



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:41 am BST

PDB ID : 6JTC
Title : Crystal structure of dipeptidyl peptidase 11 (DPP11) with SH-5 from Porphyromonas gingivalis (Space)
Authors : Sakamoto, Y.; Suzuki, Y.; Iizuka, I.; Roppongi, S.; Kushibiki, C.; Nakamura, A.; Ogasawara, W.; Tanaka, N.
Deposited on : 2019-04-10
Resolution : 2.39 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

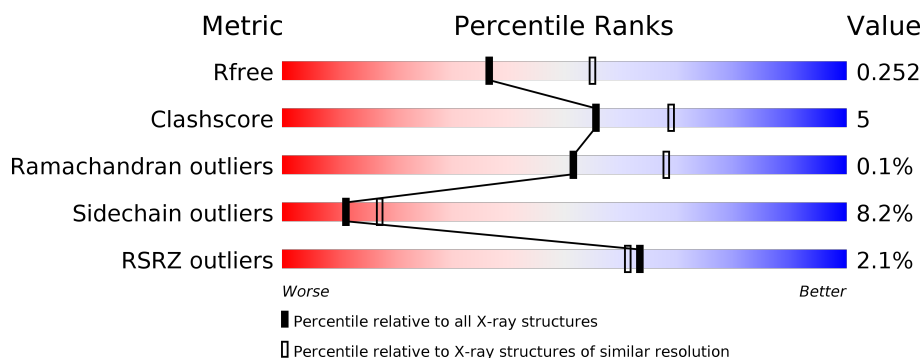
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	720	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	720	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11479 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 Asp/Glu-specific dipeptidyl-peptidase.

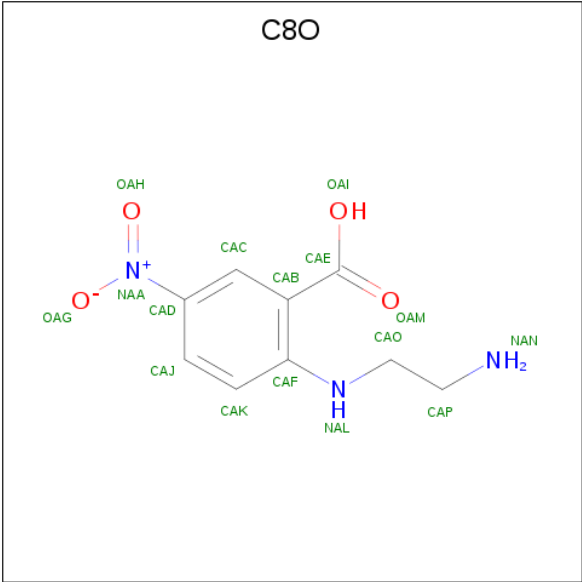
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5608	3553	970	1058	27			
1	B	699	Total	C	N	O	S	0	0	0
			5608	3553	970	1058	27			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is 2-(2-azanylethylamino)-5-nitro-benzoic acid (three-letter code: C8O) (formula: C₉H₁₁N₃O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	9	3	4		
3	B	1	Total	C	N	O	0	0
			16	9	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	134	Total	O	0	0
			134	134		

These plots are drawn for all protein, RNA and DNA 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.

- Chain A:
-
- 3% 79% 15%
- •
- Met Lys Lys Arg Leu Leu Pro Phe Ala Ala Cys Leu Ser Gln Ile Ala His Ala D22 P23 G24 K39 L50 L64 G68 G69 T70 T71 N83 H84 H85 N90 L97 E98 E103 N104 R110 D113 L139 T142 K143 D144 P145 K154 Y155 L156 L159 K163 K166 N167 F168 S169 A170 K171 G174 L175 S176 V177 M190 R200 D215 D219 L220 N221 P222 R223 H224 D227 F231 Y234 P241 F246 N258 L261 N267 D268 R281 Y282 F283 R301 R306 N310 T323 K327 R351 Q352 N353 K354 Q355 T370 T383 L390 G404 I405 E406 S410 T414 F415 D416 E417 T418 K419 A420 L421 N424 D425 A426 R429 K430 E431 K442 F443 V456 A457 M460 L461 L465 K466 P469 Y470 E471 N472 L473 L477 V480 R483 D494 R498 V516 M524 M525 L526 L538 L542 L549 L550 Q553 L560 L561 F570 N574 L575 T576 Q583 V584 K585 P589 N592 Y595 L601 D602 G603 V604 E614 D618 V624 R632 D635 R636 S637 G638 T648

- Chain B:
-
- 83% 14%
- | Label | Value |
|-------|--------|
| MET | 0.0000 |
| LYS | 0.0000 |
| ARG | 0.0000 |
| LEU | 0.0000 |
| LEU | 0.0000 |
| LEU | 0.0000 |
| PRO | 0.0000 |
| PHE | 0.0000 |
| ALA | 0.0000 |
| ALA | 0.0000 |
| LEU | 0.0000 |
| CYS | 0.0000 |
| LEU | 0.0000 |
| SER | 0.0000 |
| GLN | 0.0000 |
| ILE | 0.0000 |
| ALA | 0.0000 |
| HIS | 0.0000 |
| ALA | 0.0000 |
| D22 | 0.0000 |
| F23 | 0.0000 |
| G24 | 0.0000 |
| M25 | 0.0000 |
| W26 | 0.0000 |
| R41 | 0.0000 |
| K59 | 0.0000 |
| L64 | 0.0000 |
| T70 | 0.0000 |
| V73 | 0.0000 |
| L81 | 0.0000 |
| T82 | 0.0000 |
| N83 | 0.0000 |
| L97 | 0.0000 |
| A108 | 0.0000 |
| V122 | 0.0000 |
| K140 | 0.0000 |
| K143 | 0.0000 |
| H167 | 0.0000 |
| L187 | 0.0000 |
| I188 | 0.0000 |
| T197 | 0.0000 |
| R200 | 0.0000 |
| S207 | 0.0000 |
| S208 | 0.0000 |
| K211 | 0.0000 |
| A214 | 0.0000 |
| M218 | 0.0000 |
| W219 | 0.0000 |
| F231 | 0.0000 |
| R232 | 0.0000 |
| I233 | 0.0000 |
| Y234 | 0.0000 |
| K237 | 0.0000 |
| S245 | 0.0000 |
| P250 | 0.0000 |
| P253 | 0.0000 |
| I259 | 0.0000 |
| S260 | 0.0000 |
| L261 | 0.0000 |
| Q265 | 0.0000 |
| E266 | 0.0000 |
| Y269 | 0.0000 |
| A270 | 0.0000 |
| M271 | 0.0000 |
| I272 | 0.0000 |
| M273 | 0.0000 |
| F283 | 0.0000 |
| R306 | 0.0000 |
| K327 | 0.0000 |
| R337 | 0.0000 |
| W343 | 0.0000 |
| T347 | 0.0000 |
| R348 | 0.0000 |
| M357 | 0.0000 |
| L361 | 0.0000 |
| W364 | 0.0000 |
| K367 | 0.0000 |
| Q368 | 0.0000 |
| Y373 | 0.0000 |
| K386 | 0.0000 |
| F407 | 0.0000 |
| S410 | 0.0000 |
| P413 | 0.0000 |
| T414 | 0.0000 |
| E417 | 0.0000 |
| G423 | 0.0000 |
| M424 | 0.0000 |
| D425 | 0.0000 |
| R429 | 0.0000 |
| I433 | 0.0000 |
| F443 | 0.0000 |
| L461 | 0.0000 |
| L465 | 0.0000 |
| L475 | 0.0000 |
| H476 | 0.0000 |
| R483 | 0.0000 |
| E504 | 0.0000 |
| V513 | 0.0000 |
| L519 | 0.0000 |
| M524 | 0.0000 |
| V525 | 0.0000 |
| L526 | 0.0000 |
| V531 | 0.0000 |
| R543 | 0.0000 |
| D547 | 0.0000 |
| P548 | 0.0000 |
| L560 | 0.0000 |
| L561 | 0.0000 |
| E562 | 0.0000 |
| M563 | 0.0000 |
| D564 | 0.0000 |
| F570 | 0.0000 |
| L577 | 0.0000 |
| P589 | 0.0000 |
| V506 | 0.0000 |
| G596 | 0.0000 |
| H597 | 0.0000 |
| Q598 | 0.0000 |
| K620 | 0.0000 |
| R627 | 0.0000 |
| R632 | 0.0000 |
| D635 | 0.0000 |
| R636 | 0.0000 |
| T648 | 0.0000 |
| S655 | 0.0000 |
| P658 | 0.0000 |
| L669 | 0.0000 |
| N670 | 0.0000 |
| F671 | 0.0000 |
| D672 | 0.0000 |
| R673 | 0.0000 |
| G680 | 0.0000 |
| Q683 | 0.0000 |
| S691 | 0.0000 |
| I696 | 0.0000 |
| L700 | 0.0000 |
| R711 | 0.0000 |
| L712 | 0.0000 |
| L713 | 0.0000 |
| M716 | 0.0000 |
| P720 | 0.0000 |

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.34Å 116.96Å 148.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 2.39 39.62 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.65-2.39) 99.8 (39.62-2.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.202 , 0.253 0.208 , 0.252	Depositor DCC
R_{free} test set	3516 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11479	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, C8O

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	0.69	0/5733	0.86	0/7745
1	B	0.68	0/5733	0.85	0/7745
All	All	0.68	0/11466	0.85	0/15490

There are no bond length outliers.

There are no bond angle outliers.

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	5608	0	5491	52	0
1	B	5608	0	5491	61	0
2	A	6	0	8	0	0
3	A	16	0	0	1	0
3	B	16	0	0	4	0
4	A	91	0	0	1	0
4	B	134	0	0	1	0
All	All	11479	0	10990	113	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 5.

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)
1:B:272:ILE:HD12	1:B:648:THR:HG21	1.63	0.79
1:B:343:TRP:O	1:B:347:THR:HB	1.84	0.77
1:A:223:ARG:NH2	1:A:672:ASP:OD2	2.21	0.72
1:A:410:SER:HB3	1:A:524:MET:HE3	1.73	0.70
1:B:410:SER:CB	1:B:524:MET:CE	2.71	0.68
1:B:347:THR:HG22	1:B:348:ARG:HG2	1.76	0.68
1:B:712:LEU:O	1:B:716:MET:HG3	1.94	0.67
1:B:410:SER:CB	1:B:524:MET:HE2	2.26	0.65
3:B:801:C8O:OAM	3:B:801:C8O:CAO	2.44	0.65
1:A:410:SER:CB	1:A:524:MET:CE	2.75	0.64
1:A:410:SER:CB	1:A:524:MET:HE2	2.28	0.64
1:A:410:SER:HB3	1:A:524:MET:CE	2.28	0.63
1:A:477:LEU:O	1:A:480:VAL:HG12	1.99	0.63
1:B:410:SER:HB2	1:B:524:MET:HE2	1.80	0.63
1:A:410:SER:HB2	1:A:524:MET:HE2	1.81	0.62
1:B:343:TRP:CE2	1:B:347:THR:HG21	2.37	0.60
1:B:219:TRP:CH2	3:B:801:C8O:OAM	2.55	0.60
1:B:81:LEU:HD13	1:B:669:LEU:HD11	1.84	0.59
1:B:589:PRO:HG3	1:B:595:TYR:CE2	2.38	0.58
1:B:424:ASN:HD22	1:B:425:ASP:N	2.02	0.58
1:B:187:LEU:C	1:B:187:LEU:HD23	2.24	0.58
1:B:214:ALA:O	1:B:218:ASN:HB2	2.04	0.57
1:A:351:ARG:HH12	1:A:355:GLN:HE21	1.53	0.56
1:B:414:THR:HG22	1:B:417:GLU:H	1.70	0.56
1:A:215:ASP:HB2	1:A:614:GLU:OE2	2.04	0.56
1:A:258:ASN:CG	1:A:717:ASN:HD22	2.10	0.55
1:A:174:GLY:HA3	1:A:241:PRO:HG2	1.87	0.55
1:B:272:ILE:HD12	1:B:648:THR:CG2	2.38	0.53
1:B:410:SER:HB3	1:B:524:MET:CE	2.38	0.53
1:B:347:THR:HG23	1:B:348:ARG:NH1	2.24	0.53
1:A:221:TRP:CD2	1:A:222:PRO:HA	2.43	0.53
1:A:601:LEU:O	1:A:604:VAL:HB	2.09	0.53
1:A:461:LEU:O	1:A:465:LEU:HD22	2.09	0.52
1:A:420:ALA:O	1:A:429:ARG:HG3	2.08	0.52
1:A:83:ASN:HD21	1:A:671:PHE:HA	1.74	0.52
1:B:407:PHE:HB2	1:B:524:MET:HE3	1.91	0.52
1:B:410:SER:HB3	1:B:524:MET:HE3	1.92	0.52
1:B:410:SER:CB	1:B:524:MET:HE3	2.39	0.52
1:B:547:ASP:HB2	1:B:548:PRO:HD3	1.91	0.51
1:B:670:ASN:ND2	3:B:801:C8O:OAH	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASP:OD1	1:A:498:ARG:HD3	2.11	0.51
1:B:187:LEU:HD23	1:B:188:TYR:N	2.26	0.51
1:A:574:ASN:OD1	1:A:576:THR:HB	2.12	0.50
1:A:656:GLY:HA2	1:A:669:LEU:CD2	2.42	0.50
1:B:24:GLY:HA2	1:B:570:PHE:CD2	2.46	0.50
1:B:73:VAL:HG11	1:B:253:PRO:HG3	1.93	0.49
1:B:200:ARG:O	1:B:231:PHE:HA	2.12	0.49
1:B:24:GLY:HA3	1:B:26:TRP:CE2	2.47	0.49
1:A:457:ALA:O	1:A:461:LEU:HB2	2.13	0.49
1:A:538:LEU:O	1:A:542:LEU:HB2	2.12	0.49
1:B:563:MET:HG2	1:B:564:ASP:OD1	2.13	0.48
1:B:327:LYS:NZ	4:B:908:HOH:O	2.47	0.48
1:A:410:SER:CB	1:A:524:MET:HE3	2.39	0.47
1:B:232:ARG:HD3	1:B:250:PRO:HB3	1.97	0.47
1:A:281:ARG:HG3	1:A:570:PHE:CE2	2.50	0.47
1:B:200:ARG:HD2	1:B:234:TYR:CE1	2.50	0.47
1:B:648:THR:HG22	1:B:691:SER:HB2	1.98	0.46
1:B:108:ALA:O	1:B:711:ARG:NH1	2.49	0.46
1:A:24:GLY:HA2	1:A:570:PHE:CD2	2.51	0.45
1:A:306:ARG:NH1	4:A:905:HOH:O	2.47	0.45
1:A:421:LEU:HB3	1:A:516:VAL:HG13	1.98	0.45
1:A:673:ARG:NH1	1:A:681:ASP:OD1	2.50	0.45
1:B:561:LEU:HA	1:B:561:LEU:HD12	1.88	0.45
1:A:390:LEU:HB3	1:A:542:LEU:HD13	1.98	0.45
1:A:110:ARG:HG3	1:A:113:ASP:OD2	2.17	0.44
1:A:353:ASN:HB2	1:A:683:GLN:NE2	2.31	0.44
1:B:476:HIS:CD2	1:B:526:LEU:HB3	2.52	0.44
1:B:680:GLY:HA2	1:B:683:GLN:O	2.17	0.44
1:B:259:ILE:HG21	1:B:700:LEU:HD11	1.98	0.44
1:B:364:TRP:O	1:B:368:GLN:HG3	2.17	0.44
1:A:635:ASP:O	1:A:638:GLY:N	2.40	0.44
1:A:306:ARG:HD3	1:A:404:GLY:HA2	1.99	0.44
1:A:383:THR:HG21	1:A:549:ILE:HG13	1.98	0.44
1:B:483:ARG:HG2	1:B:483:ARG:HH11	1.83	0.43
1:B:483:ARG:CG	1:B:483:ARG:HH11	2.30	0.43
1:B:361:LEU:HD21	1:B:373:TYR:HB3	2.00	0.43
1:B:265:GLN:O	1:B:266:GLU:C	2.56	0.43
1:B:424:ASN:ND2	1:B:425:ASP:N	2.66	0.43
1:B:122:VAL:HG21	1:B:233:ILE:HG12	1.99	0.43
1:B:83:ASN:HD22	1:B:655:SER:HB3	1.83	0.43
1:A:268:ASP:O	1:A:583:GLN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HD21	1:A:585:LYS:NZ	2.17	0.43
1:B:211:LYS:HB3	1:B:214:ALA:HB2	2.01	0.43
1:A:200:ARG:HD2	1:A:234:TYR:CE1	2.52	0.42
1:A:589:PRO:HG3	1:A:595:TYR:CE2	2.55	0.42
1:B:273:MET:O	1:B:658:PRO:HD2	2.19	0.42
1:B:443:PHE:CE2	1:B:524:MET:HE1	2.54	0.42
1:A:673:ARG:HB2	3:A:802:C8O:OAH	2.19	0.42
1:B:218:ASN:OD1	3:B:801:C8O:NAN	2.53	0.42
1:B:269:TYR:CE2	1:B:271:MET:HB2	2.55	0.42
1:B:357:MET:CE	1:B:560:LEU:HD13	2.50	0.42
1:B:696:ILE:HA	1:B:696:ILE:HD12	1.89	0.42
1:A:84:HIS:N	1:A:227:ASP:OD1	2.52	0.42
1:B:59:LYS:HG3	1:B:577:LEU:HD21	2.01	0.42
1:A:405:ILE:HD11	1:A:461:LEU:HD13	2.02	0.42
1:B:413:PRO:HB3	1:B:519:LEU:HD13	2.02	0.42
1:B:343:TRP:CZ2	1:B:347:THR:HG21	2.55	0.41
1:A:592:ASN:OD1	1:B:596:GLY:CA	2.69	0.41
1:A:90:MET:HG3	1:A:231:PHE:CZ	2.56	0.41
1:A:469:PRO:HG2	1:A:472:ASN:ND2	2.35	0.41
1:A:224:HIS:CD2	1:A:603:GLY:HA3	2.56	0.41
1:A:443:PHE:CE2	1:A:524:MET:HE1	2.56	0.41
1:B:272:ILE:CD1	1:B:648:THR:HG21	2.41	0.41
1:A:83:ASN:HD22	1:A:85:HIS:CE1	2.38	0.41
1:B:232:ARG:HD2	1:B:234:TYR:CE1	2.56	0.41
1:B:83:ASN:HD21	1:B:671:PHE:HA	1.86	0.41
1:A:327:LYS:CE	1:A:406:GLU:OE2	2.69	0.40
1:A:426:ALA:HA	1:A:429:ARG:NE	2.36	0.40
1:A:456:VAL:O	1:A:460:MET:HG2	2.21	0.40
1:B:589:PRO:HG3	1:B:595:TYR:CZ	2.56	0.40
1:A:177:VAL:HB	1:A:190:MET:HE3	2.03	0.40
1:A:470:TYR:HA	1:A:473:LEU:HD12	2.02	0.40
1:A:648:THR:HG22	1:A:691:SER:HB2	2.03	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	697/720 (97%)	670 (96%)	26 (4%)	1 (0%)	51	68
1	B	697/720 (97%)	664 (95%)	33 (5%)	0	100	100
All	All	1394/1440 (97%)	1334 (96%)	59 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY

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	590/607 (97%)	530 (90%)	60 (10%)	7	10
1	B	590/607 (97%)	553 (94%)	37 (6%)	18	28
All	All	1180/1214 (97%)	1083 (92%)	97 (8%)	11	17

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	39	LYS
1	A	50	LEU
1	A	90	MET
1	A	97	LEU
1	A	98	GLU
1	A	103	GLU
1	A	104	ASN
1	A	110	ARG
1	A	139	LEU
1	A	154	LYS

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Mol	Chain	Res	Type
1	A	156	LEU
1	A	159	LEU
1	A	163	LYS
1	A	169	SER
1	A	175	LEU
1	A	219	TRP
1	A	261	LEU
1	A	281	ARG
1	A	283	PHE
1	A	301	ARG
1	A	310	MET
1	A	370	THR
1	A	390	LEU
1	A	414	THR
1	A	416	ASP
1	A	418	THR
1	A	419	LYS
1	A	421	LEU
1	A	429	ARG
1	A	431	GLU
1	A	442	LYS
1	A	461	LEU
1	A	465	LEU
1	A	466	LYS
1	A	471	GLU
1	A	477	LEU
1	A	483	ARG
1	A	526	LEU
1	A	542	LEU
1	A	550	LEU
1	A	553	GLN
1	A	560	LEU
1	A	561	LEU
1	A	575	LEU
1	A	576	THR
1	A	583	GLN
1	A	602	ASP
1	A	618	ASP
1	A	632	ARG
1	A	635	ASP
1	A	636	ARG
1	A	648	THR

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Mol	Chain	Res	Type
1	A	669	LEU
1	A	673	ARG
1	A	700	LEU
1	A	705	LYS
1	A	709	CYS
1	A	713	LEU
1	A	719	VAL
1	B	41	ARG
1	B	140	LYS
1	B	197	THR
1	B	207	SER
1	B	208	SER
1	B	237	LYS
1	B	245	SER
1	B	261	LEU
1	B	283	PHE
1	B	306	ARG
1	B	337	ARG
1	B	347	THR
1	B	367	LYS
1	B	386	LYS
1	B	414	THR
1	B	424	ASN
1	B	429	ARG
1	B	433	ILE
1	B	461	LEU
1	B	465	LEU
1	B	475	LEU
1	B	483	ARG
1	B	504	GLU
1	B	513	VAL
1	B	526	LEU
1	B	531	VAL
1	B	543	ARG
1	B	561	LEU
1	B	598	GLN
1	B	620	LYS
1	B	627	ARG
1	B	632	ARG
1	B	635	ASP
1	B	636	ARG
1	B	648	THR

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Mol	Chain	Res	Type
1	B	673	ARG
1	B	713	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	117	ASN
1	A	218	ASN
1	A	267	ASN
1	A	353	ASN
1	A	355	GLN
1	A	472	ASN
1	A	569	GLN
1	A	683	GLN
1	A	710	GLN
1	A	717	ASN
1	B	83	ASN
1	B	117	ASN
1	B	172	ASN
1	B	186	ASN
1	B	240	ASN
1	B	307	GLN
1	B	424	ASN
1	B	472	ASN
1	B	506	GLN
1	B	553	GLN
1	B	569	GLN
1	B	598	GLN
1	B	710	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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$
2	GOL	A	801	-	5,5,5	0.23	0	5,5,5	0.44	0
3	C8O	A	802	-	13,16,16	2.29	4 (30%)	13,21,21	2.29	3 (23%)
3	C8O	B	801	-	13,16,16	2.96	4 (30%)	13,21,21	2.98	7 (53%)

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
2	GOL	A	801	-	-	4/4/4/4	-
3	C8O	A	802	-	-	1/6/12/12	0/1/1/1
3	C8O	B	801	-	-	5/6/12/12	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	C8O	CAB-CAE	-8.37	1.39	1.47
3	B	801	C8O	CAD-NAA	-5.45	1.32	1.45
3	A	802	C8O	CAB-CAE	-4.91	1.42	1.47
3	A	802	C8O	OAH-NAA	4.56	1.30	1.22
3	A	802	C8O	CAD-NAA	-3.69	1.36	1.45
3	B	801	C8O	OAH-NAA	2.42	1.26	1.22
3	B	801	C8O	CAB-CAF	2.27	1.43	1.40
3	A	802	C8O	CAO-NAL	2.18	1.50	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	C8O	CAC-CAD-NAA	6.07	124.10	118.75
3	B	801	C8O	CAJ-CAD-NAA	-5.66	115.11	119.38
3	B	801	C8O	CAK-CAF-NAL	-5.37	112.65	121.80
3	B	801	C8O	CAC-CAD-NAA	4.17	122.42	118.75
3	B	801	C8O	CAB-CAF-NAL	3.95	125.99	121.24
3	A	802	C8O	OAH-NAA-CAD	3.23	123.36	118.80
3	B	801	C8O	OAH-NAA-CAD	-2.57	115.16	118.80
3	B	801	C8O	CAO-NAL-CAF	2.41	129.18	123.39
3	A	802	C8O	CAJ-CAD-CAC	-2.37	117.09	120.09
3	B	801	C8O	CAO-CAP-NAN	-2.18	97.84	114.13

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	C1-C2-C3-O3
3	B	801	C8O	CAK-CAF-NAL-CAO
3	B	801	C8O	CAB-CAF-NAL-CAO
2	A	801	GOL	O1-C1-C2-O2
2	A	801	GOL	O2-C2-C3-O3
3	A	802	C8O	CAP-CAO-NAL-CAF
3	B	801	C8O	NAL-CAO-CAP-NAN
3	B	801	C8O	CAC-CAD-NAA-OAH
3	B	801	C8O	CAJ-CAD-NAA-OAH

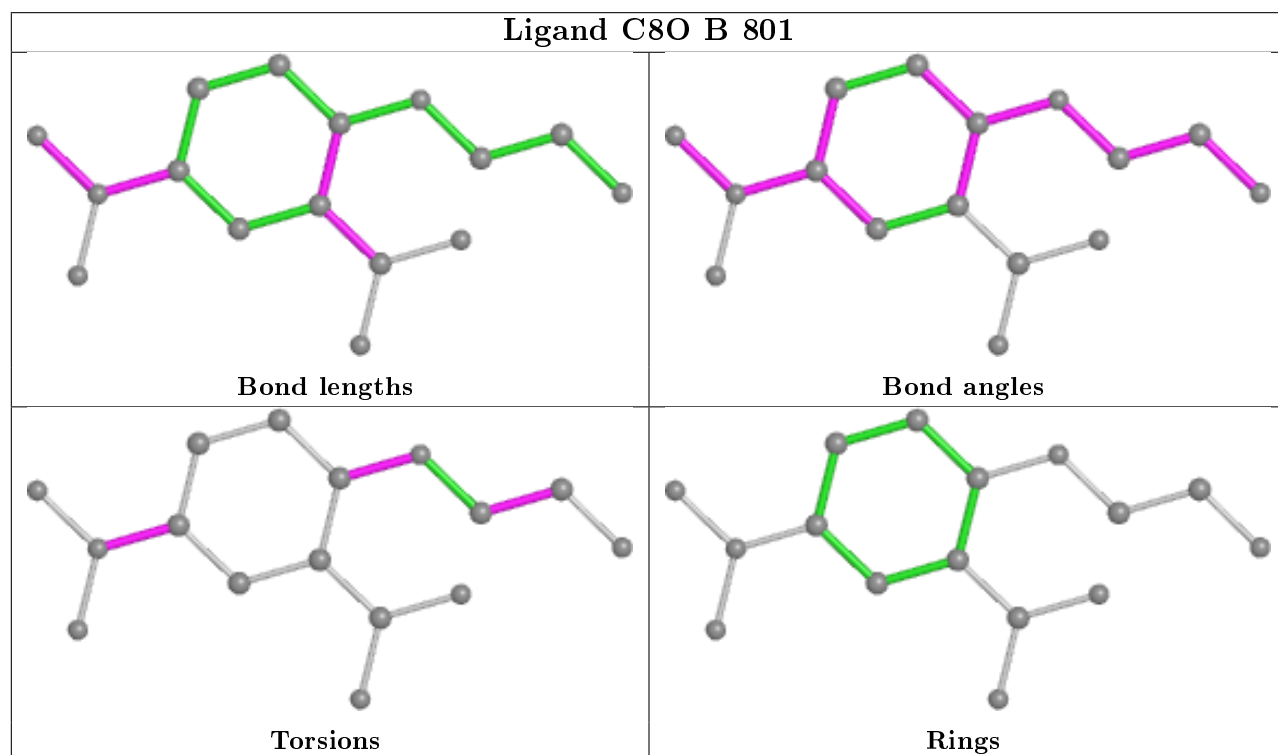
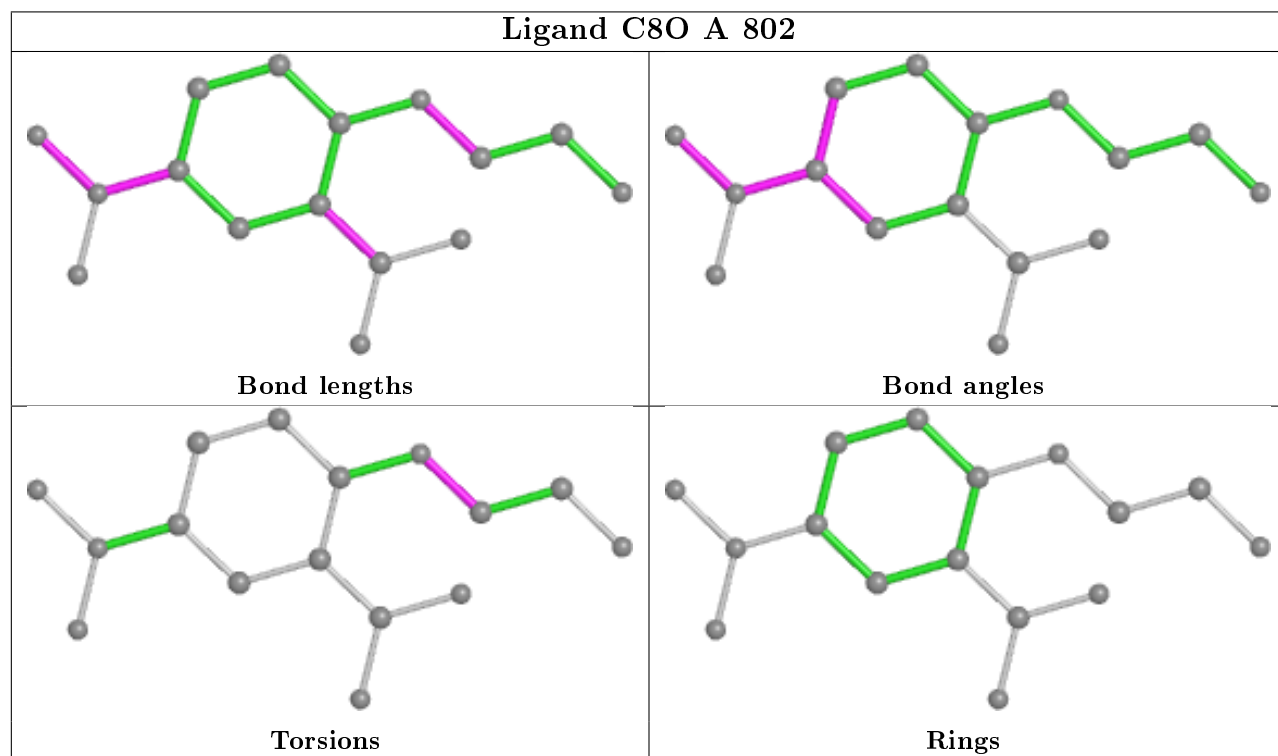
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	C8O	1	0
3	B	801	C8O	4	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	699/720 (97%)	0.26	20 (2%) 51 50	27, 43, 73, 107	0
1	B	699/720 (97%)	0.15	10 (1%) 75 73	25, 41, 71, 120	0
All	All	1398/1440 (97%)	0.20	30 (2%) 63 61	25, 42, 73, 120	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	ASN	5.3
1	A	143	LYS	4.9
1	A	97	LEU	4.7
1	A	636	ARG	4.6
1	A	624	VAL	3.8
1	B	97	LEU	3.8
1	B	424	ASN	3.5
1	B	636	ARG	3.2
1	A	98	GLU	3.2
1	A	424	ASN	3.2
1	A	142	ILE	3.1
1	A	246	GLU	3.0
1	A	166	LYS	3.0
1	A	170	ALA	2.7
1	B	632	ARG	2.5
1	B	64	LEU	2.4
1	A	145	PRO	2.4
1	B	423	GLY	2.3
1	A	71	GLY	2.3
1	A	70	THR	2.3
1	A	575	LEU	2.2
1	B	70	THR	2.2
1	A	64	LEU	2.2
1	B	143	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	245	SER	2.1
1	A	171	LYS	2.1
1	A	635	ASP	2.1
1	A	322	ILE	2.1
1	A	576	THR	2.0
1	B	167	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

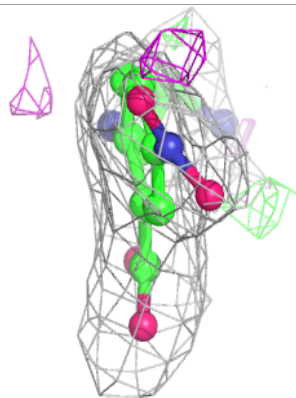
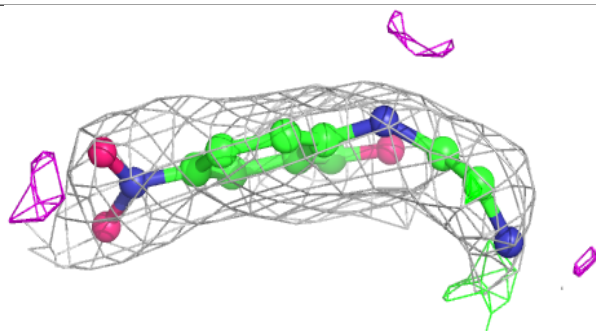
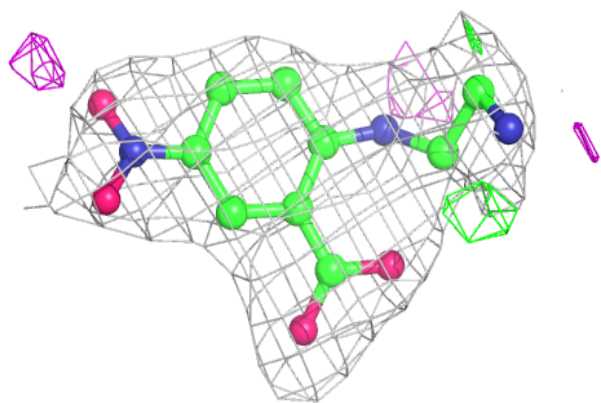
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	801	6/6	0.81	0.23	56,66,71,72	0
3	C8O	B	801	16/16	0.90	0.20	38,48,54,61	0
3	C8O	A	802	16/16	0.95	0.20	41,47,59,61	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.

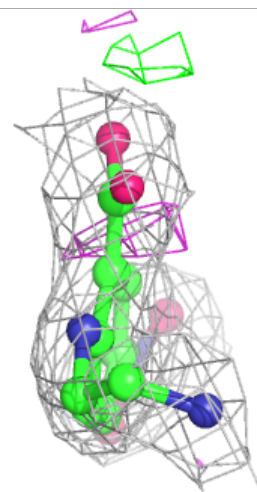
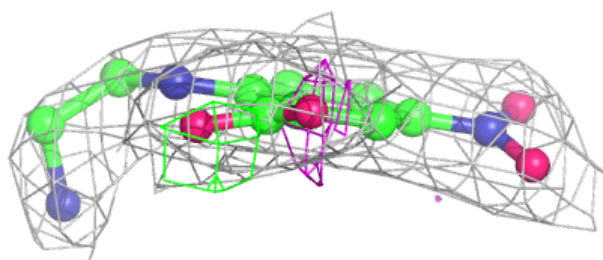
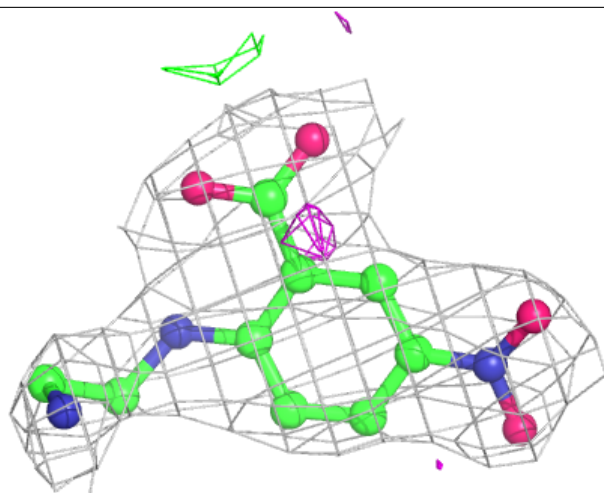
Electron density around C8O B 801:

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



Electron density around C8O A 802:

$2mF_o-DF_c$ (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.