



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:09 AM UTC

PDB ID : 6R4Q / pdb_00006r4q
Title : Crystal structure of the periplasmic nickel-binding protein NikA from Escherichia coli in complex with Ru(bpza)CO H₂O Cl
Authors : Cavazza, C.; Menage, S.
Deposited on : 2019-03-22
Resolution : 1.90 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

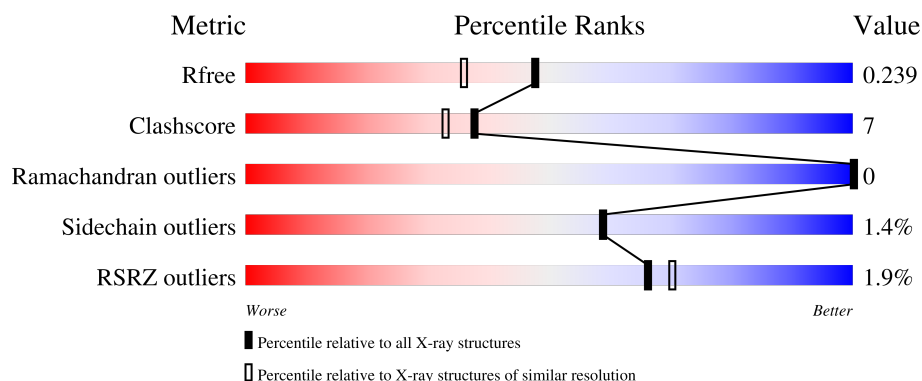
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	B	502	

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
4	CL	A	603	-	-	X	-
5	GOL	A	607	-	-	X	-
5	GOL	A	608	-	-	X	-
5	GOL	A	619	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 8848 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.

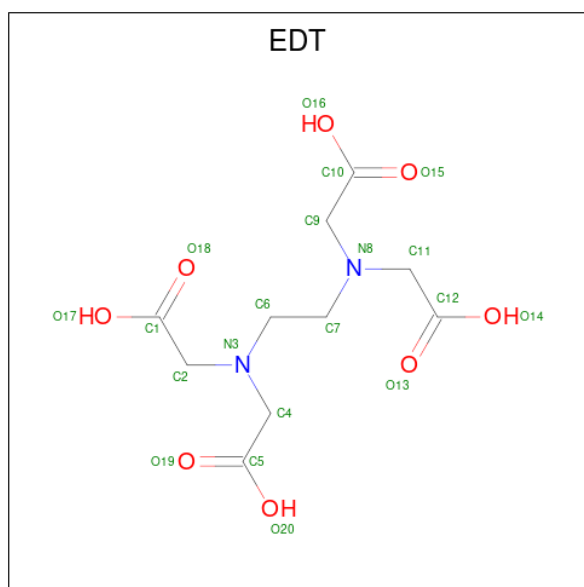
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	6	1
			3969	2547	669	743	10			
1	B	497	Total	C	N	O	S	0	7	0
			3955	2538	662	743	12			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (CCD ID: EDT) (formula: C₁₀H₁₆N₂O₈).

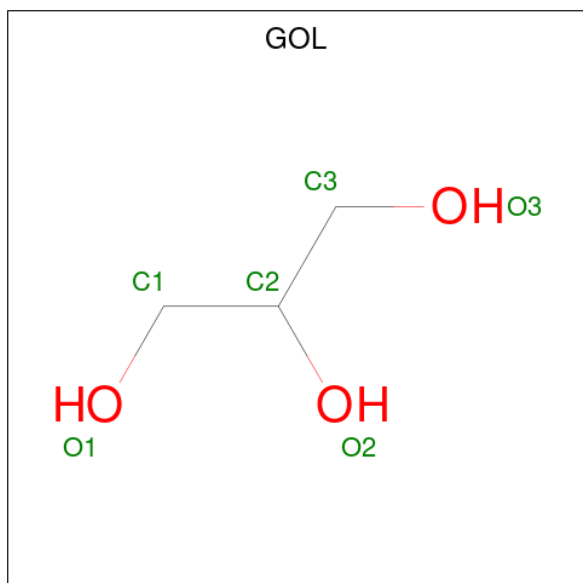


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	10	2	8		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



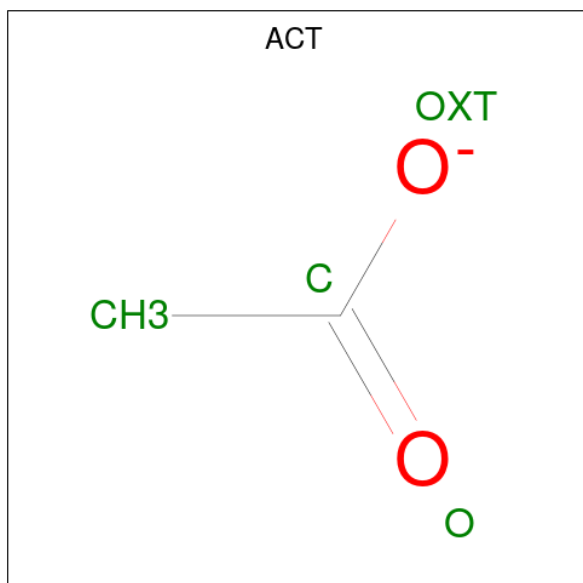
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

Continued on next page...

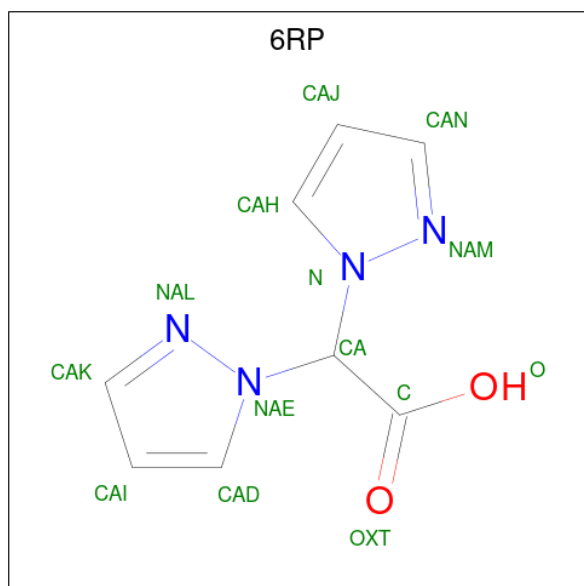
Continued from previous page...

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

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

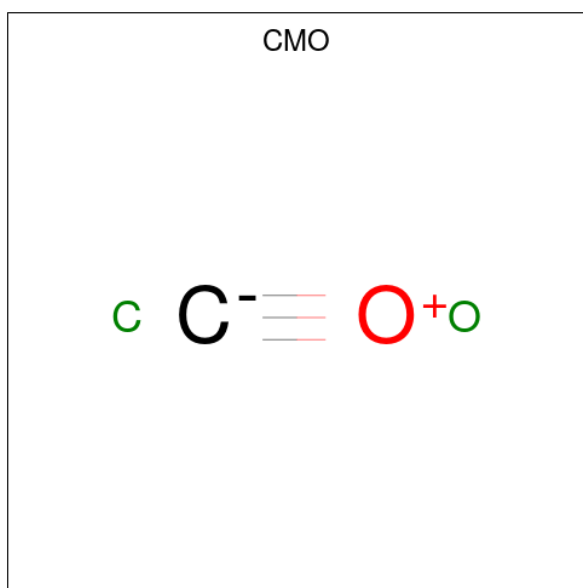
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ru	0	0
			1	1		

- Molecule 8 is bis(pyrzol-1-yl)acetate scorpionate (CCD ID: 6RP) (formula: C₈H₈N₄O₂).



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

- Molecule 9 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

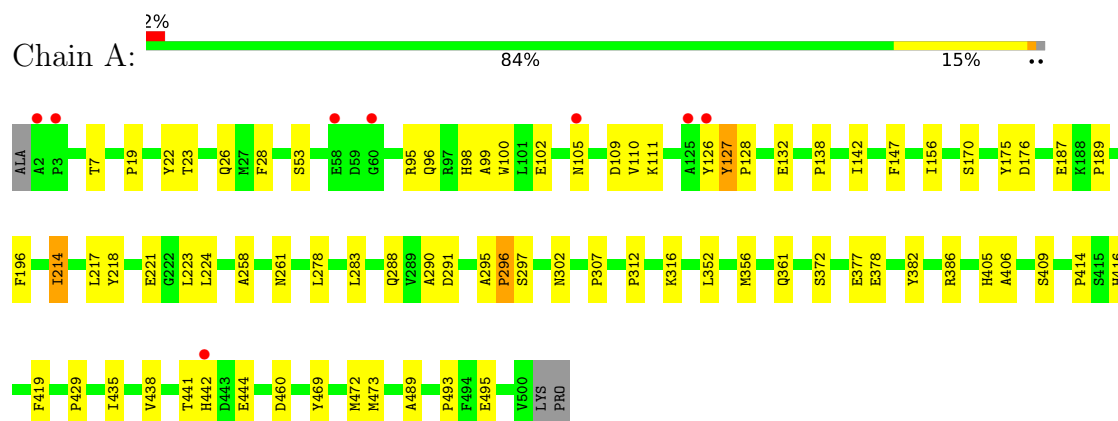
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	412	Total	O	0	0
			412	412		
10	B	326	Total	O	0	0
			326	326		

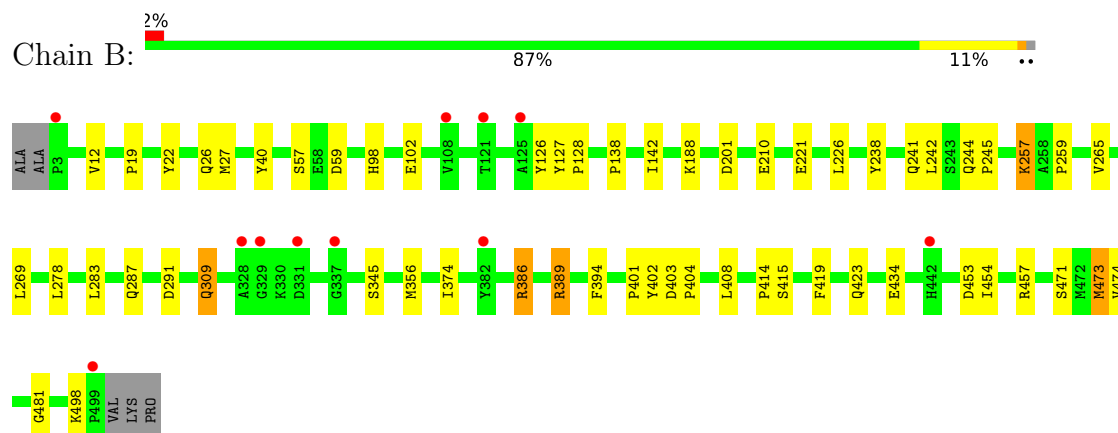
3 Residue-property plots [i](#)

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	86.63Å 94.10Å 124.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.52 – 1.90 44.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.52-1.90) 99.9 (44.52-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.178 , 0.232 0.187 , 0.239	Depositor DCC
R_{free} test set	4031 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8848	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: RU, EDT, CMO, 6RP, GOL, CL, FE, ACT

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	1/4088 (0.0%)	1.30	8/5572 (0.1%)
1	B	1.02	0/4077	1.27	2/5558 (0.0%)
All	All	1.02	1/8165 (0.0%)	1.28	10/11130 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	PRO	C-O	-5.55	1.16	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	THR	CA-C-N	6.65	129.19	120.28
1	A	441	THR	C-N-CA	6.65	129.19	120.28
1	A	147	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	214	ILE	CA-C-O	-5.64	115.75	121.67
1	A	493	PRO	N-CA-CB	-5.47	98.18	102.28
1	A	377	GLU	CA-C-N	5.21	127.58	120.54
1	A	377	GLU	C-N-CA	5.21	127.58	120.54
1	B	12	VAL	CA-C-O	-5.18	116.50	121.63
1	A	7	THR	CA-CB-OG1	-5.10	101.94	109.60
1	B	201	ASP	CA-CB-CG	5.09	117.69	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	3969	0	3912	65	0
1	B	3955	0	3892	47	0
2	A	1	0	0	0	0
3	A	20	0	12	0	0
4	A	1	0	0	2	0
4	B	1	0	0	0	0
5	A	66	0	88	19	0
5	B	48	0	64	5	0
6	A	24	0	18	0	0
6	B	8	0	6	0	0
7	B	1	0	0	0	0
8	B	14	0	0	0	0
9	B	2	0	0	0	0
10	A	412	0	0	10	1
10	B	326	0	0	4	1
All	All	8848	0	7992	112	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (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:96:GLN:CD	10:A:702:HOH:O	2.05	0.98
1:B:287:GLN:HE22	1:B:473[B]:MET:HE1	1.38	0.87
1:A:409:SER:HG	5:A:608:GOL:HO1	0.91	0.86
1:A:96:GLN:NE2	10:A:702:HOH:O	2.14	0.81
1:B:287:GLN:NE2	1:B:473[B]:MET:HE1	2.00	0.77
1:A:416:HIS:HB2	10:A:866:HOH:O	1.86	0.75
1:A:372:SER:HA	5:A:605:GOL:H2	1.70	0.73
1:B:287:GLN:HE22	1:B:473[B]:MET:CE	2.02	0.73
1:A:218:TYR:CE1	1:A:472:MET:HE2	2.24	0.73
1:A:110:VAL:N	5:A:607:GOL:O1	2.24	0.71
1:A:23:THR:OG1	5:A:619:GOL:H32	1.90	0.70
1:B:22:TYR:OH	1:B:98:HIS:HD2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:HA	1:B:473[B]:MET:HE3	1.74	0.70
1:A:105:ASN:ND2	5:A:608:GOL:O3	2.25	0.69
1:B:242:LEU:HD12	1:B:473[B]:MET:SD	2.33	0.69
1:B:226:LEU:CD2	1:B:473[A]:MET:HE1	2.22	0.69
1:B:27:MET:HE1	1:B:402:TYR:OH	1.94	0.67
1:B:471:SER:O	1:B:473[B]:MET:HE2	1.95	0.66
1:B:102:GLU:HB3	1:B:126:TYR:OH	1.96	0.65
1:A:221:GLU:O	4:A:603:CL:CL	2.52	0.65
1:B:291:ASP:OD1	10:B:701:HOH:O	2.14	0.64
1:B:242:LEU:CD1	1:B:473[B]:MET:SD	2.85	0.64
1:B:414:PRO:HA	1:B:419:PHE:CD1	2.34	0.62
1:A:189:PRO:HB3	1:A:495:GLU:HA	1.82	0.62
1:B:389:ARG:CG	1:B:389:ARG:HH11	2.14	0.59
1:A:22:TYR:OH	1:A:98:HIS:HD2	1.85	0.59
1:A:102:GLU:OE1	5:A:608:GOL:H32	2.03	0.59
5:B:614:GOL:H2	10:B:857:HOH:O	2.03	0.58
1:A:283[B]:LEU:HD12	1:A:352:LEU:HD11	1.87	0.57
1:A:23:THR:OG1	5:A:619:GOL:C3	2.53	0.57
1:B:57:SER:OG	1:B:59:ASP:OD1	2.18	0.57
1:A:223:LEU:HB3	1:A:473:MET:CE	2.35	0.57
1:A:386:ARG:HD2	10:A:1027:HOH:O	2.05	0.56
1:A:218:TYR:HE1	1:A:472:MET:HE2	1.71	0.55
1:A:288[A]:GLN:HE21	1:A:469:TYR:HD2	1.54	0.55
1:A:218:TYR:CE1	1:A:472:MET:CE	2.90	0.54
1:A:99:ALA:O	5:A:608:GOL:H31	2.08	0.53
1:A:53:SER:OG	10:A:703:HOH:O	2.19	0.53
1:B:244[A]:GLN:HE21	1:B:245:PRO:CD	2.22	0.53
1:B:419:PHE:CE1	1:B:423:GLN:NE2	2.77	0.53
1:B:265:VAL:O	1:B:269:LEU:HG	2.10	0.51
1:A:291:ASP:HB3	1:A:307:PRO:HB3	1.92	0.51
1:A:132:GLU:OE2	1:A:405:HIS:NE2	2.43	0.51
1:A:473:MET:HG2	10:A:828:HOH:O	2.10	0.51
1:A:170[B]:SER:OG	1:A:176:ASP:OD1	2.21	0.51
1:B:356:MET:HE1	5:B:606:GOL:O1	2.10	0.51
1:B:287:GLN:NE2	1:B:473[B]:MET:CE	2.69	0.50
1:A:489:ALA:HB3	10:A:807:HOH:O	2.11	0.50
1:B:226:LEU:HD12	1:B:283:LEU:HA	1.94	0.50
1:A:95:ARG:NH2	5:A:607:GOL:O3	2.46	0.49
1:A:278:LEU:HD23	1:A:278:LEU:C	2.38	0.48
1:A:223:LEU:HB3	1:A:473:MET:HE3	1.95	0.48
1:B:26:GLN:HA	5:B:609:GOL:H11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.80	0.47
1:A:361:GLN:HE22	5:A:605:GOL:H12	1.80	0.47
1:A:442:HIS:ND1	1:A:442:HIS:N	2.61	0.47
1:B:389:ARG:HH11	1:B:389:ARG:HG2	1.79	0.47
1:A:460:ASP:OD1	5:A:604:GOL:H11	2.15	0.47
1:B:40:TYR:CE1	1:B:401:PRO:HB3	2.50	0.47
1:A:23:THR:CB	5:A:619:GOL:H32	2.44	0.46
1:B:394:PHE:HB3	5:B:606:GOL:H32	1.97	0.46
1:A:126:TYR:CD2	1:A:128:PRO:HD2	2.50	0.46
1:A:100:TRP:HA	5:A:608:GOL:H12	1.96	0.46
1:B:309:GLN:CD	1:B:309:GLN:H	2.23	0.46
1:A:111:LYS:NZ	10:A:726:HOH:O	2.49	0.46
1:A:297:SER:HA	1:B:242:LEU:O	2.16	0.46
1:B:498:LYS:CE	10:B:731:HOH:O	2.64	0.46
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.97	0.46
1:A:109:ASP:HA	5:A:607:GOL:O1	2.16	0.46
1:B:345:SER:HA	1:B:374:ILE:O	2.15	0.45
1:A:100:TRP:O	5:A:608:GOL:O1	2.35	0.45
1:B:244[A]:GLN:HE21	1:B:245:PRO:HD2	1.81	0.45
1:A:444:GLU:CG	1:B:481:GLY:HA2	2.47	0.45
1:A:127:TYR:N	1:A:128:PRO:CD	2.80	0.45
1:B:434:GLU:OE1	1:B:453:ASP:OD2	2.35	0.45
1:A:175:TYR:HA	1:A:196:PHE:O	2.17	0.44
1:A:290:ALA:HA	1:A:469:TYR:CE2	2.51	0.44
1:B:19:PRO:HG3	1:B:142:ILE:HB	2.00	0.44
1:A:312:PRO:O	1:A:316:LYS:HG3	2.17	0.44
5:A:607:GOL:H12	10:A:1008:HOH:O	2.16	0.44
1:A:214:ILE:CD1	1:A:217:LEU:HD21	2.47	0.44
1:A:100:TRP:O	10:A:704:HOH:O	2.21	0.44
1:A:495:GLU:H	1:A:495:GLU:CD	2.25	0.44
1:B:498:LYS:HE3	10:B:731:HOH:O	2.18	0.44
1:B:403:ASP:HA	1:B:404:PRO:HA	1.81	0.44
1:B:408:LEU:HD13	1:B:454:ILE:HG21	2.00	0.43
1:A:435:ILE:O	1:A:438:VAL:HG12	2.18	0.43
1:B:127:TYR:N	1:B:128:PRO:CD	2.81	0.43
1:B:278:LEU:C	1:B:278:LEU:HD23	2.44	0.43
1:A:378:GLU:CG	1:A:382:TYR:CE2	3.02	0.43
1:A:414:PRO:HA	1:A:419:PHE:CG	2.54	0.42
1:A:99:ALA:O	5:A:608:GOL:C3	2.68	0.42
1:A:224:LEU:O	4:A:603:CL:CL	2.74	0.42
1:A:278:LEU:HD21	1:A:356:MET:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:HH22	5:B:607:GOL:C1	2.33	0.42
1:B:419:PHE:CZ	1:B:423:GLN:NE2	2.88	0.42
1:B:241:GLN:HB2	1:B:474:VAL:HB	2.02	0.42
1:B:127:TYR:N	1:B:128:PRO:HD3	2.35	0.41
1:B:210:GLU:HG3	1:B:238:TYR:OH	2.20	0.41
1:A:405:HIS:CG	1:A:406:ALA:N	2.88	0.41
1:B:386:ARG:HA	1:B:415:SER:O	2.21	0.41
1:A:429:PRO:HG3	5:A:617:GOL:H31	2.02	0.41
1:B:244[A]:GLN:NE2	1:B:244[A]:GLN:HA	2.35	0.41
1:A:258:ALA:HA	1:A:261:ASN:OD1	2.20	0.41
1:A:102:GLU:HB3	1:A:126:TYR:OH	2.21	0.41
1:A:283[B]:LEU:CD1	1:A:352:LEU:HD11	2.49	0.41
1:A:28:PHE:CD1	1:A:28:PHE:C	2.99	0.40
1:B:257:LYS:HE3	1:B:257:LYS:HB2	1.99	0.40
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.56	0.40
1:B:242:LEU:HD11	1:B:473[B]:MET:SD	2.61	0.40
1:A:26:GLN:HE22	5:A:619:GOL:C1	2.35	0.40
1:A:295:ALA:HA	1:A:296:PRO:HD3	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:816:HOH:O	10:B:934:HOH:O[3_545]	2.16	0.04

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	503/502 (100%)	491 (98%)	12 (2%)	0	100	100
1	B	501/502 (100%)	489 (98%)	12 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1004/1004 (100%)	980 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	422/425 (99%)	418 (99%)	4 (1%)	70	73
1	B	422/425 (99%)	413 (98%)	9 (2%)	47	44
All	All	844/850 (99%)	831 (98%)	13 (2%)	59	56

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	TYR
1	A	138	PRO
1	A	156	ILE
1	A	187	GLU
1	B	138	PRO
1	B	188	LYS
1	B	257	LYS
1	B	259	PRO
1	B	309	GLN
1	B	386	ARG
1	B	389	ARG
1	B	473[A]	MET
1	B	473[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	105	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	ASN
1	A	150	HIS
1	A	168	GLN
1	A	302	ASN
1	A	361	GLN
1	A	385	GLN
1	B	41	GLN
1	B	94	ASN
1	B	98	HIS
1	B	106	GLN
1	B	168	GLN
1	B	173	ASN
1	B	361	GLN
1	B	423	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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
5	GOL	A	606	-	5,5,5	0.09	0	5,5,5	0.27	0
5	GOL	A	615	-	5,5,5	0.09	0	5,5,5	0.34	0
5	GOL	B	610	-	5,5,5	0.12	0	5,5,5	0.50	0
9	CMO	B	604	-	0,1,1	-	-	-		
5	GOL	B	605	-	5,5,5	0.12	0	5,5,5	0.33	0
5	GOL	B	607	-	5,5,5	0.20	0	5,5,5	0.66	0
6	ACT	B	611	-	3,3,3	1.00	0	3,3,3	0.80	0
6	ACT	A	618	-	3,3,3	1.06	0	3,3,3	0.88	0
5	GOL	B	608	-	5,5,5	0.14	0	5,5,5	0.38	0
5	GOL	A	607	-	5,5,5	0.05	0	5,5,5	0.32	0
5	GOL	A	609	-	5,5,5	0.18	0	5,5,5	0.39	0
6	ACT	A	616	-	3,3,3	1.23	0	3,3,3	0.64	0
3	EDT	A	602	2	19,19,19	0.98	0	24,24,24	1.37	4 (16%)
5	GOL	A	604	-	5,5,5	0.10	0	5,5,5	0.32	0
6	ACT	A	612	-	3,3,3	1.14	0	3,3,3	0.69	0
6	ACT	A	613	-	3,3,3	0.95	0	3,3,3	0.67	0
5	GOL	A	610	-	5,5,5	0.10	0	5,5,5	0.23	0
5	GOL	A	608	-	5,5,5	0.10	0	5,5,5	0.34	0
5	GOL	A	619	-	5,5,5	0.37	0	5,5,5	0.32	0
5	GOL	B	609	-	5,5,5	0.15	0	5,5,5	0.45	0
6	ACT	A	620	-	3,3,3	1.07	0	3,3,3	0.77	0
6	ACT	B	612	-	3,3,3	1.28	0	3,3,3	1.05	0
5	GOL	A	617	-	5,5,5	0.23	0	5,5,5	0.47	0
5	GOL	B	614	-	5,5,5	0.12	0	5,5,5	0.25	0
6	ACT	A	611	-	3,3,3	1.02	0	3,3,3	0.86	0
8	6RP	B	602	7	14,15,15	0.77	0	13,20,20	1.34	3 (23%)
5	GOL	B	613	-	5,5,5	0.20	0	5,5,5	0.54	0
5	GOL	B	606	-	5,5,5	0.19	0	5,5,5	0.46	0
5	GOL	A	614	-	5,5,5	0.17	0	5,5,5	0.39	0
5	GOL	A	605	-	5,5,5	0.15	0	5,5,5	0.46	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
5	GOL	A	606	-	-	0/4/4/4	-
5	GOL	A	615	-	-	2/4/4/4	-
5	GOL	B	610	-	-	2/4/4/4	-
5	GOL	B	605	-	-	0/4/4/4	-
5	GOL	B	607	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	608	-	-	2/4/4/4	-
5	GOL	A	607	-	-	2/4/4/4	-
5	GOL	A	609	-	-	3/4/4/4	-
3	EDT	A	602	2	-	3/21/21/21	-
5	GOL	A	604	-	-	4/4/4/4	-
5	GOL	A	610	-	-	2/4/4/4	-
5	GOL	A	608	-	-	2/4/4/4	-
5	GOL	A	619	-	-	1/4/4/4	-
5	GOL	B	609	-	-	2/4/4/4	-
5	GOL	A	617	-	-	2/4/4/4	-
5	GOL	B	614	-	-	0/4/4/4	-
8	6RP	B	602	7	-	3/12/12/12	0/2/2/2
5	GOL	B	613	-	-	3/4/4/4	-
5	GOL	B	606	-	-	2/4/4/4	-
5	GOL	A	614	-	-	0/4/4/4	-
5	GOL	A	605	-	-	0/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	EDT	C12-C11-N8	-2.80	104.90	113.77
3	A	602	EDT	O17-C1-C2	2.69	123.99	113.38
8	B	602	6RP	CAH-N-NAM	-2.63	109.92	112.15
8	B	602	6RP	CAN-NAM-N	2.39	106.17	103.86
3	A	602	EDT	C7-C6-N3	-2.31	107.49	112.98
8	B	602	6RP	CAD-NAE-NAL	-2.20	110.28	112.15
3	A	602	EDT	C11-N8-C9	-2.04	106.88	111.66

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	607	GOL	O1-C1-C2-O2
5	A	607	GOL	O1-C1-C2-C3
5	A	608	GOL	C1-C2-C3-O3
5	A	609	GOL	O1-C1-C2-C3
5	A	610	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	610	GOL	O2-C2-C3-O3
5	A	615	GOL	O1-C1-C2-O2
5	A	615	GOL	O1-C1-C2-C3
5	A	617	GOL	O1-C1-C2-C3
5	B	607	GOL	O1-C1-C2-C3
5	B	607	GOL	C1-C2-C3-O3
5	B	608	GOL	C1-C2-C3-O3
5	B	608	GOL	O2-C2-C3-O3
5	B	609	GOL	O1-C1-C2-O2
5	B	609	GOL	O1-C1-C2-C3
5	B	610	GOL	O1-C1-C2-O2
5	B	610	GOL	O1-C1-C2-C3
5	B	613	GOL	C1-C2-C3-O3
8	B	602	6RP	O-C-CA-NAE
5	A	609	GOL	O1-C1-C2-O2
5	A	617	GOL	O1-C1-C2-O2
5	A	604	GOL	O1-C1-C2-C3
5	A	604	GOL	C1-C2-C3-O3
5	B	606	GOL	O1-C1-C2-C3
5	A	608	GOL	O2-C2-C3-O3
5	B	607	GOL	O1-C1-C2-O2
5	B	607	GOL	O2-C2-C3-O3
5	B	613	GOL	O2-C2-C3-O3
5	A	604	GOL	O1-C1-C2-O2
5	A	604	GOL	O2-C2-C3-O3
5	B	606	GOL	O1-C1-C2-O2
3	A	602	EDT	C10-C9-N8-C7
3	A	602	EDT	C10-C9-N8-C11
3	A	602	EDT	C1-C2-N3-C4
5	A	619	GOL	C1-C2-C3-O3
8	B	602	6RP	O-C-CA-N
5	B	613	GOL	O1-C1-C2-O2
8	B	602	6RP	OXT-C-CA-NAE
5	A	609	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 24 short contacts:

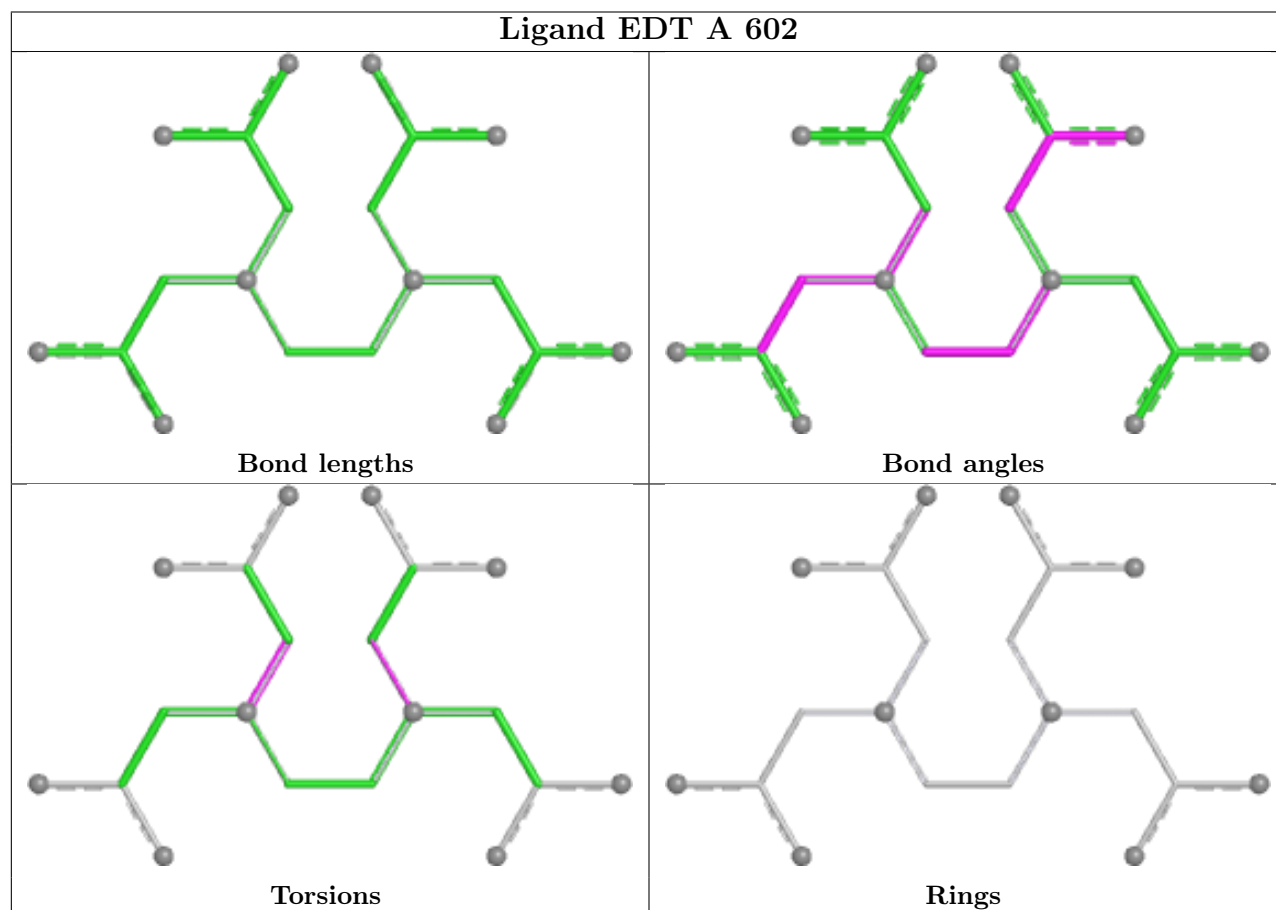
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	607	GOL	1	0
5	A	607	GOL	4	0
5	A	604	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	608	GOL	7	0
5	A	619	GOL	4	0
5	B	609	GOL	1	0
5	A	617	GOL	1	0
5	B	614	GOL	1	0
5	B	606	GOL	2	0
5	A	605	GOL	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	499/502 (99%)	0.02	8 (1%) 70 74	11, 21, 39, 61	6 (1%)
1	B	497/502 (99%)	0.20	11 (2%) 62 66	11, 25, 48, 67	6 (1%)
All	All	996/1004 (99%)	0.11	19 (1%) 66 70	11, 23, 44, 67	12 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	4.2
1	A	442	HIS	4.0
1	A	125	ALA	3.9
1	B	3	PRO	3.7
1	B	328	ALA	3.4
1	B	125	ALA	3.1
1	B	329	GLY	3.1
1	B	499	PRO	3.0
1	B	382	TYR	2.6
1	B	108	VAL	2.6
1	B	442	HIS	2.3
1	B	121	THR	2.3
1	A	126	TYR	2.3
1	A	105	ASN	2.3
1	B	337	GLY	2.2
1	A	3	PRO	2.2
1	A	58	GLU	2.1
1	A	60	GLY	2.1
1	B	331	ASP	2.1

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.

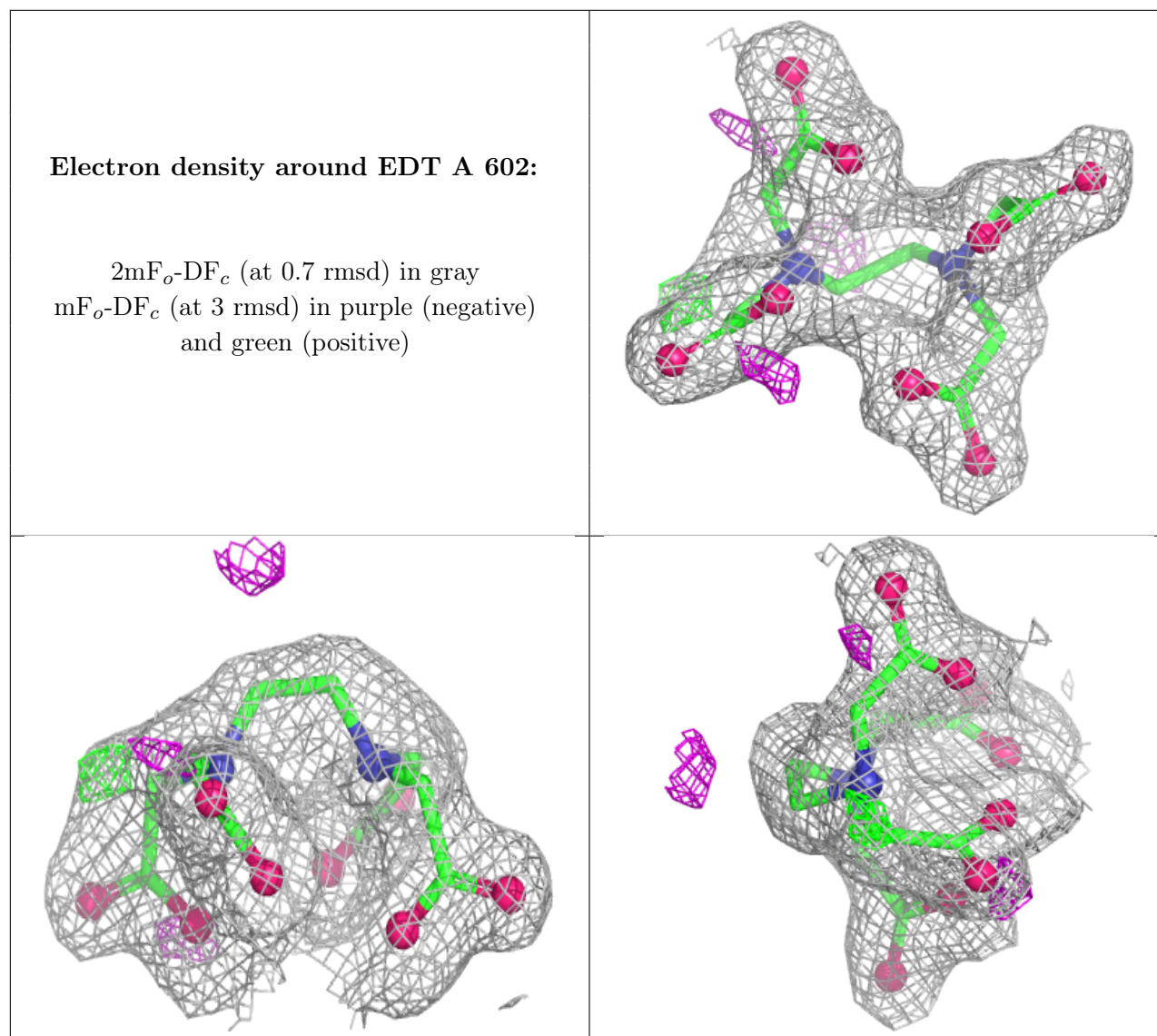
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	A	611	4/4	0.55	0.19	53,57,59,60	0
5	GOL	A	615	6/6	0.65	0.21	46,54,58,60	0
5	GOL	A	608	6/6	0.70	0.28	85,94,97,98	0
5	GOL	B	614	6/6	0.74	0.21	56,63,68,72	0
6	ACT	A	616	4/4	0.74	0.18	45,50,50,53	0
5	GOL	A	605	6/6	0.75	0.20	47,54,59,61	0
6	ACT	B	611	4/4	0.76	0.14	55,55,59,59	0
6	ACT	A	618	4/4	0.77	0.17	47,53,54,61	0
5	GOL	A	619	6/6	0.77	0.22	39,44,45,46	0
6	ACT	B	612	4/4	0.77	0.20	29,31,36,39	0
5	GOL	A	604	6/6	0.78	0.18	37,47,50,51	0
5	GOL	A	607	6/6	0.80	0.16	42,47,48,51	0
5	GOL	B	606	6/6	0.81	0.15	45,49,51,53	0
5	GOL	B	607	6/6	0.81	0.17	43,44,46,46	0
5	GOL	A	606	6/6	0.83	0.17	40,55,56,61	0
5	GOL	B	608	6/6	0.83	0.17	37,48,51,59	0
5	GOL	A	609	6/6	0.84	0.12	39,47,52,53	0
6	ACT	A	620	4/4	0.84	0.14	52,53,55,55	0
6	ACT	A	612	4/4	0.85	0.15	41,50,51,57	0
6	ACT	A	613	4/4	0.86	0.17	39,41,43,49	0
5	GOL	B	610	6/6	0.86	0.14	27,36,39,43	0
5	GOL	B	605	6/6	0.87	0.11	25,28,29,36	0
5	GOL	A	610	6/6	0.87	0.13	31,37,40,43	0
5	GOL	A	614	6/6	0.89	0.11	29,35,38,41	0
5	GOL	B	613	6/6	0.91	0.12	27,33,37,38	0
5	GOL	B	609	6/6	0.91	0.13	27,35,38,43	0
5	GOL	A	617	6/6	0.93	0.09	28,33,37,37	0
3	EDT	A	602	20/20	0.93	0.08	20,25,32,34	0
8	6RP	B	602	14/14	0.94	0.09	17,26,29,30	14
9	CMO	B	604	2/2	0.94	0.18	34,34,34,45	0
4	CL	B	603	1/1	0.95	0.14	40,40,40,40	1
4	CL	A	603	1/1	0.98	0.22	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	A	601	1/1	1.00	0.02	18,18,18,18	0
7	RU	B	601	1/1	1.00	0.03	26,26,26,26	1

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 ⓘ

There are no such residues in this entry.