



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 12:18 PM JST

PDB ID : 8ZXU / pdb_00008zxu
Title : Crystal structure of N terminal deletion mutant of Staphylococcal atypical two-cysteine thiol peroxidase complexed with substrate analog
Authors : Shukla, M.; Maji, S.; Yadav, V.K.; Bhattacharyya, S.
Deposited on : 2024-06-15
Resolution : 1.55 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

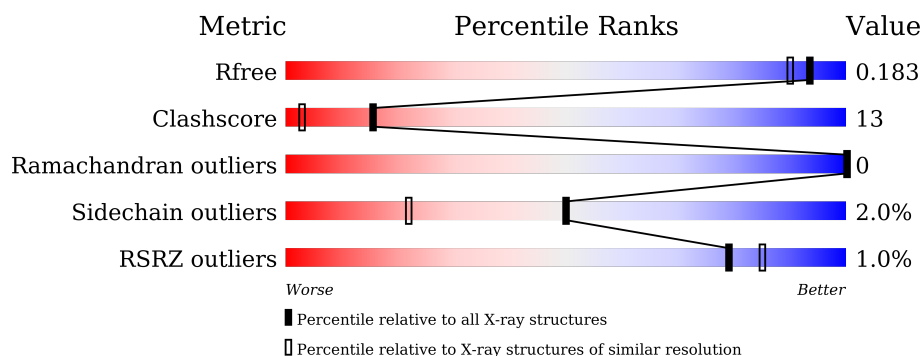
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	164625	1935 (1.56-1.56)
Clashscore	180529	2073 (1.56-1.56)
Ramachandran outliers	177936	2037 (1.56-1.56)
Sidechain outliers	177891	2034 (1.56-1.56)
RSRZ outliers	164620	1935 (1.56-1.56)

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	149	
1	B	149	
1	C	149	
1	D	149	

2 Entry composition [i](#)

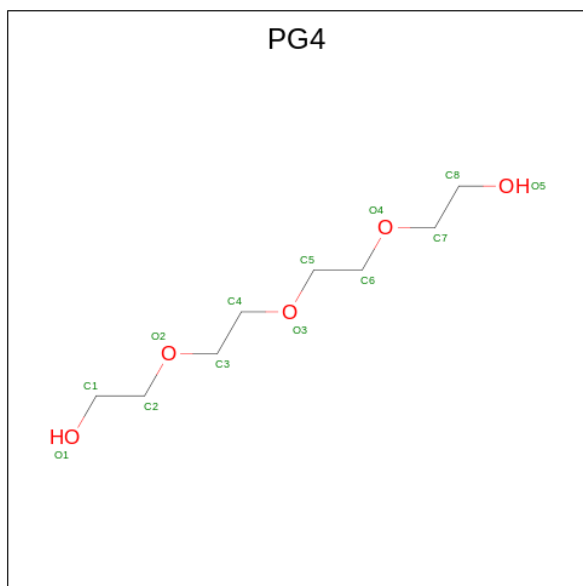
There are 8 unique types of molecules in this entry. The entry contains 10149 atoms, of which 4670 are hydrogens and 0 are deuteriums.

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 Thiol peroxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	149	Total	C	H	N	O	S	0	4	0
			2290	738	1124	190	235	3			
1	B	149	Total	C	H	N	O	S	0	3	0
			2285	736	1121	191	234	3			
1	C	149	Total	C	H	N	O	S	0	1	0
			2271	731	1111	191	235	3			
1	D	149	Total	C	H	N	O	S	0	2	0
			2285	736	1120	191	235	3			

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



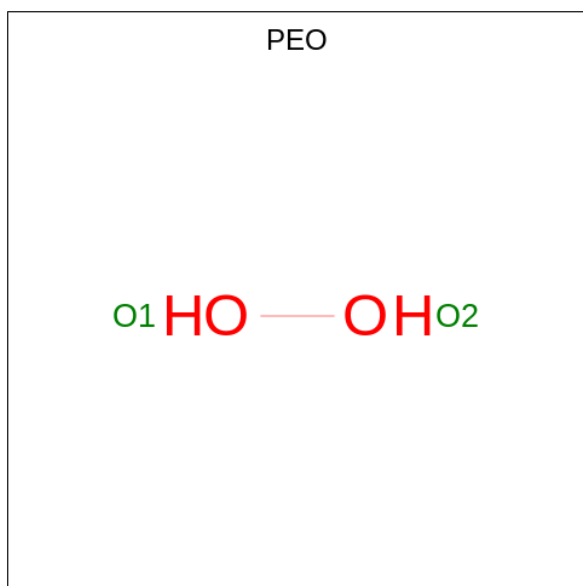
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			30	8	17	5		
2	A	1	Total	C	H	O	0	0
			30	8	17	5		

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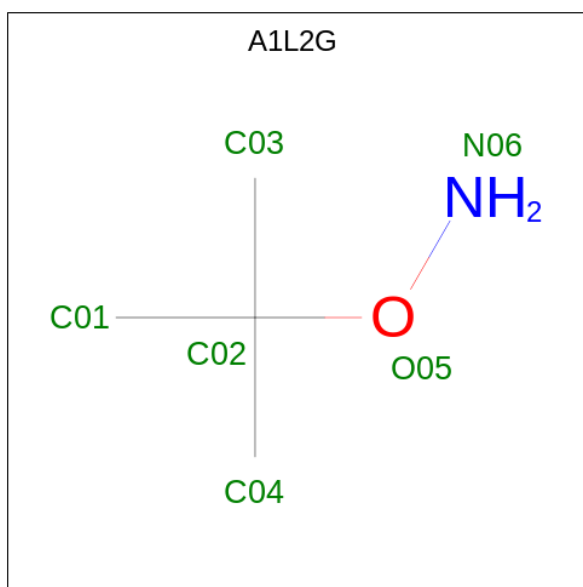
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			30	8	17	5		
2	A	1	Total	C	H	O	0	0
			30	8	17	5		
2	B	1	Total	C	H	O	0	0
			30	8	17	5		
2	B	1	Total	C	H	O	0	0
			30	8	17	5		
2	B	1	Total	C	H	O	0	0
			30	8	17	5		
2	D	1	Total	C	H	O	0	0
			30	8	17	5		

- Molecule 3 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H₂O₂).



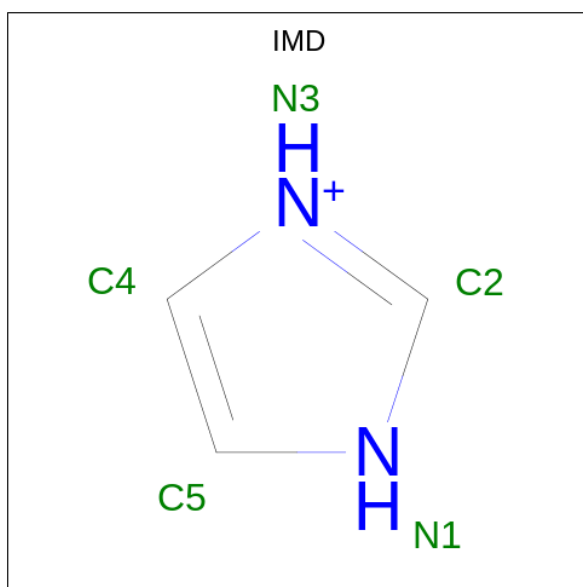
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	H	O	0	0
			3	1	2		
3	B	1	Total	H	O	0	0
			3	1	2		
3	B	1	Total	H	O	0	0
			3	1	2		

- Molecule 4 is O-tert-Butylhydroxylamine (CCD ID: A1L2G) (formula: C₄H₁₁NO) (labeled as "Ligand of Interest" by depositor).



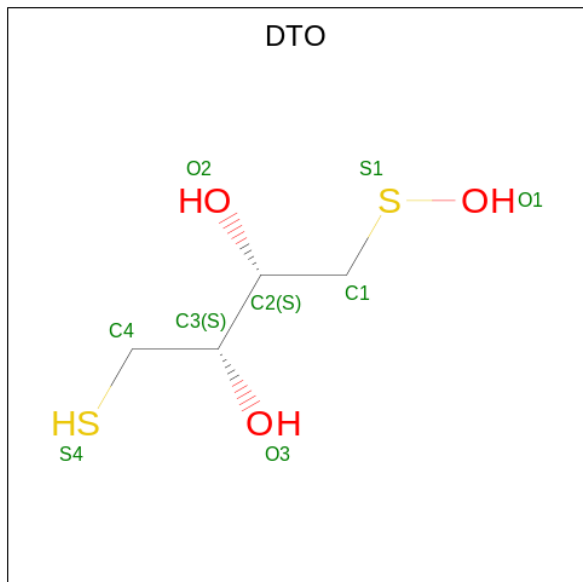
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			18	4	12	1	1		
4	C	1	Total	C	H	N	O	0	0
			18	4	12	1	1		
4	D	1	Total	C	H	N	O	0	0
			18	4	12	1	1		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



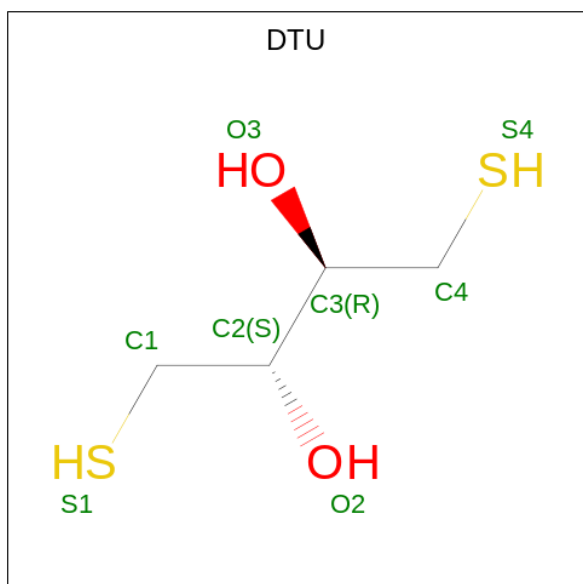
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 6 is 1-HYDROXSULFANYL-4-MERCAPTO-BUTANE-2,3-DIOL (CCD ID: DTO) (formula: $C_4H_{10}O_3S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	O	S	0	0
			15	4	7	2	2		

- Molecule 7 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (CCD ID: DTU) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	H	O	S	0	0
			15	4	7	2	2		

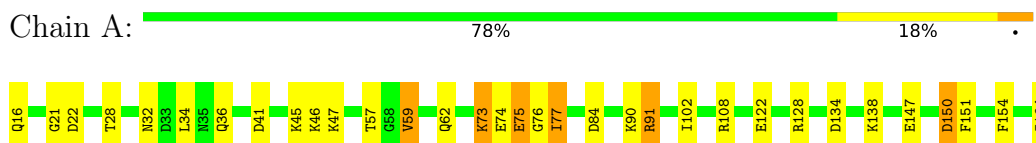
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	198	Total 198	O 198	0	0
8	B	186	Total 186	O 186	0	0
8	C	155	Total 155	O 155	0	0
8	D	136	Total 136	O 136	0	0

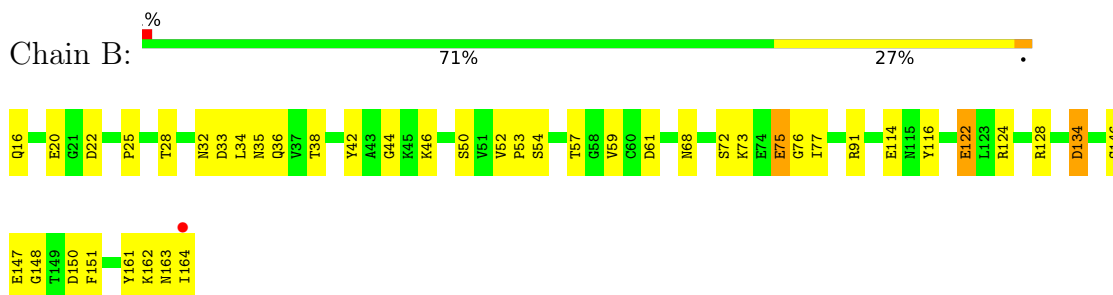
3 Residue-property plots

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.

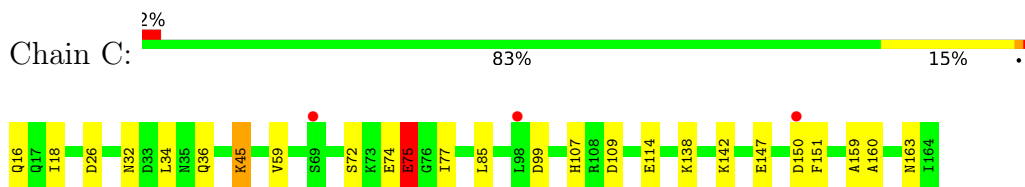
- Molecule 1: Thiol peroxidase



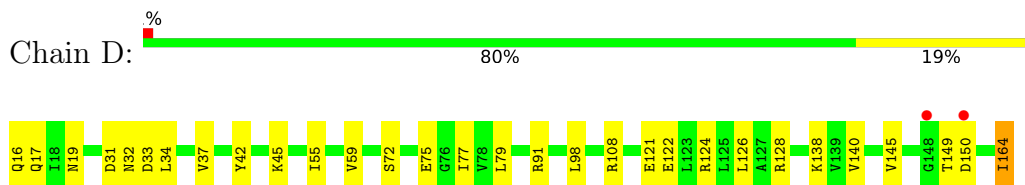
- Molecule 1: Thiol peroxidase



- Molecule 1: Thiol peroxidase



- Molecule 1: Thiol peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.27Å 148.33Å 72.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.93 – 1.55 40.93 – 1.55	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.93-1.55) 99.3 (40.93-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.163 , 0.195 0.153 , 0.183	Depositor DCC
R_{free} test set	6613 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.256 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10149	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: PG4, DTU, IMD, PEO, DTO, A1L2G

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	1.23	5/1193 (0.4%)	1.54	10/1619 (0.6%)
1	B	1.28	4/1188 (0.3%)	1.55	14/1612 (0.9%)
1	C	1.04	1/1178 (0.1%)	1.41	8/1598 (0.5%)
1	D	1.10	5/1186 (0.4%)	1.43	5/1609 (0.3%)
All	All	1.17	15/4745 (0.3%)	1.48	37/6438 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	VAL	C-O	6.57	1.28	1.24
1	D	124	ARG	NE-CZ	6.41	1.40	1.33
1	A	41	ASP	CG-OD2	-5.88	1.14	1.25
1	D	164	ILE	C-O	-5.66	1.12	1.23
1	A	108	ARG	NE-CZ	5.50	1.39	1.33
1	A	154	PHE	C-O	-5.33	1.18	1.24
1	C	107	HIS	CE1-NE2	5.31	1.37	1.32
1	D	126	LEU	C-O	5.28	1.30	1.23
1	B	50	SER	CA-CB	-5.25	1.45	1.53
1	A	77[A]	ILE	C-N	5.17	1.40	1.33
1	A	77[B]	ILE	C-N	5.17	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ARG	CD-NE	5.11	1.53	1.46
1	B	54	SER	C-N	-5.09	1.28	1.33
1	D	37	VAL	C-O	-5.07	1.19	1.24
1	D	79	LEU	C-O	-5.01	1.18	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	GLU	CB-CG-CD	8.31	126.73	112.60
1	A	150	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	150	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	91	ARG	CG-CD-NE	-6.79	97.07	112.00
1	C	107	HIS	N-CA-C	6.64	118.52	111.28
1	C	32	ASN	CA-CB-CG	6.61	119.21	112.60
1	C	150	ASP	CA-CB-CG	6.46	119.06	112.60
1	D	164	ILE	CA-C-O	-6.37	109.97	120.80
1	B	75	GLU	CA-C-N	5.92	128.80	120.57
1	B	75	GLU	C-N-CA	5.92	128.80	120.57
1	A	46	LYS	CA-C-O	-5.91	115.02	121.87
1	B	75	GLU	CB-CG-CD	5.86	122.56	112.60
1	B	128	ARG	N-CA-CB	5.67	118.37	109.69
1	A	134	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	22	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	150	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	147	GLU	CB-CA-C	5.53	118.90	109.72
1	B	32	ASN	O-C-N	5.50	130.04	122.46
1	B	61	ASP	CB-CA-C	5.44	119.52	110.81
1	A	32	ASN	CB-CG-ND2	-5.41	108.29	116.40
1	B	146	SER	CB-CA-C	5.37	119.33	109.46
1	C	75	GLU	CA-C-N	5.32	127.20	122.47
1	C	75	GLU	C-N-CA	5.32	127.20	122.47
1	D	32	ASN	O-C-N	5.32	129.79	122.46
1	B	134	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	41	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	74	GLU	N-CA-C	-5.27	106.36	112.89
1	A	59	VAL	N-CA-CB	5.25	117.68	110.54
1	A	84	ASP	CA-C-O	-5.25	115.99	121.55
1	B	33	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	73	LYS	CB-CG-CD	5.19	123.24	111.30
1	C	26	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	85	LEU	N-CA-CB	5.13	117.78	110.03
1	B	122	GLU	CB-CG-CD	5.08	121.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	THR	CB-CA-C	5.03	119.24	109.33
1	B	151	PHE	O-C-N	-5.03	118.49	121.71
1	D	124	ARG	NE-CZ-NH2	-5.00	114.70	119.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	LYS	Mainchain
1	B	34	LEU	Mainchain
1	B	53	PRO	Mainchain
1	D	16	GLN	Peptide

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	1166	1124	1148	41	0
1	B	1164	1121	1142	28	0
1	C	1160	1111	1130	21	0
1	D	1165	1120	1141	27	0
2	A	52	68	72	7	0
2	B	39	51	54	5	0
2	D	13	17	18	0	0
3	A	2	1	0	0	0
3	B	4	2	0	0	0
4	A	6	12	0	3	0
4	C	6	12	0	2	0
4	D	6	12	0	1	0
5	B	5	5	5	0	0
6	B	8	7	8	1	0
7	D	8	7	10	1	0
8	A	198	0	0	18	2
8	B	186	0	0	16	3
8	C	155	0	0	15	0
8	D	136	0	0	15	1
All	All	5479	4670	4728	126	3

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 13.

All (126) 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:A:206:A1L2G:N06	4:A:206:A1L2G:O05	1.59	1.35
4:C:201:A1L2G:N06	4:C:201:A1L2G:O05	1.66	1.27
1:D:121:GLU:OE2	8:D:301:HOH:O	1.58	1.20
1:A:28[A]:THR:HG21	1:A:36:GLN:NE2	1.56	1.19
1:A:77[B]:ILE:HD11	1:A:102:ILE:CD1	1.74	1.17
1:A:122:GLU:O	8:A:301:HOH:O	1.72	1.07
1:A:28[A]:THR:CG2	1:A:36:GLN:HE21	1.71	1.03
1:C:109:ASP:OD2	8:C:301:HOH:O	1.77	1.00
7:D:203:DTU:H4C2	7:D:203:DTU:S1	2.01	1.00
1:A:77[B]:ILE:HD11	1:A:102:ILE:HD12	1.40	1.00
1:D:108:ARG:HD2	8:D:385:HOH:O	1.64	0.98
1:A:77[B]:ILE:HD11	1:A:102:ILE:HD11	1.46	0.94
1:D:17:GLN:OE1	1:D:19:ASN:OD1	1.88	0.91
1:A:122:GLU:C	8:A:301:HOH:O	2.11	0.90
1:C:18:ILE:O	1:C:142:LYS:NZ	2.05	0.89
1:A:91:ARG:NE	1:D:91:ARG:CZ	2.39	0.86
1:C:36:GLN:NE2	8:C:302:HOH:O	2.00	0.84
1:B:147:GLU:OE2	8:B:302:HOH:O	1.94	0.84
1:A:90:LYS:NZ	8:A:305:HOH:O	2.11	0.82
1:A:59:VAL:HG22	8:A:360:HOH:O	1.78	0.82
1:B:42:TYR:CD1	1:B:77[B]:ILE:HD12	2.15	0.82
1:A:28[A]:THR:HG21	1:A:36:GLN:HE21	0.75	0.82
1:C:16:GLN:NE2	8:C:303:HOH:O	2.14	0.79
1:C:138:LYS:HD3	8:C:379:HOH:O	1.83	0.76
1:A:147:GLU:HA	8:A:315:HOH:O	1.85	0.75
1:B:35[A]:ASN:ND2	8:B:308:HOH:O	2.21	0.74
1:A:22:ASP:OD1	8:A:303:HOH:O	2.08	0.71
1:B:75:GLU:O	8:B:304:HOH:O	2.09	0.71
1:B:122:GLU:OE1	8:B:303:HOH:O	2.08	0.71
1:A:122:GLU:O	1:D:108:ARG:NH1	2.24	0.70
1:B:114:GLU:OE2	8:B:305:HOH:O	2.10	0.70
1:A:77[B]:ILE:CD1	1:A:102:ILE:HD12	2.21	0.69
1:D:45:LYS:NZ	8:D:302:HOH:O	2.01	0.69
1:A:36:GLN:OE1	8:A:304:HOH:O	2.10	0.68
1:A:75:GLU:O	8:A:307:HOH:O	2.12	0.68
1:A:28[A]:THR:CG2	1:A:36:GLN:HG3	2.24	0.68
1:B:38:THR:OG1	8:B:306:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLN:NE2	1:B:38:THR:HG23	2.09	0.67
1:A:150:ASP:OD2	8:A:306:HOH:O	2.12	0.66
1:A:77[B]:ILE:CD1	1:A:102:ILE:CD1	2.66	0.66
8:A:301:HOH:O	1:D:108:ARG:HD3	1.95	0.66
2:A:203:PG4:C2	2:A:203:PG4:O3	2.44	0.65
4:A:206:A1L2G:N06	4:A:206:A1L2G:C02	2.60	0.65
1:D:33:ASP:OD1	8:D:303:HOH:O	2.14	0.65
1:B:164:ILE:HA	8:B:428:HOH:O	1.95	0.64
1:A:59:VAL:CG2	8:A:360:HOH:O	2.40	0.64
1:B:162:LYS:HD2	8:B:460:HOH:O	1.98	0.63
1:A:21:GLY:O	1:A:138:LYS:HD2	1.98	0.63
1:A:62:GLN:HE22	2:A:202:PG4:H82	1.62	0.63
1:C:75:GLU:O	8:C:304:HOH:O	2.15	0.63
1:C:72:SER:C	8:C:310:HOH:O	2.42	0.63
1:A:91:ARG:HE	1:D:91:ARG:CZ	2.10	0.62
1:A:28[A]:THR:HG23	1:A:36:GLN:HG3	1.81	0.61
1:C:99:ASP:C	8:C:345:HOH:O	2.44	0.61
1:A:138:LYS:NZ	8:A:302:HOH:O	1.99	0.61
1:B:72:SER:HB3	1:B:75:GLU:HB2	1.83	0.60
1:D:128:ARG:NH2	8:D:306:HOH:O	2.33	0.60
1:D:17:GLN:N	8:D:304:HOH:O	2.15	0.60
1:B:46:LYS:HE2	8:B:304:HOH:O	2.02	0.60
1:A:91:ARG:HE	1:D:91:ARG:NH2	2.00	0.59
1:B:28:THR:HG23	1:B:36:GLN:HG3	1.84	0.59
1:C:160:ALA:HA	1:C:163:ASN:OD1	2.03	0.58
4:D:201:A1L2G:N06	8:D:309:HOH:O	2.32	0.58
2:B:203:PG4:H51	8:B:360:HOH:O	2.03	0.57
1:A:28[A]:THR:CG2	1:A:36:GLN:NE2	2.47	0.57
1:B:124:ARG:HH21	6:B:205:DTO:H11	1.68	0.57
1:D:77[B]:ILE:HG13	8:D:346:HOH:O	2.04	0.56
1:B:28:THR:HG23	1:B:36:GLN:CG	2.36	0.56
1:C:160:ALA:HB2	8:C:434:HOH:O	2.05	0.56
2:B:201:PG4:O5	8:B:301:HOH:O	1.90	0.54
1:C:75:GLU:N	1:C:75:GLU:OE1	2.42	0.53
1:A:62:GLN:NE2	2:A:202:PG4:H82	2.22	0.53
1:B:134:ASP:HA	1:B:164:ILE:HD13	1.91	0.52
1:D:72:SER:HB3	1:D:75:GLU:HB2	1.91	0.52
2:A:203:PG4:C6	2:A:203:PG4:H22	2.40	0.51
1:B:20:GLU:OE2	8:B:307:HOH:O	2.18	0.51
1:A:59:VAL:HG23	1:A:151:PHE:CE1	2.45	0.51
1:B:42:TYR:HB3	1:B:77[B]:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28[A]:THR:CG2	1:A:36:GLN:CG	2.89	0.50
1:C:74:GLU:N	8:C:310:HOH:O	2.37	0.50
1:B:42:TYR:CD1	1:B:77[B]:ILE:CD1	2.93	0.50
1:D:55:ILE:CG2	8:D:340:HOH:O	2.60	0.50
1:A:57:THR:HB	2:A:204:PG4:H51	1.94	0.49
1:C:59:VAL:HG23	1:C:151:PHE:CE1	2.47	0.49
2:B:202:PG4:H71	8:B:314:HOH:O	2.14	0.47
1:C:114:GLU:OE1	8:C:305:HOH:O	2.20	0.47
4:C:201:A1L2G:N06	4:C:201:A1L2G:C02	2.71	0.47
2:B:203:PG4:H42	2:B:203:PG4:O4	2.15	0.46
1:C:34:LEU:HG	8:C:416:HOH:O	2.14	0.46
1:C:75:GLU:C	8:C:304:HOH:O	2.57	0.46
1:B:16:GLN:N	8:B:317:HOH:O	2.48	0.46
1:B:28:THR:CG2	1:B:36:GLN:HG3	2.44	0.46
4:A:206:A1L2G:N06	4:A:206:A1L2G:C01	2.78	0.46
1:B:46:LYS:HG3	1:B:161:TYR:CE1	2.51	0.46
1:B:68:ASN:O	1:B:73:LYS:HE3	2.16	0.45
2:A:203:PG4:H61	8:A:338:HOH:O	2.16	0.45
1:D:149:THR:O	8:D:306:HOH:O	2.21	0.45
1:A:45:LYS:HE2	8:A:312:HOH:O	2.17	0.44
1:D:121:GLU:HG3	8:D:343:HOH:O	2.17	0.44
1:D:31:ASP:OD1	1:D:31:ASP:C	2.60	0.44
1:C:159:ALA:O	1:C:163:ASN:OD1	2.36	0.44
1:C:163:ASN:ND2	8:C:316:HOH:O	2.50	0.44
1:D:17:GLN:NE2	8:D:307:HOH:O	2.30	0.44
1:A:164:ILE:C	8:A:446:HOH:O	2.61	0.44
1:B:44:GLY:O	2:B:201:PG4:H52	2.18	0.43
1:A:76:GLY:HA2	8:A:307:HOH:O	2.18	0.43
1:C:138:LYS:CD	8:C:379:HOH:O	2.53	0.43
1:A:164:ILE:HA	8:A:446:HOH:O	2.18	0.42
1:A:91:ARG:CD	1:D:91:ARG:NH1	2.83	0.42
2:A:203:PG4:O3	2:A:203:PG4:H21	2.20	0.42
1:D:17:GLN:CA	8:D:304:HOH:O	2.64	0.42
1:B:148:GLY:N	8:B:318:HOH:O	2.48	0.42
1:A:91:ARG:HD3	1:D:91:ARG:NH1	2.35	0.41
1:A:28[A]:THR:HG23	1:A:36:GLN:CG	2.48	0.41
1:C:45:LYS:HD2	1:C:77:ILE:HD11	2.00	0.41
1:B:25:PRO:HG2	1:B:116:TYR:CE1	2.55	0.41
1:C:163:ASN:HB2	8:C:312:HOH:O	2.20	0.41
1:D:55:ILE:HG23	8:D:340:HOH:O	2.19	0.41
1:A:22:ASP:OD1	8:A:308:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:TYR:CD1	1:D:77[B]:ILE:HD13	2.56	0.41
1:B:163:ASN:OD1	8:B:309:HOH:O	2.22	0.41
1:D:98:LEU:HD23	1:D:98:LEU:HA	1.89	0.41
1:B:46:LYS:HG2	1:B:76:GLY:HA3	2.03	0.41
1:D:145:VAL:HG12	8:D:306:HOH:O	2.21	0.40
1:A:59:VAL:HG21	1:A:128:ARG:NH1	2.36	0.40
1:D:140:VAL:HG21	1:D:164:ILE:HD11	2.02	0.40

All (3) 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)
8:A:446:HOH:O	8:B:349:HOH:O[1_655]	1.99	0.21
8:B:414:HOH:O	8:D:320:HOH:O[2_555]	2.12	0.08
8:A:382:HOH:O	8:B:433:HOH:O[1_655]	2.15	0.05

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	150/149 (101%)	149 (99%)	1 (1%)	0	100	100
1	B	149/149 (100%)	148 (99%)	1 (1%)	0	100	100
1	C	148/149 (99%)	148 (100%)	0	0	100	100
1	D	149/149 (100%)	149 (100%)	0	0	100	100
All	All	596/596 (100%)	594 (100%)	2 (0%)	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	129/126 (102%)	125 (97%)	4 (3%)	35	9
1	B	128/126 (102%)	127 (99%)	1 (1%)	79	63
1	C	127/126 (101%)	125 (98%)	2 (2%)	58	31
1	D	128/126 (102%)	125 (98%)	3 (2%)	45	17
All	All	512/504 (102%)	502 (98%)	10 (2%)	50	22

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	34	LEU
1	A	73	LYS
1	A	75	GLU
1	B	59	VAL
1	C	45	LYS
1	C	75	GLU
1	D	34	LEU
1	D	59	VAL
1	D	138	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	19	ASN
1	A	36	GLN
1	A	62	GLN
1	A	100	ASN
1	B	36	GLN
1	B	62	GLN
1	B	163	ASN
1	C	62	GLN

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Mol	Chain	Res	Type
1	C	107	HIS
1	D	19	ASN
1	D	62	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	$\# Z > 2$
7	DTU	D	203	-	7,7,7	0.28	0	4,8,8	1.04	0
2	PG4	A	204	-	12,12,12	0.40	0	11,11,11	0.36	0
3	PEO	B	207	-	1,1,1	0.54	0	-		
2	PG4	A	201	-	12,12,12	0.54	0	11,11,11	0.36	0
2	PG4	B	201	-	12,12,12	0.29	0	11,11,11	0.26	0
2	PG4	A	202	-	12,12,12	0.39	0	11,11,11	0.30	0
2	PG4	B	202	-	12,12,12	0.29	0	11,11,11	0.25	0
4	A1L2G	C	201	-	4,5,5	2.31	3 (75%)	6,7,7	1.72	2 (33%)
5	IMD	B	204	-	3,5,5	0.35	0	4,5,5	0.66	0
2	PG4	A	203	-	12,12,12	0.38	0	11,11,11	0.37	0
2	PG4	B	203	-	12,12,12	0.40	0	11,11,11	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1L2G	A	206	-	4,5,5	2.77	1 (25%)	6,7,7	1.43	1 (16%)
4	A1L2G	D	201	-	4,5,5	7.63	1 (25%)	6,7,7	1.03	0
6	DTO	B	205	-	7,7,8	1.45	1 (14%)	4,8,9	1.49	1 (25%)
3	PEO	B	206	-	1,1,1	0.42	0	-	-	-
3	PEO	A	205	-	1,1,1	0.38	0	-	-	-
2	PG4	D	202	-	12,12,12	0.31	0	11,11,11	0.26	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
7	DTU	D	203	-	-	6/8/8/8	-
2	PG4	A	204	-	-	6/10/10/10	-
2	PG4	A	201	-	-	3/10/10/10	-
2	PG4	B	201	-	-	5/10/10/10	-
2	PG4	A	202	-	-	4/10/10/10	-
2	PG4	B	202	-	-	6/10/10/10	-
5	IMD	B	204	-	-	-	0/1/1/1
2	PG4	A	203	-	-	8/10/10/10	-
2	PG4	B	203	-	-	5/10/10/10	-
4	A1L2G	A	206	-	-	0/0/3/3	-
4	A1L2G	D	201	-	-	0/0/3/3	-
6	DTO	B	205	-	-	6/8/8/9	-
4	A1L2G	C	201	-	-	0/0/3/3	-
2	PG4	D	202	-	-	8/10/10/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	A1L2G	O05-C02	-15.11	1.32	1.48
4	A	206	A1L2G	O05-C02	-4.85	1.43	1.48
6	B	205	DTO	O3-C3	-3.61	1.35	1.43
4	C	201	A1L2G	O05-C02	-3.22	1.45	1.48
4	C	201	A1L2G	C04-C02	2.49	1.58	1.51
4	C	201	A1L2G	C03-C02	2.03	1.57	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	206	A1L2G	C03-C02-C01	-2.91	103.53	111.16
6	B	205	DTO	C2-C1-S1	-2.84	106.22	114.47
4	C	201	A1L2G	C03-C02-C01	-2.73	104.00	111.16
4	C	201	A1L2G	C04-C02-C03	2.50	117.72	111.16

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	205	DTO	S1-C1-C2-O2
6	B	205	DTO	S1-C1-C2-C3
6	B	205	DTO	C1-C2-C3-O3
6	B	205	DTO	C1-C2-C3-C4
6	B	205	DTO	O2-C2-C3-O3
6	B	205	DTO	O2-C2-C3-C4
7	D	203	DTU	C1-C2-C3-O3
7	D	203	DTU	C1-C2-C3-C4
7	D	203	DTU	O2-C2-C3-O3
7	D	203	DTU	O2-C2-C3-C4
7	D	203	DTU	C2-C3-C4-S4
7	D	203	DTU	O3-C3-C4-S4
2	A	201	PG4	C5-C6-O4-C7
2	A	204	PG4	C3-C4-O3-C5
2	D	202	PG4	O3-C5-C6-O4
2	B	201	PG4	O1-C1-C2-O2
2	B	203	PG4	O1-C1-C2-O2
2	D	202	PG4	O4-C7-C8-O5
2	A	204	PG4	O3-C5-C6-O4
2	B	203	PG4	C1-C2-O2-C3
2	D	202	PG4	O2-C3-C4-O3
2	A	202	PG4	O1-C1-C2-O2
2	A	203	PG4	O1-C1-C2-O2
2	D	202	PG4	O1-C1-C2-O2
2	D	202	PG4	C4-C3-O2-C2
2	A	203	PG4	O2-C3-C4-O3
2	B	202	PG4	O4-C7-C8-O5
2	A	202	PG4	O3-C5-C6-O4
2	B	203	PG4	O2-C3-C4-O3
2	B	202	PG4	O3-C5-C6-O4
2	B	202	PG4	C6-C5-O3-C4
2	A	201	PG4	O3-C5-C6-O4
2	B	203	PG4	C4-C3-O2-C2
2	A	203	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	B	202	PG4	C3-C4-O3-C5
2	A	203	PG4	C8-C7-O4-C6
2	B	201	PG4	C1-C2-O2-C3
2	D	202	PG4	C8-C7-O4-C6
2	D	202	PG4	C5-C6-O4-C7
2	A	202	PG4	C5-C6-O4-C7
2	B	201	PG4	O3-C5-C6-O4
2	B	201	PG4	C5-C6-O4-C7
2	A	203	PG4	C3-C4-O3-C5
2	A	204	PG4	C8-C7-O4-C6
2	A	203	PG4	C4-C3-O2-C2
2	A	203	PG4	C6-C5-O3-C4
2	A	204	PG4	O2-C3-C4-O3
2	B	202	PG4	C8-C7-O4-C6
2	B	201	PG4	C3-C4-O3-C5
2	A	201	PG4	C6-C5-O3-C4
2	D	202	PG4	C3-C4-O3-C5
2	A	204	PG4	C6-C5-O3-C4
2	A	203	PG4	O3-C5-C6-O4
2	A	202	PG4	C8-C7-O4-C6
2	B	203	PG4	C6-C5-O3-C4
2	B	202	PG4	O2-C3-C4-O3
2	A	204	PG4	C1-C2-O2-C3

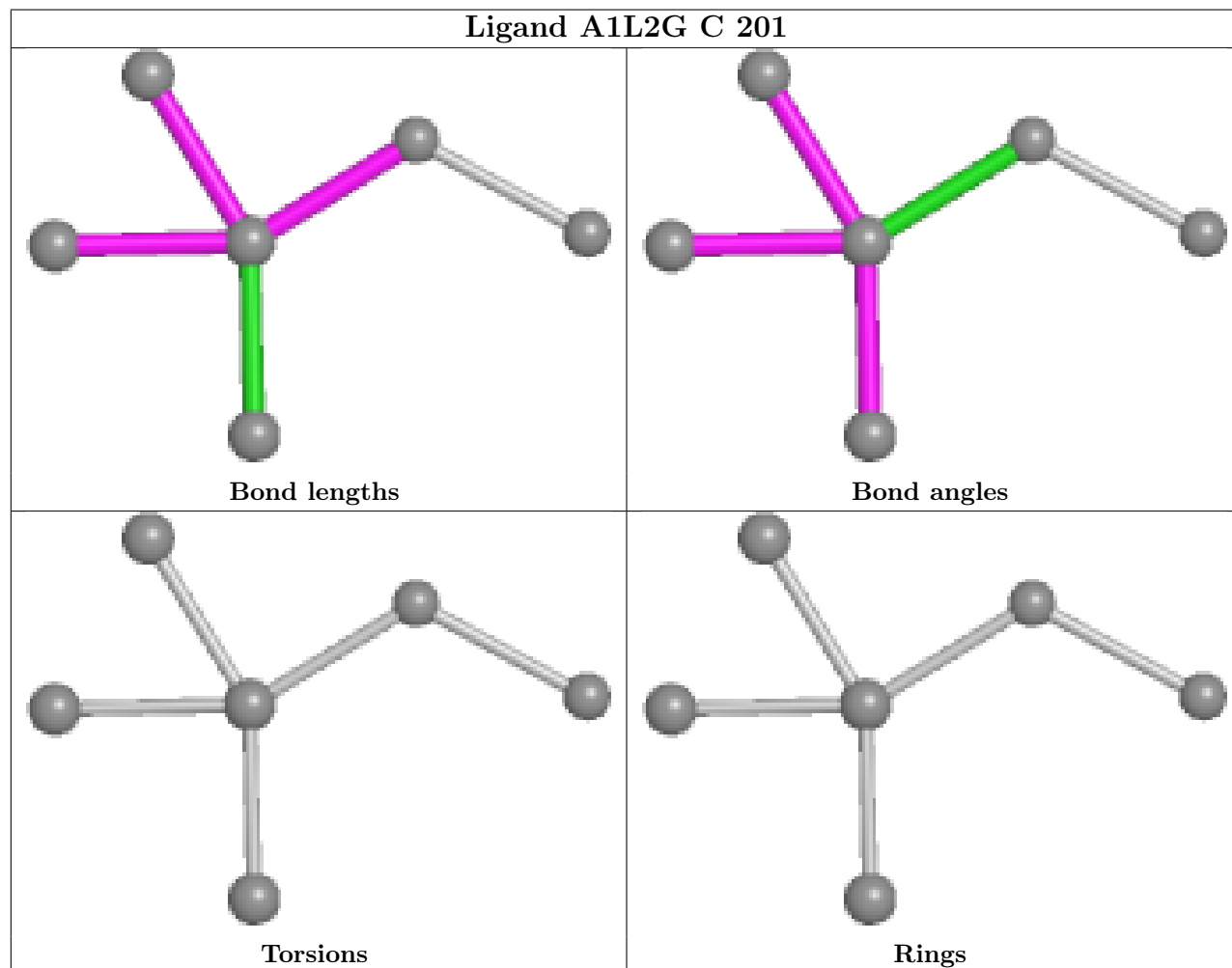
There are no ring outliers.

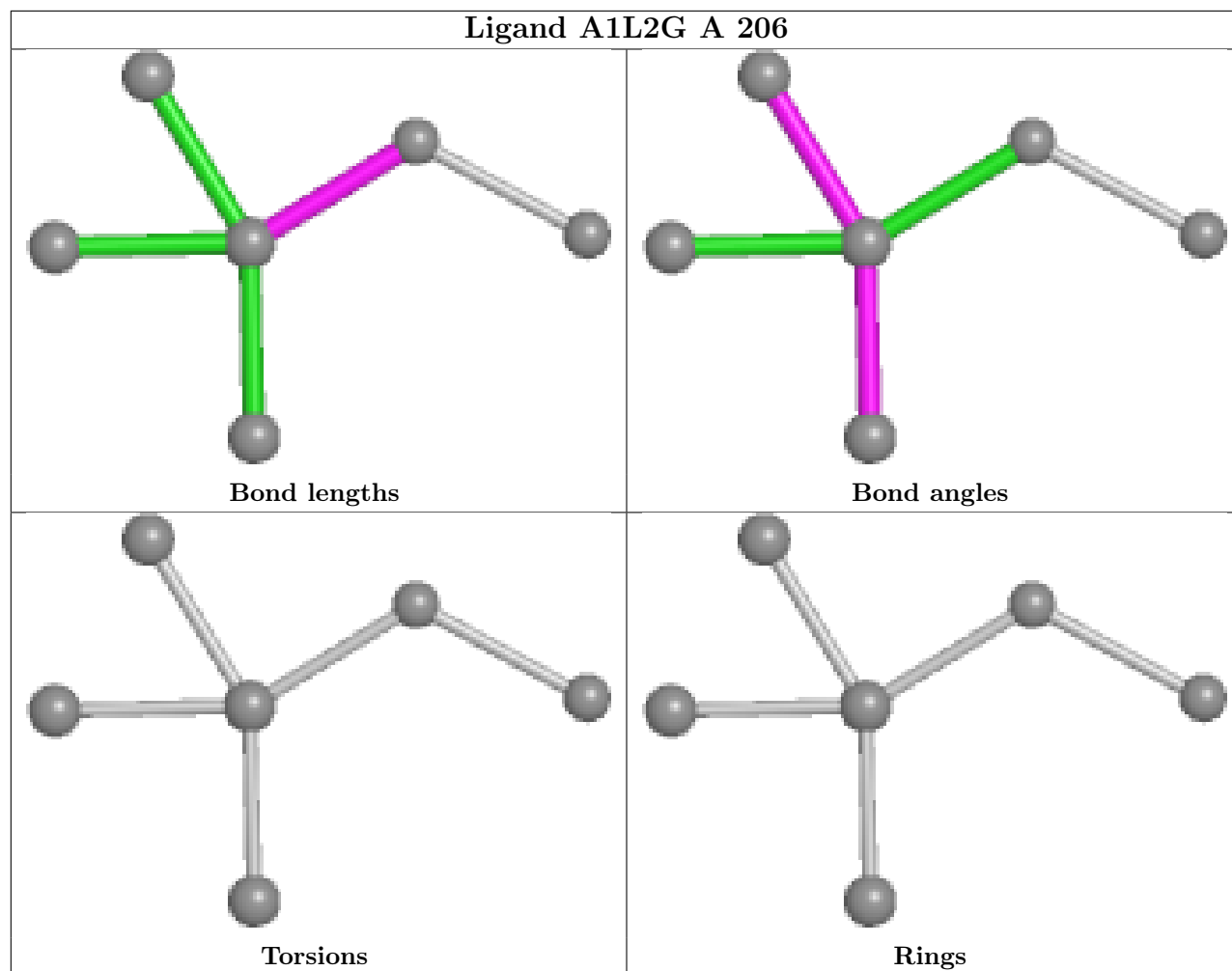
11 monomers are involved in 20 short contacts:

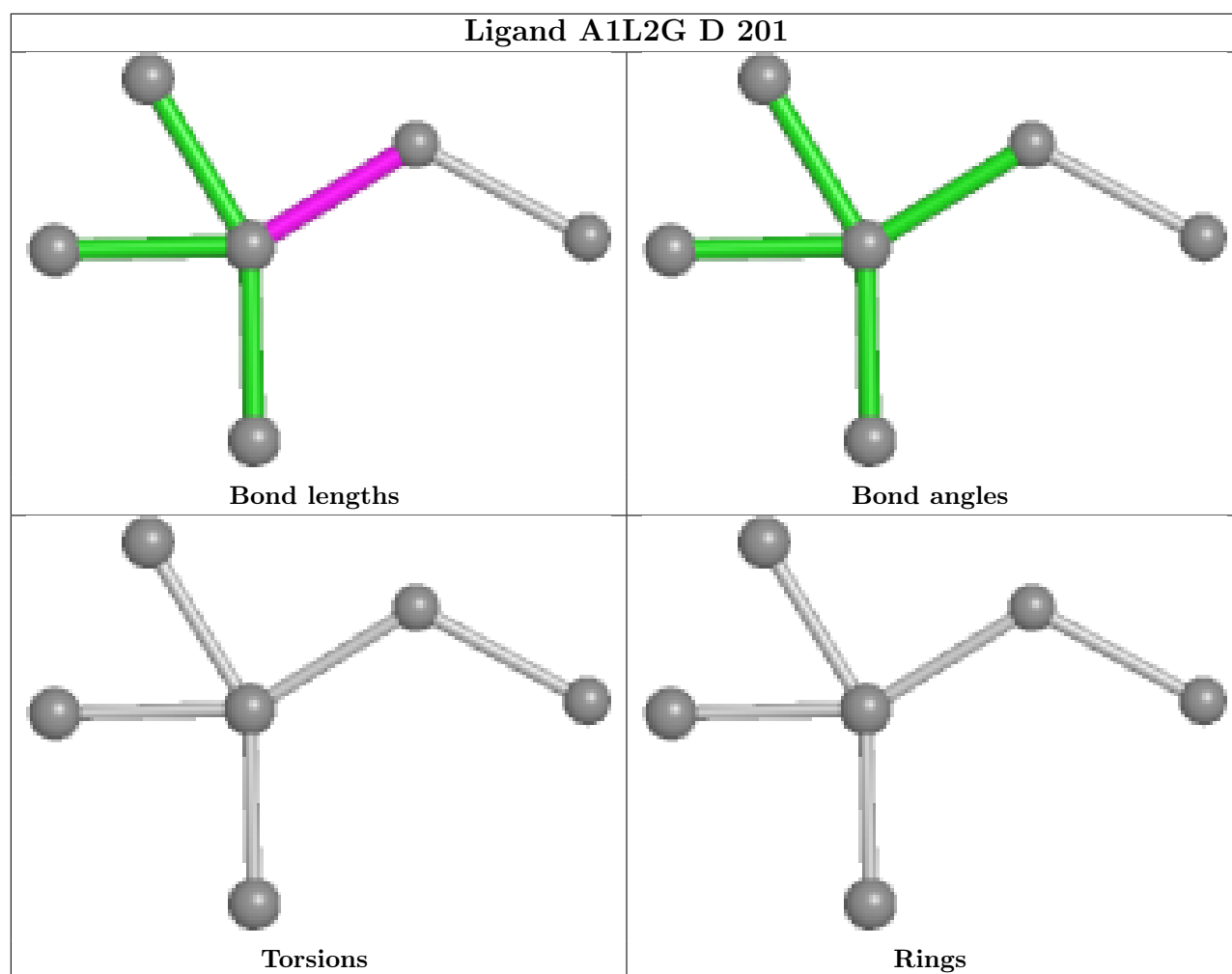
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	203	DTU	1	0
2	A	204	PG4	1	0
2	B	201	PG4	2	0
2	A	202	PG4	2	0
2	B	202	PG4	1	0
4	C	201	A1L2G	2	0
2	A	203	PG4	4	0
2	B	203	PG4	2	0
4	A	206	A1L2G	3	0
4	D	201	A1L2G	1	0
6	B	205	DTO	1	0

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 [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	149/149 (100%)	-0.50	0 100 100	9, 15, 26, 48	3 (2%)
1	B	149/149 (100%)	-0.57	1 (0%) 84 89	7, 15, 26, 40	2 (1%)
1	C	149/149 (100%)	-0.26	3 (2%) 64 73	10, 19, 41, 62	1 (0%)
1	D	149/149 (100%)	-0.25	2 (1%) 74 82	10, 19, 38, 52	2 (1%)
All	All	596/596 (100%)	-0.40	6 (1%) 79 85	7, 17, 36, 62	8 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	69[A]	SER	3.2
1	D	150	ASP	2.8
1	B	164	ILE	2.8
1	D	148	GLY	2.5
1	C	98	LEU	2.4
1	C	150	ASP	2.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

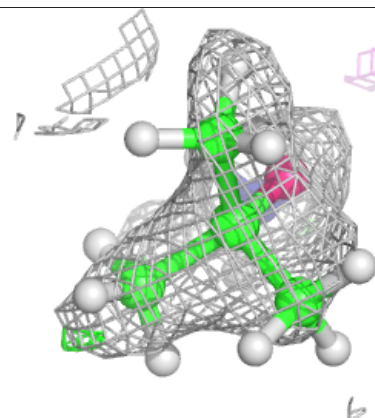
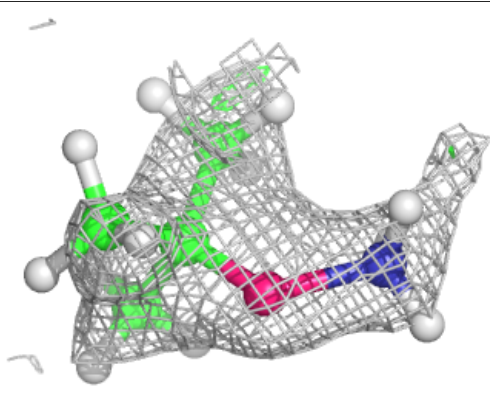
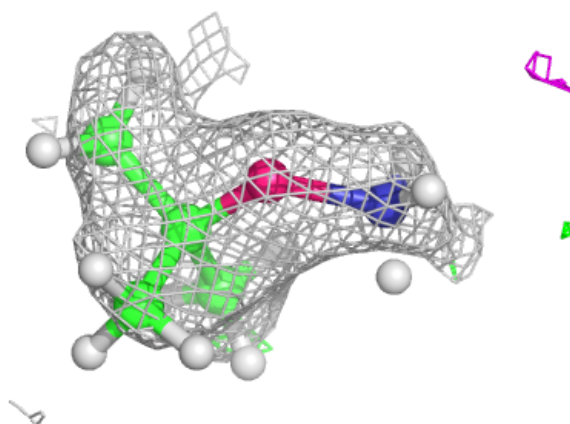
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A1L2G	C	201	6/6	0.84	0.17	40,43,47,48	0
2	PG4	B	202	13/13	0.89	0.13	45,50,53,54	0
2	PG4	A	204	13/13	0.89	0.11	32,37,41,42	0
2	PG4	D	202	13/13	0.90	0.11	37,40,42,45	0
2	PG4	A	203	13/13	0.90	0.11	32,45,50,52	0
2	PG4	A	202	13/13	0.91	0.11	32,35,42,44	0
2	PG4	A	201	13/13	0.91	0.10	33,36,40,41	0
4	A1L2G	D	201	6/6	0.91	0.11	34,36,36,37	0
2	PG4	B	203	13/13	0.93	0.10	29,34,42,43	0
4	A1L2G	A	206	6/6	0.93	0.11	31,35,38,39	0
6	DTO	B	205	8/9	0.93	0.10	27,34,40,46	0
5	IMD	B	204	5/5	0.95	0.08	29,31,32,33	0
2	PG4	B	201	13/13	0.95	0.08	28,31,37,38	0
7	DTU	D	203	8/8	0.95	0.10	39,45,48,49	0
3	PEO	B	206	2/2	0.97	0.06	18,18,20,23	0
3	PEO	A	205	2/2	0.98	0.05	21,21,22,25	0
3	PEO	B	207	2/2	0.98	0.04	20,20,22,22	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.

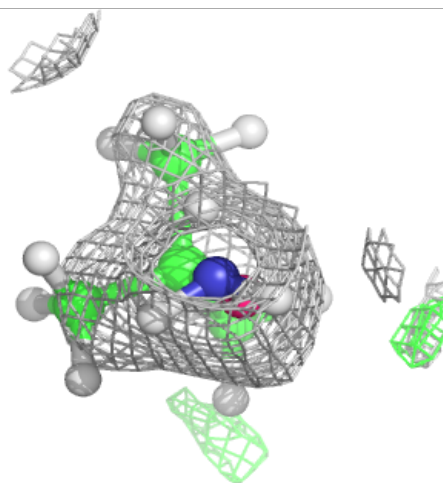
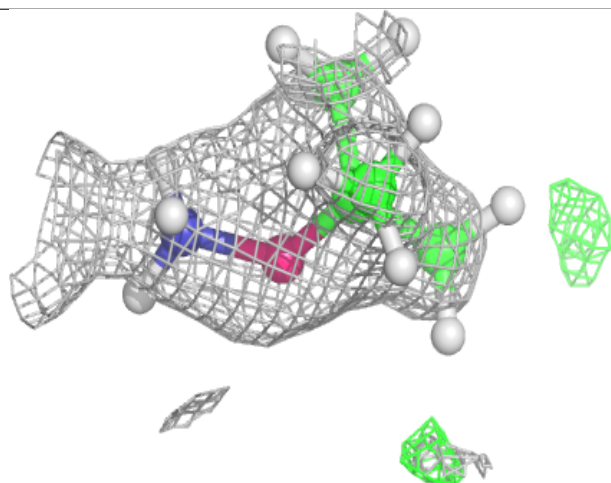
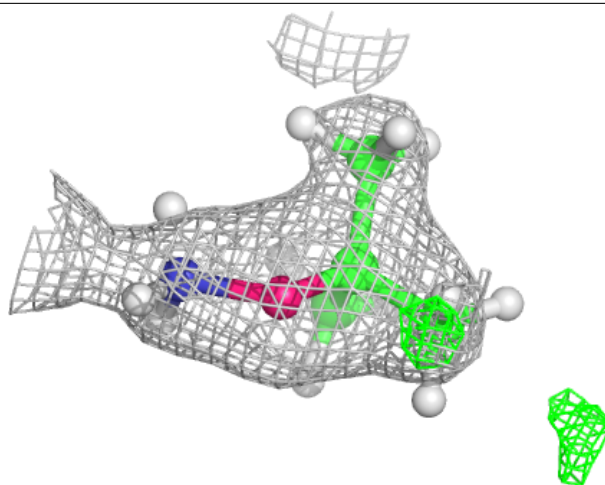
Electron density around A1L2G C 201:

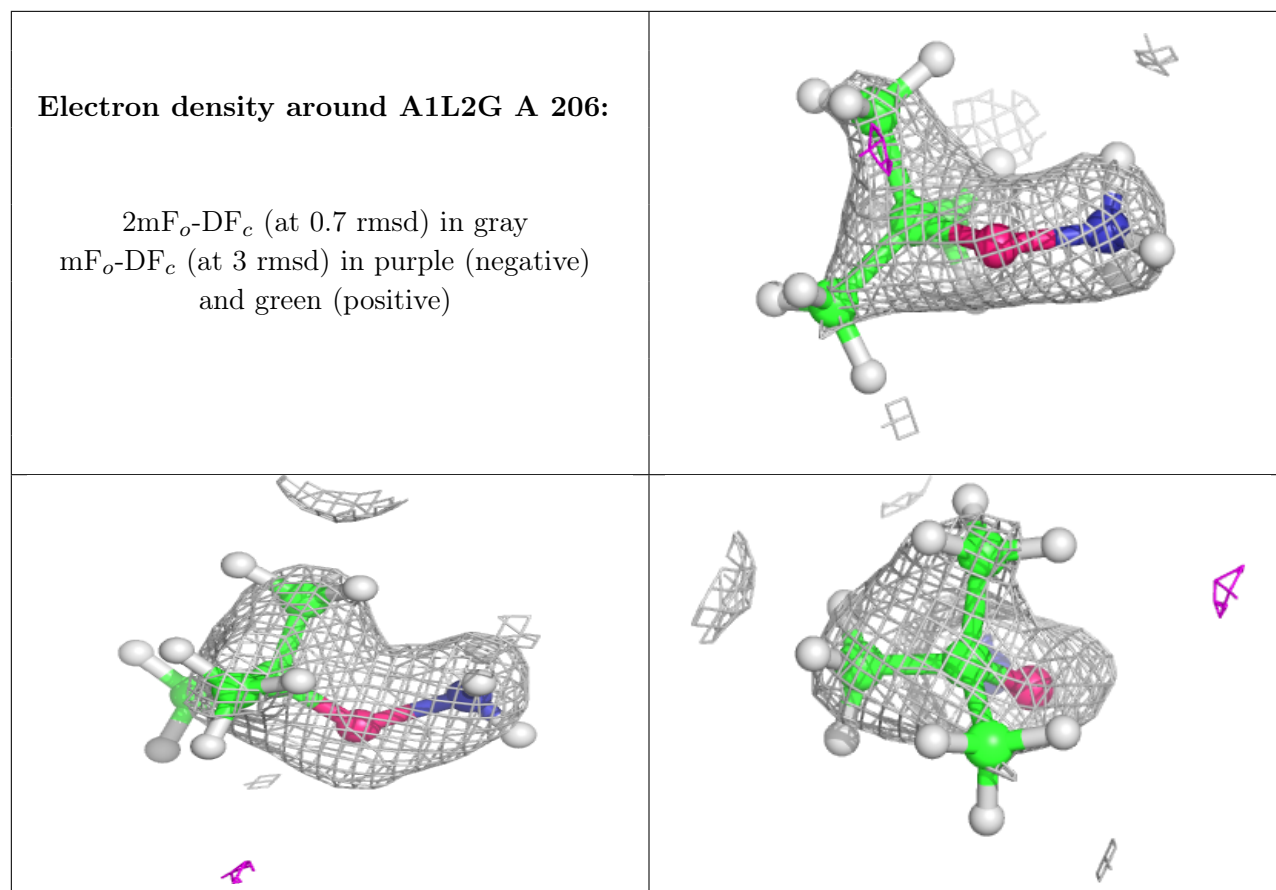
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1L2G D 201:

$2mF_o-DF_c$ (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.