



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:01 PM UTC

PDB ID : 3C6G / pdb_00003c6g
Title : Crystal structure of CYP2R1 in complex with vitamin D3
Authors : Strushkevich, N.V.; Min, J.; Loppnau, P.; Tempel, W.; Arrowsmith, C.H.;
Edwards, A.M.; Sundstrom, M.; Weigelt, J.; Bochkarev, A.; Plotnikov, A.N.;
Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2008-02-04
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

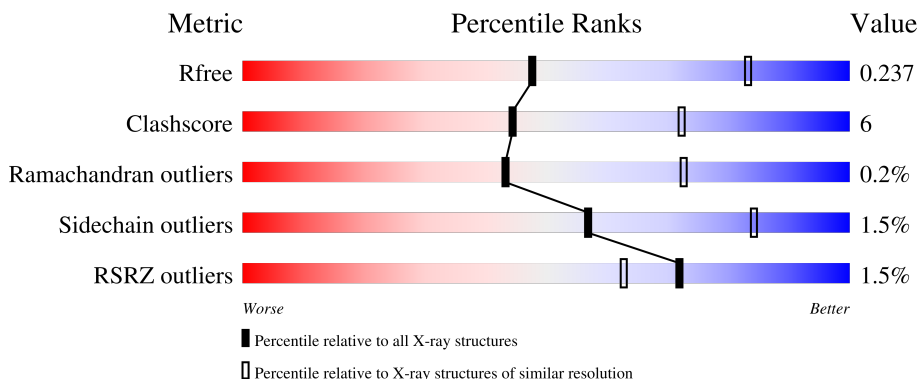
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

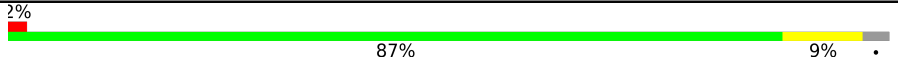
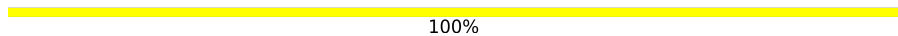
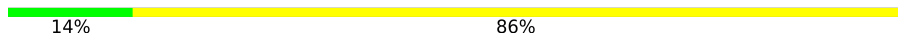
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	479	
1	B	479	
2	C	7	
2	D	7	

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
3	UNX	A	1	-	-	-	X
3	UNX	A	2	-	-	-	X
3	UNX	A	3	-	-	-	X
3	UNX	B	4	-	-	-	X
3	UNX	B	5	-	-	-	X
3	UNX	B	6	-	-	-	X
3	UNX	B	7	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7955 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.

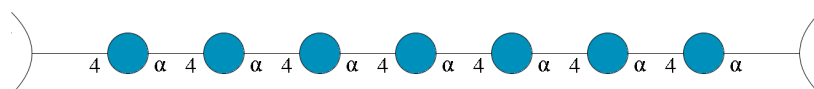
- Molecule 1 is a protein called Cytochrome P450 2R1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3763	2444	632	669	18			
1	B	467	Total	C	N	O	S	0	0	0
			3793	2462	641	672	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q6VVX0
A	28	ALA	-	expression tag	UNP Q6VVX0
A	29	LYS	-	expression tag	UNP Q6VVX0
A	30	LYS	-	expression tag	UNP Q6VVX0
A	31	THR	-	expression tag	UNP Q6VVX0
A	502	HIS	-	expression tag	UNP Q6VVX0
A	503	HIS	-	expression tag	UNP Q6VVX0
A	504	HIS	-	expression tag	UNP Q6VVX0
A	505	HIS	-	expression tag	UNP Q6VVX0
B	27	MET	-	expression tag	UNP Q6VVX0
B	28	ALA	-	expression tag	UNP Q6VVX0
B	29	LYS	-	expression tag	UNP Q6VVX0
B	30	LYS	-	expression tag	UNP Q6VVX0
B	31	THR	-	expression tag	UNP Q6VVX0
B	502	HIS	-	expression tag	UNP Q6VVX0
B	503	HIS	-	expression tag	UNP Q6VVX0
B	504	HIS	-	expression tag	UNP Q6VVX0
B	505	HIS	-	expression tag	UNP Q6VVX0

- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).

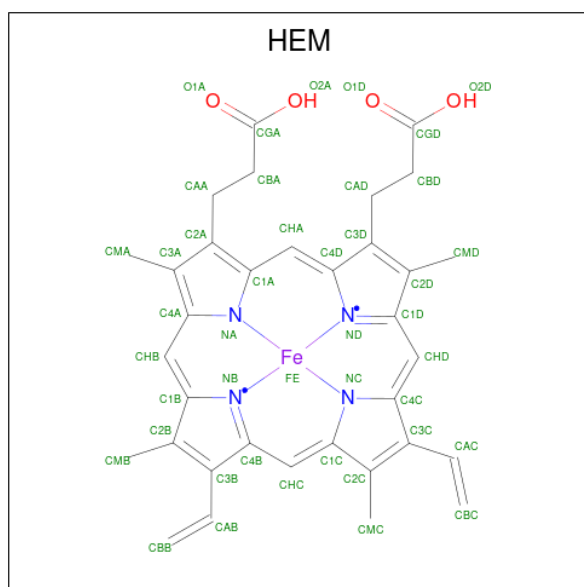


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total 77	C 42	O 35	0	0	0
2	D	7	Total 77	C 42	O 35	0	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

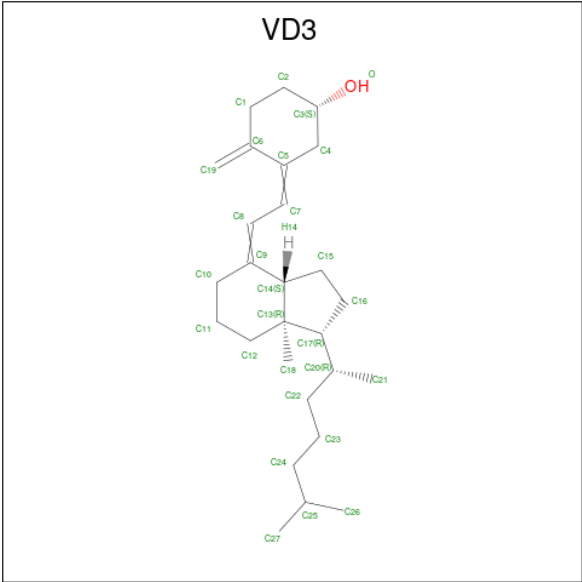
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total X 3 3	0	0
3	B	4	Total X 4 4	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is (1S,3Z)-3-[(2E)-2-[(1R,3AR,7AS)-7A-METHYL-1-[(2R)-6-METHYLHEPTA N-2-YL]-2,3,3A,5,6,7-HEXAHYDRO-1H-INDEN-4-YLIDENE]ETHYLIDENE]-4-METHYLIDENE-CYCLOHEXAN-1-OL (CCD ID: VD3) (formula: C₂₇H₄₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			28	27	1		
5	B	1	Total	C	O	0	0
			28	27	1		

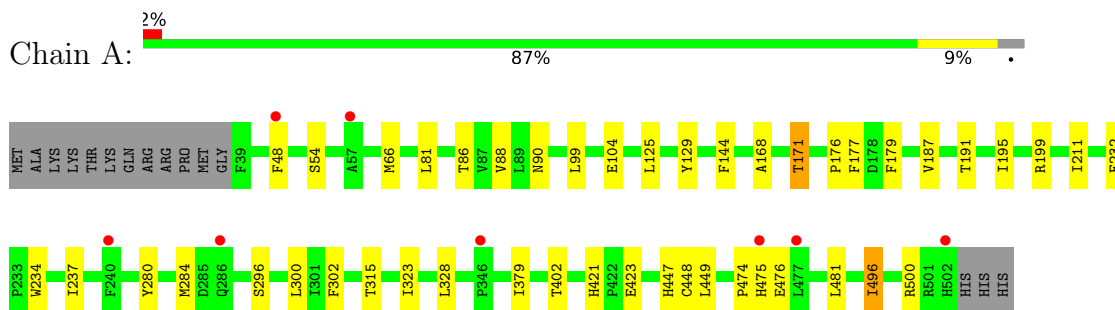
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total	O	0	0
			59	59		
6	B	37	Total	O	0	0
			37	37		

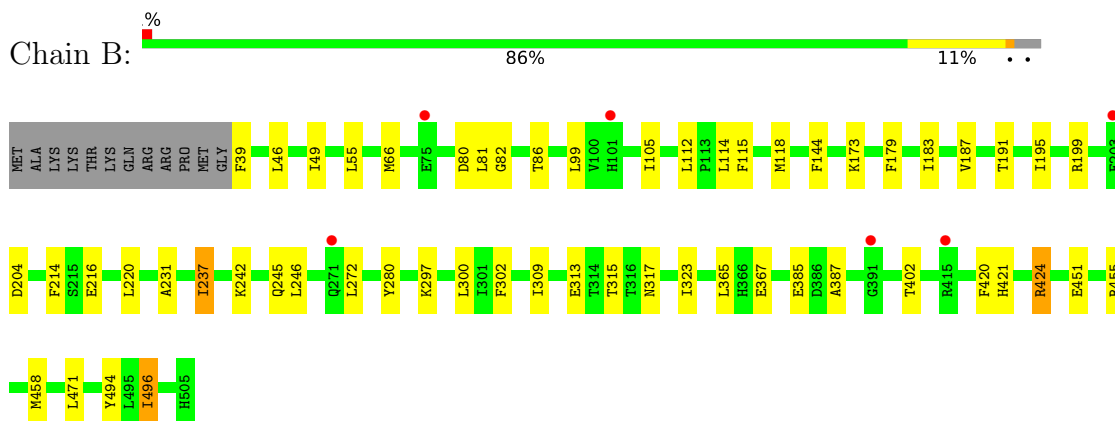
3 Residue-property plots [i](#)

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: Cytochrome P450 2R1



- Molecule 1: Cytochrome P450 2R1



- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	137.68Å 163.05Å 152.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.34 – 2.80 29.34 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.34-2.80) 99.5 (29.34-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.193 , 0.231 0.203 , 0.237	Depositor DCC
R_{free} test set	2132 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7955	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, GLC, VD3, HEM

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	0.86	0/3872	0.80	0/5247
1	B	0.82	0/3905	0.79	3/5292 (0.1%)
All	All	0.84	0/7777	0.80	3/10539 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ILE	CB-CA-C	-6.76	103.18	112.04
1	B	39	PHE	CA-C-N	5.18	123.44	119.66
1	B	39	PHE	C-N-CA	5.18	123.44	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3763	0	3704	39	0
1	B	3793	0	3724	37	0
2	C	77	0	63	0	0
2	D	77	0	63	0	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	30	8	0
4	B	43	0	30	6	0
5	A	28	0	44	4	0
5	B	28	0	44	10	0
6	A	59	0	0	0	0
6	B	37	0	0	0	0
All	All	7955	0	7702	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (93) 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)
5:B:700:VD3:H212	5:B:700:VD3:H183	1.39	1.02
4:A:601:HEM:HMB1	4:A:601:HEM:HBB2	1.44	0.97
4:B:601:HEM:HMB1	4:B:601:HEM:HBB2	1.54	0.90
1:A:66:MET:HE3	1:A:88:VAL:CG1	2.08	0.83
4:A:601:HEM:HMC2	4:A:601:HEM:HBC2	1.59	0.83
4:B:601:HEM:HBC2	4:B:601:HEM:HMC2	1.62	0.81
1:B:46:LEU:HD12	1:B:49:ILE:HD11	1.68	0.76
4:A:601:HEM:HBB2	4:A:601:HEM:CMB	2.14	0.75
5:B:700:VD3:H213	5:B:700:VD3:H121	1.70	0.73
1:A:99:LEU:HD11	1:A:402:THR:HG21	1.71	0.72
1:A:191:THR:HG22	1:A:195:ILE:HD12	1.71	0.71
1:B:99:LEU:HD11	1:B:402:THR:HG21	1.72	0.70
1:B:55:LEU:HD11	1:B:66:MET:HE3	1.72	0.70
1:A:66:MET:HE3	1:A:88:VAL:HG13	1.72	0.69
1:B:323:ILE:HG22	1:B:496:ILE:CD1	2.22	0.67
4:B:601:HEM:HBB2	4:B:601:HEM:CMB	2.24	0.67
1:B:191:THR:HG22	1:B:195:ILE:HD12	1.78	0.66
1:A:66:MET:HE3	1:A:88:VAL:HG11	1.76	0.66
4:A:601:HEM:HBC2	4:A:601:HEM:CMC	2.27	0.65
5:A:701:VD3:H212	5:A:701:VD3:H121	1.79	0.65
5:B:700:VD3:H121	5:B:700:VD3:C21	2.28	0.63
1:A:323:ILE:HG22	1:A:496:ILE:HD12	1.81	0.62
1:A:302:PHE:HD1	5:A:701:VD3:H12	1.64	0.61
1:A:81:LEU:HD12	1:A:86:THR:HG21	1.83	0.60
1:A:144:PHE:CE2	4:A:601:HEM:HBC1	2.37	0.60
1:B:302:PHE:HD1	5:B:700:VD3:H12	1.65	0.60
1:B:81:LEU:HD12	1:B:86:THR:HG21	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:CE1	1:A:232:PHE:CE2	2.90	0.59
4:B:601:HEM:HBC2	4:B:601:HEM:CMC	2.31	0.59
1:B:220:LEU:HD22	1:B:242:LYS:HB3	1.86	0.57
1:A:280:TYR:CG	1:A:300:LEU:HD13	2.39	0.57
1:A:237:ILE:HD11	1:B:237:ILE:HD11	1.86	0.57
5:B:700:VD3:H212	5:B:700:VD3:C18	2.23	0.56
1:A:302:PHE:CD1	5:A:701:VD3:H12	2.40	0.56
1:A:104:GLU:OE2	1:A:129:TYR:OH	2.20	0.56
1:B:144:PHE:CE2	4:B:601:HEM:HBC1	2.42	0.55
1:B:421:HIS:O	1:B:424:ARG:HB3	2.07	0.54
1:B:82:GLY:HA3	1:B:231:ALA:HB1	1.90	0.54
1:A:421:HIS:CE1	1:A:423:GLU:HB3	2.43	0.54
1:A:323:ILE:CG2	1:A:496:ILE:HD12	2.37	0.53
1:A:176:PRO:HB3	1:A:474:PRO:HG3	1.91	0.53
1:A:449:LEU:O	1:A:449:LEU:HD23	2.10	0.52
1:A:66:MET:CE	1:A:88:VAL:HG13	2.38	0.52
1:A:323:ILE:HG22	1:A:496:ILE:CD1	2.39	0.51
1:A:66:MET:CE	1:A:88:VAL:CG1	2.84	0.51
1:B:82:GLY:HA3	1:B:231:ALA:CB	2.40	0.51
1:A:284:MET:HE3	1:A:296:SER:HA	1.92	0.50
1:B:451:GLU:O	1:B:455:ARG:HG3	2.11	0.50
1:A:168:ALA:O	1:A:171:THR:HB	2.12	0.50
4:A:601:HEM:HHA	4:A:601:HEM:HBA2	1.92	0.49
1:B:112:LEU:HD12	1:B:115:PHE:CE1	2.48	0.49
1:B:302:PHE:CD1	5:B:700:VD3:H12	2.44	0.49
5:B:700:VD3:H183	5:B:700:VD3:C21	2.24	0.48
1:A:191:THR:HG22	1:A:195:ILE:CD1	2.43	0.48
1:B:216:GLU:OE1	1:B:245:GLN:NE2	2.47	0.47
1:A:187:VAL:HG11	1:A:315:THR:HB	1.96	0.46
1:B:187:VAL:HG11	1:B:315:THR:HB	1.97	0.46
1:B:105:ILE:HG23	1:B:385:GLU:HG2	1.97	0.46
1:B:105:ILE:HG21	1:B:387:ALA:HB2	1.97	0.46
1:B:323:ILE:HG23	1:B:471:LEU:HD13	1.97	0.46
1:B:280:TYR:CG	1:B:300:LEU:HD13	2.52	0.45
1:B:191:THR:CG2	1:B:195:ILE:HD12	2.46	0.45
1:B:80:ASP:OD1	1:B:82:GLY:O	2.35	0.44
1:B:313:GLU:O	1:B:317:ASN:ND2	2.50	0.44
1:B:367:GLU:HG3	1:B:420:PHE:CD1	2.51	0.44
1:B:214:PHE:HB3	1:B:309:ILE:HD13	1.99	0.44
1:A:66:MET:CE	1:A:88:VAL:HG11	2.45	0.44
1:A:237:ILE:HD11	1:B:237:ILE:CD1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:CZ	4:A:601:HEM:HBC1	2.53	0.43
1:B:494:TYR:HE1	1:B:496:ILE:HD12	1.84	0.43
1:A:125:LEU:HD21	1:A:379:ILE:HD13	2.01	0.43
1:B:365:LEU:HD22	1:B:458:MET:HE2	2.01	0.43
1:B:118:MET:HE3	1:B:246:LEU:HD22	2.00	0.43
1:A:177:PHE:CZ	1:A:179:PHE:CE2	3.07	0.43
1:A:302:PHE:HD1	5:A:701:VD3:C1	2.31	0.43
1:A:449:LEU:HD23	1:A:449:LEU:C	2.44	0.43
4:A:601:HEM:HMB1	4:A:601:HEM:CBB	2.30	0.42
1:B:323:ILE:CG2	1:B:496:ILE:CD1	2.94	0.42
1:A:48:PHE:CZ	1:A:232:PHE:CE2	3.07	0.42
1:A:232:PHE:HB3	1:A:234:TRP:CE2	2.55	0.42
1:B:144:PHE:HE2	4:B:601:HEM:HBC1	1.85	0.41
5:B:700:VD3:C21	5:B:700:VD3:C12	2.96	0.41
1:B:323:ILE:HG22	1:B:496:ILE:HD12	2.00	0.41
1:A:88:VAL:HG12	1:A:90:ASN:HD21	1.84	0.41
1:A:447:HIS:O	1:A:448:CYS:C	2.60	0.41
1:A:474:PRO:O	1:A:475:HIS:C	2.63	0.41
1:B:114:LEU:O	1:B:118:MET:HG2	2.20	0.41
1:A:328:LEU:CD2	1:A:481:LEU:HD11	2.50	0.41
1:B:365:LEU:HD22	1:B:458:MET:CE	2.51	0.40
1:B:179:PHE:HB3	1:B:183:ILE:CD1	2.51	0.40
5:B:700:VD3:H7	5:B:700:VD3:C15	2.51	0.40
5:B:700:VD3:H42	5:B:700:VD3:H8	1.90	0.40
1:A:179:PHE:CE2	1:A:496:ILE:HG22	2.57	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	462/479 (96%)	446 (96%)	15 (3%)	1 (0%)	43 72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	465/479 (97%)	450 (97%)	14 (3%)	1 (0%)	43	72
All	All	927/958 (97%)	896 (97%)	29 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	GLU
1	B	204	ASP

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	409/422 (97%)	403 (98%)	6 (2%)	57	84
1	B	412/422 (98%)	406 (98%)	6 (2%)	57	84
All	All	821/844 (97%)	809 (98%)	12 (2%)	57	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	171	THR
1	A	199	ARG
1	A	211	ILE
1	A	496	ILE
1	A	500	ARG
1	B	173	LYS
1	B	199	ARG
1	B	272	LEU
1	B	297	LYS
1	B	424	ARG
1	B	496	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	181	GLN
1	A	243	HIS
1	B	63	HIS
1	B	181	GLN
1	B	335	GLN
1	B	470	HIS
1	B	492	GLN
1	B	503	HIS

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 ⓘ

14 monosaccharides 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	$\# Z > 2$
2	GLC	C	1	2	11,11,12	0.59	0	15,15,17	2.02	4 (26%)
2	GLC	C	2	2	11,11,12	0.54	0	15,15,17	1.14	2 (13%)
2	GLC	C	3	2	11,11,12	0.80	0	15,15,17	1.42	1 (6%)
2	GLC	C	4	2	11,11,12	0.77	0	15,15,17	1.92	4 (26%)
2	GLC	C	5	2	11,11,12	0.80	0	15,15,17	1.17	1 (6%)
2	GLC	C	6	2	11,11,12	0.66	0	15,15,17	1.70	3 (20%)
2	GLC	C	7	2	11,11,12	0.58	0	15,15,17	1.71	2 (13%)
2	GLC	D	1	2	11,11,12	0.49	0	15,15,17	1.99	2 (13%)
2	GLC	D	2	2	11,11,12	0.62	0	15,15,17	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	D	3	2	11,11,12	0.43	0	15,15,17	1.16	1 (6%)
2	GLC	D	4	2	11,11,12	0.31	0	15,15,17	1.23	2 (13%)
2	GLC	D	5	2	11,11,12	0.69	0	15,15,17	1.66	3 (20%)
2	GLC	D	6	2	11,11,12	0.71	0	15,15,17	0.89	1 (6%)
2	GLC	D	7	2	11,11,12	0.61	0	15,15,17	1.87	4 (26%)

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
2	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	C	5	2	-	2/2/19/22	0/1/1/1
2	GLC	C	6	2	-	1/2/19/22	0/1/1/1
2	GLC	C	7	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/19/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	5	2	-	2/2/19/22	0/1/1/1
2	GLC	D	6	2	-	1/2/19/22	0/1/1/1
2	GLC	D	7	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	C1-O5-C5	6.07	120.32	112.19
2	C	7	GLC	C1-O5-C5	5.62	119.72	112.19
2	C	1	GLC	C1-O5-C5	5.13	119.07	112.19
2	D	5	GLC	C1-C2-C3	4.79	116.62	109.64
2	C	3	GLC	C1-O5-C5	4.35	118.02	112.19
2	C	1	GLC	C1-C2-C3	4.11	115.62	109.64
2	C	4	GLC	C1-C2-C3	3.95	115.39	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	GLC	C1-O5-C5	3.86	117.36	112.19
2	C	6	GLC	C1-O5-C5	3.65	117.08	112.19
2	C	6	GLC	C1-C2-C3	3.62	114.92	109.64
2	D	7	GLC	C3-C4-C5	3.48	116.55	110.23
2	C	4	GLC	O4-C4-C3	-3.29	102.63	110.38
2	C	4	GLC	C2-C3-C4	3.09	116.30	110.86
2	D	7	GLC	C2-C3-C4	2.94	116.03	110.86
2	D	5	GLC	C2-C3-C4	2.91	115.97	110.86
2	D	1	GLC	C1-C2-C3	2.88	113.83	109.64
2	C	4	GLC	C1-O5-C5	2.72	115.84	112.19
2	C	5	GLC	C1-O5-C5	2.69	115.79	112.19
2	D	4	GLC	C1-O5-C5	2.68	115.77	112.19
2	C	6	GLC	O5-C5-C6	2.67	112.86	107.66
2	D	3	GLC	C1-O5-C5	2.63	115.71	112.19
2	D	6	GLC	C1-O5-C5	2.60	115.67	112.19
2	C	2	GLC	C1-C2-C3	2.53	113.32	109.64
2	D	4	GLC	C1-C2-C3	2.52	113.31	109.64
2	C	1	GLC	C2-C3-C4	2.50	115.26	110.86
2	D	7	GLC	C1-C2-C3	2.40	113.13	109.64
2	C	2	GLC	C2-C3-C4	2.22	114.76	110.86
2	C	7	GLC	O5-C5-C4	2.17	116.11	110.83
2	D	5	GLC	O5-C5-C6	2.16	111.86	107.66
2	C	1	GLC	O4-C4-C3	-2.00	105.65	110.38

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	7	GLC	O5-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	C	5	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	C	5	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6

Continued on next page...

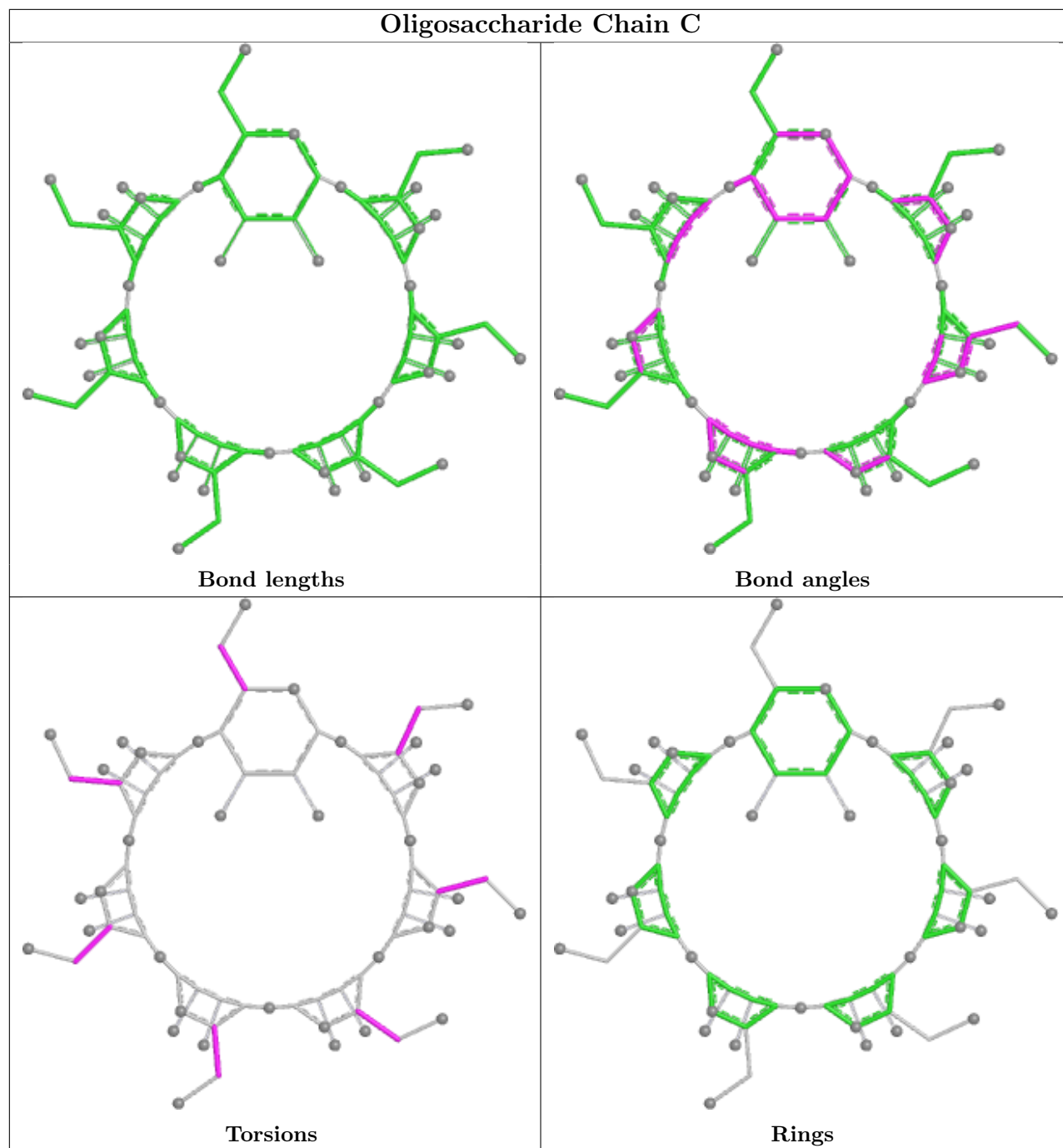
Continued from previous page...

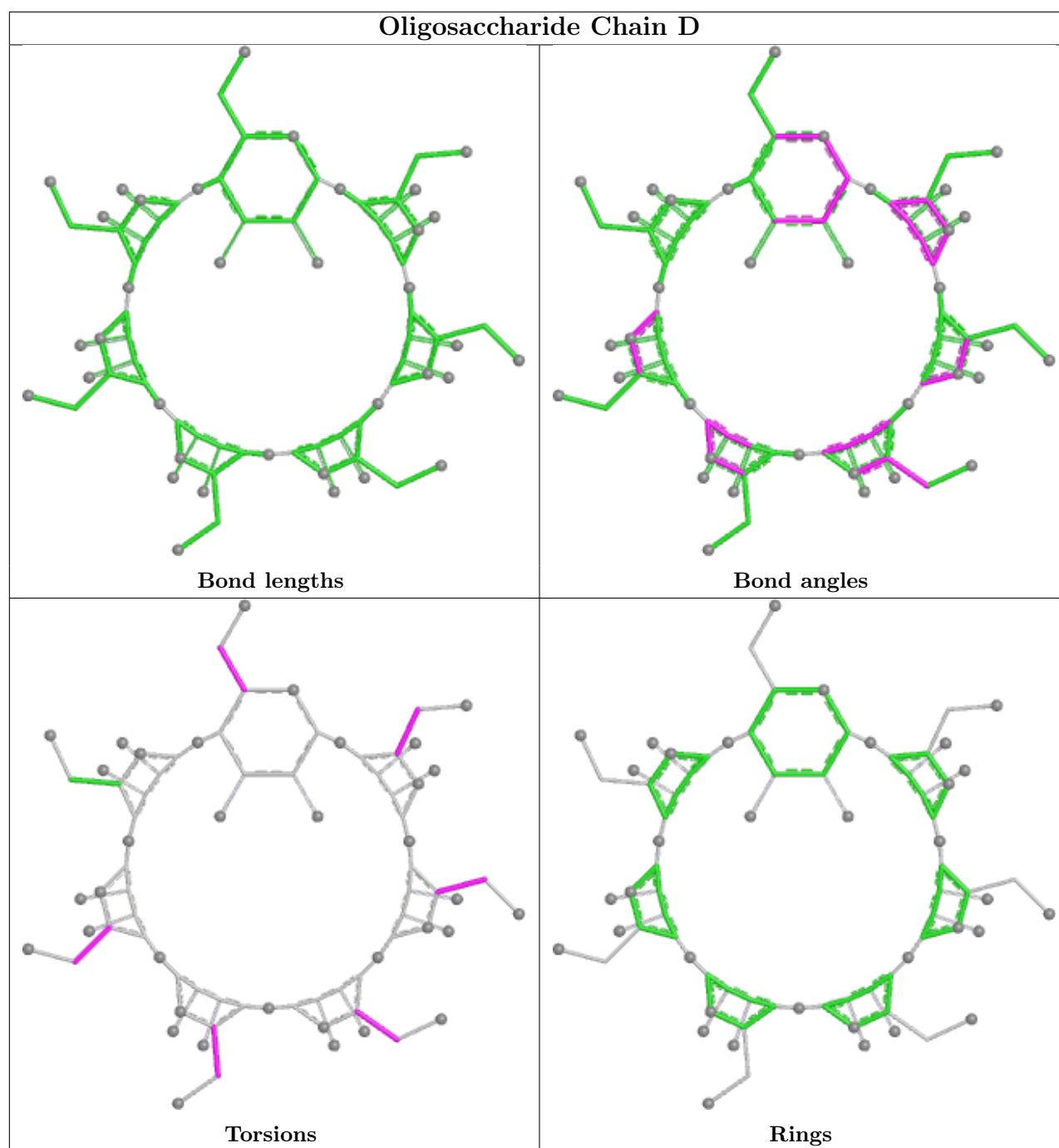
Mol	Chain	Res	Type	Atoms
2	C	4	GLC	C4-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	C	7	GLC	C4-C5-C6-O6
2	D	6	GLC	O5-C5-C6-O6
2	D	7	GLC	O5-C5-C6-O6
2	C	6	GLC	O5-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
2	D	5	GLC	C4-C5-C6-O6
2	D	5	GLC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 7 are unknown - leaving 4 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	VD3	B	700	-	30,30,30	1.82	6 (20%)	43,43,43	2.82	16 (37%)
4	HEM	A	601	1	50,50,50	1.72	11 (22%)	67,82,82	1.36	10 (14%)
5	VD3	A	701	-	30,30,30	1.81	9 (30%)	43,43,43	2.70	12 (27%)
4	HEM	B	601	1	50,50,50	1.97	11 (22%)	67,82,82	1.24	6 (8%)

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	VD3	B	700	-	-	9/15/56/56	0/3/3/3
4	HEM	A	601	1	-	4/14/54/54	-
5	VD3	A	701	-	-	3/15/56/56	0/3/3/3
4	HEM	B	601	1	-	3/14/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C3D-C2D	6.75	1.51	1.36
4	A	601	HEM	C3D-C2D	6.22	1.50	1.36
4	B	601	HEM	FE-NB	5.97	2.13	1.94
5	B	700	VD3	C6-C5	-5.81	1.38	1.48
5	A	701	VD3	C6-C5	-5.36	1.39	1.48
4	B	601	HEM	FE-NA	3.99	2.08	1.95
5	A	701	VD3	C8-C9	3.65	1.39	1.34
4	A	601	HEM	FE-ND	3.55	2.05	1.94
5	B	700	VD3	C8-C9	3.49	1.39	1.34
5	A	701	VD3	C19-C6	3.09	1.38	1.32
4	A	601	HEM	CMC-C2C	3.08	1.57	1.50
4	B	601	HEM	CAB-C3B	2.78	1.54	1.47
4	B	601	HEM	CMC-C2C	2.71	1.56	1.50
4	A	601	HEM	C2A-C3A	-2.68	1.31	1.38
4	A	601	HEM	CAB-C3B	2.64	1.54	1.47
5	B	700	VD3	C14-C9	2.64	1.56	1.51
4	B	601	HEM	CMB-C2B	2.63	1.56	1.50
5	B	700	VD3	C4-C5	2.57	1.55	1.51
5	A	701	VD3	C4-C5	2.53	1.55	1.51
4	B	601	HEM	CAA-C2A	2.51	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	VD3	C4-C3	2.51	1.56	1.52
4	A	601	HEM	CAC-C3C	2.33	1.53	1.47
4	B	601	HEM	CAC-C3C	2.31	1.53	1.47
4	B	601	HEM	CHD-C1D	-2.30	1.33	1.39
5	A	701	VD3	C12-C13	-2.30	1.50	1.54
5	B	700	VD3	C19-C6	2.27	1.37	1.32
4	A	601	HEM	C3C-C2C	-2.26	1.32	1.37
4	A	601	HEM	CMA-C3A	2.24	1.55	1.50
4	A	601	HEM	CMB-C2B	2.20	1.55	1.50
5	A	701	VD3	C13-C14	-2.18	1.52	1.56
4	B	601	HEM	C3C-C4C	-2.14	1.42	1.46
5	A	701	VD3	C14-C9	2.12	1.55	1.51
5	A	701	VD3	C7-C5	2.09	1.42	1.36
4	A	601	HEM	CMD-C2D	2.06	1.55	1.50
4	B	601	HEM	CMD-C2D	2.05	1.55	1.50
4	A	601	HEM	O2A-CGA	-2.05	1.24	1.30
5	B	700	VD3	C13-C17	-2.03	1.51	1.55

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	700	VD3	C10-C9-C8	-11.39	112.96	125.27
5	A	701	VD3	C10-C9-C8	-10.07	114.39	125.27
5	A	701	VD3	C7-C5-C6	-6.70	118.27	125.15
5	B	700	VD3	C7-C5-C6	-5.78	119.22	125.15
5	A	701	VD3	C2-C1-C6	-5.49	103.95	111.45
5	A	701	VD3	C14-C9-C8	4.98	131.43	123.56
5	B	700	VD3	C13-C17-C20	-4.30	112.86	119.50
5	B	700	VD3	C12-C13-C17	-4.28	110.29	116.60
5	A	701	VD3	C4-C5-C6	4.23	118.67	113.86
5	B	700	VD3	C14-C9-C8	4.21	130.21	123.56
5	B	700	VD3	C4-C5-C6	3.90	118.30	113.86
5	B	700	VD3	C1-C6-C5	3.82	119.96	114.51
5	A	701	VD3	C11-C12-C13	-3.72	108.82	113.19
4	A	601	HEM	C4D-ND-C1D	3.69	109.58	105.21
4	B	601	HEM	C4D-ND-C1D	3.47	109.31	105.21
5	A	701	VD3	C16-C15-C14	-3.37	99.75	105.25
5	B	700	VD3	C8-C7-C5	-3.35	121.30	126.54
5	B	700	VD3	C2-C3-C4	3.21	114.80	110.29
4	A	601	HEM	C4C-C3C-C2C	3.14	109.54	106.81
5	A	701	VD3	C13-C17-C20	-3.09	114.73	119.50
5	A	701	VD3	C1-C6-C5	3.09	118.91	114.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	VD3	C12-C13-C17	-3.08	112.07	116.60
4	B	601	HEM	C1D-C2D-C3D	-3.04	103.78	106.98
5	A	701	VD3	C1-C6-C19	-2.92	117.76	122.42
4	B	601	HEM	CHD-C4C-NC	2.83	127.53	124.45
5	B	700	VD3	C1-C6-C19	-2.81	117.94	122.42
5	B	700	VD3	C13-C14-C9	-2.70	108.89	113.09
5	B	700	VD3	C11-C12-C13	-2.68	110.04	113.19
4	A	601	HEM	CHD-C4C-NC	2.66	127.34	124.45
5	B	700	VD3	C21-C20-C22	-2.59	106.33	110.34
5	B	700	VD3	C16-C15-C14	-2.46	101.24	105.25
5	A	701	VD3	C8-C7-C5	-2.46	122.70	126.54
4	B	601	HEM	CBD-CAD-C3D	-2.45	105.75	112.53
4	A	601	HEM	CAA-C2A-C1A	2.44	129.71	124.94
4	A	601	HEM	CAA-CBA-CGA	-2.37	107.38	113.67
4	A	601	HEM	C1D-C2D-C3D	-2.35	104.51	106.98
4	A	601	HEM	C4B-C3B-C2B	2.20	109.31	107.28
5	B	700	VD3	C16-C17-C13	-2.19	101.27	103.84
4	A	601	HEM	CBD-CAD-C3D	-2.17	106.54	112.53
4	B	601	HEM	CMD-C2D-C1D	2.16	128.41	125.03
4	B	601	HEM	CHC-C4B-NB	2.16	126.74	124.42
5	B	700	VD3	C15-C14-C13	-2.13	102.31	104.21
4	A	601	HEM	CAD-C3D-C4D	2.10	128.35	124.70
4	A	601	HEM	CMD-C2D-C1D	2.03	128.21	125.03

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	HEM	C1A-C2A-CAA-CBA
5	A	701	VD3	C7-C8-C9-C10
5	A	701	VD3	C7-C8-C9-C14
5	B	700	VD3	C7-C8-C9-C10
5	B	700	VD3	C7-C8-C9-C14
5	B	700	VD3	C13-C17-C20-C21
5	B	700	VD3	C16-C17-C20-C21
5	B	700	VD3	C16-C17-C20-C22
5	B	700	VD3	C13-C17-C20-C22
4	A	601	HEM	C3A-C2A-CAA-CBA
5	B	700	VD3	C23-C24-C25-C26
5	A	701	VD3	C22-C23-C24-C25
5	B	700	VD3	C23-C24-C25-C27
5	B	700	VD3	C21-C20-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	601	HEM	CAA-CBA-CGA-O2A
4	B	601	HEM	CAA-CBA-CGA-O1A
4	A	601	HEM	CAA-CBA-CGA-O2A
4	A	601	HEM	CAA-CBA-CGA-O1A
4	B	601	HEM	C2C-C3C-CAC-CBC

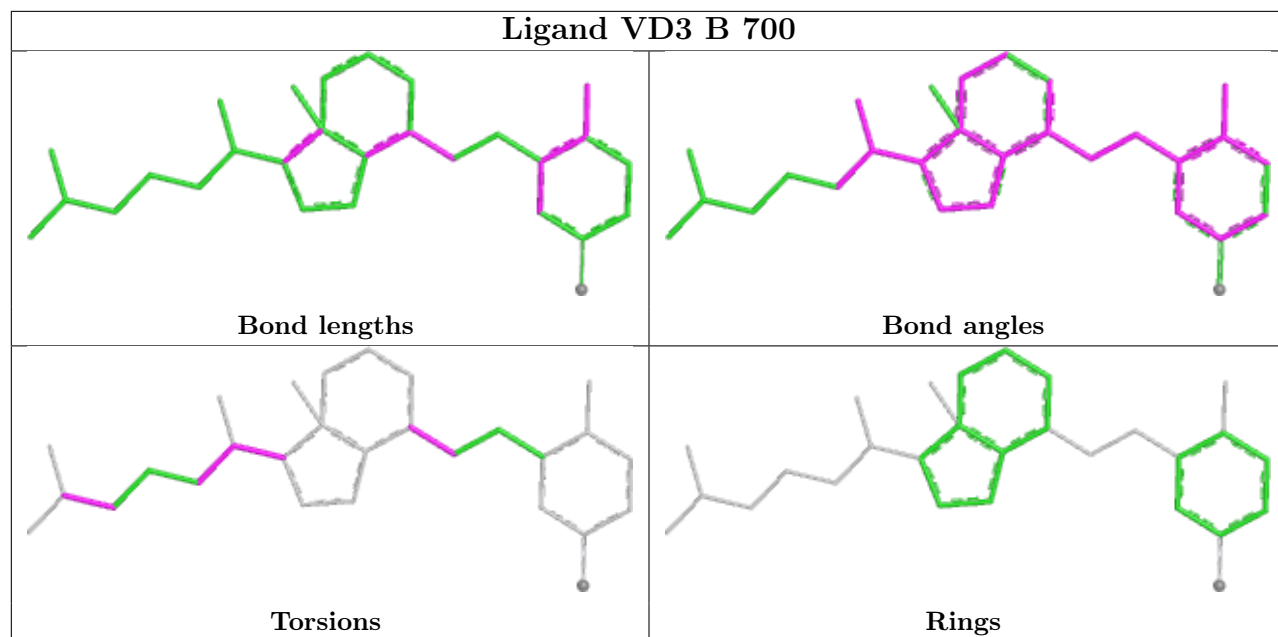
There are no ring outliers.

4 monomers are involved in 28 short contacts:

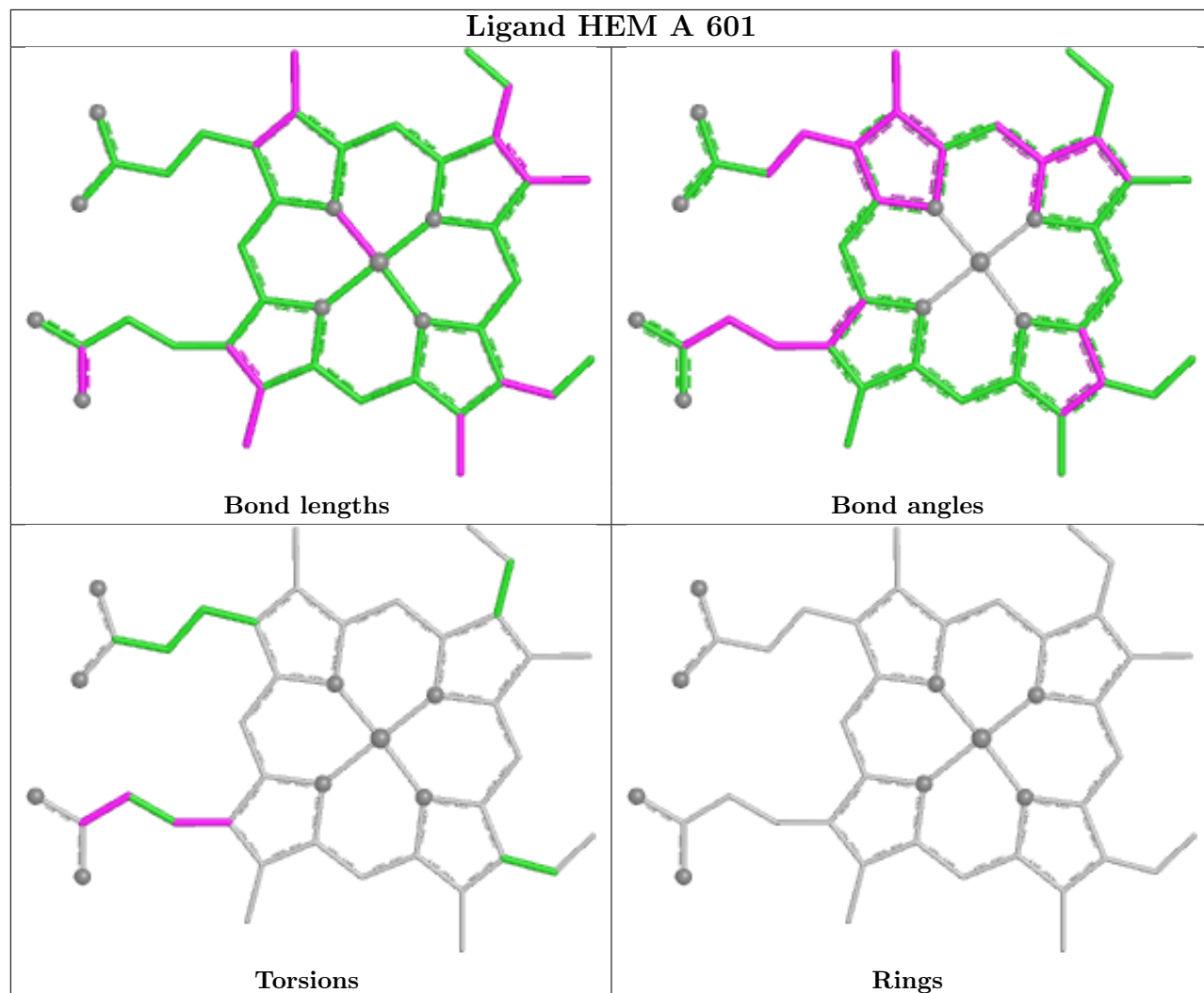
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	VD3	10	0
4	A	601	HEM	8	0
5	A	701	VD3	4	0
4	B	601	HEM	6	0

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.

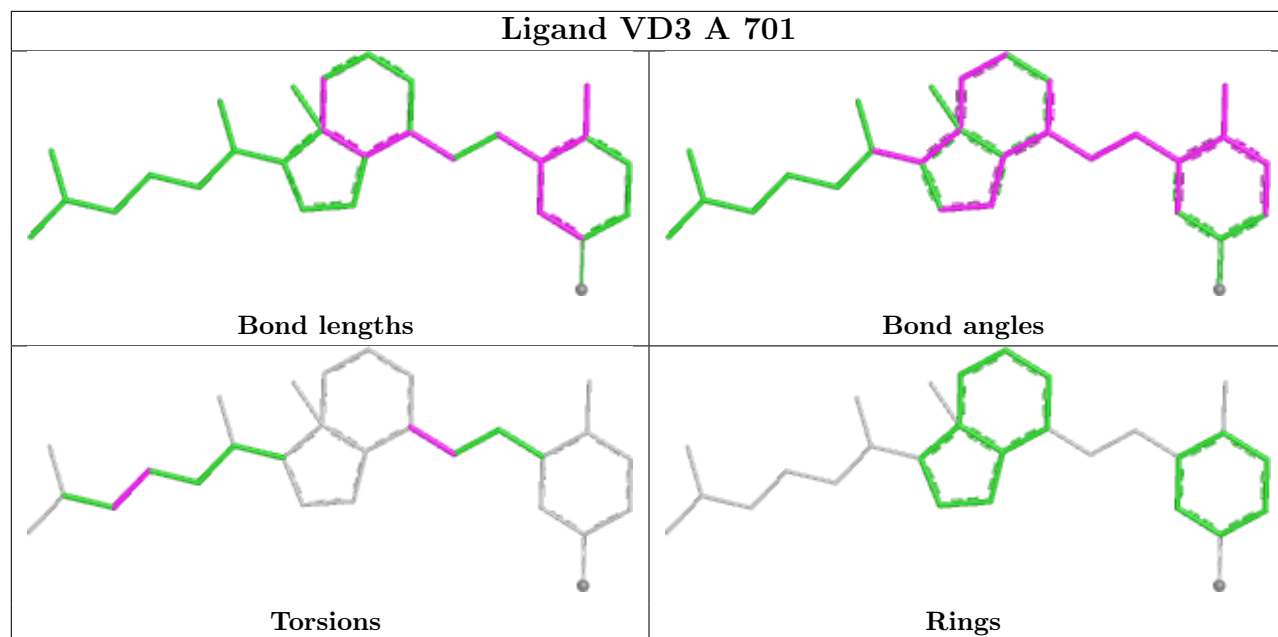
Ligand VD3 B 700



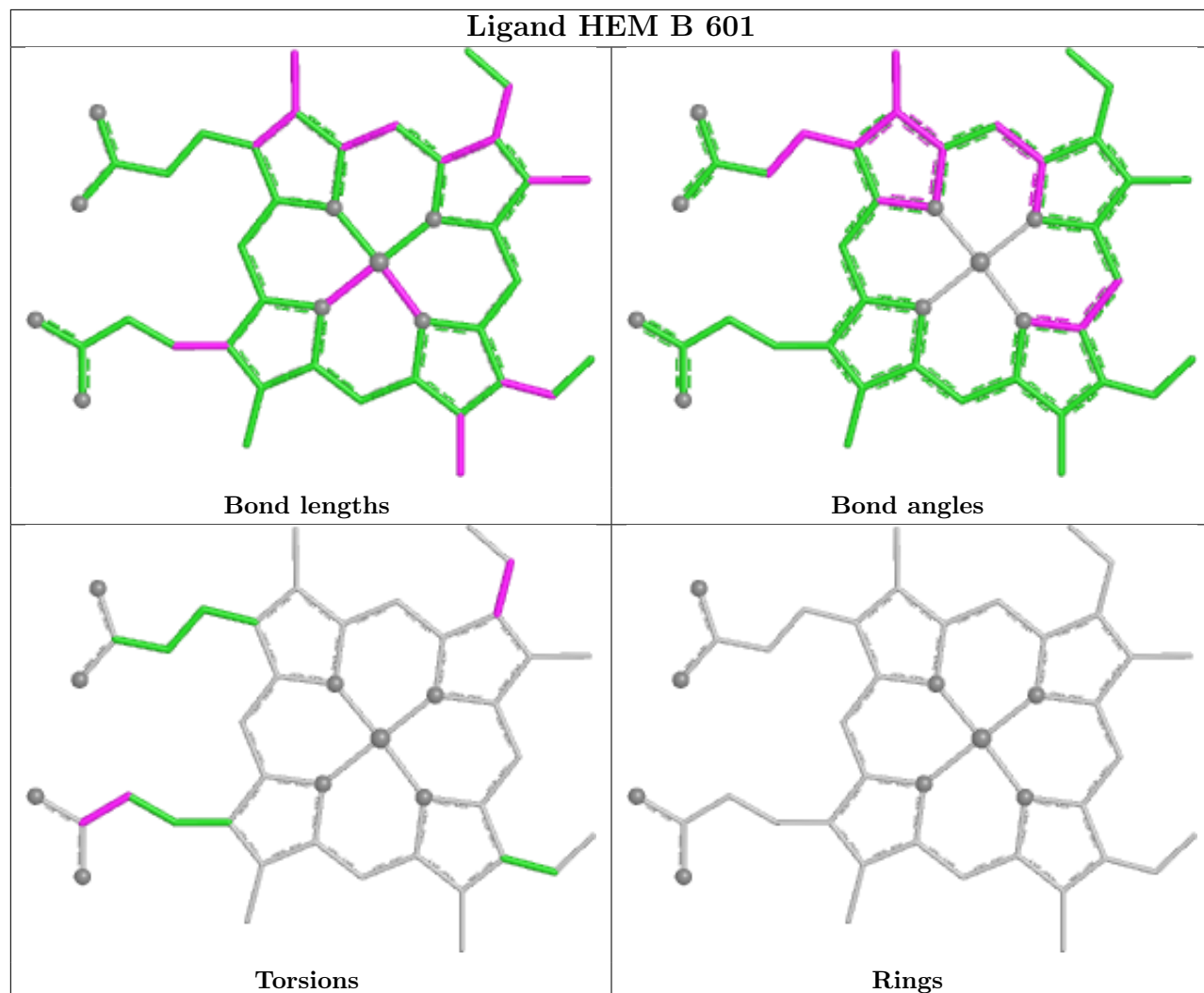
Ligand HEM A 601



Ligand VD3 A 701



Ligand HEM B 601



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	464/479 (96%)	-0.22	8 (1%) 69 60	17, 33, 57, 77	0
1	B	467/479 (97%)	-0.05	6 (1%) 75 66	21, 41, 61, 79	0
All	All	931/958 (97%)	-0.14	14 (1%) 72 63	17, 37, 60, 79	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	HIS	4.5
1	A	48	PHE	3.4
1	A	502	HIS	3.4
1	B	203	GLU	3.2
1	A	57	ALA	3.0
1	B	271	GLN	2.7
1	A	477	LEU	2.7
1	B	75	GLU	2.5
1	A	286	GLN	2.4
1	A	346	PRO	2.3
1	A	240	PHE	2.2
1	B	415	ARG	2.1
1	B	101	HIS	2.1
1	B	391	GLY	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](#)

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

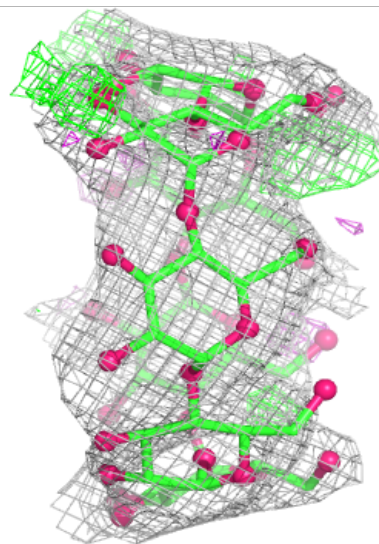
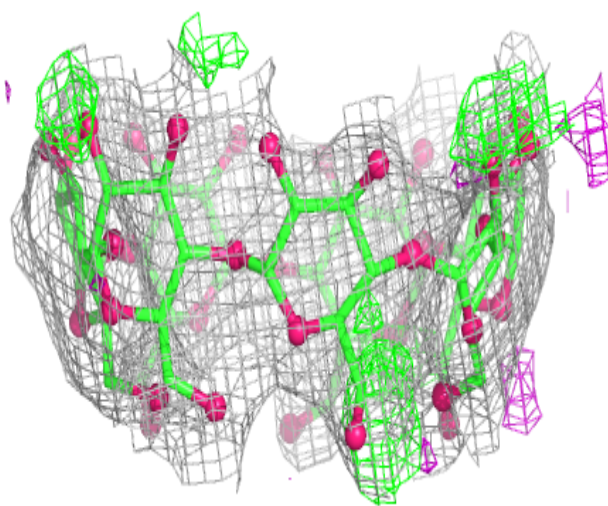
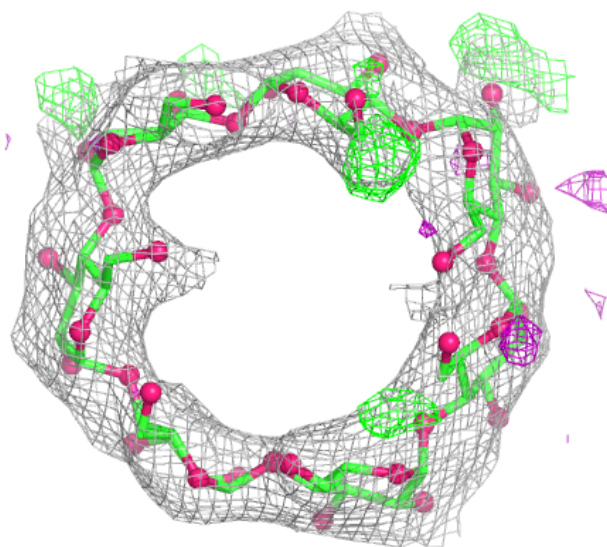
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

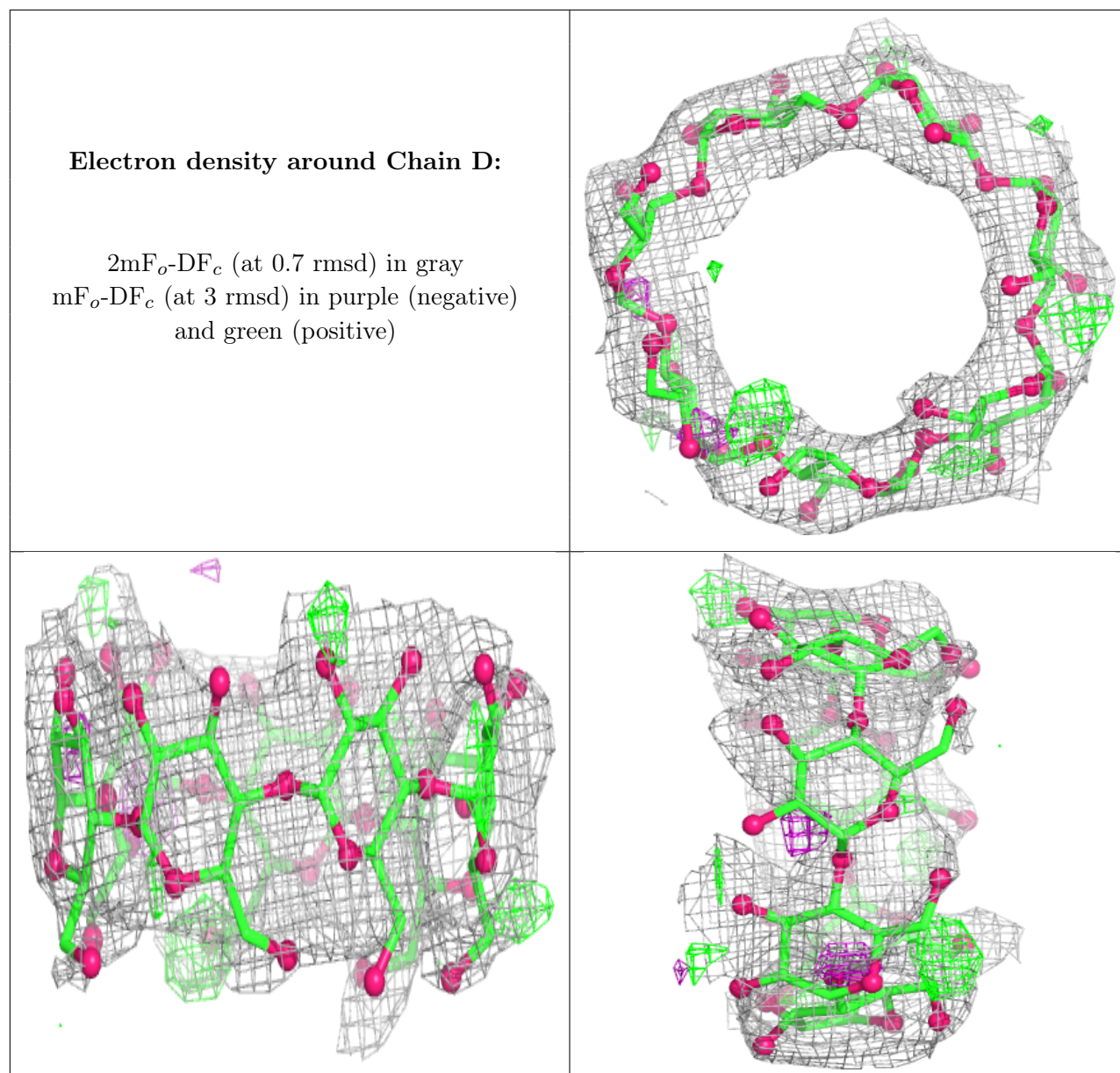
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	6	11/12	0.56	0.21	97,98,99,100	0
2	GLC	C	5	11/12	0.68	0.22	74,76,76,78	0
2	GLC	D	7	11/12	0.70	0.17	93,95,97,97	0
2	GLC	C	4	11/12	0.73	0.17	68,70,72,73	0
2	GLC	D	2	11/12	0.73	0.16	86,89,90,92	0
2	GLC	D	3	11/12	0.75	0.16	89,90,91,91	0
2	GLC	C	2	11/12	0.76	0.14	70,71,71,72	0
2	GLC	C	6	11/12	0.77	0.17	76,76,77,78	0
2	GLC	D	1	11/12	0.79	0.15	89,90,90,91	0
2	GLC	D	5	11/12	0.79	0.17	89,91,93,96	0
2	GLC	C	3	11/12	0.80	0.15	62,67,69,69	0
2	GLC	C	7	11/12	0.82	0.15	71,72,74,74	0
2	GLC	D	4	11/12	0.88	0.16	85,87,88,89	0
2	GLC	C	1	11/12	0.88	0.12	73,74,74,74	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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





6.4 Ligands ⓘ

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

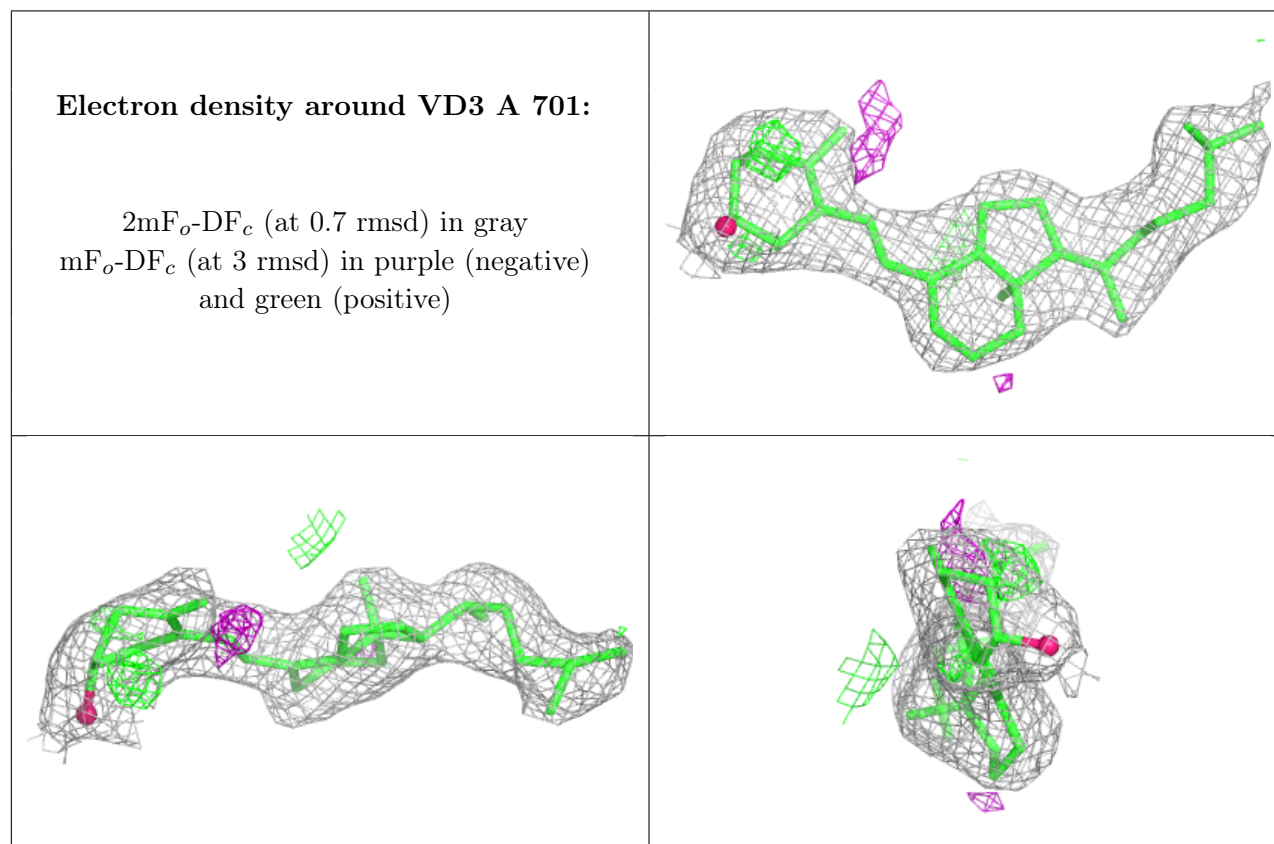
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UNX	B	6	1/1	-0.44	2.22	2,2,2,2	1
3	UNX	B	7	1/1	-0.21	1.51	2,2,2,2	1
3	UNX	A	3	1/1	0.05	1.56	2,2,2,2	1
3	UNX	B	5	1/1	0.29	1.50	2,2,2,2	1

Continued on next page...

Continued from previous page...

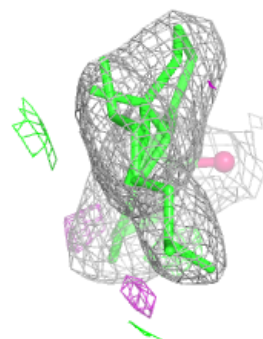
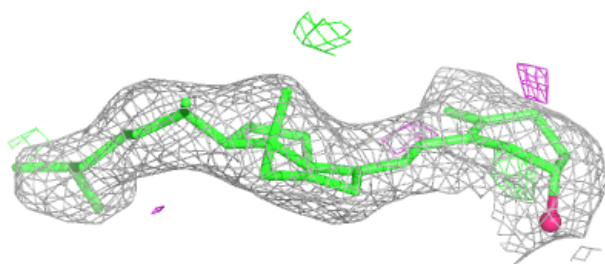
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNX	A	2	1/1	0.42	1.32	2,2,2,2	1
3	UNX	A	1	1/1	0.51	1.45	2,2,2,2	1
3	UNX	B	4	1/1	0.66	1.98	2,2,2,2	1
5	VD3	A	701	28/28	0.92	0.13	31,35,37,38	0
5	VD3	B	700	28/28	0.93	0.12	28,34,39,40	0
4	HEM	A	601	43/43	0.98	0.07	19,24,26,28	0
4	HEM	B	601	43/43	0.98	0.06	22,26,31,35	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.



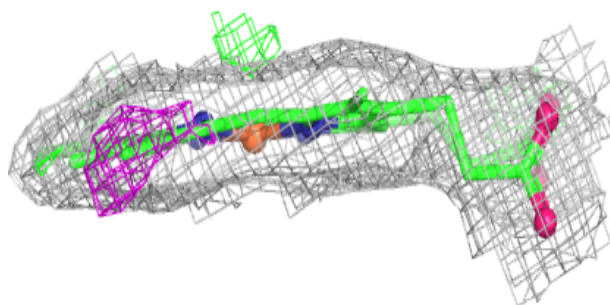
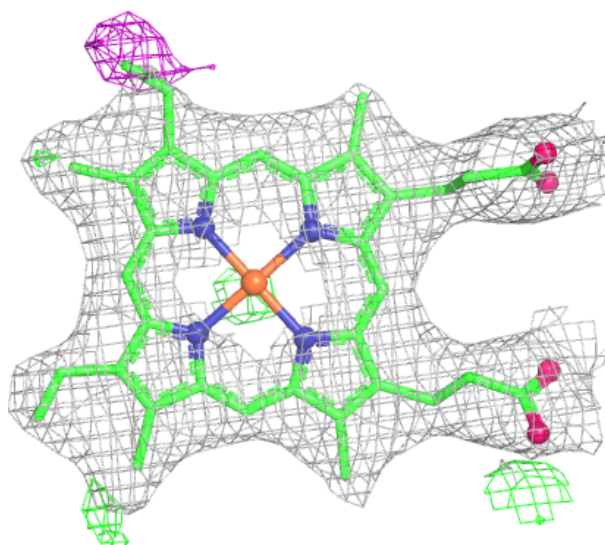
Electron density around VD3 B 700:

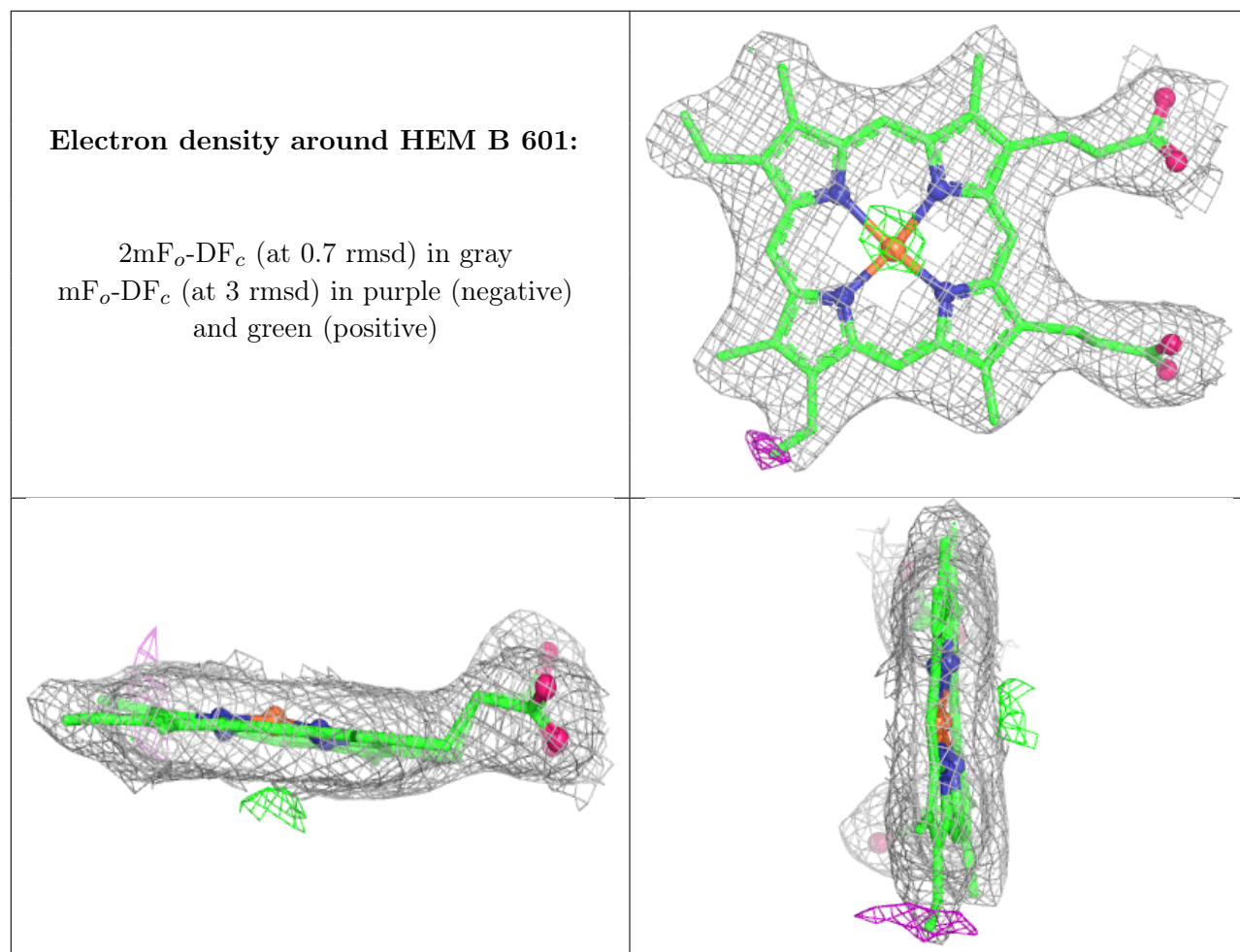
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 601:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.