



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:54 PM EDT

PDB ID : 6JTC / pdb_00006jtc
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 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

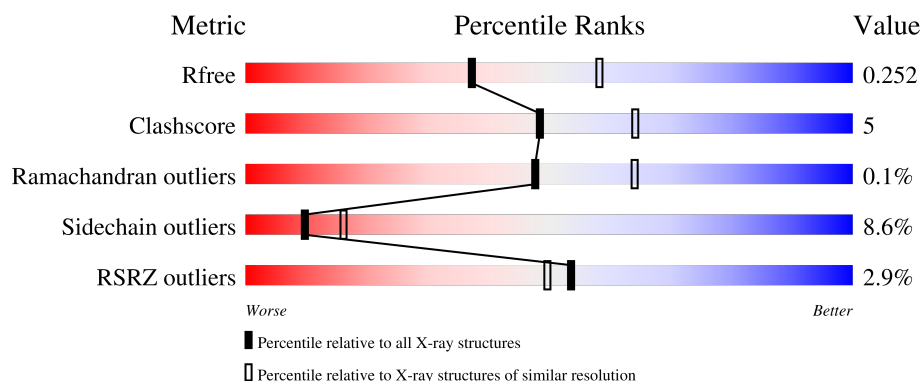
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

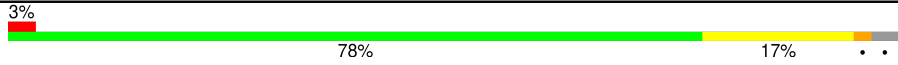
The reported resolution of this entry is 2.39 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	720	
1	B	720	

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.

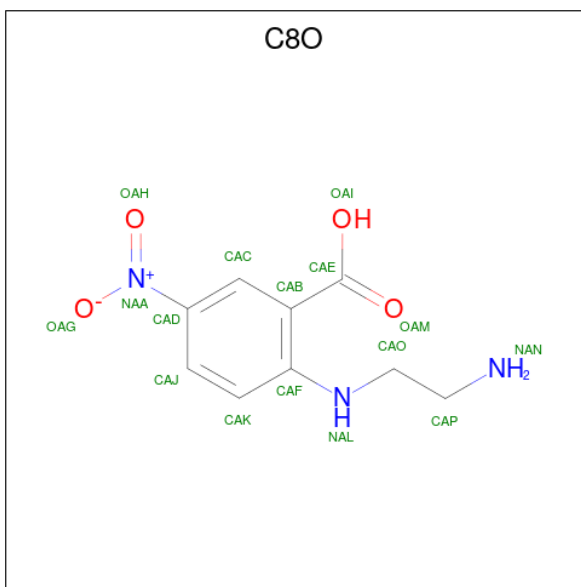
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5608	3553	970	1058	27			
1	B	699	Total	C	N	O	S	0	0	0
			5608	3553	970	1058	27			

- Molecule 2 is GLYCEROL (CCD ID: 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 (CCD ID: C8O) (formula: C₉H₁₁N₃O₄) (labeled as "Ligand of Interest" by depositor).



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		

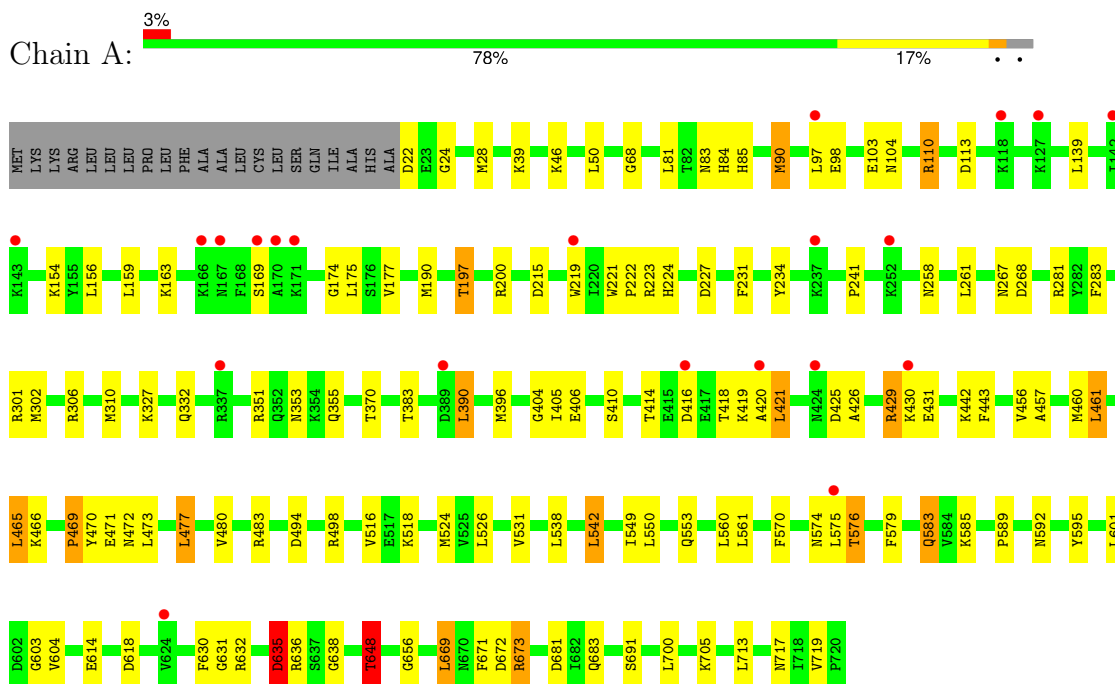
- Molecule 4 is water.

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

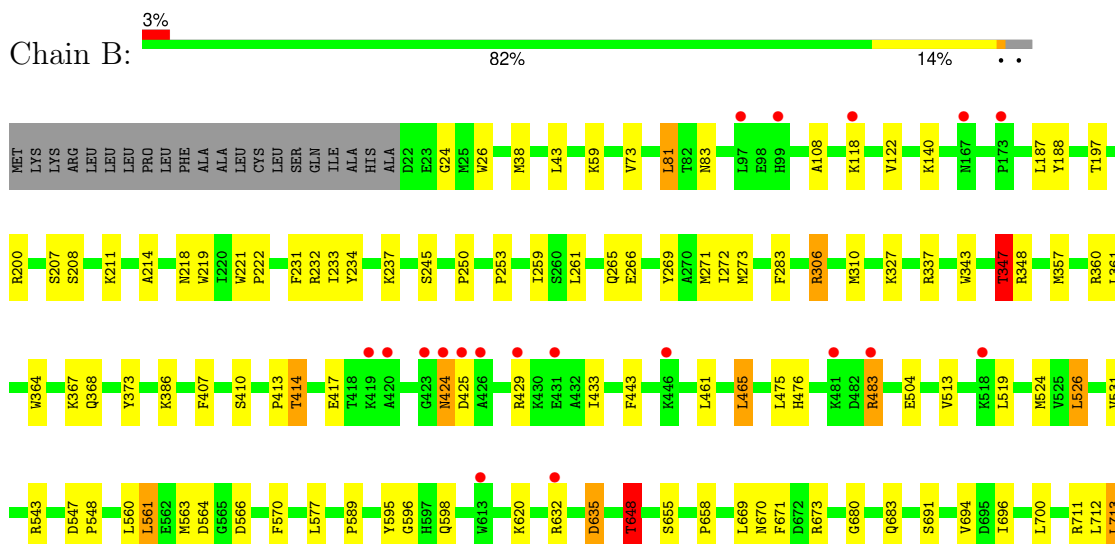
3 Residue-property plots [i](#)

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: Asp/Glu-specific dipeptidyl-peptidase



• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase





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 39.65 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.65-2.39) 99.7 (39.65-2.39)	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 (4.95%)	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)	0.35 , 25.9	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	1.03	0/5733	1.46	6/7745 (0.1%)
1	B	1.02	0/5733	1.45	12/7745 (0.2%)
All	All	1.03	0/11466	1.45	18/15490 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	648	THR	CB-CA-C	7.60	123.53	109.54
1	A	648	THR	CB-CA-C	7.19	124.52	109.65
1	A	648	THR	N-CA-CB	-6.61	100.81	110.26
1	A	197	THR	CB-CA-C	6.23	118.85	109.13
1	B	635	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	347	THR	N-CA-CB	-5.64	102.47	110.81
1	A	635	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	714	ASP	CA-C-N	5.41	127.52	120.28
1	B	714	ASP	C-N-CA	5.41	127.52	120.28
1	B	465	LEU	CA-C-N	5.39	127.50	120.28
1	B	465	LEU	C-N-CA	5.39	127.50	120.28
1	B	713	LEU	CA-C-N	5.29	127.32	120.44
1	B	713	LEU	C-N-CA	5.29	127.32	120.44
1	B	648	THR	N-CA-CB	-5.26	102.59	110.17
1	A	469	PRO	CA-C-N	5.23	127.55	120.38
1	A	469	PRO	C-N-CA	5.23	127.55	120.38
1	B	347	THR	CB-CA-C	5.17	118.36	109.15
1	B	566	ASP	CA-CB-CG	5.03	117.63	112.60

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	56	0
1	B	5608	0	5491	66	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	122	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 (122) 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:410:SER:HB3	1:A:524:MET:HE3	1.66	0.76
1:A:223:ARG:NH2	1:A:672:ASP:OD2	2.21	0.72
1:B:410:SER:CB	1:B:524:MET:CE	2.71	0.68
1:B:410:SER:CB	1:B:524:MET:HE2	2.22	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
3:B:801:C8O:OAM	3:B:801:C8O:CAO	2.44	0.65
1:A:410:SER:CB	1:A:524:MET:HE3	2.27	0.65
1:A:410:SER:CB	1:A:524:MET:CE	2.75	0.64
1:B:410:SER:HB2	1:B:524:MET:HE2	1.79	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:187:LEU:C	1:B:187:LEU:HD23	2.24	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:A:258:ASN:CG	1:A:717:ASN:HD22	2.10	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASN:HD22	1:B:425:ASP:N	2.02	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:B:407:PHE:HB2	1:B:524:MET:HE3	1.87	0.55
1:A:174:GLY:HA3	1:A:241:PRO:HG2	1.87	0.55
1:B:38:MET:HE2	1:B:43:LEU:HD22	1.90	0.53
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:410:SER:HB2	1:A:524:MET:HE2	1.90	0.52
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: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
1:A:177:VAL:HB	1:A:190:MET:HE2	1.93	0.51
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:410:SER:HB3	1:B:524:MET:HE3	1.94	0.50
1:A:410:SER:CB	1:A:524:MET:HE2	2.40	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:357:MET:HE3	1:B:560:LEU:HD13	1.95	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:410:SER:CB	1:B:524:MET:HE3	2.43	0.48
1:B:265:GLN:O	1:B:266:GLU:C	2.56	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:302:MET:HE2	1:A:396:MET:SD	2.56	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:HD12	1:B:561:LEU:HA	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:360:ARG:NH1	1:B:563:MET:HE3	2.32	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:HH11	1:B:483:ARG:CG	2.30	0.43
1:B:361:LEU:HD21	1:B:373:TYR:HB3	2.00	0.43
1:A:443:PHE:CE2	1:A:524:MET:HE1	2.54	0.43
1:B:424:ASN:ND2	1:B:425:ASP:N	2.66	0.43
1:B:83:ASN:HD22	1:B:655:SER:HB3	1.83	0.43
1:B:122:VAL:HG21	1:B:233:ILE:HG12	1.99	0.43
1:A:267:ASN:HD21	1:A:585:LYS:NZ	2.17	0.43
1:A:268:ASP:O	1:A:583:GLN:HA	2.18	0.43
1:B:211:LYS:HB3	1:B:214:ALA:HB2	2.01	0.43
1:B:306:ARG:HD2	1:B:310:MET:HE2	2.00	0.43
1:A:200:ARG:HD2	1:A:234:TYR:CE1	2.52	0.42
1:B:443:PHE:CE2	1:B:524:MET:HE1	2.53	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: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:HD12	1:B:696:ILE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PRO:HB3	1:B:519:LEU:HD13	2.02	0.42
1:B:221:TRP:HA	1:B:222:PRO:C	2.45	0.42
1:B:343:TRP:CZ2	1:B:347:THR:HG21	2.55	0.41
1:A:90:MET:HG3	1:A:231:PHE:CZ	2.56	0.41
1:A:592:ASN:OD1	1:B:596:GLY:CA	2.69	0.41
1:A:425:ASP:OD1	1:A:425:ASP:C	2.62	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: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:83:ASN:HD21	1:B:671:PHE:HA	1.86	0.41
1:B:232:ARG:HD2	1:B:234:TYR:CE1	2.56	0.41
1:A:28:MET:HE1	1:A:579:PHE:HB3	2.02	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:630:PHE:O	1:A:631:GLY:C	2.63	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%)	48	64
1	B	697/720 (97%)	664 (95%)	33 (5%)	0	100	100
All	All	1394/1440 (97%)	1334 (96%)	59 (4%)	1 (0%)	48	64

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%)	526 (89%)	64 (11%)	6	9
1	B	590/607 (97%)	553 (94%)	37 (6%)	16	29
All	All	1180/1214 (97%)	1079 (91%)	101 (9%)	10	16

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	39	LYS
1	A	46	LYS
1	A	50	LEU
1	A	81	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
1	A	156	LEU
1	A	159	LEU
1	A	163	LYS
1	A	169	SER
1	A	175	LEU
1	A	197	THR
1	A	219	TRP
1	A	261	LEU
1	A	283	PHE
1	A	301	ARG

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Mol	Chain	Res	Type
1	A	310	MET
1	A	332	GLN
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	430	LYS
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	518	LYS
1	A	526	LEU
1	A	531	VAL
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	618	ASP
1	A	632	ARG
1	A	635	ASP
1	A	636	ARG
1	A	648	THR
1	A	669	LEU
1	A	673	ARG
1	A	700	LEU
1	A	705	LYS
1	A	713	LEU
1	A	719	VAL
1	B	81	LEU

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Mol	Chain	Res	Type
1	B	118	LYS
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	632	ARG
1	B	635	ASP
1	B	648	THR
1	B	673	ARG
1	B	694	VAL
1	B	713	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	157	GLN
1	A	218	ASN
1	A	248	ASN
1	A	267	ASN
1	A	307	GLN
1	A	319	GLN
1	A	332	GLN
1	A	353	ASN
1	A	355	GLN
1	A	472	ASN
1	A	489	GLN
1	A	567	GLN
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	186	ASN
1	B	240	ASN
1	B	307	GLN
1	B	422	GLN
1	B	424	ASN
1	B	472	ASN
1	B	506	GLN
1	B	553	GLN
1	B	569	GLN
1	B	597	HIS
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 oligosaccharides 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$
3	C8O	A	802	-	16,16,16	1.95	4 (25%)	19,21,21	2.00	3 (15%)
2	GOL	A	801	-	5,5,5	0.23	0	5,5,5	0.44	0
3	C8O	B	801	-	16,16,16	2.05	3 (18%)	19,21,21	2.66	10 (52%)

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	C8O	A	802	-	-	1/10/12/12	0/1/1/1
2	GOL	A	801	-	-	4/4/4/4	-
3	C8O	B	801	-	-	4/10/12/12	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	C8O	CAD-NAA	-5.52	1.32	1.45
3	B	801	C8O	CAB-CAE	-4.80	1.39	1.49
3	A	802	C8O	OAH-NAA	4.49	1.30	1.22
3	A	802	C8O	CAD-NAA	-3.75	1.36	1.45
3	A	802	C8O	CAB-CAE	-3.24	1.42	1.49
3	B	801	C8O	OAH-NAA	2.38	1.26	1.22
3	A	802	C8O	CAO-NAL	2.28	1.50	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	C8O	CAC-CAD-NAA	6.22	124.10	118.74
3	B	801	C8O	CAK-CAF-NAL	-5.51	112.65	121.75
3	B	801	C8O	CAJ-CAD-NAA	-4.84	115.11	119.34
3	B	801	C8O	CAC-CAD-NAA	4.28	122.42	118.74
3	B	801	C8O	CAB-CAF-NAL	3.80	125.99	121.37
3	A	802	C8O	OAH-NAA-CAD	3.30	123.36	118.82
3	B	801	C8O	CAF-CAB-CAE	2.68	124.70	121.72
3	B	801	C8O	OAH-NAA-CAD	-2.66	115.16	118.82
3	B	801	C8O	OAM-CAE-CAB	-2.53	115.92	121.97
3	B	801	C8O	OAI-CAE-CAB	2.52	122.43	115.28
3	B	801	C8O	CAO-NAL-CAF	2.41	129.18	123.35
3	A	802	C8O	CAJ-CAD-CAC	-2.35	117.09	120.11
3	B	801	C8O	CAO-CAP-NAN	-2.25	97.84	113.83

There are no chirality outliers.

All (9) 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	CAB-CAF-NAL-CAO
3	B	801	C8O	CAK-CAF-NAL-CAO
2	A	801	GOL	O1-C1-C2-O2
2	A	801	GOL	O2-C2-C3-O3
3	B	801	C8O	NAL-CAO-CAP-NAN
3	A	802	C8O	CAP-CAO-NAL-CAF
3	B	801	C8O	CAC-CAD-NAA-OAH

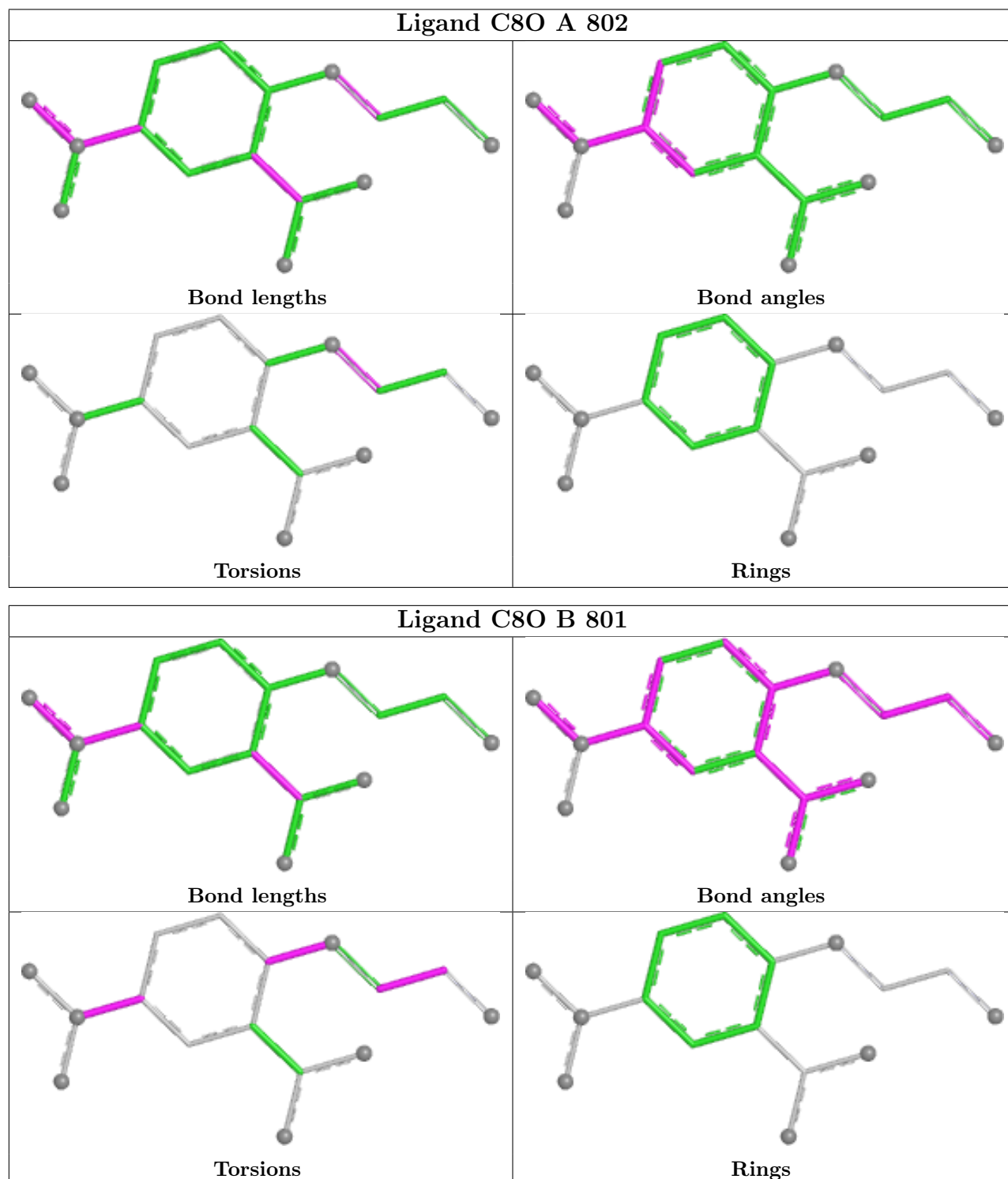
There are no ring outliers.

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 [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	699/720 (97%)	0.11	21 (3%)	52	48	27, 43, 73, 107	0
1	B	699/720 (97%)	0.04	19 (2%)	56	52	25, 41, 71, 120	0
All	All	1398/1440 (97%)	0.08	40 (2%)	53	50	25, 42, 73, 120	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	LYS	4.4
1	A	424	ASN	3.9
1	A	97	LEU	3.6
1	B	97	LEU	3.6
1	A	416	ASP	3.6
1	B	424	ASN	3.5
1	B	419	LYS	3.3
1	B	426	ALA	2.9
1	A	142	ILE	2.8
1	A	575	LEU	2.6
1	B	420	ALA	2.6
1	B	429	ARG	2.5
1	B	481	LYS	2.5
1	B	425	ASP	2.4
1	B	173	PRO	2.4
1	A	143	LYS	2.4
1	A	166	LYS	2.4
1	A	219	TRP	2.4
1	A	624	VAL	2.3
1	A	337	ARG	2.3
1	A	389	ASP	2.3
1	B	118	LYS	2.3
1	A	420	ALA	2.2
1	A	430	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	518	LYS	2.2
1	A	127	LYS	2.2
1	B	613	TRP	2.2
1	B	167	ASN	2.2
1	B	99	HIS	2.2
1	B	423	GLY	2.1
1	A	252	LYS	2.1
1	A	171	LYS	2.1
1	B	483	ARG	2.1
1	B	632	ARG	2.1
1	A	169	SER	2.0
1	B	431	GLU	2.0
1	B	446	LYS	2.0
1	A	170	ALA	2.0
1	A	167	ASN	2.0
1	A	237	LYS	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](#)

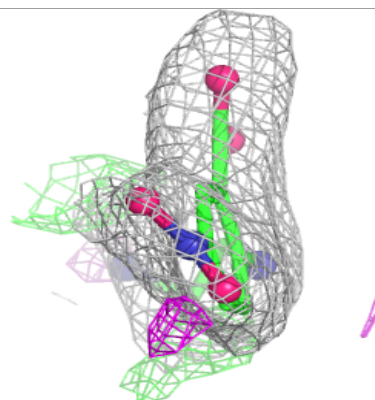
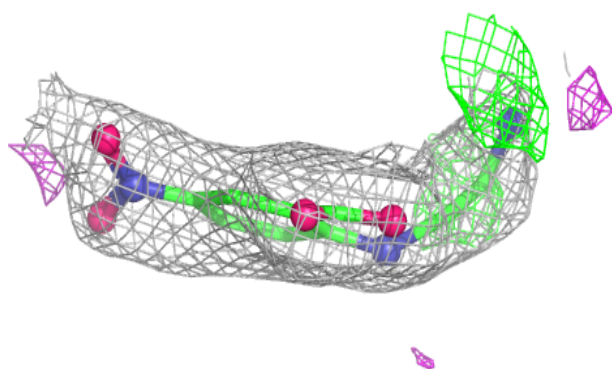
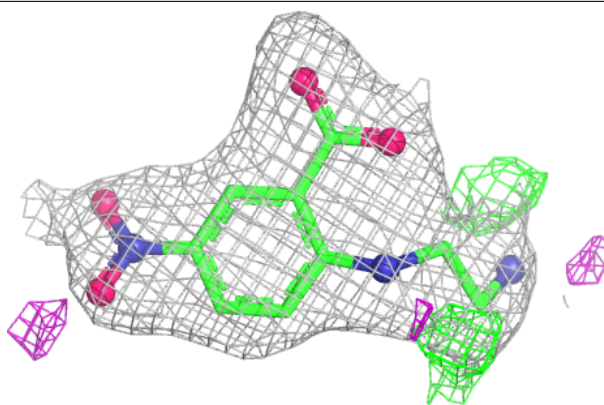
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	801	6/6	0.78	0.24	56,66,71,72	0
3	C8O	B	801	16/16	0.84	0.14	38,48,54,61	0
3	C8O	A	802	16/16	0.91	0.11	41,47,59,61	0

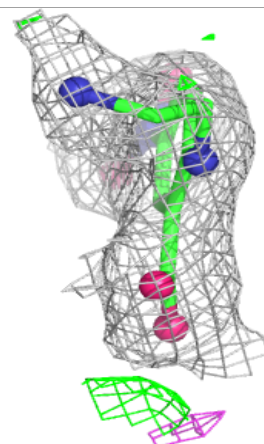
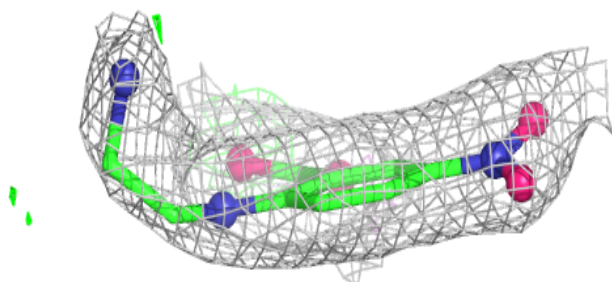
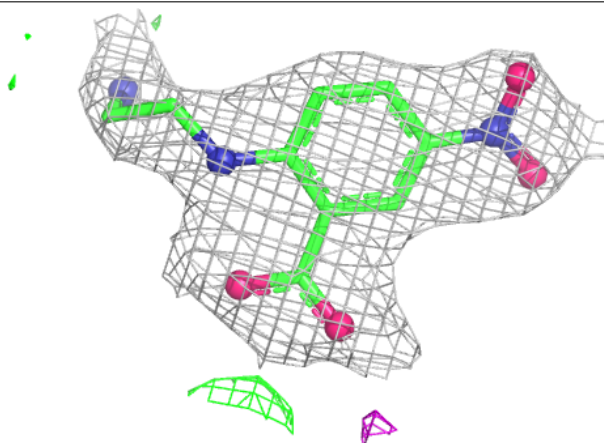
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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