



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:36 PM UTC

PDB ID : 6DWI / pdb_00006dwi
Title : Structure of the 4462 Antibody Fab fragment bound to a Staphylococcus aureus wall teichoic acid analog
Authors : Fong, R.; Lupardus, P.J.
Deposited on : 2018-06-26
Resolution : 2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

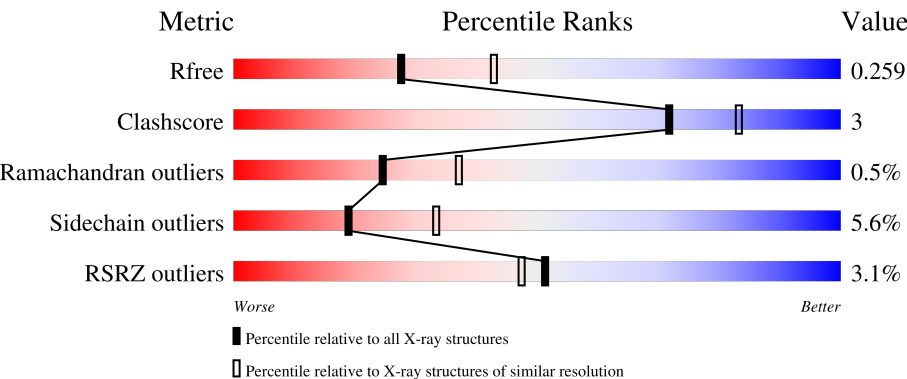
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	% 82%8%9%
1	C	233	8% 72%15%12%
1	E	233	5% 73%13%12%
1	G	233	82%8%9%
1	I	233	% 80%10%9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	233	% 79% 12% 9%
1	M	233	2% 76% 13% 11%
1	O	233	76% 13% 9%
2	B	243	2% 72% 10% 17%
2	D	243	5% 75% 10% 13%
2	F	243	4% 73% 9% 18%
2	H	243	% 74% 12% 13%
2	J	243	4% 79% 9% 12%
2	L	243	7% 72% 13% 13%
2	N	243	% 75% 9% 14%
2	P	243	2% 73% 9% 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26175 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 4462 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1619	1011	278	324	6			
1	C	206	Total	C	N	O	S	0	0	0
			1569	983	266	314	6			
1	E	205	Total	C	N	O	S	0	0	0
			1583	990	271	316	6			
1	G	211	Total	C	N	O	S	0	0	0
			1613	1008	275	324	6			
1	I	211	Total	C	N	O	S	3	0	0
			1613	1008	275	324	6			
1	K	211	Total	C	N	O	S	0	0	0
			1613	1008	275	324	6			
1	M	207	Total	C	N	O	S	0	0	0
			1582	990	272	314	6			
1	O	211	Total	C	N	O	S	0	0	0
			1619	1011	278	324	6			

- Molecule 2 is a protein called 4462 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	202	Total	C	N	O	S	4	0	0
			1523	962	259	295	7			
2	D	212	Total	C	N	O	S	4	0	0
			1579	993	270	309	7			
2	F	200	Total	C	N	O	S	4	1	0
			1508	952	256	293	7			
2	H	212	Total	C	N	O	S	0	1	0
			1586	998	270	311	7			
2	J	214	Total	C	N	O	S	0	1	0
			1601	1007	273	314	7			
2	L	211	Total	C	N	O	S	0	0	0
			1578	994	269	308	7			

Continued on next page...

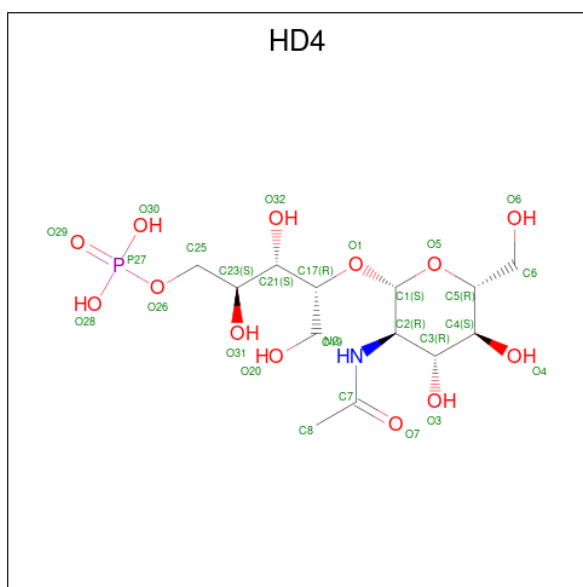
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	209	Total	C	N	O	S	0	0	0
			1571	989	267	308	7			
2	P	204	Total	C	N	O	S	0	0	0
			1537	969	261	300	7			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	O	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 4-O-[2-acetamido-2-deoxy-beta-D-glucopyranosyl]-1-O-phosphono-D-ribose (CCD ID: HD4) (formula: C₁₃H₂₆NO₁₃P).



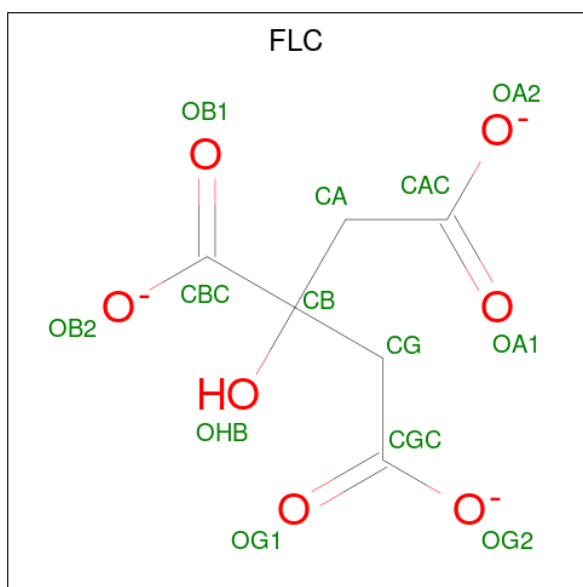
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			28	13	1	13	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			28	13	1	13	1		
4	J	1	Total	C	N	O	P	0	0
			28	13	1	13	1		
4	L	1	Total	C	N	O	P	0	0
			28	13	1	13	1		

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	44	Total	O	0	0
			44	44		
7	B	81	Total	O	0	0
			81	81		
7	C	24	Total	O	0	0
			24	24		
7	D	39	Total	O	0	0
			39	39		
7	E	9	Total	O	0	0
			9	9		
7	F	36	Total	O	0	0
			36	36		
7	G	65	Total	O	0	0
			65	65		
7	H	74	Total	O	0	0
			74	74		
7	I	66	Total	O	0	0
			66	66		
7	J	64	Total	O	0	0
			64	64		

Continued on next page...

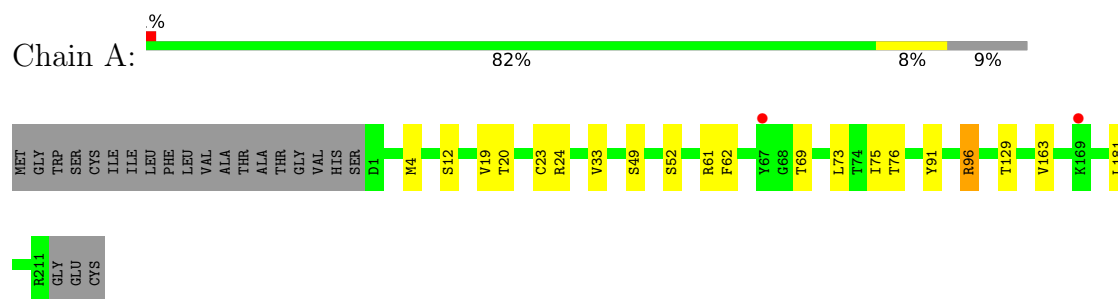
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	32	Total 32	O 32	0	0
7	L	33	Total 33	O 33	0	0
7	M	26	Total 26	O 26	0	0
7	N	42	Total 42	O 42	0	0
7	O	28	Total 28	O 28	0	0
7	P	75	Total 75	O 75	0	0

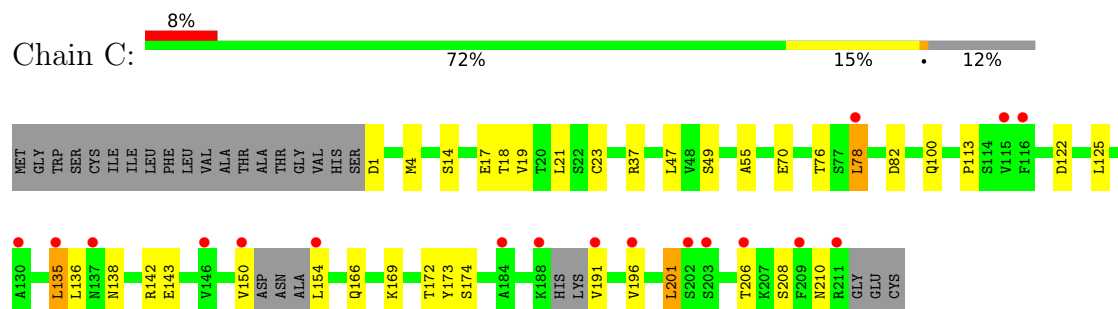
3 Residue-property plots [i](#)

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.

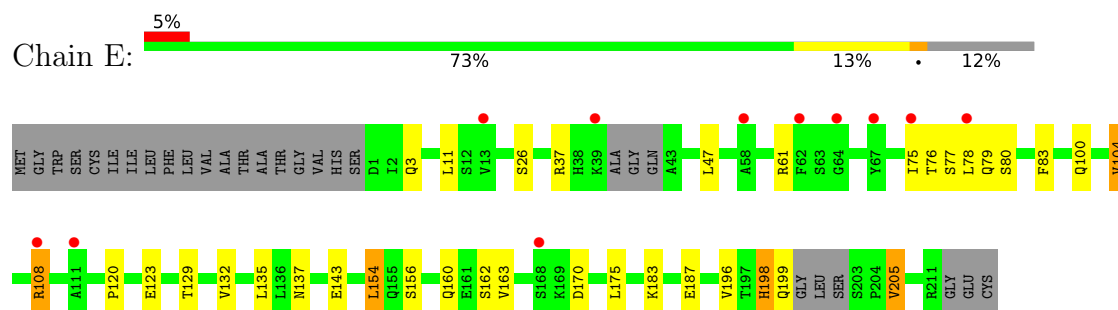
- Molecule 1: 4462 Fab Light Chain



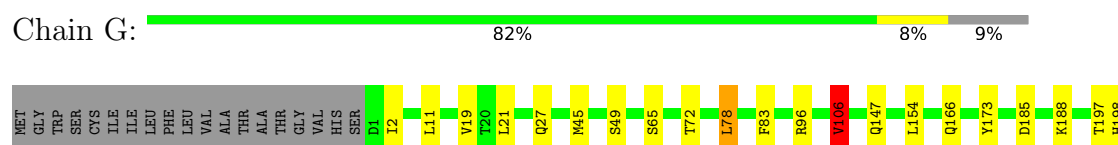
- Molecule 1: 4462 Fab Light Chain

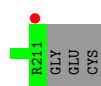


- Molecule 1: 4462 Fab Light Chain

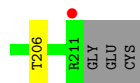
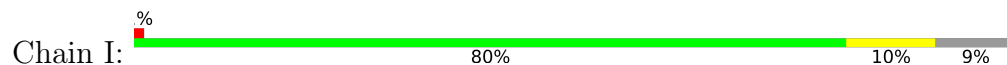


- Molecule 1: 4462 Fab Light Chain

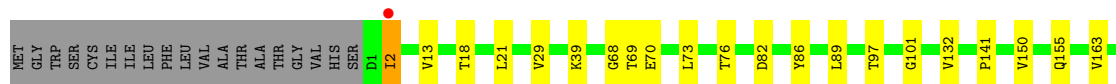
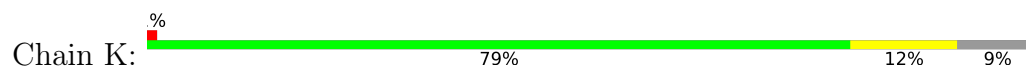




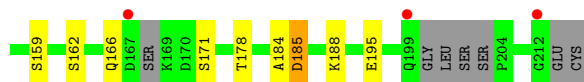
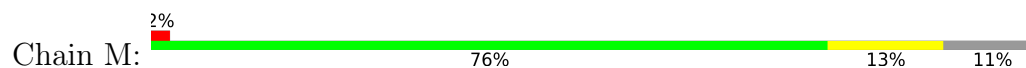
• Molecule 1: 4462 Fab Light Chain



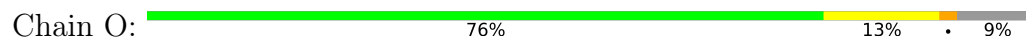
• Molecule 1: 4462 Fab Light Chain



• Molecule 1: 4462 Fab Light Chain

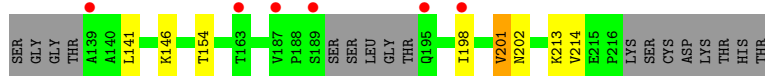


• Molecule 1: 4462 Fab Light Chain

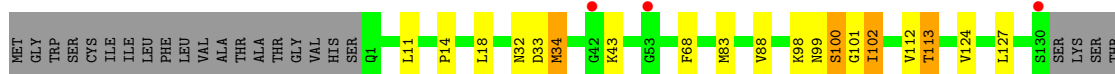
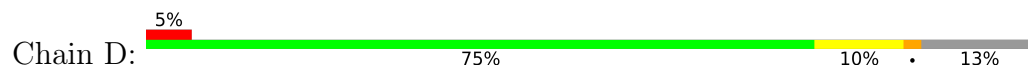


• Molecule 2: 4462 Fab Heavy chain

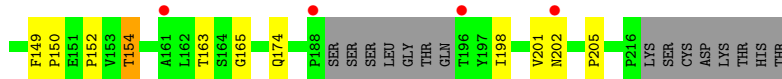
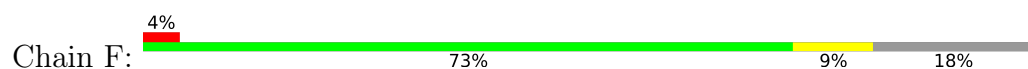




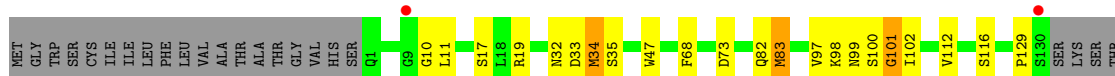
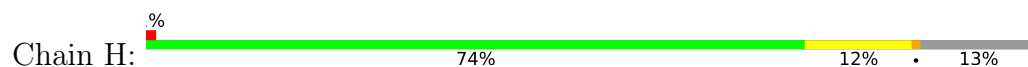
• Molecule 2: 4462 Fab Heavy chain



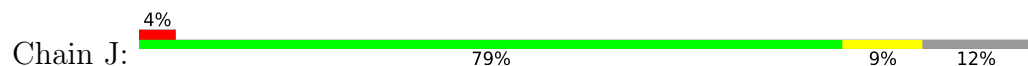
• Molecule 2: 4462 Fab Heavy chain



• Molecule 2: 4462 Fab Heavy chain

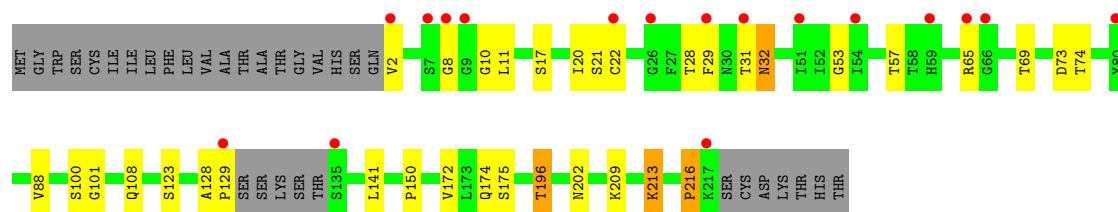


• Molecule 2: 4462 Fab Heavy chain



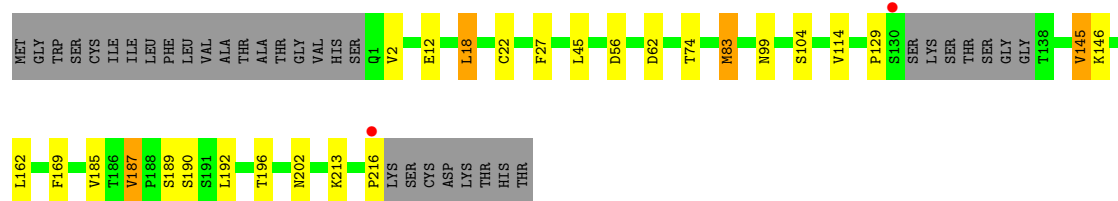
- Molecule 2: 4462 Fab Heavy chain

Chain L: 



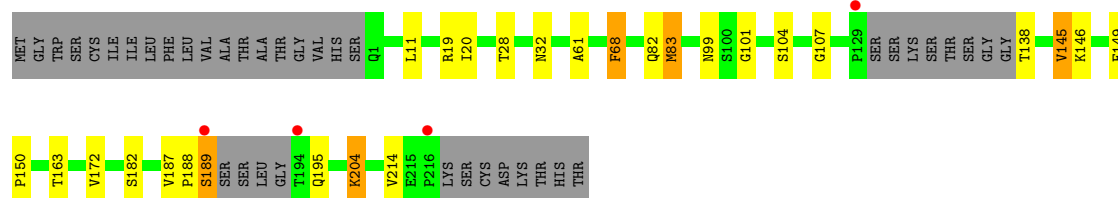
- Molecule 2: 4462 Fab Heavy chain

Chain N: 



- Molecule 2: 4462 Fab Heavy chain

Chain P: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.57Å 114.10Å 128.30Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	29.89 – 2.39 29.89 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.89-2.39) 99.0 (29.89-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.203 , 0.249 0.207 , 0.259	Depositor DCC
R_{free} test set	6979 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for l,k,-h 0.037 for h,-k,-l 0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26175	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: HD4, CL, GOL, FLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.82	0/1654	1.16	1/2249 (0.0%)
1	C	0.82	0/1601	1.21	3/2176 (0.1%)
1	E	0.78	0/1616	1.20	3/2195 (0.1%)
1	G	0.84	0/1648	1.21	3/2242 (0.1%)
1	I	0.86	0/1648	1.19	0/2242
1	K	0.79	0/1648	1.21	2/2242 (0.1%)
1	M	0.81	0/1615	1.17	2/2194 (0.1%)
1	O	0.86	1/1654 (0.1%)	1.20	1/2249 (0.0%)
2	B	0.86	0/1558	1.22	5/2122 (0.2%)
2	D	0.89	2/1615 (0.1%)	1.22	5/2201 (0.2%)
2	F	0.80	0/1545	1.21	5/2106 (0.2%)
2	H	0.92	3/1625 (0.2%)	1.24	7/2214 (0.3%)
2	J	0.89	0/1640	1.23	6/2234 (0.3%)
2	L	0.84	0/1614	1.23	11/2198 (0.5%)
2	N	0.87	1/1607 (0.1%)	1.27	4/2190 (0.2%)
2	P	0.91	1/1572 (0.1%)	1.22	5/2143 (0.2%)
All	All	0.85	8/25860 (0.0%)	1.21	63/35197 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	4	MET	SD-CE	-8.67	1.57	1.79
2	H	34	MET	SD-CE	-7.74	1.60	1.79
2	D	34	MET	SD-CE	-6.78	1.62	1.79
2	P	83	MET	SD-CE	-6.71	1.62	1.79
2	H	83	MET	SD-CE	-6.56	1.63	1.79
2	N	83	MET	SD-CE	-5.45	1.66	1.79
2	H	100	SER	CA-C	5.32	1.60	1.52
2	D	187	VAL	CA-C	5.30	1.57	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	187	VAL	N-CA-CB	-7.48	103.64	111.87
2	H	68	PHE	CA-CB-CG	7.10	120.90	113.80
2	H	101	GLY	CA-C-N	6.84	131.44	122.95
2	H	101	GLY	C-N-CA	6.84	131.44	122.95
2	P	68	PHE	CA-CB-CG	6.51	120.31	113.80
2	H	100	SER	N-CA-C	6.32	121.18	112.90
2	L	10	GLY	N-CA-C	6.28	120.98	110.56
2	L	128	ALA	N-CA-C	6.12	118.42	110.40
2	N	145	VAL	CB-CA-C	6.04	119.38	111.53
2	H	73	ASP	CA-C-N	5.90	128.78	120.28
2	H	73	ASP	C-N-CA	5.90	128.78	120.28
1	E	104	VAL	N-CA-CB	5.90	118.11	111.21
2	D	68	PHE	CA-CB-CG	5.89	119.69	113.80
2	B	68	PHE	CA-CB-CG	5.87	119.67	113.80
2	D	100	SER	N-CA-C	5.82	120.50	113.41
2	J	135	SER	N-CA-C	-5.69	106.26	113.43
1	C	70	GLU	CB-CG-CD	5.69	122.27	112.60
2	L	53	GLY	N-CA-C	5.67	120.69	114.40
2	J	8	GLY	N-CA-C	-5.66	102.53	112.77
1	O	167	ASP	CA-CB-CG	5.64	118.24	112.60
2	J	29	PHE	CA-C-N	5.64	128.61	120.38
2	J	29	PHE	C-N-CA	5.64	128.61	120.38
2	B	128	ALA	N-CA-C	5.63	116.92	109.93
2	F	90	ASP	CA-CB-CG	5.63	118.23	112.60
2	B	96	CYS	N-CA-C	-5.62	101.31	110.20
2	P	146	LYS	N-CA-C	5.60	118.53	109.40
2	J	73	ASP	CA-C-N	5.58	127.76	120.28
2	J	73	ASP	C-N-CA	5.58	127.76	120.28
2	P	107	GLY	N-CA-C	-5.54	105.17	112.82
2	L	216	PRO	CA-C-N	5.48	131.56	121.70
2	L	216	PRO	C-N-CA	5.48	131.56	121.70
1	M	185	ASP	CA-CB-CG	5.43	118.03	112.60
1	G	106	VAL	N-CA-CB	5.42	117.02	110.95
2	B	90	ASP	CA-CB-CG	5.37	117.97	112.60
2	F	62	ASP	CA-C-N	5.37	127.47	120.28
2	F	62	ASP	C-N-CA	5.37	127.47	120.28
2	N	189	SER	CA-C-N	5.33	127.42	120.28
2	N	189	SER	C-N-CA	5.33	127.42	120.28
1	A	96	ARG	N-CA-C	-5.33	102.39	110.28
1	K	141	PRO	CA-C-N	5.28	127.89	120.28
1	K	141	PRO	C-N-CA	5.28	127.89	120.28
2	L	174	GLN	CA-C-N	5.25	127.58	120.38
2	L	174	GLN	C-N-CA	5.25	127.58	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	137	ASN	N-CA-C	5.21	117.47	109.07
2	L	31	THR	CA-C-N	5.18	128.07	120.71
2	L	31	THR	C-N-CA	5.18	128.07	120.71
2	F	165	GLY	CA-C-N	5.16	127.50	120.63
2	F	165	GLY	C-N-CA	5.16	127.50	120.63
2	H	10	GLY	N-CA-C	5.14	116.97	110.38
2	D	127	LEU	CA-C-N	5.11	128.13	120.83
2	D	127	LEU	C-N-CA	5.11	128.13	120.83
2	L	73	ASP	CA-C-N	5.09	127.60	120.28
2	L	73	ASP	C-N-CA	5.09	127.60	120.28
2	B	90	ASP	N-CA-C	-5.07	107.10	113.28
2	D	102	ILE	N-CA-CB	-5.04	107.17	112.06
2	P	61	ALA	N-CA-C	-5.04	103.03	110.48
1	C	55	ALA	CA-C-N	5.02	127.31	120.54
1	C	55	ALA	C-N-CA	5.02	127.31	120.54
1	E	198	HIS	CA-C-N	5.02	130.73	121.70
1	E	198	HIS	C-N-CA	5.02	130.73	121.70
1	G	198	HIS	CA-C-N	5.00	127.29	120.54
1	G	198	HIS	C-N-CA	5.00	127.29	120.54
2	P	145	VAL	CB-CA-C	5.00	118.66	111.81

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	1619	0	1577	6	0
1	C	1569	0	1516	16	0
1	E	1583	0	1540	18	0
1	G	1613	0	1566	9	0
1	I	1613	0	1566	9	0
1	K	1613	0	1566	11	0
1	M	1582	0	1531	15	0
1	O	1619	0	1577	19	0
2	B	1523	0	1489	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1579	0	1532	13	0
2	F	1508	0	1463	9	0
2	H	1586	0	1549	15	0
2	J	1601	0	1564	5	0
2	L	1578	0	1544	9	0
2	N	1571	0	1539	6	0
2	P	1537	0	1498	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	1	0
3	G	1	0	0	0	0
3	O	1	0	0	0	0
4	D	28	0	0	0	0
4	H	28	0	0	1	0
4	J	28	0	0	0	0
4	L	28	0	0	0	0
5	G	13	0	5	0	0
6	H	6	0	8	0	0
6	J	6	0	8	0	0
7	A	44	0	0	0	0
7	B	81	0	0	0	0
7	C	24	0	0	1	0
7	D	39	0	0	0	0
7	E	9	0	0	0	0
7	F	36	0	0	0	0
7	G	65	0	0	1	0
7	H	74	0	0	0	0
7	I	66	0	0	0	0
7	J	64	0	0	0	0
7	K	32	0	0	1	0
7	L	33	0	0	0	0
7	M	26	0	0	0	0
7	N	42	0	0	0	0
7	O	28	0	0	0	0
7	P	75	0	0	0	0
All	All	26175	0	24638	165	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 3.

All (165) 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)
2:B:47:TRP:HE1	2:B:50:THR:HG22	1.35	0.90
2:H:33:ASP:O	2:H:34:MET:HE2	1.85	0.76
1:O:13:VAL:HG21	1:O:19:VAL:HG11	1.71	0.71
1:E:198:HIS:CG	1:E:199:GLN:H	2.09	0.70
1:O:29:VAL:HG11	1:O:90:GLN:HG2	1.72	0.70
2:L:11:LEU:HD21	2:L:150:PRO:HG3	1.74	0.70
2:D:11:LEU:HD21	2:D:150:PRO:HG3	1.77	0.66
2:L:129:PRO:HG2	2:L:216:PRO:HB3	1.77	0.66
1:C:17:GLU:HG2	1:E:154:LEU:HB3	1.80	0.64
7:G:455:HOH:O	2:H:167:HIS:HD2	1.81	0.63
1:K:18:THR:HG23	1:K:76:THR:HA	1.81	0.63
2:F:154:THR:HB	2:F:202:ASN:HB3	1.81	0.63
2:D:88:VAL:HG22	2:L:196:THR:HG23	1.81	0.62
1:I:2:ILE:O	1:I:97:THR:HG21	2.00	0.62
1:M:185:ASP:HA	1:M:188:LYS:HE2	1.84	0.60
1:O:29:VAL:HG11	1:O:90:GLN:CG	2.31	0.60
2:D:14:PRO:HB2	2:L:213:LYS:HE3	1.83	0.60
1:M:29:VAL:HG11	1:M:90:GLN:HG3	1.82	0.60
1:E:120:PRO:HD3	1:E:132:VAL:HG22	1.85	0.59
1:E:61:ARG:NH1	1:E:79:GLN:HB2	2.18	0.58
2:D:33:ASP:O	2:D:34:MET:HE2	2.04	0.58
2:D:11:LEU:HD23	2:D:113:THR:HB	1.86	0.58
2:B:154:THR:O	2:B:201:VAL:HA	2.04	0.57
2:B:97:VAL:HG21	2:B:103:TYR:HB3	1.85	0.57
1:G:78:LEU:HD23	1:G:83:PHE:CZ	2.39	0.57
1:C:172:THR:HG23	7:C:421:HOH:O	2.04	0.57
2:H:34:MET:HE1	2:H:98:LYS:HG3	1.86	0.56
1:O:2:ILE:HG22	1:O:4:MET:CE	2.35	0.56
1:O:123:GLU:HA	1:O:126:LYS:HE2	1.86	0.56
1:C:4:MET:HE3	1:C:23:CYS:SG	2.45	0.56
2:H:147:ASP:HB3	2:H:178:LEU:HD13	1.89	0.55
2:B:97:VAL:CG2	2:B:103:TYR:HB3	2.36	0.54
1:O:2:ILE:HD13	1:O:27:GLN:HB2	1.90	0.54
1:K:69:THR:HG23	1:K:70:GLU:HG2	1.90	0.53
2:H:35:SER:HB2	2:H:97:VAL:HG23	1.90	0.53
1:G:83:PHE:CG	1:G:106:VAL:HG22	2.44	0.52
1:O:37:ARG:HB2	1:O:47:LEU:HD11	1.90	0.52
2:B:47:TRP:HE1	2:B:50:THR:CG2	2.17	0.52
1:O:33:VAL:HA	1:O:89:LEU:O	2.10	0.51
1:A:4:MET:HE3	1:A:23:CYS:SG	2.50	0.51
1:M:61:ARG:HB2	1:M:76:THR:O	2.11	0.51
1:M:29:VAL:HG11	1:M:90:GLN:CG	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:108:ARG:HH12	1:I:111:ALA:HB2	1.76	0.50
2:P:188:PRO:O	2:P:189:SER:HB2	2.12	0.50
1:C:49:SER:HB2	2:D:102:ILE:HG12	1.94	0.49
2:P:187:VAL:HB	2:P:188:PRO:HD2	1.95	0.49
1:E:61:ARG:HH12	1:E:79:GLN:HB2	1.77	0.49
1:K:21:LEU:HD12	1:K:73:LEU:HD23	1.94	0.49
2:B:47:TRP:NE1	2:B:50:THR:HG22	2.16	0.49
2:F:154:THR:O	2:F:201:VAL:HA	2.13	0.48
2:F:37:VAL:HG13	2:F:95:TYR:HB2	1.95	0.48
2:F:152:PRO:HA	3:F:301:CL:CL	2.51	0.48
2:L:8:GLY:O	2:L:20:ILE:HG22	2.13	0.48
1:G:185:ASP:HA	1:G:188:LYS:HD3	1.96	0.48
2:H:116:SER:HB3	2:J:215:GLU:OE1	2.14	0.48
1:C:18:THR:HG23	1:C:76:THR:HA	1.96	0.47
1:G:49:SER:HB2	2:H:102:ILE:HG12	1.96	0.47
1:O:59:PRO:HB2	1:O:61:ARG:HG2	1.97	0.47
2:L:29:PHE:HE2	2:L:74:THR:HA	1.78	0.47
2:B:76:LYS:HB2	2:B:78:MET:HG2	1.96	0.47
1:C:19:VAL:HG12	1:E:156:SER:HB3	1.95	0.47
2:L:129:PRO:HD3	2:L:141:LEU:HD23	1.97	0.47
2:P:204:LYS:H	2:P:204:LYS:NZ	2.12	0.47
2:F:150:PRO:HD2	2:F:205:PRO:CB	2.45	0.46
2:D:100:SER:N	2:D:101:GLY:HA3	2.29	0.46
1:C:78:LEU:HG	1:C:82:ASP:HB2	1.96	0.46
1:C:19:VAL:HG22	1:C:78:LEU:HD13	1.98	0.46
1:A:62:PHE:CE1	1:A:75:ILE:HG12	2.51	0.46
1:C:169:LYS:HE2	1:M:95:PRO:HD3	1.97	0.46
1:E:135:LEU:HD21	1:E:137:ASN:HD22	1.81	0.46
1:O:4:MET:SD	1:O:90:GLN:HB2	2.56	0.46
1:E:160:GLN:HE22	2:F:174:GLN:HG2	1.80	0.46
1:K:166:GLN:HG3	1:K:173:TYR:CZ	2.51	0.45
1:M:162:SER:OG	2:N:169:PHE:HB3	2.15	0.45
2:N:162:LEU:HD21	2:N:185:VAL:HG21	1.98	0.45
1:G:96:ARG:HB2	2:H:47:TRP:CG	2.52	0.45
1:O:13:VAL:HG11	1:O:19:VAL:CG1	2.46	0.45
1:E:183:LYS:O	1:E:187:GLU:HG2	2.15	0.45
1:M:122:ASP:O	1:M:126:LYS:HG2	2.15	0.45
1:M:166:GLN:HG2	1:M:171:SER:HA	1.98	0.45
1:E:108:ARG:HH21	1:E:170:ASP:HB2	1.81	0.45
2:H:35:SER:HB2	2:H:97:VAL:CG2	2.47	0.45
1:M:33:VAL:HA	1:M:89:LEU:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:192:TYR:O	1:O:208:SER:HA	2.17	0.45
1:G:21:LEU:O	1:G:72:THR:HA	2.15	0.45
1:A:20:THR:HA	1:A:73:LEU:O	2.17	0.44
2:B:198:ILE:HG22	2:B:213:LYS:HB3	2.00	0.44
1:E:3:GLN:HB2	1:E:26:SER:HB3	1.99	0.44
1:M:5:THR:HG23	1:M:24:ARG:HB3	1.99	0.44
1:G:2:ILE:HD12	1:G:27:GLN:HB2	2.00	0.44
1:I:90:GLN:HE22	1:I:93:THR:H	1.66	0.44
1:O:13:VAL:HG11	1:O:19:VAL:HG12	2.00	0.44
1:E:198:HIS:CG	1:E:199:GLN:N	2.79	0.44
1:K:163:VAL:HG22	1:K:175:LEU:HD12	1.99	0.44
1:M:4:MET:HE3	1:M:23:CYS:SG	2.58	0.44
1:M:159:SER:HA	1:M:178:THR:O	2.18	0.44
1:O:25:ALA:HB3	1:O:69:THR:HA	1.99	0.44
1:O:29:VAL:CG1	1:O:90:GLN:HG2	2.45	0.44
2:F:37:VAL:HG11	2:F:106:TRP:CZ3	2.53	0.44
1:E:143:GLU:O	1:E:198:HIS:HD2	2.01	0.43
1:I:37:ARG:HB2	1:I:47:LEU:HD11	1.98	0.43
2:L:202:ASN:OD1	2:L:209:LYS:HG2	2.18	0.43
2:J:35:SER:HB2	2:J:97:VAL:HG23	1.99	0.43
2:N:129:PRO:HG2	2:N:216:PRO:HG3	2.00	0.43
2:P:11:LEU:HD11	2:P:149:PHE:CZ	2.53	0.43
2:D:34:MET:HE1	2:D:98:LYS:HG3	2.00	0.43
2:D:153:VAL:HG23	2:D:203:HIS:HB2	2.01	0.43
1:C:14:SER:O	1:C:17:GLU:HB2	2.19	0.43
1:G:19:VAL:HG12	1:G:78:LEU:HD13	2.00	0.43
1:C:174:SER:O	2:D:169:PHE:HE1	2.02	0.43
2:H:83:MET:HE1	2:H:112:VAL:HG21	1.99	0.43
1:M:2:ILE:HD12	1:M:27:GLN:HB2	2.01	0.43
2:J:122:PRO:HB3	2:J:148:TYR:HB3	2.00	0.43
1:C:135:LEU:HD21	2:D:184:VAL:HG21	2.00	0.42
1:A:61:ARG:HB2	1:A:76:THR:O	2.19	0.42
2:N:12:GLU:O	2:N:114:VAL:HA	2.19	0.42
1:O:161:GLU:HG2	1:O:175:LEU:HD21	2.00	0.42
1:I:90:GLN:OE1	1:I:97:THR:HG22	2.19	0.42
2:P:11:LEU:HD11	2:P:149:PHE:HZ	1.85	0.42
1:I:90:GLN:HG3	1:I:97:THR:HG23	2.01	0.42
2:P:11:LEU:HD22	2:P:150:PRO:HG3	2.01	0.42
1:E:37:ARG:HB2	1:E:47:LEU:HD11	2.02	0.42
2:N:18:LEU:HG	2:N:83:MET:HE3	2.01	0.42
1:M:184:ALA:O	1:M:188:LYS:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:MET:HE1	2:D:112:VAL:HG21	2.01	0.42
2:H:202:ASN:ND2	2:H:209:LYS:HD2	2.35	0.42
2:J:91:THR:HG23	2:J:113:THR:HA	2.02	0.42
1:K:167:ASP:O	1:K:171:SER:HA	2.20	0.42
1:E:61:ARG:HB2	1:E:76:THR:O	2.20	0.42
1:K:89:LEU:HD12	1:K:97:THR:O	2.20	0.42
1:O:85:VAL:HG22	1:O:103:LYS:HG3	2.01	0.42
1:C:113:PRO:HD2	1:C:201:LEU:HD13	2.02	0.41
2:B:5:GLN:O	2:B:22:CYS:HA	2.20	0.41
1:M:37:ARG:HB3	1:M:47:LEU:HD11	2.02	0.41
1:K:82:ASP:HA	7:K:306:HOH:O	2.20	0.41
1:O:86:TYR:O	1:O:101:GLY:HA2	2.20	0.41
1:E:196:VAL:HB	1:E:205:VAL:HG13	2.02	0.41
1:I:120:PRO:HD3	1:I:132:VAL:HG22	2.02	0.41
1:K:86:TYR:O	1:K:101:GLY:HA2	2.21	0.41
1:O:145:LYS:HB3	1:O:197:THR:HB	2.03	0.41
2:D:124:VAL:HA	2:D:144:LEU:O	2.21	0.41
2:H:11:LEU:HD11	2:H:149:PHE:HE2	1.86	0.41
2:P:68:PHE:HA	2:P:82:GLN:O	2.20	0.41
2:B:35:SER:OG	2:B:50:THR:HB	2.21	0.41
2:H:19:ARG:HB2	2:H:82:GLN:OE1	2.21	0.41
2:H:101:GLY:CA	4:H:301:HD4:O7	2.69	0.41
1:K:2:ILE:HD13	1:K:29:VAL:HG12	2.03	0.41
2:L:28:THR:O	2:L:32:ASN:HB2	2.21	0.41
1:C:37:ARG:HB2	1:C:47:LEU:HD11	2.03	0.41
1:G:166:GLN:HG3	1:G:173:TYR:CZ	2.55	0.40
1:I:3:GLN:HB2	1:I:26:SER:HB3	2.04	0.40
2:J:83:MET:HB3	2:J:86:LEU:HD21	2.03	0.40
1:K:150:VAL:HG12	1:K:155:GLN:NE2	2.36	0.40
2:P:20:ILE:HG12	2:P:83:MET:HE2	2.03	0.40
1:A:24:ARG:HA	1:A:69:THR:O	2.21	0.40
2:F:11:LEU:HD11	2:F:149:PHE:CZ	2.56	0.40
2:H:202:ASN:HD21	2:H:209:LYS:HD2	1.86	0.40
1:I:90:GLN:NE2	1:I:92:ASN:H	2.20	0.40
2:N:2:VAL:HG13	2:N:27:PHE:CD1	2.57	0.40
1:A:91:TYR:HA	1:A:96:ARG:HD2	2.04	0.40
1:C:166:GLN:HG3	1:C:173:TYR:CE1	2.57	0.40
1:E:83:PHE:HA	1:E:104:VAL:HG23	2.03	0.40
2:F:2:VAL:HG13	2:F:27:PHE:HD2	1.87	0.40
1:C:150:VAL:HA	1:C:191:VAL:O	2.21	0.40
1:E:163:VAL:HG22	1:E:175:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/233 (90%)	202 (97%)	7 (3%)	0	100	100
1	C	200/233 (86%)	189 (94%)	9 (4%)	2 (1%)	12	20
1	E	199/233 (85%)	188 (94%)	9 (4%)	2 (1%)	12	20
1	G	209/233 (90%)	203 (97%)	6 (3%)	0	100	100
1	I	209/233 (90%)	201 (96%)	8 (4%)	0	100	100
1	K	209/233 (90%)	200 (96%)	8 (4%)	1 (0%)	24	37
1	M	201/233 (86%)	191 (95%)	10 (5%)	0	100	100
1	O	209/233 (90%)	203 (97%)	6 (3%)	0	100	100
2	B	196/243 (81%)	193 (98%)	2 (1%)	1 (0%)	24	37
2	D	208/243 (86%)	199 (96%)	8 (4%)	1 (0%)	24	37
2	F	195/243 (80%)	187 (96%)	8 (4%)	0	100	100
2	H	209/243 (86%)	202 (97%)	5 (2%)	2 (1%)	12	20
2	J	211/243 (87%)	206 (98%)	3 (1%)	2 (1%)	14	22
2	L	207/243 (85%)	196 (95%)	9 (4%)	2 (1%)	12	20
2	N	205/243 (84%)	199 (97%)	5 (2%)	1 (0%)	24	37
2	P	198/243 (82%)	192 (97%)	4 (2%)	2 (1%)	12	20
All	All	3274/3808 (86%)	3151 (96%)	107 (3%)	16 (0%)	24	37

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	138	ASN
2	D	99	ASN
2	H	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	129	PRO
2	J	99	ASN
1	K	68	GLY
2	N	99	ASN
2	L	65	ARG
1	E	77	SER
2	L	101	GLY
1	C	143	GLU
1	E	80	SER
2	P	99	ASN
2	B	101	GLY
2	J	101	GLY
2	P	101	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/199 (92%)	174 (96%)	8 (4%)	25	43
1	C	174/199 (87%)	159 (91%)	15 (9%)	10	16
1	E	179/199 (90%)	169 (94%)	10 (6%)	19	33
1	G	181/199 (91%)	173 (96%)	8 (4%)	25	43
1	I	181/199 (91%)	169 (93%)	12 (7%)	15	26
1	K	181/199 (91%)	175 (97%)	6 (3%)	33	55
1	M	175/199 (88%)	170 (97%)	5 (3%)	37	60
1	O	182/199 (92%)	173 (95%)	9 (5%)	22	39
2	B	172/207 (83%)	160 (93%)	12 (7%)	14	24
2	D	176/207 (85%)	167 (95%)	9 (5%)	21	37
2	F	169/207 (82%)	162 (96%)	7 (4%)	27	46
2	H	179/207 (86%)	172 (96%)	7 (4%)	28	48
2	J	181/207 (87%)	172 (95%)	9 (5%)	22	38
2	L	178/207 (86%)	163 (92%)	15 (8%)	10	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	179/207 (86%)	164 (92%)	15 (8%)	10	17
2	P	174/207 (84%)	161 (92%)	13 (8%)	12	21
All	All	2843/3248 (88%)	2683 (94%)	160 (6%)	19	33

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	19	VAL
1	A	33	VAL
1	A	49	SER
1	A	52	SER
1	A	129	THR
1	A	163	VAL
1	A	181	LEU
2	B	1	GLN
2	B	32	ASN
2	B	50	THR
2	B	56	ASP
2	B	76	LYS
2	B	88	VAL
2	B	127	LEU
2	B	141	LEU
2	B	146	LYS
2	B	201	VAL
2	B	202	ASN
2	B	214	VAL
1	C	1	ASP
1	C	21	LEU
1	C	78	LEU
1	C	100	GLN
1	C	122	ASP
1	C	125	LEU
1	C	135	LEU
1	C	136	LEU
1	C	142	ARG
1	C	154	LEU
1	C	196	VAL
1	C	201	LEU
1	C	206	THR
1	C	208	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	210	ASN
2	D	18	LEU
2	D	32	ASN
2	D	43	LYS
2	D	113	THR
2	D	141	LEU
2	D	153	VAL
2	D	182	SER
2	D	186	THR
2	D	196	THR
1	E	11	LEU
1	E	75	ILE
1	E	78	LEU
1	E	100	GLN
1	E	108	ARG
1	E	123	GLU
1	E	129	THR
1	E	154	LEU
1	E	162	SER
1	E	205	VAL
2	F	32	ASN
2	F	56	ASP
2	F	88	VAL
2	F	97	VAL
2	F	154	THR
2	F	163	THR
2	F	198	ILE
1	G	11	LEU
1	G	45	MET
1	G	65	SER
1	G	78	LEU
1	G	106	VAL
1	G	147	GLN
1	G	154	LEU
1	G	197	THR
2	H	17	SER
2	H	32	ASN
2	H	141	LEU
2	H	146	LYS
2	H	153	VAL
2	H	194	THR
2	H	204	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	1	ASP
1	I	10	THR
1	I	13	VAL
1	I	69	THR
1	I	70	GLU
1	I	90	GLN
1	I	154	LEU
1	I	161	GLU
1	I	191	VAL
1	I	197	THR
1	I	202	SER
1	I	206	THR
2	J	11	LEU
2	J	21	SER
2	J	32	ASN
2	J	88	VAL
2	J	134	THR
2	J	153	VAL
2	J	172	VAL
2	J	215	GLU
2	J	217	LYS
1	K	2	ILE
1	K	13	VAL
1	K	39	LYS
1	K	132	VAL
1	K	183	LYS
1	K	188	LYS
2	L	2	VAL
2	L	17	SER
2	L	21	SER
2	L	22	CYS
2	L	32	ASN
2	L	57	THR
2	L	69	THR
2	L	88	VAL
2	L	100	SER
2	L	108	GLN
2	L	123	SER
2	L	172	VAL
2	L	175	SER
2	L	196	THR
2	L	213	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	1	ASP
1	M	42	GLN
1	M	105	GLU
1	M	107	LYS
1	M	195	GLU
2	N	18	LEU
2	N	22	CYS
2	N	45	LEU
2	N	56	ASP
2	N	62	ASP
2	N	74	THR
2	N	104	SER
2	N	145	VAL
2	N	146	LYS
2	N	187	VAL
2	N	190	SER
2	N	192	LEU
2	N	196	THR
2	N	202	ASN
2	N	213	LYS
1	O	2	ILE
1	O	19	VAL
1	O	27	GLN
1	O	78	LEU
1	O	80	SER
1	O	105	GLU
1	O	106	VAL
1	O	143	GLU
1	O	191	VAL
2	P	19	ARG
2	P	28	THR
2	P	32	ASN
2	P	104	SER
2	P	138	THR
2	P	145	VAL
2	P	163	THR
2	P	172	VAL
2	P	182	SER
2	P	189	SER
2	P	195	GLN
2	P	204	LYS
2	P	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
1	C	160	GLN
1	C	199	GLN
2	D	77	ASN
2	D	82	GLN
1	E	3	GLN
1	E	32	ASN
1	E	152	ASN
2	F	82	GLN
2	F	84	ASN
2	F	202	ASN
1	G	3	GLN
1	G	27	GLN
1	G	210	ASN
2	H	13	GLN
2	H	32	ASN
2	H	39	GLN
2	H	77	ASN
2	H	99	ASN
1	I	32	ASN
1	I	160	GLN
1	K	32	ASN
1	K	138	ASN
1	K	147	GLN
1	K	152	ASN
1	K	199	GLN
2	L	5	GLN
2	L	32	ASN
2	L	82	GLN
2	L	84	ASN
2	L	108	GLN
2	L	167	HIS
1	M	32	ASN
1	M	92	ASN
1	M	160	GLN
1	M	210	ASN
2	N	39	GLN
2	N	77	ASN
2	N	99	ASN
2	N	195	GLN
1	O	38	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	79	GLN
1	O	137	ASN
1	O	138	ASN
1	O	147	GLN
1	O	210	ASN
2	P	30	ASN
2	P	32	ASN
2	P	77	ASN
2	P	82	GLN
2	P	99	ASN
2	P	167	HIS

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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	FLC	G	302	-	12,12,12	1.07	0	17,17,17	1.14	1 (5%)
6	GOL	J	302	-	5,5,5	0.17	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HD4	H	301	-	28,28,28	0.99	1 (3%)	38,40,40	1.09	3 (7%)
4	HD4	D	301	-	28,28,28	1.03	1 (3%)	38,40,40	1.08	0
6	GOL	H	302	-	5,5,5	0.12	0	5,5,5	0.19	0
4	HD4	J	301	-	28,28,28	1.12	1 (3%)	38,40,40	1.15	4 (10%)
4	HD4	L	301	-	28,28,28	1.00	1 (3%)	38,40,40	0.93	1 (2%)

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	FLC	G	302	-	-	0/16/16/16	-
6	GOL	J	302	-	-	2/4/4/4	-
4	HD4	H	301	-	-	2/26/46/46	0/1/1/1
4	HD4	D	301	-	-	2/26/46/46	0/1/1/1
6	GOL	H	302	-	-	0/4/4/4	-
4	HD4	J	301	-	-	7/26/46/46	0/1/1/1
4	HD4	L	301	-	-	7/26/46/46	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	HD4	P27-O29	3.71	1.62	1.50
4	L	301	HD4	P27-O29	3.69	1.61	1.50
4	D	301	HD4	P27-O29	3.54	1.61	1.50
4	J	301	HD4	P27-O29	3.49	1.61	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	301	HD4	C1-O1-C17	2.74	119.86	115.27
4	J	301	HD4	C1-O1-C17	2.60	119.61	115.27
4	H	301	HD4	O5-C1-C2	-2.58	105.72	110.59
5	G	302	FLC	OB1-CBC-CB	-2.54	117.17	122.09
4	J	301	HD4	O1-C17-C21	2.40	112.02	107.47
4	J	301	HD4	C1-O5-C5	2.31	118.23	113.72
4	L	301	HD4	C3-C2-N2	-2.28	106.41	110.62
4	H	301	HD4	C3-C4-C5	-2.13	106.38	110.23
4	J	301	HD4	C6-C5-C4	-2.10	107.87	113.02

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	301	HD4	O1-C17-C19-O20
4	J	301	HD4	C21-C17-C19-O20
4	L	301	HD4	C17-C21-C23-C25
4	L	301	HD4	C17-C21-C23-O31
4	L	301	HD4	O32-C21-C23-C25
4	L	301	HD4	O32-C21-C23-O31
4	L	301	HD4	C21-C23-C25-O26
4	L	301	HD4	O31-C23-C25-O26
6	J	302	GOL	C1-C2-C3-O3
6	J	302	GOL	O2-C2-C3-O3
4	J	301	HD4	C17-C21-C23-O31
4	J	301	HD4	C17-C21-C23-C25
4	D	301	HD4	C17-C21-C23-O31
4	J	301	HD4	O5-C1-O1-C17
4	D	301	HD4	C21-C17-C19-O20
4	H	301	HD4	C25-O26-P27-O29
4	J	301	HD4	C4-C5-C6-O6
4	L	301	HD4	O1-C17-C21-C23
4	J	301	HD4	O32-C21-C23-O31
4	H	301	HD4	O5-C1-O1-C17

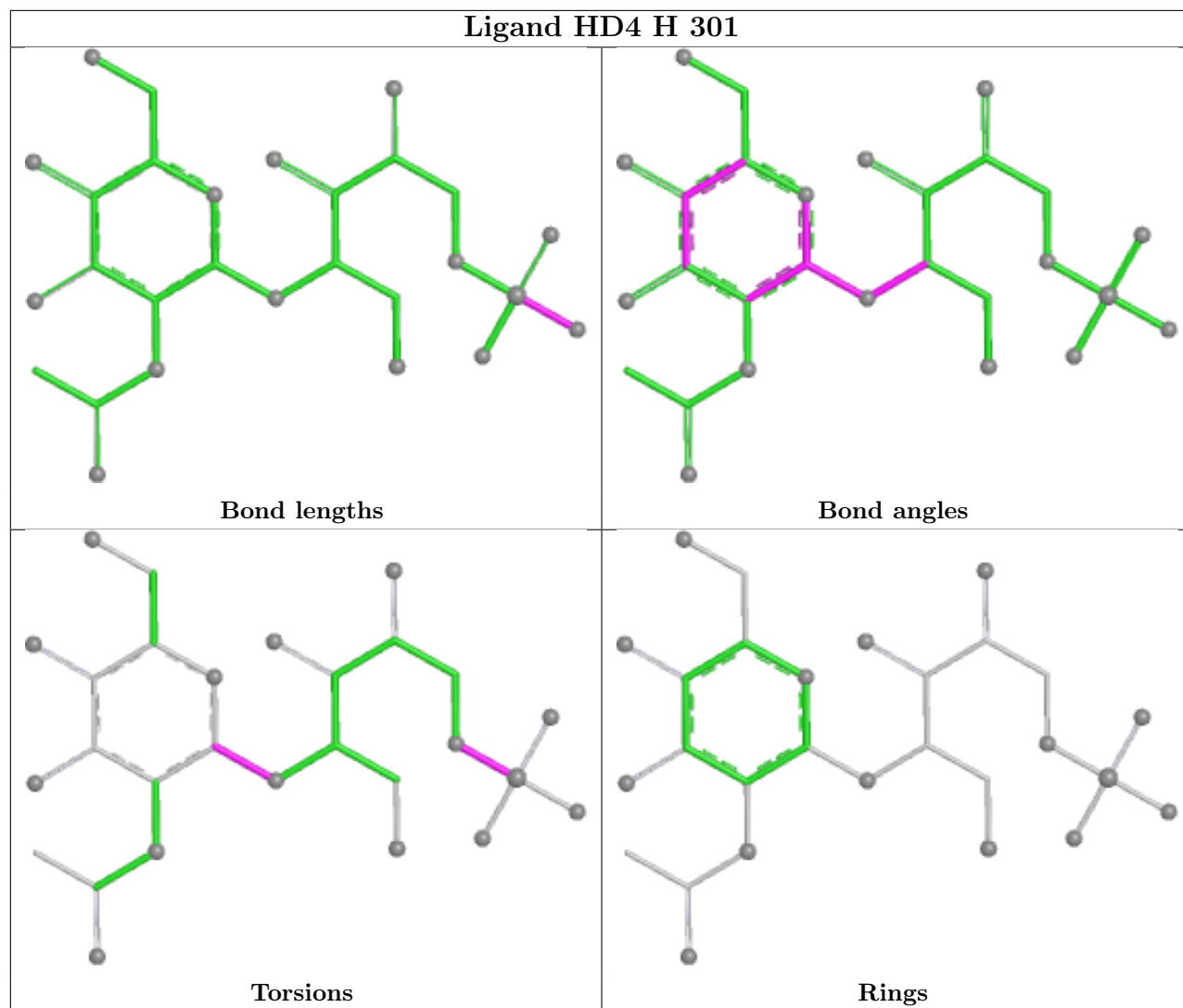
There are no ring outliers.

1 monomer is involved in 1 short contact:

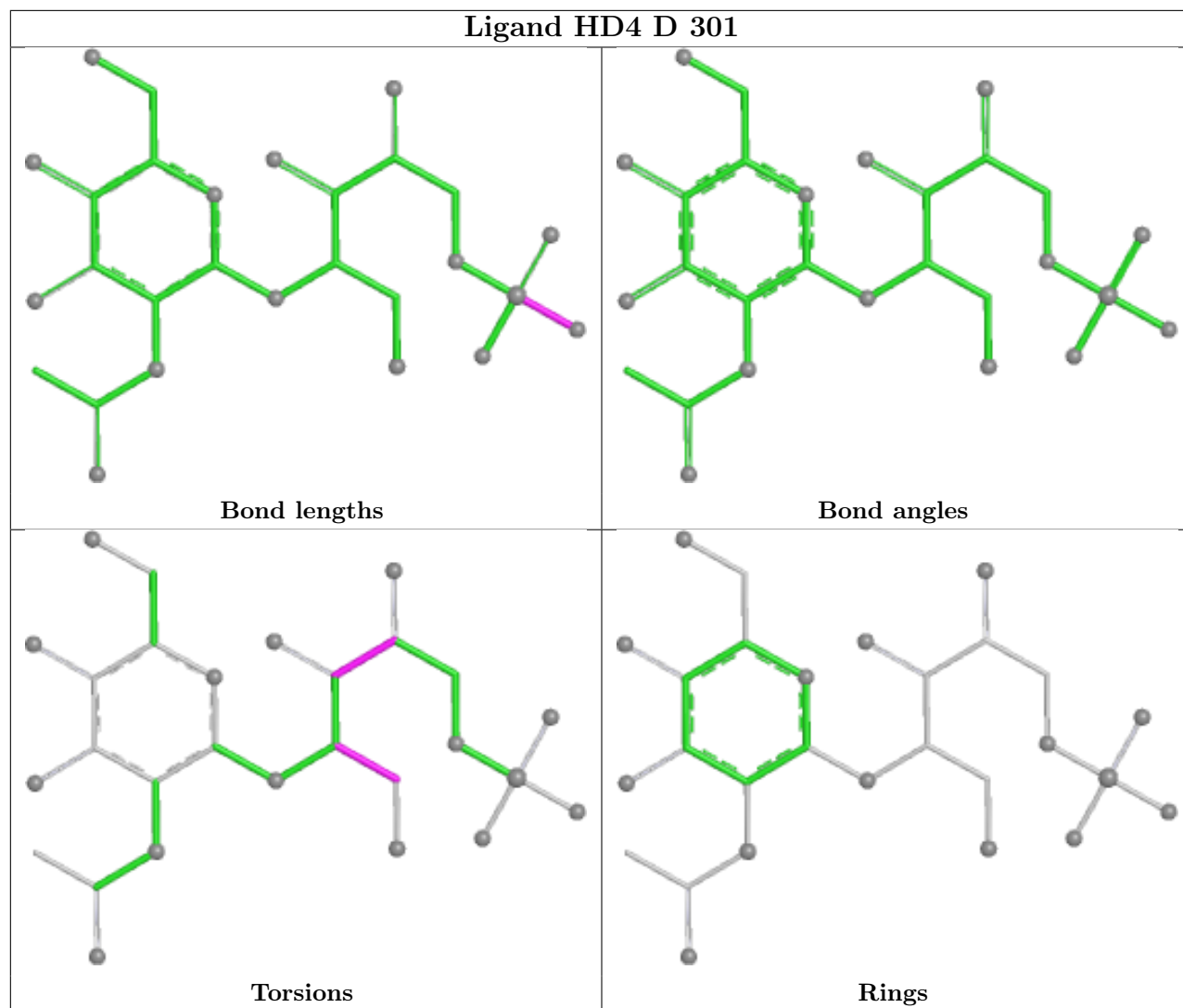
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	HD4	1	0

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.

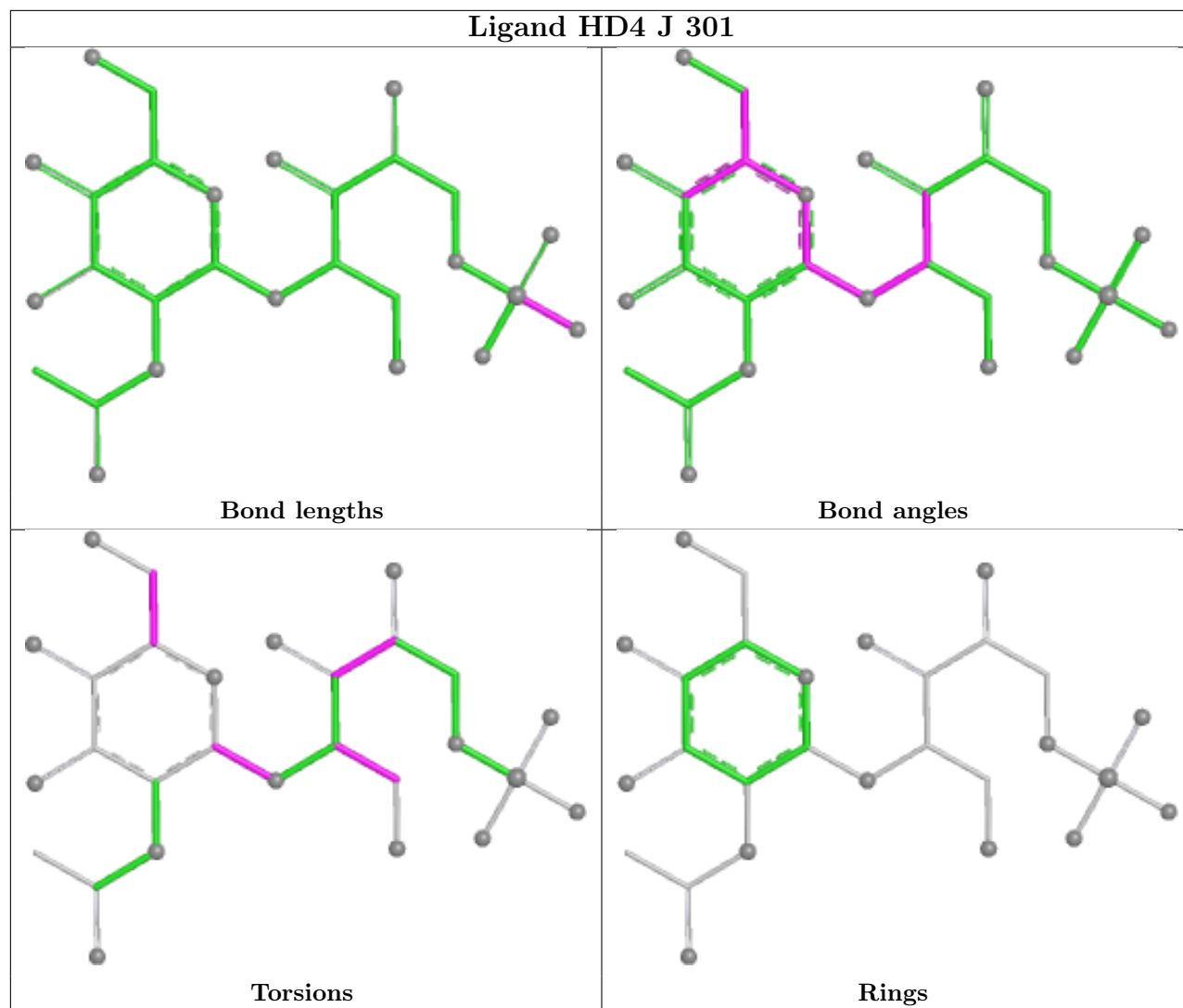
Ligand HD4 H 301

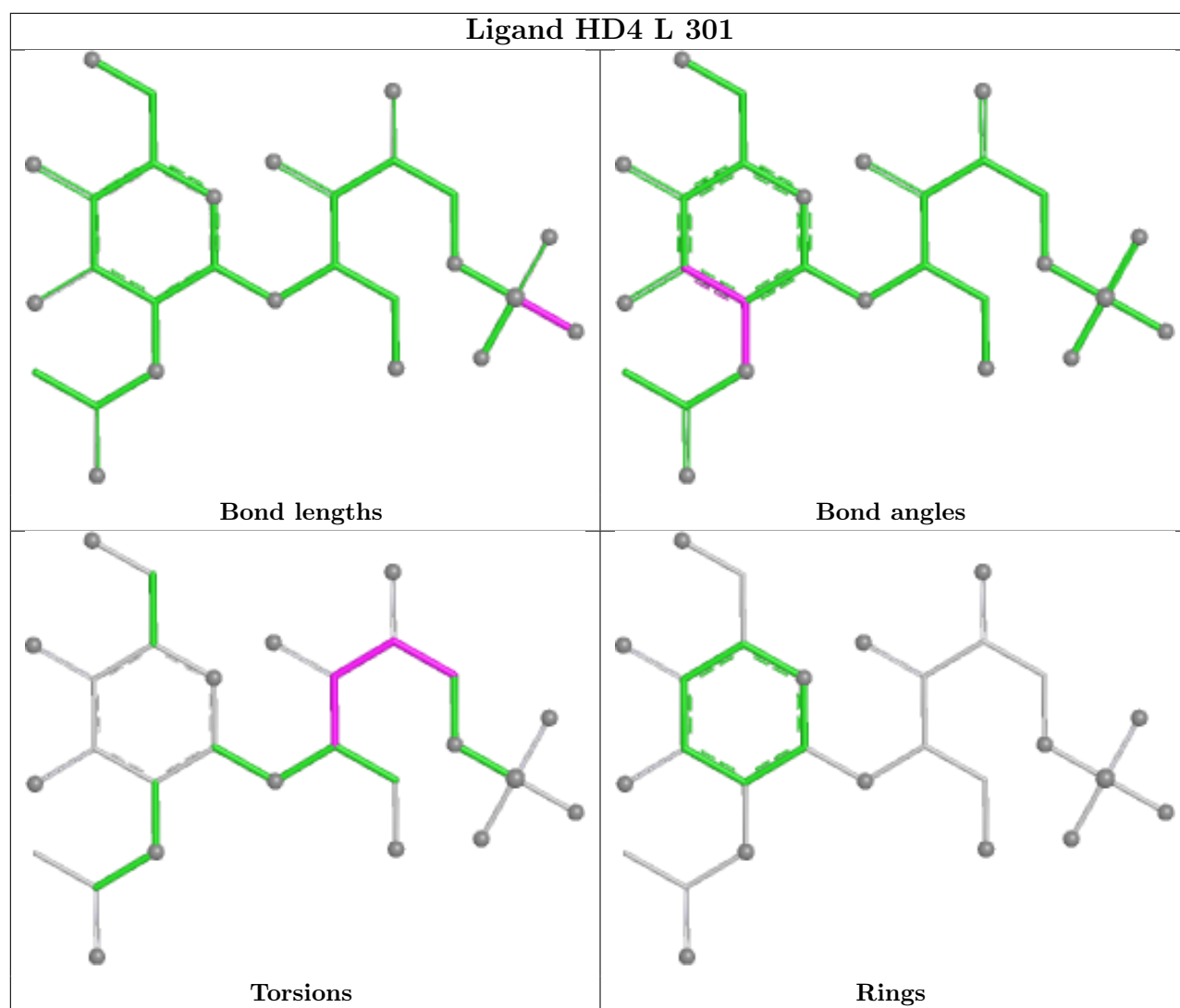


Ligand HD4 D 301



Ligand HD4 J 301





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	211/233 (90%)	0.22	2 (0%) 81 78	28, 46, 64, 78	0
1	C	206/233 (88%)	0.67	18 (8%) 16 13	32, 53, 84, 97	0
1	E	205/233 (87%)	0.74	11 (5%) 31 28	40, 60, 81, 96	0
1	G	211/233 (90%)	-0.01	1 (0%) 87 85	19, 40, 66, 81	0
1	I	211/233 (90%)	-0.02	2 (0%) 81 78	23, 38, 67, 74	1 (0%)
1	K	211/233 (90%)	0.39	2 (0%) 81 78	32, 49, 69, 88	0
1	M	207/233 (88%)	0.09	4 (1%) 66 62	25, 41, 66, 79	0
1	O	211/233 (90%)	0.12	1 (0%) 87 85	26, 45, 67, 79	0
2	B	202/243 (83%)	-0.04	6 (2%) 52 48	20, 34, 63, 88	1 (0%)
2	D	212/243 (87%)	0.38	12 (5%) 29 25	22, 43, 68, 86	1 (0%)
2	F	200/243 (82%)	0.47	9 (4%) 38 34	32, 48, 69, 85	2 (1%)
2	H	212/243 (87%)	-0.10	3 (1%) 73 69	22, 35, 54, 91	1 (0%)
2	J	214/243 (88%)	0.00	9 (4%) 40 36	21, 35, 57, 76	1 (0%)
2	L	211/243 (86%)	0.48	17 (8%) 18 14	28, 44, 81, 101	0
2	N	209/243 (86%)	-0.00	2 (0%) 79 76	27, 40, 63, 84	0
2	P	204/243 (83%)	-0.07	4 (1%) 65 60	22, 35, 59, 81	0
All	All	3337/3808 (87%)	0.21	103 (3%) 51 47	19, 43, 71, 101	7 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	VAL	5.5
2	L	2	VAL	4.7
1	C	184	ALA	4.2
1	M	212	GLY	4.1
2	D	130	SER	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	129	PRO	3.9
2	F	188	PRO	3.7
1	C	135	LEU	3.6
1	M	167	ASP	3.5
2	H	136	GLY	3.4
1	K	2	ILE	3.4
1	C	116	PHE	3.4
1	M	199	GLN	3.4
2	F	138	THR	3.3
1	C	154	LEU	3.3
2	H	130	SER	3.3
2	J	134	THR	3.3
1	G	211	ARG	3.2
2	L	135	SER	3.1
2	P	216	PRO	3.1
2	L	217	LYS	3.1
2	B	189	SER	3.1
2	L	129	PRO	3.0
1	C	188	LYS	3.0
2	P	194	THR	3.0
2	F	161	ALA	2.9
2	L	8	GLY	2.9
1	E	39	LYS	2.9
2	D	139	ALA	2.9
1	C	191	VAL	2.9
1	E	13	VAL	2.9
2	F	128	ALA	2.9
1	I	1	ASP	2.9
2	L	29	PHE	2.8
2	F	202	ASN	2.8
1	C	211	ARG	2.8
1	E	62	PHE	2.8
1	K	211	ARG	2.8
2	D	138	THR	2.7
2	L	54	ILE	2.7
2	D	136	GLY	2.7
1	E	168	SER	2.7
1	A	67	TYR	2.7
1	C	146	VAL	2.7
1	E	78	LEU	2.7
1	C	206	THR	2.7
2	F	196	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	7	SER	2.7
2	N	216	PRO	2.7
1	M	67	TYR	2.6
2	B	198	ILE	2.6
2	B	195	GLN	2.6
2	L	66	GLY	2.6
1	E	111	ALA	2.5
1	C	115	VAL	2.5
2	N	130	SER	2.5
2	D	198	ILE	2.5
2	D	42	GLY	2.5
1	I	211	ARG	2.4
2	D	53	GLY	2.4
2	L	59	HIS	2.4
2	H	9	GLY	2.3
2	L	9	GLY	2.3
1	C	209	PHE	2.3
2	P	129	PRO	2.3
1	E	64	GLY	2.3
2	D	137	GLY	2.3
2	L	26	GLY	2.3
1	E	58	ALA	2.3
1	C	202	SER	2.3
2	J	135	SER	2.3
2	L	7	SER	2.3
2	F	105	PHE	2.3
2	D	165	GLY	2.3
2	D	214	VAL	2.3
2	B	139	ALA	2.3
2	L	31	THR	2.3
2	P	189	SER	2.3
2	D	217	LYS	2.3
2	D	187	VAL	2.3
1	C	130	ALA	2.2
2	B	187	VAL	2.2
2	J	2	VAL	2.2
2	J	137	GLY	2.2
2	F	23	ALA	2.2
2	F	76	LYS	2.2
2	L	51	ILE	2.2
2	L	80	TYR	2.2
1	C	78	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	75	ILE	2.2
1	C	203	SER	2.1
1	O	18	THR	2.1
1	E	108	ARG	2.1
1	C	137	ASN	2.1
2	J	136	GLY	2.1
2	J	132	LYS	2.1
2	J	116	SER	2.0
1	E	67	TYR	2.0
1	C	196	VAL	2.0
2	L	65	ARG	2.0
1	A	169	LYS	2.0
2	B	163	THR	2.0
2	L	22	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	J	302	6/6	0.79	0.15	42,46,49,50	0
5	FLC	G	302	13/13	0.84	0.13	56,64,77,78	0
6	GOL	H	302	6/6	0.84	0.16	65,66,67,67	0
4	HD4	L	301	28/28	0.84	0.13	54,67,98,99	0
4	HD4	J	301	28/28	0.90	0.09	32,44,68,69	0
4	HD4	D	301	28/28	0.91	0.08	38,46,69,71	0
3	CL	O	301	1/1	0.92	0.09	43,43,43,43	0
3	CL	F	301	1/1	0.93	0.07	51,51,51,51	0
4	HD4	H	301	28/28	0.94	0.07	26,38,52,53	0

Continued on next page...

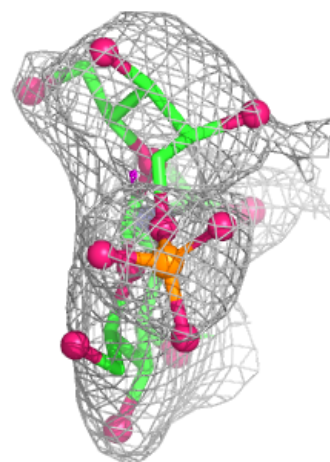
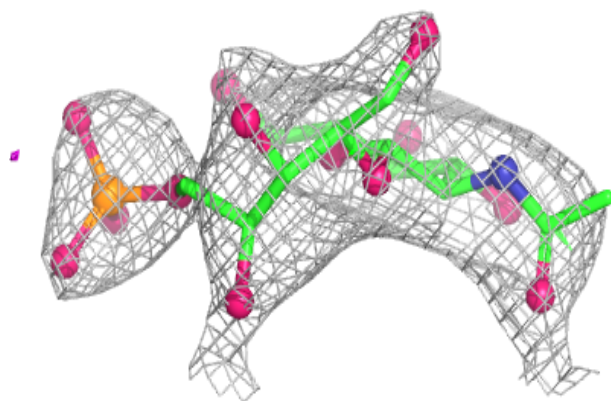
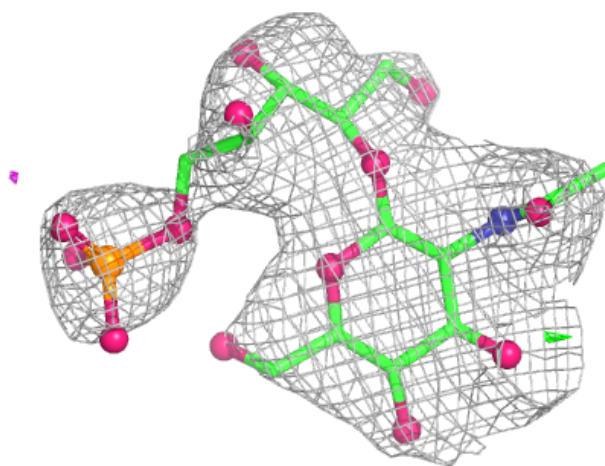
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	G	301	1/1	0.98	0.04	30,30,30,30	0
3	CL	A	301	1/1	0.99	0.05	50,50,50,50	0
3	CL	B	301	1/1	0.99	0.03	38,38,38,38	0
3	CL	C	301	1/1	1.00	0.02	35,35,35,35	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.

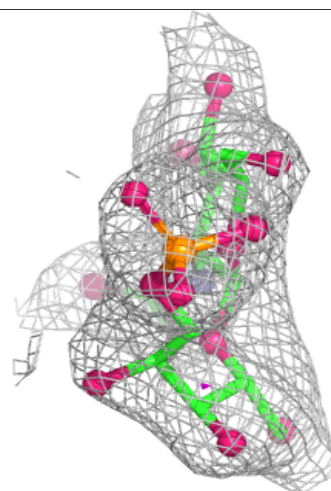
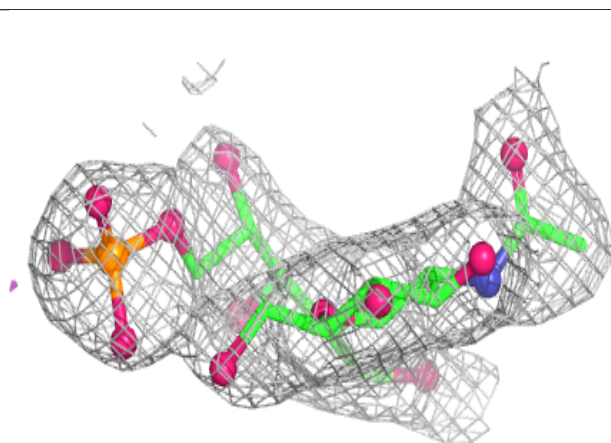
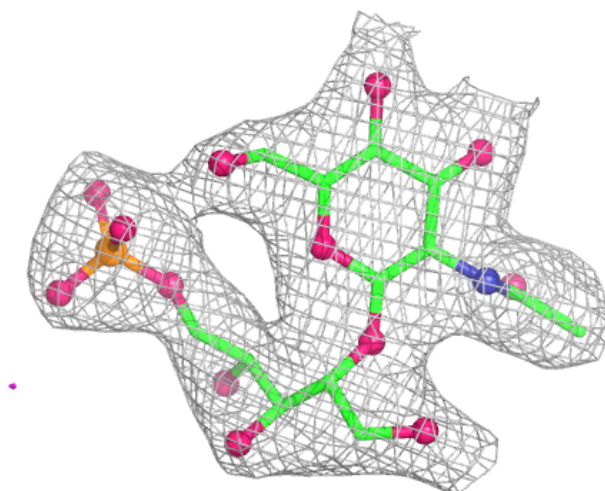
Electron density around HD4 L 301:

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



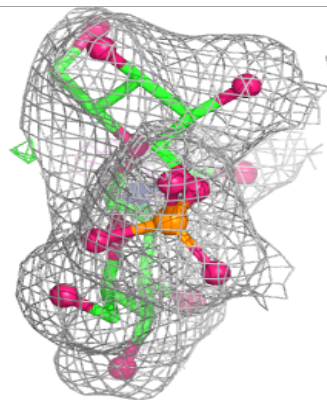
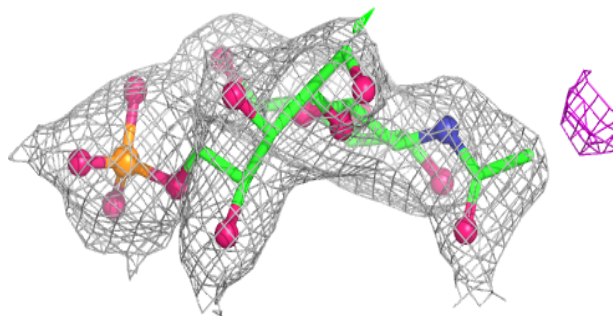
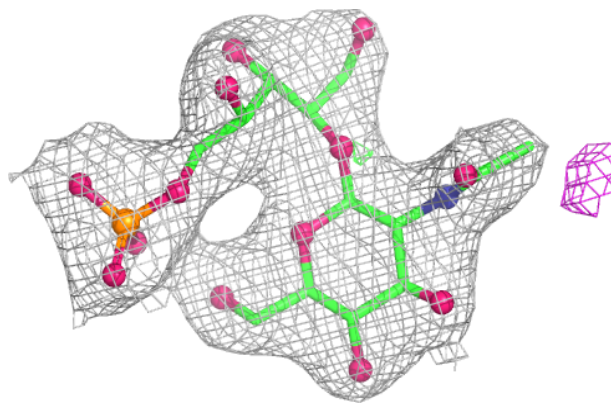
Electron density around HD4 J 301:

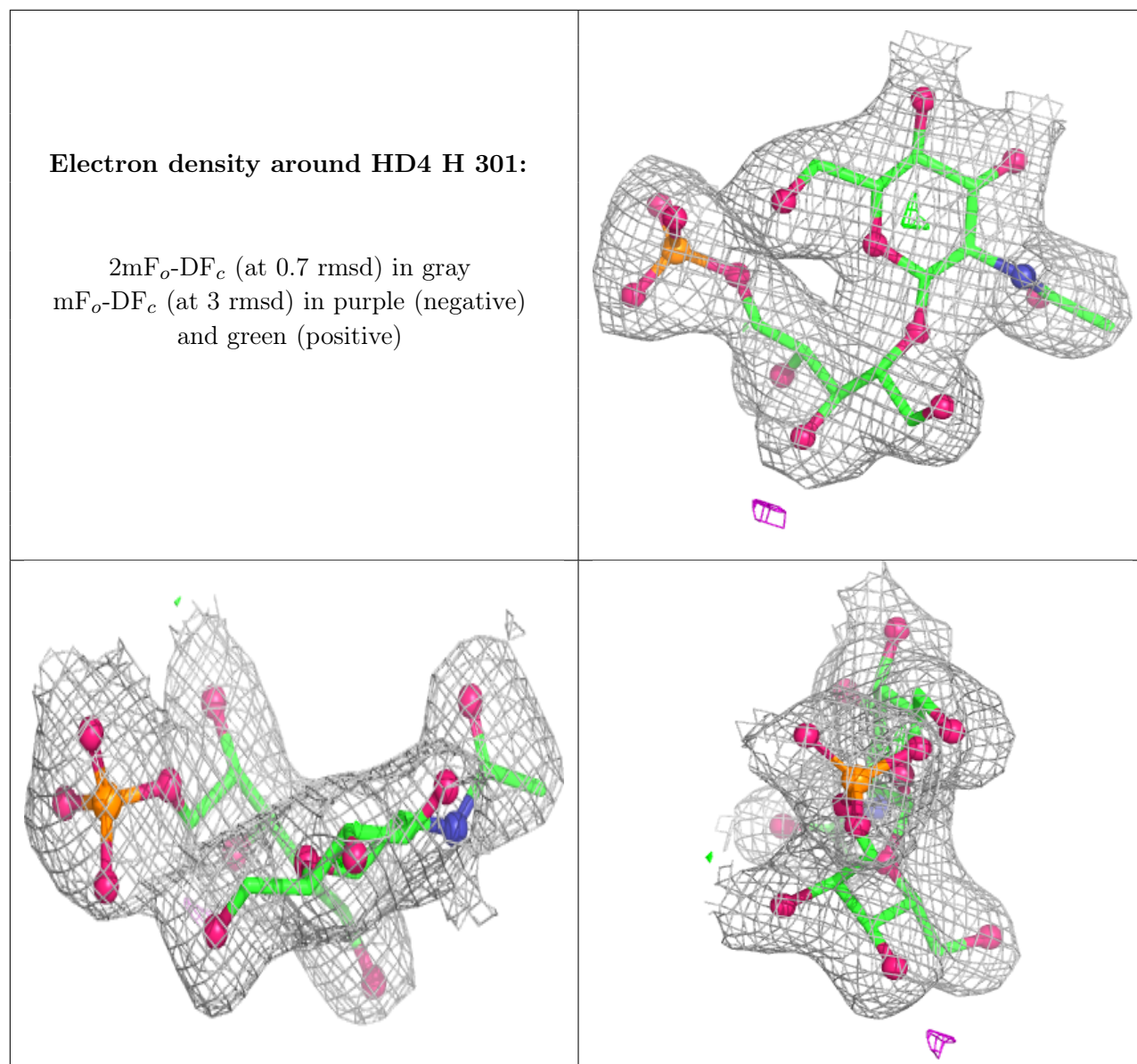
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HD4 D 301:

$2mF_o - DF_c$ (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.