



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:54 PM UTC

PDB ID : 5L8D / pdb_00005l8d
Title : X-ray structure of NikA from Escherichia coli in complex with Ru(bis(pyrz-1-yl)acetate scorpionate)(CO)₂Cl
Authors : Menage, S.; Cavazza, C.
Deposited on : 2016-06-07
Resolution : 1.80 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

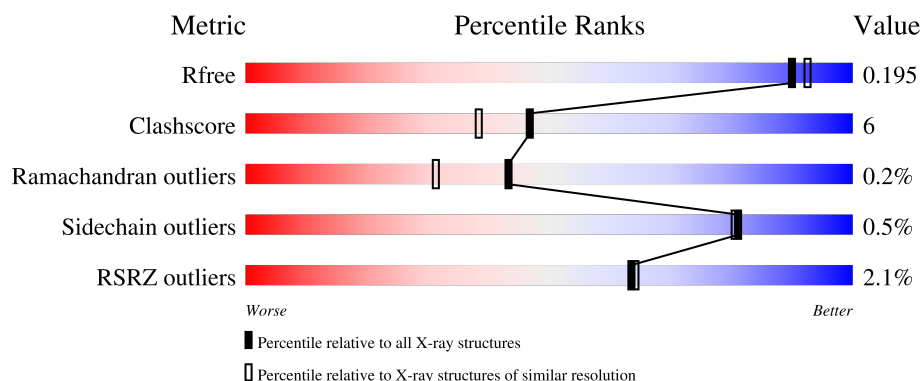
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	502	% 87% 12% .
1	B	502	3% 91% 8% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	613	-	-	X	-
4	GOL	B	614	-	-	X	-

2 Entry composition [i](#)

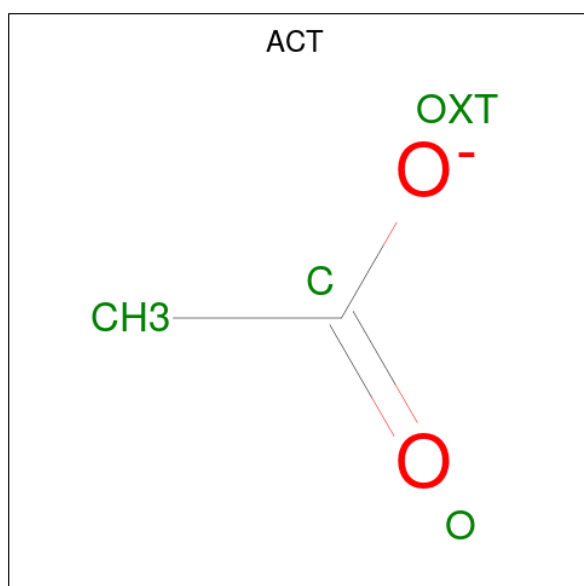
There are 11 unique types of molecules in this entry. The entry contains 8824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	18	0
			4031	2590	673	754	14			
1	B	498	Total	C	N	O	S	0	13	0
			3968	2555	660	741	12			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



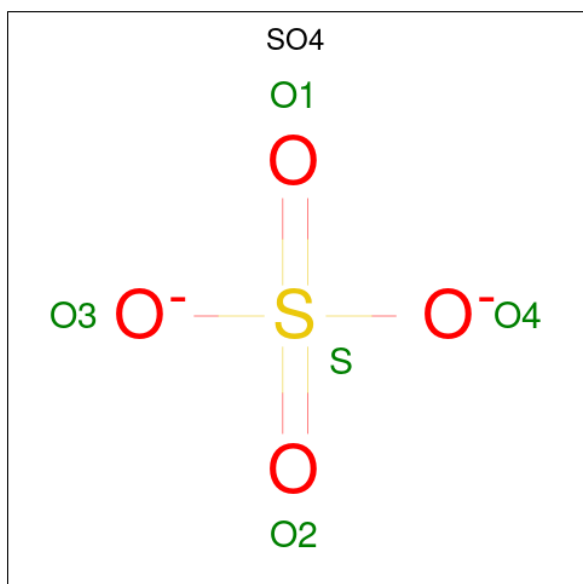
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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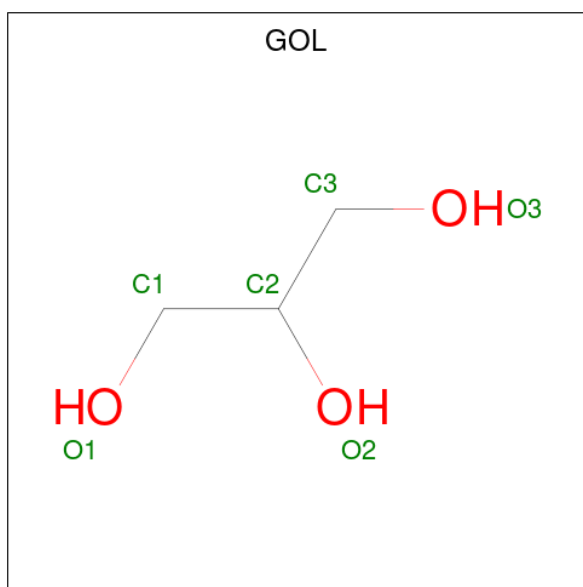
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

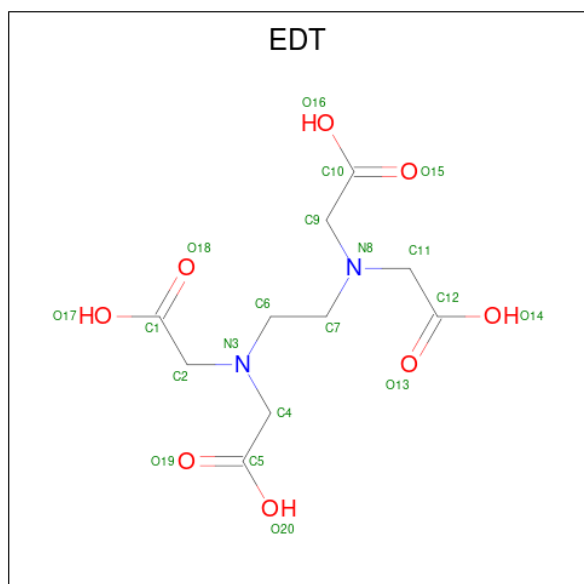


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe 1 1	0	0

- Molecule 6 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (CCD ID: EDT) (formula: C₁₀H₁₆N₂O₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 20 10 2 8	0	0

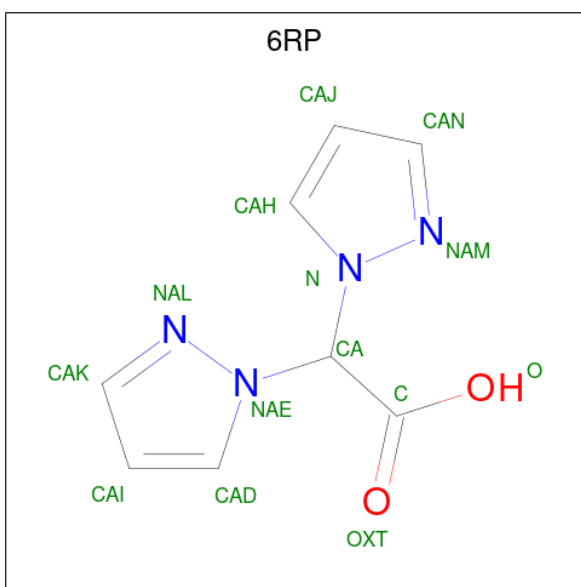
- Molecule 7 is RUTHENIUM ION (CCD ID: RU) (formula: Ru).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ru 1 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

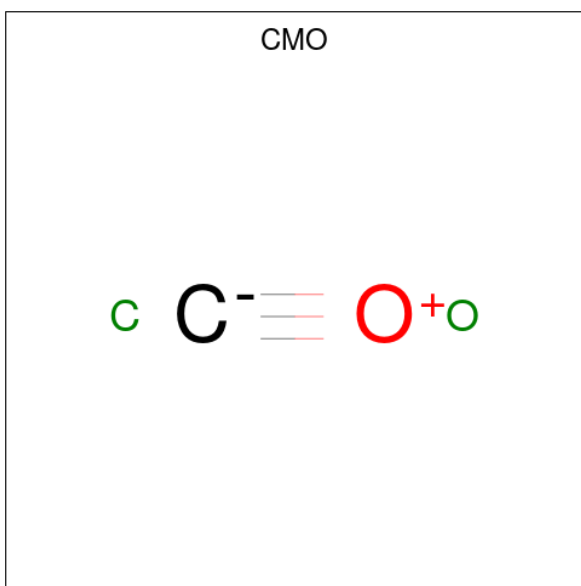
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total Cl 2 2	0	0

- Molecule 9 is bis(pyrzol-1-yl)acetate scorpionate (CCD ID: 6RP) (formula: C₈H₈N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 10 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			2	1	1		
10	B	1	Total	C	O	0	0
			2	1	1		

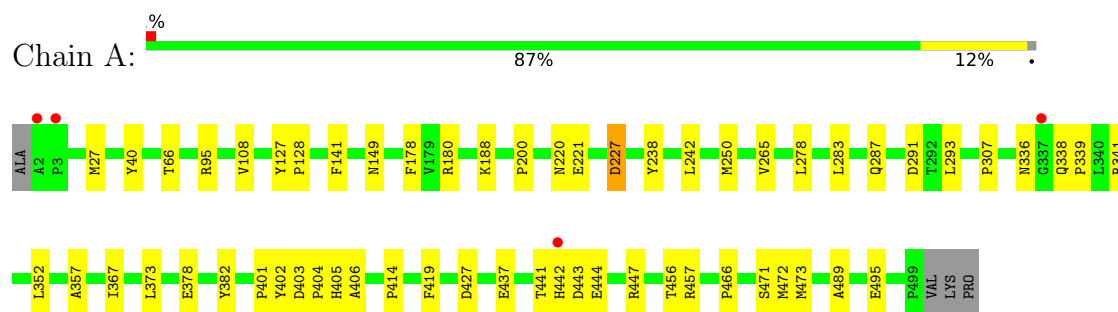
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	365	Total 365	O 365	0	0
11	B	301	Total 301	O 301	0	0

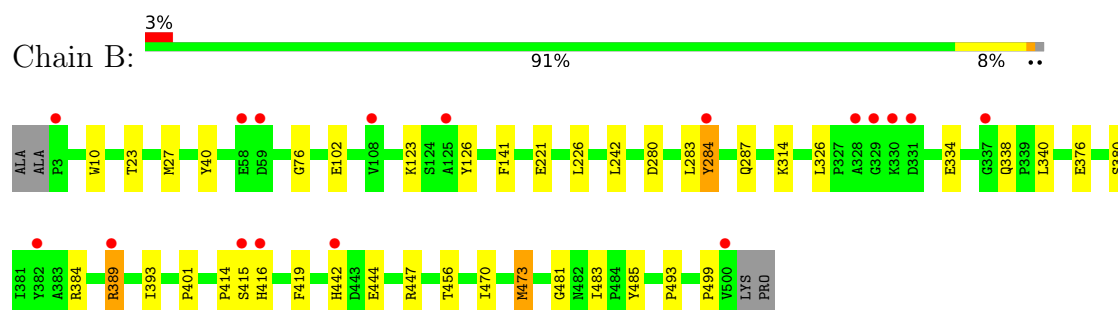
3 Residue-property plots [i](#)

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: Nickel-binding periplasmic protein



- Molecule 1: Nickel-binding periplasmic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.30Å 93.61Å 124.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 1.80 46.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.80-1.80) 98.8 (46.80-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.168 , 0.208 0.179 , 0.195	Depositor DCC
R_{free} test set	4628 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8824	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: SO4, FE, CMO, GOL, 6RP, RU, ACT, EDT, CL

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	1.29	11/4187 (0.3%)	1.09	2/5701 (0.0%)
1	B	1.30	6/4112 (0.1%)	1.10	7/5609 (0.1%)
All	All	1.29	17/8299 (0.2%)	1.10	9/11310 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389[A]	ARG	C-O	14.87	1.43	1.24
1	B	389[B]	ARG	C-O	14.87	1.43	1.24
1	A	456	THR	N-CA	-6.14	1.39	1.46
1	B	340	LEU	C-O	-5.93	1.17	1.23
1	A	178	PHE	N-CA	-5.78	1.38	1.45
1	A	227	ASP	C-O	-5.49	1.17	1.24
1	A	66	THR	CA-CB	5.37	1.60	1.53
1	A	27[A]	MET	C-O	5.37	1.30	1.24
1	A	27[B]	MET	C-O	5.37	1.30	1.24
1	A	200	PRO	C-O	-5.31	1.18	1.24
1	A	466	PRO	N-CA	-5.21	1.40	1.47
1	A	447	ARG	C-O	-5.17	1.18	1.24
1	B	456	THR	N-CA	-5.15	1.40	1.46
1	A	265	VAL	N-CA	-5.10	1.40	1.46
1	A	238	TYR	N-CA	5.09	1.52	1.45
1	B	393	ILE	C-O	5.08	1.29	1.23
1	B	493	PRO	CA-C	5.08	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	LEU	CA-C-N	-7.01	112.74	119.89
1	B	326	LEU	C-N-CA	-7.01	112.74	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	ILE	CA-C-N	-6.36	114.08	120.31
1	B	483	ILE	C-N-CA	-6.36	114.08	120.31
1	B	76	GLY	N-CA-C	6.17	123.55	115.40
1	B	27	MET	CG-SD-CE	-5.73	88.29	100.90
1	B	141	PHE	N-CA-C	5.06	116.66	108.41
1	A	402	TYR	N-CA-C	5.05	116.86	111.36
1	A	141	PHE	N-CA-C	5.05	116.64	108.41

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	4031	0	3999	47	0
1	B	3968	0	3894	42	0
2	A	28	0	21	1	0
2	B	12	0	9	2	0
3	A	5	0	0	0	0
4	A	42	0	56	3	0
4	B	30	0	40	12	0
5	A	1	0	0	0	0
6	A	20	0	12	0	0
7	B	1	0	0	0	0
8	B	2	0	0	0	0
9	B	14	0	0	0	0
10	B	4	0	0	0	0
11	A	365	0	0	10	0
11	B	301	0	0	10	0
All	All	8824	0	8031	92	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 6.

All (92) 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)
4:B:604:GOL:H31	11:B:706:HOH:O	1.23	1.35
1:A:287:GLN:HE22	1:A:473[B]:MET:HE1	1.33	0.91
1:B:314:LYS:HZ3	4:B:614:GOL:H2	1.44	0.82
1:B:287:GLN:HE22	1:B:473[B]:MET:HE1	1.45	0.82
1:B:314:LYS:NZ	4:B:614:GOL:H2	1.93	0.82
1:B:242:LEU:HD12	1:B:473[B]:MET:SD	2.22	0.80
1:A:341:ARG:NH1	11:A:701:HOH:O	2.16	0.77
1:A:472[B]:MET:CE	11:A:1001:HOH:O	2.32	0.77
1:A:472[B]:MET:HE3	11:A:1001:HOH:O	1.85	0.76
1:B:23[B]:THR:HG23	11:B:920:HOH:O	1.87	0.74
1:B:242:LEU:CD1	1:B:473[B]:MET:SD	2.76	0.73
1:A:442[B]:HIS:CD2	1:A:443:ASP:H	2.07	0.72
1:B:287:GLN:HE22	1:B:473[B]:MET:CE	2.04	0.70
1:A:149:ASN:ND2	2:A:611:ACT:H3	2.08	0.69
1:B:287:GLN:NE2	1:B:473[B]:MET:HE1	2.09	0.68
1:A:287:GLN:HE22	1:A:473[B]:MET:CE	2.04	0.68
1:A:287:GLN:NE2	1:A:473[B]:MET:HE1	2.06	0.67
1:A:442[B]:HIS:HD2	1:A:443:ASP:H	1.42	0.66
1:B:314:LYS:HZ3	4:B:614:GOL:C2	2.09	0.66
4:B:604:GOL:C3	11:B:706:HOH:O	2.04	0.65
1:A:242:LEU:CD1	1:A:473[B]:MET:SD	2.85	0.65
1:B:485:TYR:HB3	4:B:602:GOL:H11	1.78	0.64
1:B:23[B]:THR:HG22	2:B:613:ACT:OXT	1.98	0.62
1:A:221:GLU:HA	1:A:473[B]:MET:HE3	1.79	0.62
1:A:336:ASN:N	11:A:705:HOH:O	2.31	0.62
1:A:95:ARG:HD3	11:A:876:HOH:O	2.01	0.59
1:B:123:LYS:NZ	11:B:705:HOH:O	2.36	0.59
1:A:471:SER:O	1:A:473[B]:MET:HE2	2.02	0.59
1:A:242:LEU:HD12	1:A:473[B]:MET:SD	2.42	0.59
1:B:416:HIS:HB2	11:B:833:HOH:O	2.03	0.57
1:A:283[B]:LEU:HD12	1:A:352:LEU:HD11	1.87	0.56
1:B:280:ASP:O	1:B:284[B]:TYR:HA	2.06	0.55
1:B:414:PRO:O	1:B:415:SER:CB	2.53	0.54
1:A:414:PRO:HA	1:A:419:PHE:CG	2.43	0.53
1:B:314:LYS:HZ3	4:B:614:GOL:H31	1.72	0.53
1:A:220:ASN:HB3	4:A:605:GOL:H11	1.91	0.52
1:B:23[B]:THR:HG23	11:B:951:HOH:O	2.08	0.52
4:B:614:GOL:O3	11:B:701:HOH:O	1.97	0.52
1:A:278:LEU:HD23	1:A:278:LEU:C	2.35	0.52
1:A:378:GLU:HG2	1:A:382:TYR:CE2	2.45	0.51
1:B:314:LYS:HZ3	4:B:614:GOL:C3	2.23	0.51
1:B:416:HIS:CB	11:B:833:HOH:O	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLU:OE1	1:B:447:ARG:NH1	2.44	0.51
1:B:10:TRP:CZ3	4:B:603:GOL:H31	2.47	0.50
1:A:472[A]:MET:HG3	11:A:1001:HOH:O	2.10	0.50
1:B:314:LYS:HZ1	4:B:614:GOL:H2	1.76	0.50
1:B:414:PRO:HA	1:B:419:PHE:CD2	2.47	0.49
1:A:338:GLN:NE2	1:A:339:PRO:HD2	2.28	0.49
1:A:40:TYR:CE1	1:A:401:PRO:HB3	2.47	0.49
1:A:283[B]:LEU:CD1	1:A:352:LEU:HD11	2.42	0.49
2:B:613:ACT:H1	11:B:951:HOH:O	2.12	0.49
1:B:23[B]:THR:CG2	11:B:951:HOH:O	2.60	0.48
1:A:227:ASP:OD2	4:A:607:GOL:H12	2.14	0.47
1:B:473[A]:MET:HB3	1:B:473[A]:MET:HE2	1.65	0.47
1:A:291:ASP:HB3	1:A:307:PRO:HB3	1.97	0.47
1:A:180:ARG:HD2	1:A:188:LYS:HG2	1.97	0.47
1:A:250[B]:MET:SD	1:A:293:LEU:CD1	3.03	0.47
1:A:495:GLU:H	1:A:495:GLU:CD	2.24	0.46
1:B:221:GLU:HA	1:B:473[B]:MET:HE3	1.97	0.46
1:B:40:TYR:CE1	1:B:401:PRO:HB3	2.51	0.45
1:A:437:GLU:OE1	11:A:702:HOH:O	2.20	0.45
4:A:613:GOL:H32	11:A:759:HOH:O	2.16	0.44
1:A:427:ASP:OD2	1:A:457:ARG:NH1	2.51	0.44
1:A:442[B]:HIS:CD2	1:A:442[B]:HIS:H	2.32	0.44
1:B:102:GLU:HB3	1:B:126:TYR:OH	2.18	0.44
1:B:334:GLU:HA	1:B:338:GLN:O	2.17	0.44
1:B:384:ARG:NH1	1:B:389[B]:ARG:HD2	2.33	0.44
1:A:441:THR:OG1	1:A:442[B]:HIS:CD2	2.71	0.44
1:A:472[B]:MET:HE2	11:A:1001:HOH:O	2.08	0.43
1:A:180:ARG:HD2	1:A:188:LYS:CG	2.49	0.43
1:A:489:ALA:HB3	11:A:901:HOH:O	2.19	0.43
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.54	0.43
1:A:441:THR:OG1	1:A:442[B]:HIS:HD2	2.00	0.42
1:B:376:GLU:OE1	1:B:380:SER:OG	2.36	0.42
1:A:378:GLU:CG	1:A:382:TYR:CE2	3.02	0.42
1:A:403:ASP:HA	1:A:404:PRO:HA	1.87	0.42
1:B:242:LEU:HD11	1:B:473[B]:MET:SD	2.59	0.42
1:A:357:ALA:HB1	1:A:373:LEU:HD22	2.02	0.42
1:A:444:GLU:HG2	1:B:481:GLY:HA2	2.01	0.42
1:A:127:TYR:N	1:A:128:PRO:CD	2.84	0.41
1:A:405:HIS:CG	1:A:406:ALA:N	2.87	0.41
1:B:314:LYS:NZ	4:B:614:GOL:C2	2.70	0.41
1:A:283[A]:LEU:HD13	1:A:352:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HD12	1:B:283:LEU:HA	2.03	0.41
1:A:444:GLU:CG	1:B:481:GLY:HA2	2.52	0.40
1:B:470:ILE:HD12	1:B:470:ILE:C	2.46	0.40

There are no symmetry-related clashes.

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	A	514/502 (102%)	499 (97%)	15 (3%)	0	100	100
1	B	508/502 (101%)	493 (97%)	12 (2%)	3 (1%)	21	11
All	All	1022/1004 (102%)	992 (97%)	27 (3%)	3 (0%)	43	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284[A]	TYR
1	B	284[B]	TYR
1	B	499	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	435/425 (102%)	433 (100%)	2 (0%)	81	80
1	B	420/425 (99%)	417 (99%)	3 (1%)	76	73
All	All	855/850 (101%)	850 (99%)	5 (1%)	81	77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	367	ILE
1	B	442	HIS
1	B	473[A]	MET
1	B	473[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	150	HIS
1	A	168	GLN
1	A	174	GLN
1	A	244	GLN
1	A	302	ASN
1	A	309	GLN
1	A	385	GLN
1	A	416	HIS
1	A	482	ASN

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](#)

Of 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 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
2	ACT	A	602	-	3,3,3	1.18	1 (33%)	3,3,3	0.73	0
9	6RP	B	608	7	14,15,15	2.26	4 (28%)	13,20,20	5.70	9 (69%)
4	GOL	A	607	-	5,5,5	0.77	0	5,5,5	0.62	0
4	GOL	B	609	-	5,5,5	0.41	0	5,5,5	0.58	0
4	GOL	A	605	-	5,5,5	0.74	0	5,5,5	0.65	0
4	GOL	B	603	-	5,5,5	0.97	0	5,5,5	1.66	2 (40%)
2	ACT	B	601	-	3,3,3	1.17	0	3,3,3	0.26	0
4	GOL	B	604	-	5,5,5	0.52	0	5,5,5	0.81	0
10	CMO	B	611	-	0,1,1	-	-	-	-	-
4	GOL	A	606	-	5,5,5	0.61	0	5,5,5	1.42	0
4	GOL	A	615	-	5,5,5	0.34	0	5,5,5	0.76	0
2	ACT	B	605	-	3,3,3	1.01	0	3,3,3	0.40	0
4	GOL	B	614	-	5,5,5	1.17	0	5,5,5	1.27	1 (20%)
4	GOL	A	614	-	5,5,5	0.61	0	5,5,5	0.75	0
2	ACT	A	603	-	3,3,3	1.42	1 (33%)	3,3,3	1.41	0
4	GOL	A	616	-	5,5,5	0.35	0	5,5,5	0.85	0
4	GOL	B	602	-	5,5,5	0.54	0	5,5,5	1.31	1 (20%)
6	EDT	A	609	5	19,19,19	1.24	2 (10%)	24,24,24	1.38	3 (12%)
2	ACT	A	611	-	3,3,3	0.81	0	3,3,3	0.52	0
2	ACT	A	617	-	3,3,3	1.72	1 (33%)	3,3,3	1.94	1 (33%)
3	SO4	A	604	-	4,4,4	0.52	0	6,6,6	0.63	0
2	ACT	A	612	-	3,3,3	0.89	0	3,3,3	0.59	0
2	ACT	A	601	-	3,3,3	0.99	0	3,3,3	0.28	0
2	ACT	B	613	-	3,3,3	0.98	0	3,3,3	1.34	0
10	CMO	B	612	-	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	613	-	5,5,5	0.96	0	5,5,5	1.48	1 (20%)
2	ACT	A	610	-	3,3,3	1.20	0	3,3,3	0.71	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	A	614	-	-	1/4/4/4	-
9	6RP	B	608	7	-	4/12/12/12	0/2/2/2
4	GOL	B	604	-	-	0/4/4/4	-
6	EDT	A	609	5	-	3/21/21/21	-
4	GOL	A	616	-	-	2/4/4/4	-
4	GOL	A	607	-	-	1/4/4/4	-
4	GOL	B	602	-	-	0/4/4/4	-
4	GOL	B	609	-	-	0/4/4/4	-
4	GOL	A	605	-	-	2/4/4/4	-
4	GOL	A	606	-	-	3/4/4/4	-
4	GOL	A	615	-	-	2/4/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	A	613	-	-	4/4/4/4	-
4	GOL	B	614	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	608	6RP	NAE-NAL	-6.33	1.24	1.36
9	B	608	6RP	CAD-NAE	-2.80	1.31	1.35
2	A	603	ACT	O-C	2.38	1.32	1.22
9	B	608	6RP	CAJ-CAN	-2.37	1.32	1.39
2	A	617	ACT	OXT-C	-2.31	1.20	1.30
6	A	609	EDT	C4-C5	-2.04	1.47	1.51
9	B	608	6RP	CAD-CAI	-2.01	1.32	1.37
6	A	609	EDT	O18-C1	2.01	1.28	1.22
2	A	602	ACT	OXT-C	-2.00	1.21	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	608	6RP	CAH-N-NAM	-9.80	103.85	112.15
9	B	608	6RP	CA-N-NAM	9.77	133.64	120.02
9	B	608	6RP	CAN-NAM-N	9.15	112.70	103.86
9	B	608	6RP	CAK-NAL-NAE	7.90	111.49	103.86
9	B	608	6RP	CA-NAE-NAL	5.96	128.34	120.02
9	B	608	6RP	CAD-NAE-NAL	-3.85	108.89	112.15
9	B	608	6RP	CAI-CAK-NAL	-3.59	104.43	111.72
6	A	609	EDT	C6-C7-N8	-3.52	104.61	112.98
9	B	608	6RP	CAJ-CAN-NAM	-3.26	105.10	111.72
4	A	613	GOL	O2-C2-C3	2.70	120.35	109.18
2	A	617	ACT	OXT-C-CH3	2.60	125.94	115.05
9	B	608	6RP	CAH-CAJ-CAN	2.53	110.40	105.44
4	B	603	GOL	C3-C2-C1	-2.41	102.94	111.80
6	A	609	EDT	O19-C5-C4	-2.36	112.51	122.38
6	A	609	EDT	O20-C5-O19	2.17	128.91	123.33
4	B	603	GOL	O2-C2-C3	2.14	118.04	109.18
4	B	602	GOL	C3-C2-C1	-2.10	104.09	111.80
4	B	614	GOL	O1-C1-C2	-2.05	101.13	110.38

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	GOL	C1-C2-C3-O3
4	A	606	GOL	O2-C2-C3-O3
4	A	613	GOL	O1-C1-C2-C3
4	A	616	GOL	O1-C1-C2-O2
4	A	616	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
4	B	614	GOL	C1-C2-C3-O3
9	B	608	6RP	O-C-CA-NAE
9	B	608	6RP	O-C-CA-N
4	A	615	GOL	O1-C1-C2-C3
4	B	614	GOL	O1-C1-C2-C3
4	A	613	GOL	O1-C1-C2-O2
4	B	603	GOL	O1-C1-C2-O2
4	B	614	GOL	O2-C2-C3-O3
4	A	615	GOL	O1-C1-C2-O2
4	A	614	GOL	O2-C2-C3-O3
4	B	614	GOL	O1-C1-C2-O2
4	A	613	GOL	C1-C2-C3-O3
4	A	605	GOL	O1-C1-C2-C3
4	A	607	GOL	O2-C2-C3-O3

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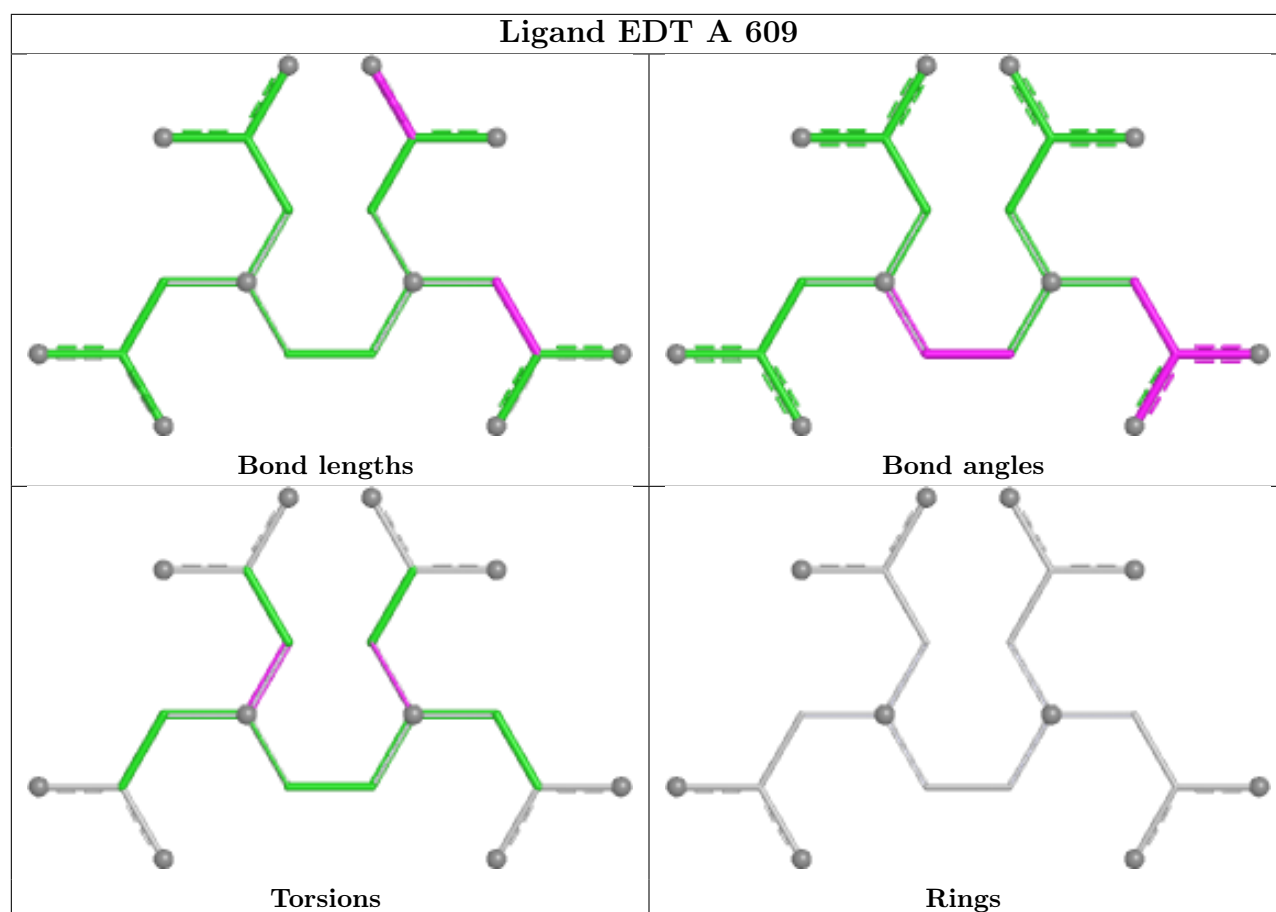
Mol	Chain	Res	Type	Atoms
4	A	613	GOL	O2-C2-C3-O3
6	A	609	EDT	C1-C2-N3-C4
6	A	609	EDT	C10-C9-N8-C11
4	A	606	GOL	O1-C1-C2-O2
4	A	605	GOL	O1-C1-C2-O2
9	B	608	6RP	OXT-C-CA-NAE
6	A	609	EDT	C1-C2-N3-C6
9	B	608	6RP	C-CA-NAE-CAD

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	GOL	1	0
4	A	605	GOL	1	0
4	B	603	GOL	1	0
4	B	604	GOL	2	0
4	B	614	GOL	8	0
4	B	602	GOL	1	0
2	A	611	ACT	1	0
2	B	613	ACT	2	0
4	A	613	GOL	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	498/502 (99%)	-0.15	4 (0%) 82 83	11, 23, 40, 62	18 (3%)
1	B	498/502 (99%)	0.06	17 (3%) 48 48	11, 25, 48, 77	12 (2%)
All	All	996/1004 (99%)	-0.05	21 (2%) 63 64	11, 24, 44, 77	30 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	VAL	6.2
1	B	329	GLY	4.3
1	B	328	ALA	3.7
1	B	389[A]	ARG	3.6
1	A	3	PRO	3.5
1	B	3	PRO	3.4
1	B	284[A]	TYR	3.0
1	A	2	ALA	3.0
1	B	330	LYS	2.7
1	B	337	GLY	2.7
1	A	442[A]	HIS	2.5
1	B	416	HIS	2.5
1	B	442	HIS	2.5
1	B	382	TYR	2.3
1	B	331	ASP	2.3
1	B	108	VAL	2.3
1	B	415	SER	2.2
1	B	59	ASP	2.2
1	A	337	GLY	2.1
1	B	58	GLU	2.0
1	B	125	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

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.

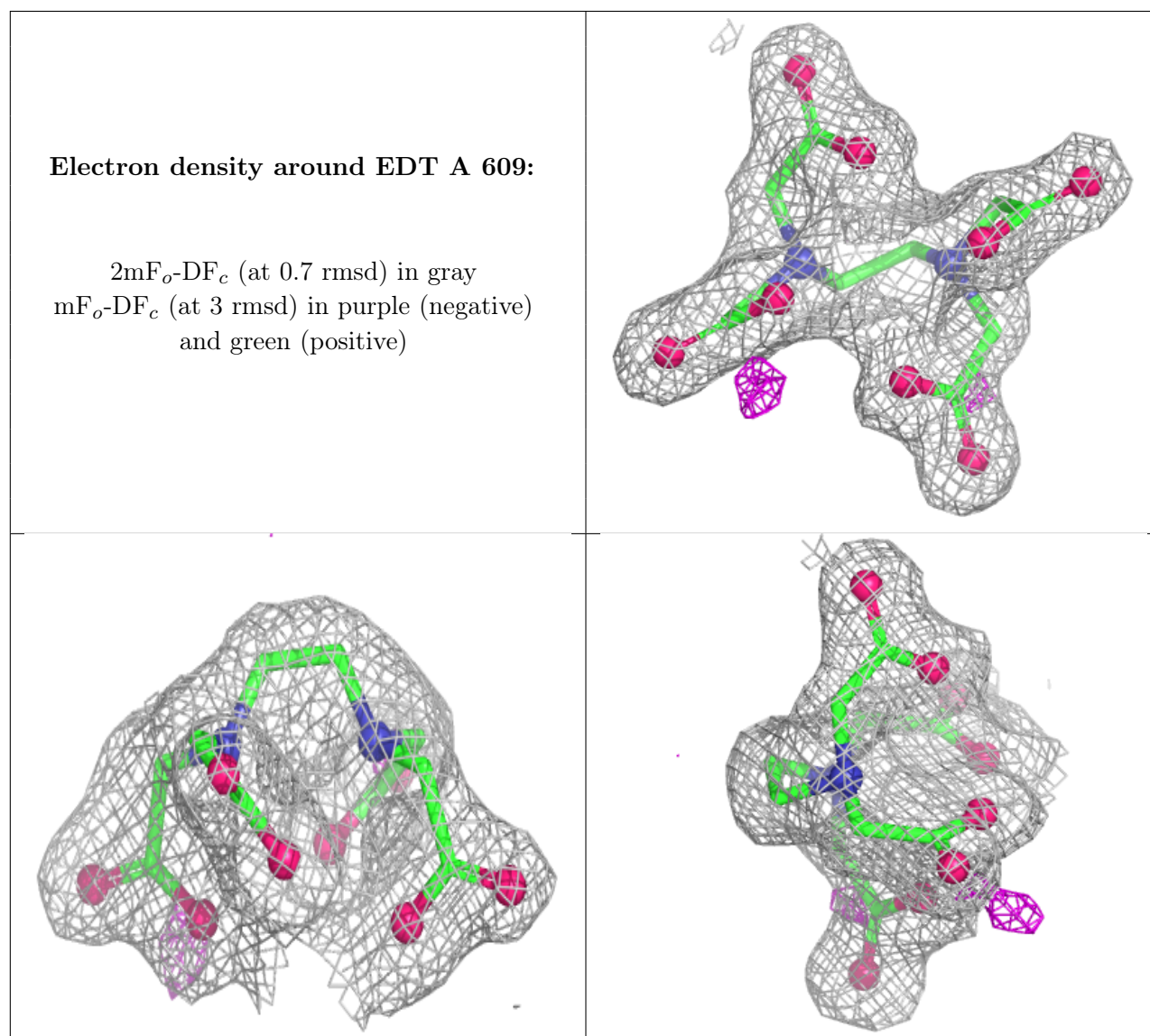
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	B	601	4/4	0.66	0.21	43,59,59,61	0
4	GOL	B	614	6/6	0.67	0.15	28,32,34,34	0
4	GOL	B	609	6/6	0.70	0.19	53,60,63,65	0
4	GOL	A	614	6/6	0.71	0.19	61,74,79,82	0
2	ACT	B	605	4/4	0.72	0.19	54,65,68,79	0
4	GOL	A	615	6/6	0.73	0.18	57,65,71,74	0
4	GOL	A	607	6/6	0.74	0.17	47,52,54,55	0
2	ACT	A	601	4/4	0.75	0.15	48,49,59,62	0
2	ACT	B	613	4/4	0.81	0.19	45,46,50,56	0
4	GOL	B	602	6/6	0.81	0.17	37,50,54,64	0
2	ACT	A	612	4/4	0.82	0.14	43,54,55,62	0
2	ACT	A	610	4/4	0.83	0.15	36,43,44,48	0
2	ACT	A	603	4/4	0.85	0.13	31,35,41,43	0
4	GOL	A	606	6/6	0.86	0.14	27,38,42,43	0
4	GOL	B	603	6/6	0.86	0.14	31,42,45,53	0
2	ACT	A	602	4/4	0.87	0.11	33,35,42,50	0
4	GOL	A	613	6/6	0.89	0.15	35,46,46,58	0
4	GOL	A	616	6/6	0.89	0.12	46,53,55,60	0
4	GOL	A	605	6/6	0.89	0.13	25,41,47,52	0
3	SO4	A	604	5/5	0.91	0.08	53,56,58,59	0
10	CMO	B	612	2/2	0.91	0.15	32,32,32,39	2
2	ACT	A	617	4/4	0.92	0.13	27,31,32,32	0
8	CL	B	607	1/1	0.94	0.13	42,42,42,42	0
8	CL	B	610	1/1	0.94	0.23	46,46,46,46	0
9	6RP	B	608	14/14	0.94	0.09	19,28,32,33	0
2	ACT	A	611	4/4	0.94	0.10	39,48,52,58	0
4	GOL	B	604	6/6	0.95	0.09	22,31,32,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDT	A	609	20/20	0.95	0.07	21,27,31,33	0
10	CMO	B	611	2/2	0.96	0.15	34,34,34,42	0
7	RU	B	606	1/1	1.00	0.04	28,28,28,28	0
5	FE	A	608	1/1	1.00	0.02	23,23,23,23	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.