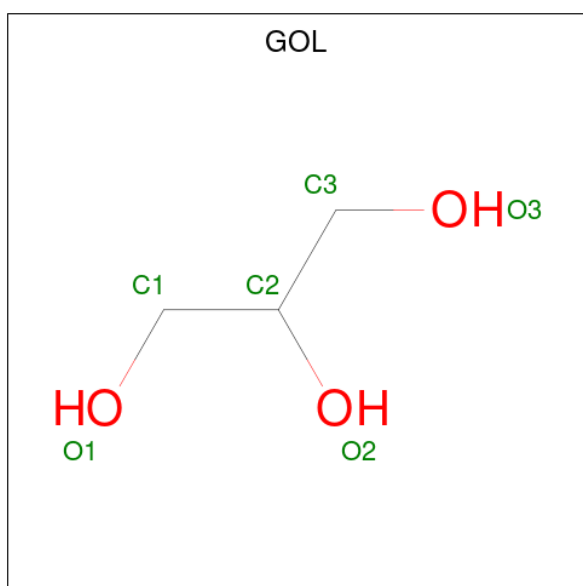
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



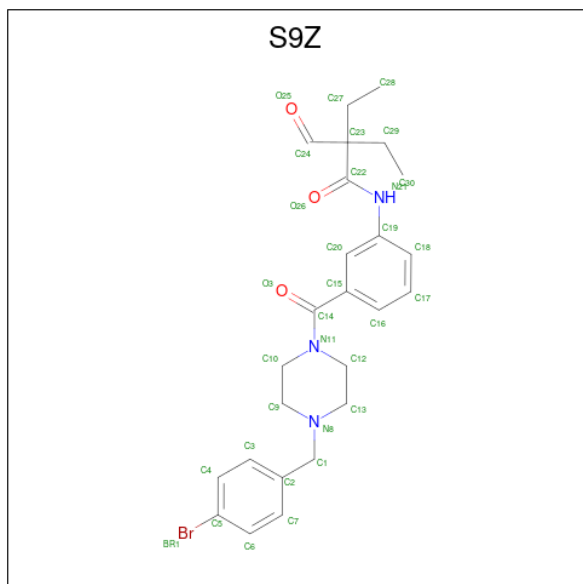
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

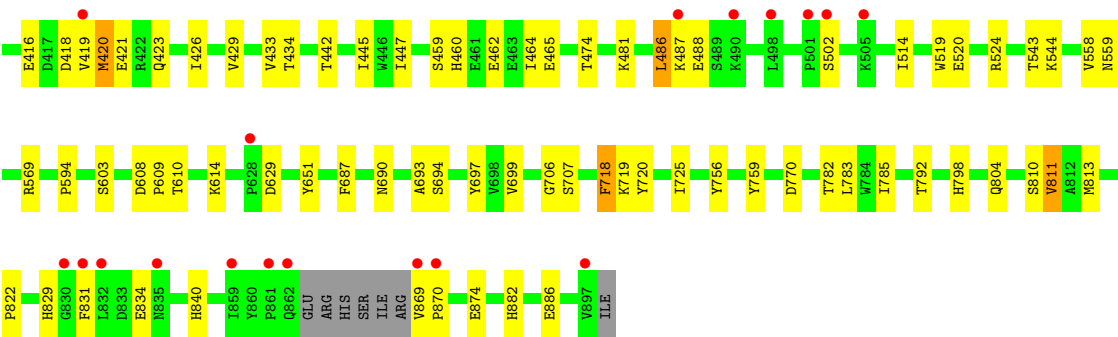
- Molecule 5 is {N}-[3-[4-[(4-bromophenyl)methyl]piperazin-1-yl]carbonylphenyl]-2-ethyl-2-methanoyl-butanamide (CCD ID: S9Z) (formula: C₂₅H₃₀BrN₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Br	C	N	O	0	0
			32	1	25	3	3		
5	B	1	Total	Br	C	N	O	0	0
			32	1	25	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	108	Total	O	0	0
			108	108		
6	B	57	Total	O	0	0
			57	57		



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	149.50Å 149.50Å 269.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.94 – 2.45 48.94 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.94-2.45) 100.0 (48.94-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.228 0.198 , 0.231	Depositor DCC
R_{free} test set	6228 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13428	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: PO4, GOL, S9Z, TMO

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	1.04	0/6774	1.30	6/9191 (0.1%)
1	B	1.05	3/6768 (0.0%)	1.32	9/9185 (0.1%)
All	All	1.05	3/13542 (0.0%)	1.31	15/18376 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	GLU	CA-CB	-5.69	1.44	1.53
1	B	798	HIS	CE1-NE2	5.08	1.37	1.32
1	B	810	SER	CA-CB	-5.07	1.46	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	HIS	CA-C-N	6.16	128.86	120.54
1	A	172	HIS	C-N-CA	6.16	128.86	120.54
1	B	594	PRO	CA-C-N	5.88	129.07	120.71
1	B	594	PRO	C-N-CA	5.88	129.07	120.71
1	B	609	PRO	CA-C-N	5.79	129.71	120.44
1	B	609	PRO	C-N-CA	5.79	129.71	120.44
1	B	133	LYS	CB-CA-C	5.45	116.06	109.85
1	B	486	LEU	CA-C-N	5.30	128.23	120.71
1	B	486	LEU	C-N-CA	5.30	128.23	120.71
1	B	97	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	519	TRP	CA-C-O	-5.23	115.83	121.38
1	A	444	ASP	N-CA-C	-5.19	106.63	113.17
1	A	396	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	517	GLY	CA-C-O	-5.12	117.96	122.16
1	B	707	SER	CA-C-O	-5.12	116.24	121.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6584	0	6395	61	0
1	B	6583	0	6385	55	0
2	A	5	0	9	0	0
2	B	5	0	9	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	32	0	0	1	0
5	B	32	0	0	1	0
6	A	108	0	0	0	0
6	B	57	0	0	0	0
All	All	13428	0	12814	112	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 4.

All (112) 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:829:HIS:HD2	1:A:841:THR:OG1	1.64	0.81
1:A:334:THR:CG2	1:A:785:ILE:HA	2.13	0.78
1:A:173:GLN:HE22	1:A:579:GLN:HE22	1.40	0.70
1:B:376:GLU:HG2	1:B:397:ARG:HB2	1.75	0.69
1:A:882:HIS:CE1	1:B:822:PRO:HG3	2.28	0.68
1:A:705:ARG:HD3	1:A:729:ASP:OD2	1.96	0.66
1:A:317:THR:HB	1:A:832:LEU:HD21	1.78	0.65
1:B:304:GLU:CD	1:B:306:ASN:HD21	2.05	0.64
1:A:123:ASN:ND2	1:A:125:ALA:H	2.00	0.59
1:B:423:GLN:HA	1:B:426:ILE:HD12	1.85	0.59
1:A:348:ILE:HG22	1:A:350:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:TYR:HB2	1:B:699:VAL:HB	1.85	0.58
1:A:822:PRO:HG3	1:B:882:HIS:CE1	2.39	0.57
1:A:348:ILE:HG22	1:A:350:ILE:CD1	2.34	0.57
1:A:500:ALA:HB1	1:A:501:PRO:HD2	1.86	0.57
1:A:767:GLN:O	1:A:768:ARG:HD2	2.05	0.56
1:B:211:CYS:HB3	1:B:232:HIS:CD2	2.40	0.56
1:B:252:VAL:HG13	1:B:264:ARG:HB3	1.87	0.56
1:A:402:LEU:C	1:A:402:LEU:HD23	2.31	0.55
1:B:481:LYS:HB2	1:B:514:ILE:HD11	1.90	0.53
1:B:687:PHE:O	1:B:690:ASN:HB3	2.09	0.53
1:B:164:VAL:HG21	1:B:183:GLY:CA	2.38	0.53
1:B:487:LYS:HG3	1:B:488:GLU:O	2.08	0.53
1:A:421:GLU:HA	1:A:421:GLU:OE1	2.08	0.52
1:A:719:LYS:HE3	1:A:720:TYR:CZ	2.45	0.52
1:B:629:ASP:OD1	1:B:629:ASP:N	2.38	0.51
1:B:78:LYS:HB2	1:B:104:MET:HE3	1.92	0.51
1:A:123:ASN:C	1:A:123:ASN:HD22	2.18	0.51
1:A:123:ASN:ND2	1:A:123:ASN:C	2.67	0.51
1:B:259:MET:HE1	1:B:328:SER:O	2.09	0.51
1:A:519:TRP:CG	1:A:544:LYS:HA	2.46	0.50
1:A:123:ASN:HD21	1:A:125:ALA:HB3	1.76	0.50
1:B:462:GLU:HA	1:B:486:LEU:HB2	1.93	0.50
1:A:351:ASP:OD1	1:A:353:GLU:HG2	2.10	0.50
1:A:252:VAL:CG1	1:A:264:ARG:HB3	2.42	0.50
1:B:882:HIS:CE1	1:B:886:GLU:HG3	2.48	0.49
1:A:271:PHE:CZ	1:A:275:GLU:HG3	2.47	0.49
1:A:719:LYS:HE3	1:A:720:TYR:CE2	2.47	0.49
1:B:69:ARG:CZ	1:B:874:GLU:HG2	2.42	0.49
1:A:273:LEU:HD22	1:A:279:ARG:NH2	2.28	0.48
1:A:627:LEU:HB2	1:A:630:TYR:HB3	1.96	0.48
1:A:99:ILE:O	1:A:115:TYR:HA	2.13	0.48
1:A:252:VAL:HG13	1:A:264:ARG:HB3	1.95	0.48
1:A:536:ARG:HA	1:A:557:TYR:CE2	2.48	0.48
1:B:376:GLU:CG	1:B:397:ARG:HB2	2.42	0.48
1:A:473:LYS:NZ	1:A:511:GLU:OE2	2.30	0.48
1:B:400:THR:O	1:B:442:THR:HA	2.14	0.48
1:B:519:TRP:CG	1:B:544:LYS:HA	2.49	0.48
5:A:904:S9Z:C12	5:A:904:S9Z:C16	2.91	0.47
1:B:756:TYR:O	1:B:759:TYR:HB3	2.14	0.47
1:A:303:TYR:CZ	1:A:344:LYS:HB2	2.49	0.47
1:B:258:ASN:HD22	1:B:258:ASN:N	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:VAL:HG22	1:B:870:PRO:HD2	1.95	0.47
1:B:365:ILE:HD12	1:B:429:VAL:HG21	1.96	0.47
1:A:782:THR:H	1:A:840:HIS:CD2	2.33	0.46
1:A:782:THR:H	1:A:840:HIS:HD2	1.61	0.46
1:A:882:HIS:CE1	1:A:886:GLU:HG3	2.51	0.46
1:B:192:GLY:HA2	1:B:197:PHE:CE1	2.51	0.46
1:A:49:GLU:O	1:A:660:LYS:HA	2.15	0.46
1:B:286:CYS:HB2	1:B:383:TRP:CZ2	2.51	0.46
1:B:460:HIS:CE1	1:B:462:GLU:HG2	2.51	0.45
1:B:465:GLU:OE1	1:B:481:LYS:HE2	2.17	0.45
1:B:782:THR:H	1:B:840:HIS:HD2	1.64	0.45
1:A:882:HIS:CE1	1:B:822:PRO:CG	2.98	0.45
5:B:904:S9Z:C12	5:B:904:S9Z:C16	2.94	0.45
1:A:69:ARG:CZ	1:A:874:GLU:HG2	2.47	0.45
1:A:734:LEU:HD12	1:A:734:LEU:HA	1.81	0.45
1:A:829:HIS:HE1	1:A:836:VAL:O	1.99	0.45
1:A:882:HIS:NE2	1:B:822:PRO:HG3	2.32	0.44
1:A:400:THR:O	1:A:442:THR:HA	2.18	0.44
1:A:334:THR:HG22	1:A:785:ILE:HA	1.96	0.44
1:A:422:ARG:NH1	1:A:426:ILE:HD11	2.32	0.44
1:B:433:VAL:O	1:B:433:VAL:HG12	2.18	0.44
1:A:736:TYR:OH	1:A:740:ARG:NH1	2.51	0.44
1:A:869:VAL:HG12	1:A:871:GLU:HG2	2.00	0.44
1:B:770:ASP:OD1	1:B:770:ASP:N	2.49	0.44
1:B:465:GLU:OE1	1:B:481:LYS:CE	2.66	0.44
1:A:84:MET:SD	1:A:171:TYR:CD2	3.11	0.43
1:A:353:GLU:CG	1:A:355:ARG:HG2	2.49	0.43
1:B:783:LEU:HD11	1:B:813:MET:HE3	1.99	0.43
1:B:804:GLN:NE2	1:B:804:GLN:HA	2.34	0.43
1:A:302:LEU:HD22	1:A:390:ALA:HB1	2.00	0.43
1:B:693:ALA:HA	1:B:697:TYR:O	2.19	0.43
1:A:178:PHE:O	1:A:188:HIS:HA	2.19	0.42
1:A:353:GLU:HG3	1:A:355:ARG:HG2	2.00	0.42
1:A:693:ALA:HA	1:A:697:TYR:O	2.19	0.42
1:A:706:GLY:HA3	1:A:718:PHE:CE2	2.54	0.42
1:B:706:GLY:HA3	1:B:718:PHE:CE2	2.54	0.42
1:B:719:LYS:HG2	1:B:720:TYR:CD2	2.54	0.42
1:B:782:THR:HA	1:B:811:VAL:HG13	2.01	0.42
1:B:334:THR:CG2	1:B:785:ILE:HA	2.50	0.42
1:A:211:CYS:HB3	1:A:232:HIS:CD2	2.54	0.42
1:A:273:LEU:HD22	1:A:279:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:O	1:B:115:TYR:HA	2.19	0.42
1:B:209:THR:OG1	1:B:246:GLU:OE2	2.31	0.42
1:A:418:ASP:OD1	1:A:418:ASP:C	2.63	0.41
1:B:416:GLU:HG2	1:B:421:GLU:HG3	2.02	0.41
1:B:520:GLU:H	1:B:543:THR:HG1	1.68	0.41
1:B:411:LEU:HD21	1:B:434:THR:HA	2.02	0.41
1:B:608:ASP:OD1	1:B:610:THR:HB	2.20	0.41
1:A:831:PHE:CZ	1:B:831:PHE:CZ	3.09	0.41
1:A:79:ALA:O	1:A:80:PRO:C	2.64	0.41
1:A:129:MET:HE1	1:A:622:ASP:HB2	2.03	0.41
1:A:446:TRP:HZ2	1:A:715:GLU:HG2	1.86	0.40
1:B:372:PHE:HE1	1:B:405:VAL:HG11	1.87	0.40
1:B:243:THR:O	1:B:244:ARG:HB2	2.21	0.40
1:B:402:LEU:HD12	1:B:447:ILE:HG21	2.03	0.40
1:A:766:MET:HE2	1:A:766:MET:HB3	1.92	0.40
1:A:820:SER:O	1:B:58:TRP:HB3	2.22	0.40
1:B:418:ASP:OD1	1:B:420:MET:HB2	2.22	0.40
1:A:759:TYR:CE1	1:A:763:MET:HE2	2.56	0.40
1:B:524:ARG:HA	1:B:524:ARG:HD2	1.90	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	801/898 (89%)	774 (97%)	26 (3%)	1 (0%)	48 61
1	B	804/898 (90%)	775 (96%)	28 (4%)	1 (0%)	48 61
All	All	1605/1796 (89%)	1549 (96%)	54 (3%)	2 (0%)	48 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	ILE
1	B	445	ILE

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	719/795 (90%)	700 (97%)	19 (3%)	40	55
1	B	718/795 (90%)	689 (96%)	29 (4%)	28	41
All	All	1437/1590 (90%)	1389 (97%)	48 (3%)	33	48

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	123	ASN
1	A	139	PHE
1	A	260	GLU
1	A	261	GLU
1	A	273	LEU
1	A	294	SER
1	A	312	GLU
1	A	314	ILE
1	A	419	VAL
1	A	434	THR
1	A	464	ILE
1	A	502	SER
1	A	510	GLU
1	A	524	ARG
1	A	545	ASP
1	A	718	PHE
1	A	801	GLN
1	A	892	ILE
1	B	53	VAL
1	B	110	GLU
1	B	164	VAL

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Mol	Chain	Res	Type
1	B	252	VAL
1	B	258	ASN
1	B	294	SER
1	B	304	GLU
1	B	314	ILE
1	B	350	ILE
1	B	366	GLN
1	B	376	GLU
1	B	419	VAL
1	B	420	MET
1	B	459	SER
1	B	464	ILE
1	B	474	THR
1	B	502	SER
1	B	558	VAL
1	B	559	ASN
1	B	569	ARG
1	B	603	SER
1	B	614	LYS
1	B	694	SER
1	B	718	PHE
1	B	725	ILE
1	B	792	THR
1	B	811	VAL
1	B	829	HIS
1	B	834	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	72	HIS
1	A	111	ASN
1	A	123	ASN
1	A	173	GLN
1	A	200	GLN
1	A	338	ASN
1	A	550	HIS
1	A	580	HIS
1	A	657	GLN
1	A	829	HIS
1	A	835	ASN

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Mol	Chain	Res	Type
1	A	840	HIS
1	A	858	GLN
1	A	882	HIS
1	B	72	HIS
1	B	173	GLN
1	B	199	GLN
1	B	200	GLN
1	B	258	ASN
1	B	306	ASN
1	B	315	HIS
1	B	366	GLN
1	B	460	HIS
1	B	579	GLN
1	B	580	HIS
1	B	595	HIS
1	B	835	ASN
1	B	840	HIS
1	B	858	GLN
1	B	882	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	903	-	5,5,5	0.42	0	5,5,5	0.76	0
5	S9Z	B	904	1	32,34,34	0.76	0	41,47,47	1.84	9 (21%)
3	PO4	A	902	-	4,4,4	0.65	0	6,6,6	0.52	0
2	TMO	B	901	-	4,4,4	1.06	0	6,6,6	0.62	0
3	PO4	B	902	-	4,4,4	0.66	0	6,6,6	0.60	0
5	S9Z	A	904	1	32,34,34	0.71	0	41,47,47	1.67	9 (21%)
4	GOL	B	903	-	5,5,5	0.30	0	5,5,5	0.61	0
2	TMO	A	901	-	4,4,4	1.36	0	6,6,6	0.49	0

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
4	GOL	B	903	-	-	2/4/4/4	-
4	GOL	A	903	-	-	1/4/4/4	-
5	S9Z	A	904	1	-	3/28/41/41	0/3/3/3
5	S9Z	B	904	1	-	2/28/41/41	0/3/3/3

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	S9Z	C23-C22-N21	4.87	122.11	115.68
5	B	904	S9Z	BR1-C5-C4	4.86	125.92	119.30
5	B	904	S9Z	C15-C14-N11	4.53	124.32	118.66
5	B	904	S9Z	BR1-C5-C6	-4.46	113.22	119.30
5	A	904	S9Z	C10-C9-N8	-3.65	103.29	110.65
5	B	904	S9Z	O3-C14-C15	-3.10	114.15	120.29
5	B	904	S9Z	C1-N8-C13	-2.88	104.87	111.07
5	A	904	S9Z	C7-C2-C3	2.75	122.33	118.23
5	B	904	S9Z	C1-C2-C7	-2.74	115.69	120.75
5	B	904	S9Z	C12-N11-C10	2.62	118.03	112.68
5	A	904	S9Z	C18-C19-C20	-2.53	116.59	119.66
5	A	904	S9Z	C13-N8-C9	-2.43	103.60	108.84
5	A	904	S9Z	C12-N11-C10	2.37	117.52	112.68
5	B	904	S9Z	C23-C22-N21	2.32	118.74	115.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	S9Z	C20-C19-N21	2.15	127.11	120.13
5	A	904	S9Z	C6-C7-C2	-2.13	118.19	121.00
5	B	904	S9Z	C7-C2-C3	2.05	121.28	118.23
5	A	904	S9Z	C17-C16-C15	-2.01	118.39	120.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

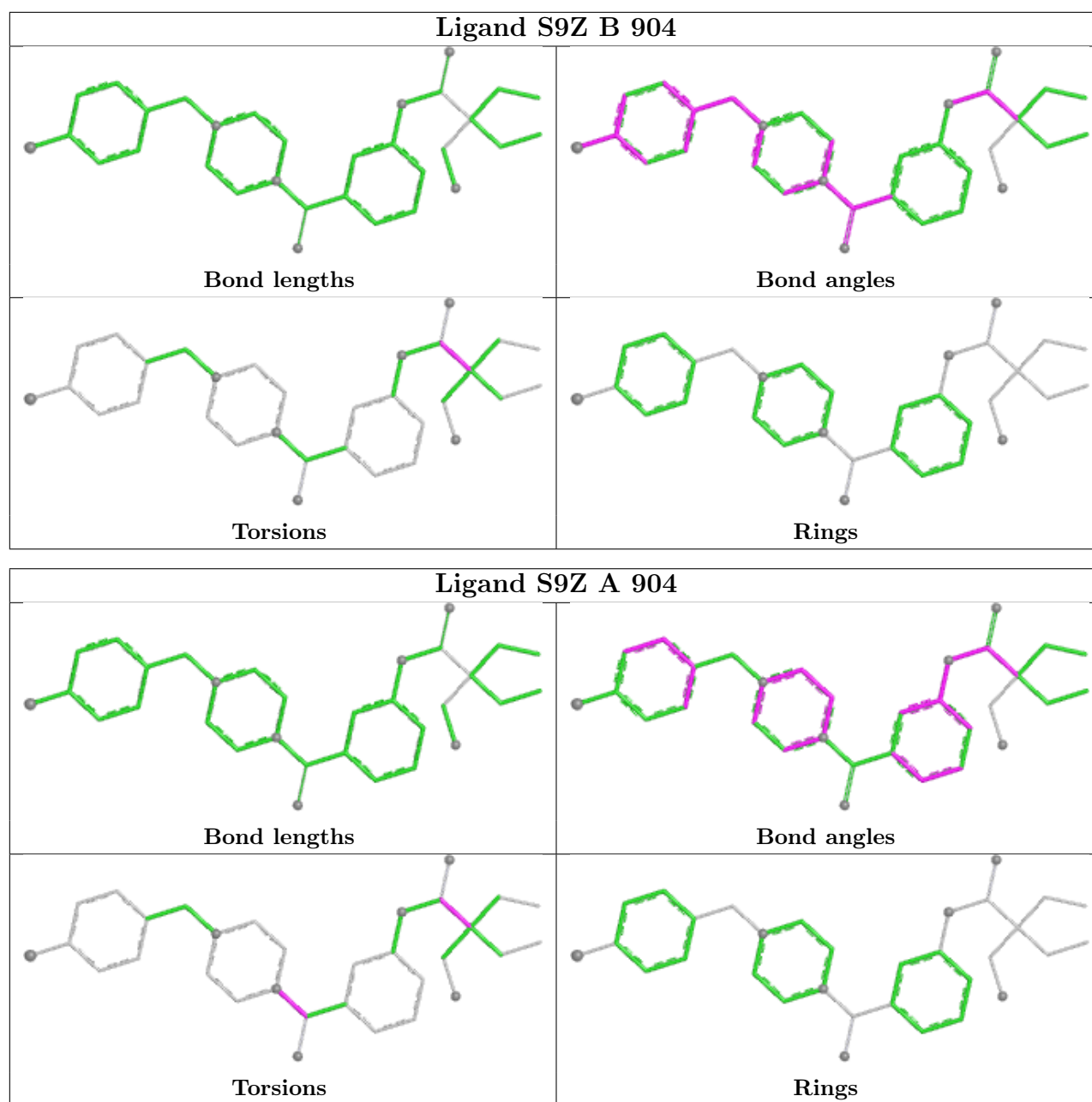
Mol	Chain	Res	Type	Atoms
4	B	903	GOL	O1-C1-C2-C3
4	B	903	GOL	O1-C1-C2-O2
5	A	904	S9Z	O3-C14-N11-C10
5	A	904	S9Z	N21-C22-C23-C27
5	B	904	S9Z	O26-C22-C23-C27
5	A	904	S9Z	O26-C22-C23-C29
5	B	904	S9Z	N21-C22-C23-C27
4	A	903	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	904	S9Z	1	0
5	A	904	S9Z	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	808/898 (89%)	0.03	34 (4%)	40 40	36, 62, 111, 154	3 (0%)
1	B	811/898 (90%)	0.17	35 (4%)	40 39	33, 67, 114, 155	3 (0%)
All	All	1619/1796 (90%)	0.10	69 (4%)	40 39	33, 64, 113, 155	6 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	7.2
1	B	317	THR	5.6
1	B	897	VAL	5.4
1	A	317	THR	5.2
1	A	259	MET	5.0
1	B	48	LEU	4.6
1	A	897	VAL	4.5
1	A	869	VAL	4.4
1	B	164	VAL	4.4
1	A	628	PRO	4.2
1	A	74	TYR	4.2
1	B	316	VAL	4.2
1	A	138	LEU	4.2
1	A	71	TYR	4.1
1	B	869	VAL	4.0
1	B	419	VAL	3.7
1	B	861	PRO	3.6
1	A	70	LYS	3.4
1	B	832	LEU	3.4
1	B	71	TYR	3.4
1	B	831	PHE	3.4
1	B	74	TYR	3.3
1	B	78	LYS	3.3
1	B	862	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	629	ASP	3.2
1	B	835	ASN	3.2
1	A	77	ALA	3.2
1	B	76	MET	3.1
1	B	259	MET	3.1
1	A	419	VAL	3.1
1	B	139	PHE	3.1
1	A	862	GLN	3.1
1	A	316	VAL	3.1
1	A	256	LEU	3.0
1	A	627	LEU	3.0
1	B	830	GLY	3.0
1	B	628	PRO	3.0
1	A	140	GLN	2.8
1	B	501	PRO	2.7
1	A	659	GLY	2.6
1	A	624	ALA	2.6
1	B	256	LEU	2.5
1	B	487	LYS	2.5
1	B	107	GLU	2.5
1	B	490	LYS	2.5
1	B	505	LYS	2.4
1	A	835	ASN	2.4
1	B	70	LYS	2.4
1	B	870	PRO	2.4
1	A	501	PRO	2.3
1	A	830	GLY	2.2
1	A	896	LYS	2.2
1	B	293	PRO	2.2
1	A	861	PRO	2.2
1	A	73	GLY	2.2
1	A	832	LEU	2.1
1	B	388	LYS	2.1
1	A	420	MET	2.1
1	A	257	ALA	2.1
1	A	105	SER	2.1
1	B	498	LEU	2.1
1	A	891	ARG	2.1
1	B	859	ILE	2.1
1	A	78	LYS	2.1
1	B	72	HIS	2.1
1	A	831	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	257	ALA	2.0
1	A	72	HIS	2.0
1	B	502	SER	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](#)

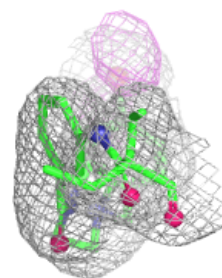
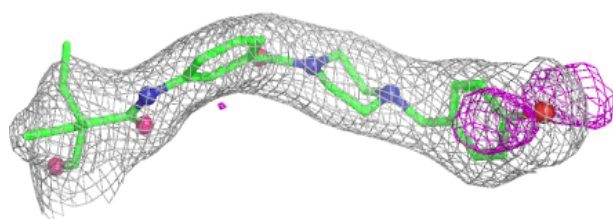
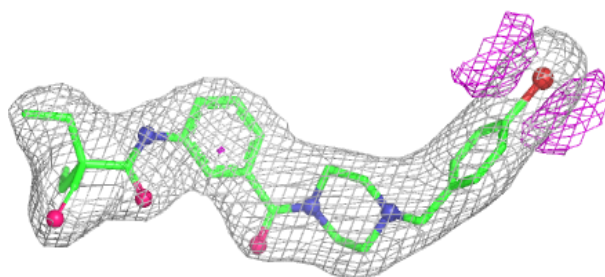
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	B	902	5/5	0.88	0.10	91,94,113,114	0
3	PO4	A	902	5/5	0.90	0.09	101,110,123,124	0
4	GOL	A	903	6/6	0.92	0.19	71,80,98,99	0
4	GOL	B	903	6/6	0.92	0.20	83,89,102,102	0
5	S9Z	A	904	32/32	0.95	0.11	53,69,79,109	0
2	TMO	A	901	5/5	0.96	0.14	57,62,70,71	0
2	TMO	B	901	5/5	0.97	0.12	61,64,72,74	0
5	S9Z	B	904	32/32	0.97	0.09	45,67,76,93	0

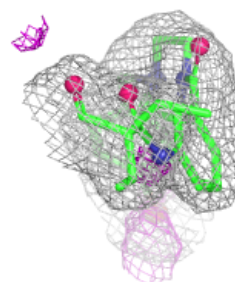
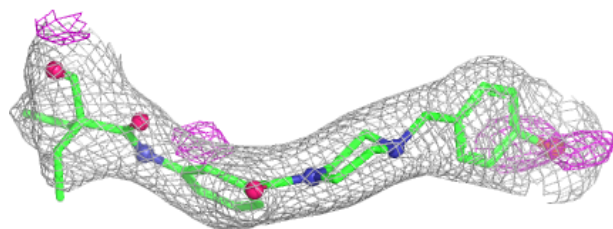
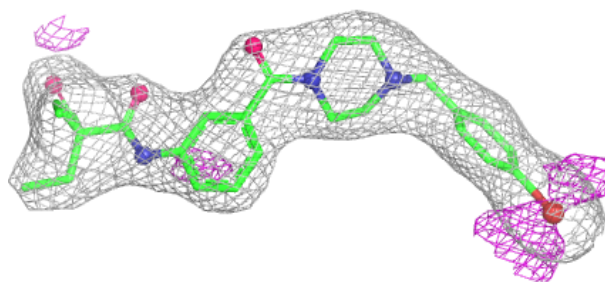
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S9Z A 904:

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

**Electron density around S9Z B 904:**

$2mF_o-DF_c$ (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.