



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:18 AM UTC

PDB ID : 8Z2U / pdb_00008z2u
Title : Crystal structure of trehalose synthase mutant E324D from *Deinococcus radiodurans* complexed with validoxylamine A (VAA)
Authors : Ye, L.C.; Chen, S.C.
Deposited on : 2024-04-13
Resolution : 2.90 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

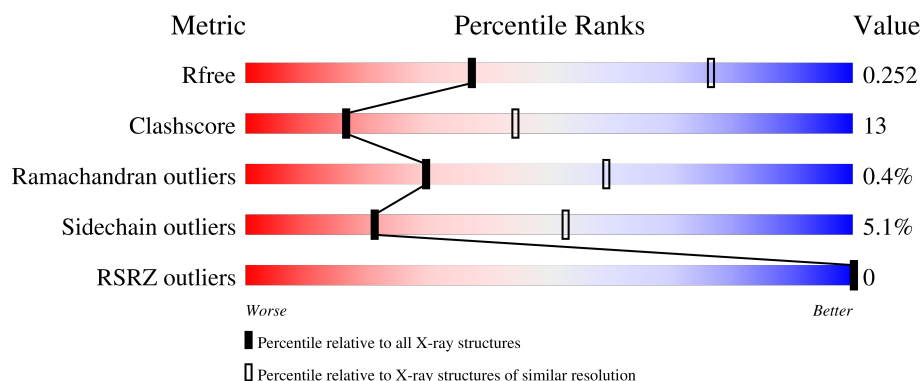
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	571	 68% 26% . .
1	B	571	 64% 30% . .
1	C	571	 65% 30% . .
1	D	571	 67% 27% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17712 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 maltose alpha-D-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4403	2817	751	819	16			
1	B	548	Total	C	N	O	S	0	0	0
			4403	2817	751	819	16			
1	C	548	Total	C	N	O	S	0	0	0
			4403	2817	751	819	16			
1	D	548	Total	C	N	O	S	0	0	0
			4403	2817	751	819	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP I3NX86
A	0	VAL	-	expression tag	UNP I3NX86
A	1	PRO	-	expression tag	UNP I3NX86
A	97	TRP	ARG	engineered mutation	UNP I3NX86
A	313	ILE	THR	engineered mutation	UNP I3NX86
A	324	ASP	GLU	engineered mutation	UNP I3NX86
A	380	VAL	ILE	engineered mutation	UNP I3NX86
A	553	SER	-	expression tag	UNP I3NX86
A	554	ARG	-	expression tag	UNP I3NX86
A	555	VAL	-	expression tag	UNP I3NX86
A	556	ASP	-	expression tag	UNP I3NX86
A	557	LYS	-	expression tag	UNP I3NX86
A	558	LEU	-	expression tag	UNP I3NX86
A	559	ALA	-	expression tag	UNP I3NX86
A	560	ALA	-	expression tag	UNP I3NX86
A	561	ALA	-	expression tag	UNP I3NX86
A	562	LEU	-	expression tag	UNP I3NX86
A	563	GLU	-	expression tag	UNP I3NX86
A	564	HIS	-	expression tag	UNP I3NX86
A	565	HIS	-	expression tag	UNP I3NX86
A	566	HIS	-	expression tag	UNP I3NX86

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Chain	Residue	Modelled	Actual	Comment	Reference
A	567	HIS	-	expression tag	UNP I3NX86
A	568	HIS	-	expression tag	UNP I3NX86
A	569	HIS	-	expression tag	UNP I3NX86
B	-1	MET	-	initiating methionine	UNP I3NX86
B	0	VAL	-	expression tag	UNP I3NX86
B	1	PRO	-	expression tag	UNP I3NX86
B	97	TRP	ARG	engineered mutation	UNP I3NX86
B	313	ILE	THR	engineered mutation	UNP I3NX86
B	324	ASP	GLU	engineered mutation	UNP I3NX86
B	380	VAL	ILE	engineered mutation	UNP I3NX86
B	553	SER	-	expression tag	UNP I3NX86
B	554	ARG	-	expression tag	UNP I3NX86
B	555	VAL	-	expression tag	UNP I3NX86
B	556	ASP	-	expression tag	UNP I3NX86
B	557	LYS	-	expression tag	UNP I3NX86
B	558	LEU	-	expression tag	UNP I3NX86
B	559	ALA	-	expression tag	UNP I3NX86
B	560	ALA	-	expression tag	UNP I3NX86
B	561	ALA	-	expression tag	UNP I3NX86
B	562	LEU	-	expression tag	UNP I3NX86
B	563	GLU	-	expression tag	UNP I3NX86
B	564	HIS	-	expression tag	UNP I3NX86
B	565	HIS	-	expression tag	UNP I3NX86
B	566	HIS	-	expression tag	UNP I3NX86
B	567	HIS	-	expression tag	UNP I3NX86
B	568	HIS	-	expression tag	UNP I3NX86
B	569	HIS	-	expression tag	UNP I3NX86
C	-1	MET	-	initiating methionine	UNP I3NX86
C	0	VAL	-	expression tag	UNP I3NX86
C	1	PRO	-	expression tag	UNP I3NX86
C	97	TRP	ARG	engineered mutation	UNP I3NX86
C	313	ILE	THR	engineered mutation	UNP I3NX86
C	324	ASP	GLU	engineered mutation	UNP I3NX86
C	380	VAL	ILE	engineered mutation	UNP I3NX86
C	553	SER	-	expression tag	UNP I3NX86
C	554	ARG	-	expression tag	UNP I3NX86
C	555	VAL	-	expression tag	UNP I3NX86
C	556	ASP	-	expression tag	UNP I3NX86
C	557	LYS	-	expression tag	UNP I3NX86
C	558	LEU	-	expression tag	UNP I3NX86
C	559	ALA	-	expression tag	UNP I3NX86
C	560	ALA	-	expression tag	UNP I3NX86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	561	ALA	-	expression tag	UNP I3NX86
C	562	LEU	-	expression tag	UNP I3NX86
C	563	GLU	-	expression tag	UNP I3NX86
C	564	HIS	-	expression tag	UNP I3NX86
C	565	HIS	-	expression tag	UNP I3NX86
C	566	HIS	-	expression tag	UNP I3NX86
C	567	HIS	-	expression tag	UNP I3NX86
C	568	HIS	-	expression tag	UNP I3NX86
C	569	HIS	-	expression tag	UNP I3NX86
D	-1	MET	-	initiating methionine	UNP I3NX86
D	0	VAL	-	expression tag	UNP I3NX86
D	1	PRO	-	expression tag	UNP I3NX86
D	97	TRP	ARG	engineered mutation	UNP I3NX86
D	313	ILE	THR	engineered mutation	UNP I3NX86
D	324	ASP	GLU	engineered mutation	UNP I3NX86
D	380	VAL	ILE	engineered mutation	UNP I3NX86
D	553	SER	-	expression tag	UNP I3NX86
D	554	ARG	-	expression tag	UNP I3NX86
D	555	VAL	-	expression tag	UNP I3NX86
D	556	ASP	-	expression tag	UNP I3NX86
D	557	LYS	-	expression tag	UNP I3NX86
D	558	LEU	-	expression tag	UNP I3NX86
D	559	ALA	-	expression tag	UNP I3NX86
D	560	ALA	-	expression tag	UNP I3NX86
D	561	ALA	-	expression tag	UNP I3NX86
D	562	LEU	-	expression tag	UNP I3NX86
D	563	GLU	-	expression tag	UNP I3NX86
D	564	HIS	-	expression tag	UNP I3NX86
D	565	HIS	-	expression tag	UNP I3NX86
D	566	HIS	-	expression tag	UNP I3NX86
D	567	HIS	-	expression tag	UNP I3NX86
D	568	HIS	-	expression tag	UNP I3NX86
D	569	HIS	-	expression tag	UNP I3NX86

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

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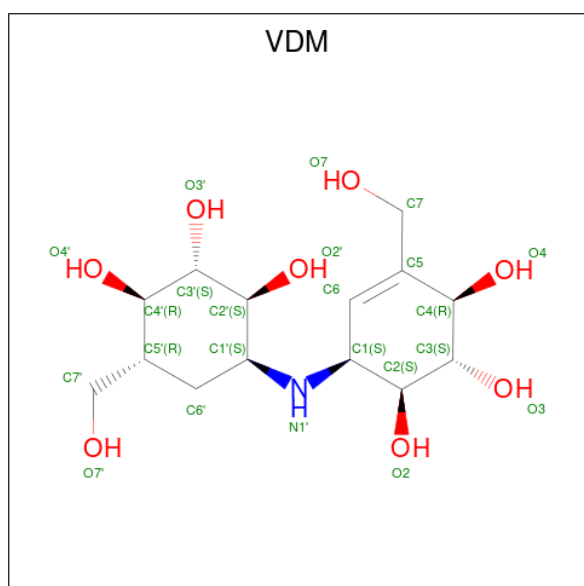
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (1S,2S,3R,6S)-4-(HYDROXYMETHYL)-6-{[(1S,2S,3S,4R,5R)-2,3,4-TRIHYDROXY-5-(HYDROXYMETHYL)CYCLOHEXYL]AMINO}CYCLOHEX-4-ENE-1,2,3-TRIOL (CCD ID: VDM) (formula: C₁₄H₂₅NO₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	14	1	8		
4	B	1	Total	C	N	O	0	0
			23	14	1	8		

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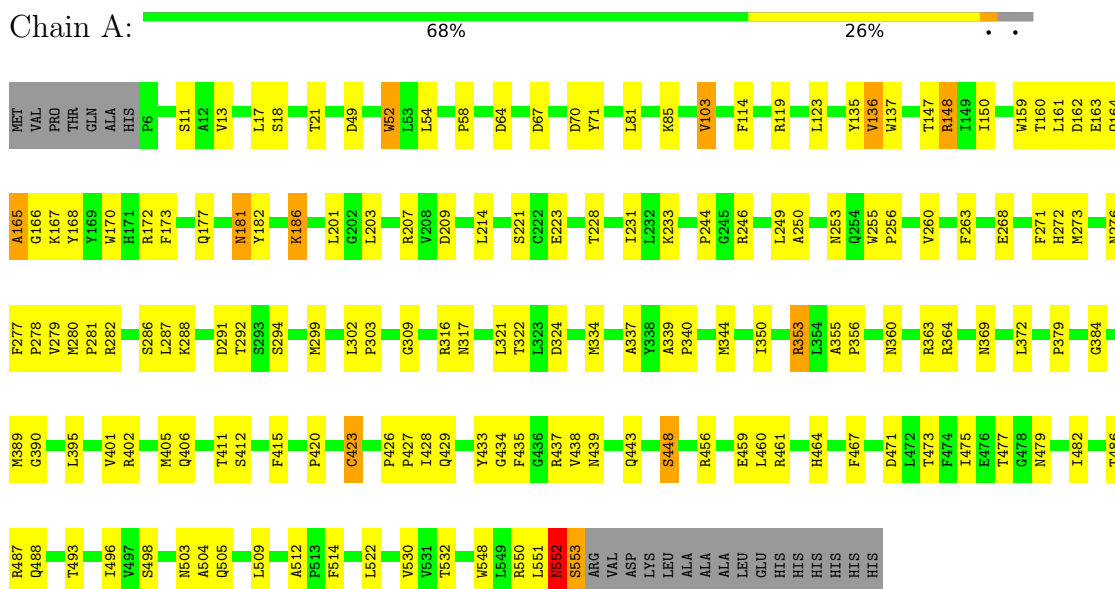
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			23	14	1	8		
4	D	1	Total	C	N	O	0	0
			23	14	1	8		

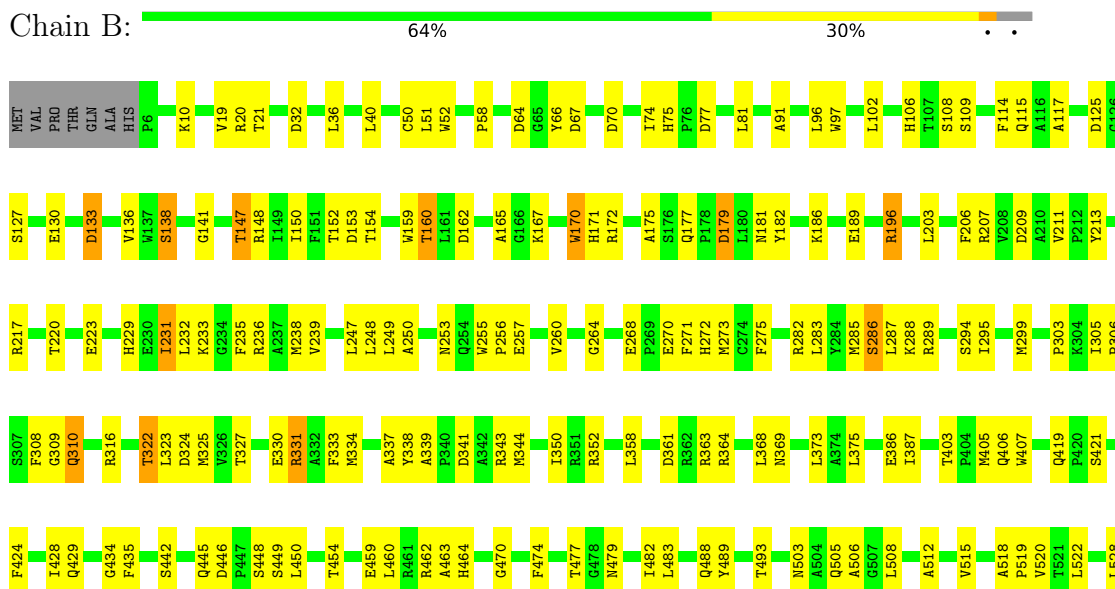
3 Residue-property plots [i](#)

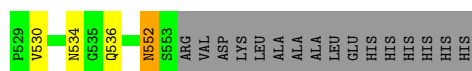
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: maltose alpha-D-glucosyltransferase



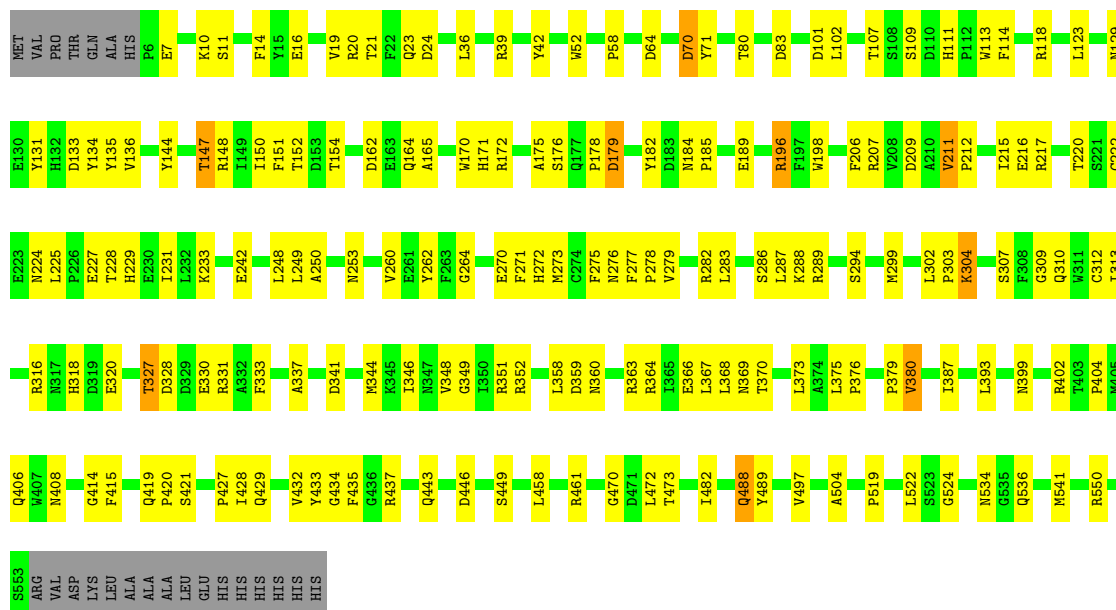
• Molecule 1: maltose alpha-D-glucosyltransferase





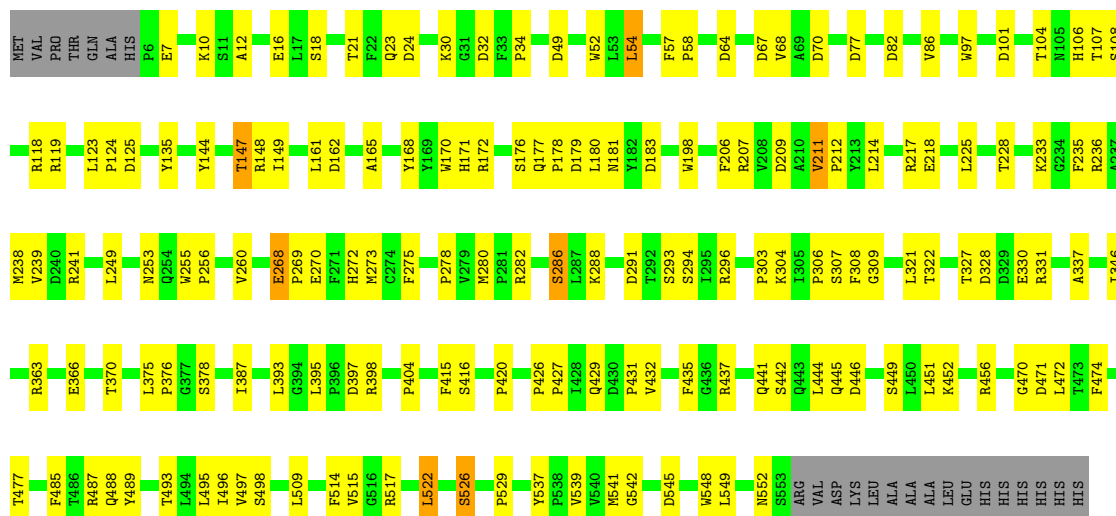
• Molecule 1: maltose alpha-D-glucosyltransferase

Chain C: 65% 30%



• Molecule 1: maltose alpha-D-glucosyltransferase

Chain D: 67% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.73Å 152.03Å 153.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.14 – 2.90 29.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.1 (29.14-2.90) 90.1 (29.14-2.90)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.180 , 0.252 0.180 , 0.252	Depositor DCC
R_{free} test set	3055 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 3.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17712	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: MG, CA, VDM

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	0.41	0/4536	0.59	0/6181
1	B	0.40	0/4536	0.59	0/6181
1	C	0.38	0/4536	0.56	0/6181
1	D	0.37	0/4536	0.55	0/6181
All	All	0.39	0/18144	0.57	0/24724

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Sidechain

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	4403	0	4199	102	0
1	B	4403	0	4199	131	0
1	C	4403	0	4199	123	0
1	D	4403	0	4199	104	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	25	1	0
4	B	23	0	25	2	0
4	C	23	0	25	1	0
4	D	23	0	25	1	0
All	All	17712	0	16896	445	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 13.

All (445) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:NH2	1:A:209:ASP:OD1	2.07	0.87
1:B:260:VAL:HG21	1:B:303:PRO:HD2	1.56	0.85
1:B:288:LYS:HG2	1:B:337:ALA:HB1	1.58	0.85
1:D:304:LYS:H	1:D:304:LYS:HE2	1.42	0.83
1:C:211:VAL:HG23	1:C:212:PRO:HD3	1.64	0.79
1:A:136:VAL:HG13	1:A:170:TRP:HB3	1.65	0.79
1:C:288:LYS:HG3	1:C:337:ALA:HB1	1.63	0.79
1:B:147:THR:HG21	1:B:170:TRP:HH2	1.48	0.78
1:A:233:LYS:HD3	1:A:268:GLU:HB3	1.64	0.78
1:D:497:VAL:HG12	1:D:541:MET:HE1	1.64	0.77
1:C:279:VAL:HG21	1:C:299:MET:HE3	1.65	0.77
1:B:52:TRP:CZ2	1:B:207:ARG:HD3	2.21	0.76
1:C:118:ARG:NH1	1:C:162:ASP:OD1	2.20	0.75
1:A:249:LEU:HD13	1:A:273:MET:HG3	1.69	0.74
1:D:207:ARG:HG3	1:D:249:LEU:HD23	1.71	0.73
1:A:287:LEU:HD21	1:A:364:ARG:HG2	1.70	0.73
1:D:214:LEU:HB2	1:D:228:THR:HG23	1.69	0.73
1:A:280:MET:HE1	1:A:321:LEU:HG	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PRO:O	1:A:282:ARG:NH1	2.22	0.71
1:A:395:LEU:HD21	1:A:426:PRO:HD2	1.73	0.71
1:B:534:ASN:HD22	1:B:534:ASN:H	1.39	0.71
1:D:288:LYS:HG2	1:D:337:ALA:HB1	1.72	0.71
1:A:477:THR:HG22	1:A:509:LEU:HD22	1.73	0.70
1:C:279:VAL:CG2	1:C:299:MET:HE3	2.22	0.70
1:C:224:ASN:OD1	1:C:262:TYR:OH	2.08	0.70
1:D:249:LEU:HD13	1:D:273:MET:HG3	1.72	0.70
1:D:514:PHE:HB3	1:D:517:ARG:HG3	1.74	0.69
1:A:475:ILE:HD11	1:A:486:THR:HG23	1.74	0.69
1:C:249:LEU:HD13	1:C:273:MET:HG3	1.73	0.69
1:A:256:PRO:HB3	1:A:302:LEU:HD23	1.74	0.69
1:B:207:ARG:HD2	1:B:275:PHE:HE2	1.58	0.68
1:D:58:PRO:HG2	1:D:70:ASP:HB3	1.75	0.68
1:B:247:LEU:HD11	1:B:273:MET:HG2	1.77	0.67
1:D:477:THR:HG22	1:D:509:LEU:HD22	1.77	0.66
1:B:171:HIS:CD2	1:B:175:ALA:HA	2.30	0.66
1:B:518:ALA:HB3	1:B:552:ASN:HD21	1.60	0.66
1:B:287:LEU:HD21	1:B:364:ARG:HG2	1.78	0.65
1:B:260:VAL:HG13	1:B:305:ILE:HG22	1.77	0.65
1:C:233:LYS:HG2	1:C:270:GLU:HG3	1.77	0.65
1:D:147:THR:HG21	1:D:170:TRP:HH2	1.61	0.65
1:D:497:VAL:CG1	1:D:541:MET:HE1	2.26	0.64
1:C:147:THR:HG21	1:C:170:TRP:HH2	1.62	0.64
1:B:446:ASP:HB3	1:B:449:SER:HB3	1.78	0.64
1:B:58:PRO:HG2	1:B:70:ASP:HB3	1.80	0.64
1:C:58:PRO:HG2	1:C:70:ASP:HB3	1.80	0.64
1:A:162:ASP:HB3	1:A:165:ALA:HB3	1.80	0.64
1:B:148:ARG:NH2	1:B:223:GLU:OE1	2.31	0.64
1:B:282:ARG:O	1:B:286:SER:HB3	1.97	0.64
1:D:488:GLN:HG3	1:D:493:THR:HG23	1.80	0.64
1:A:260:VAL:HG21	1:A:303:PRO:HD2	1.81	0.63
1:B:147:THR:HG21	1:B:170:TRP:CH2	2.32	0.63
1:A:255:TRP:HE3	1:A:256:PRO:HD3	1.63	0.63
1:C:428:ILE:HG22	1:C:434:GLY:HA2	1.80	0.62
1:C:16:GLU:OE2	1:C:318:HIS:ND1	2.32	0.62
1:C:171:HIS:O	1:C:171:HIS:ND1	2.31	0.62
1:D:67:ASP:HB3	1:D:177:GLN:HE21	1.64	0.62
1:C:217:ARG:HE	1:C:227:GLU:HG2	1.63	0.62
1:A:286:SER:HB2	1:A:291:ASP:O	1.99	0.62
1:A:456:ARG:NH1	1:B:343:ARG:HD3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASP:HB3	1:B:344:MET:HG3	1.80	0.62
1:D:446:ASP:HB3	1:D:449:SER:HB3	1.81	0.62
1:A:214:LEU:HB2	1:A:228:THR:HG23	1.82	0.62
1:A:464:HIS:CE1	1:A:522:LEU:HD22	2.36	0.61
1:C:346:ILE:HB	1:C:351:ARG:HD3	1.83	0.61
1:A:503:ASN:HD22	1:C:524:GLY:HA3	1.66	0.61
1:A:148:ARG:NH1	1:A:223:GLU:OE1	2.35	0.60
1:C:198:TRP:HB2	1:C:206:PHE:HZ	1.66	0.60
1:A:550:ARG:HH12	1:A:552:ASN:HD22	1.47	0.60
1:D:444:LEU:O	1:D:452:LYS:NZ	2.32	0.60
1:B:363:ARG:HE	1:D:363:ARG:HH21	1.48	0.60
1:C:123:LEU:HG	1:C:129:ASN:HB2	1.84	0.60
1:A:136:VAL:CG1	1:A:170:TRP:HB3	2.31	0.60
1:A:437:ARG:HG3	1:C:437:ARG:HA	1.83	0.60
1:D:249:LEU:HD21	1:D:275:PHE:CZ	2.37	0.60
1:C:299:MET:HE2	1:C:302:LEU:HD12	1.83	0.59
1:C:260:VAL:HG21	1:C:303:PRO:HD2	1.82	0.59
1:D:282:ARG:HG3	1:D:294:SER:HB2	1.83	0.59
1:B:125:ASP:OD1	1:B:127:SER:OG	2.14	0.59
1:C:80:THR:H	1:C:83:ASP:HB2	1.68	0.59
1:C:327:THR:HG23	1:C:330:GLU:CD	2.28	0.59
1:A:488:GLN:HG2	1:A:493:THR:HG23	1.84	0.59
1:C:250:ALA:HB2	1:C:271:PHE:CG	2.38	0.59
1:D:529:PRO:O	1:D:537:TYR:OH	2.19	0.59
1:D:67:ASP:HB2	1:D:108:SER:HB2	1.85	0.58
1:C:406:GLN:HG2	1:C:435:PHE:HB3	1.85	0.58
1:A:406:GLN:NE2	1:A:438:VAL:O	2.36	0.58
1:B:508:LEU:HD21	1:B:536:GLN:HB3	1.85	0.58
1:C:341:ASP:OD1	1:D:456:ARG:NH1	2.37	0.58
1:C:399:ASN:HA	1:C:402:ARG:HD2	1.86	0.57
1:C:216:GLU:HG3	1:C:222:CYS:HB3	1.86	0.57
1:C:277:PHE:N	1:C:278:PRO:HD2	2.19	0.57
1:B:182:TYR:HB3	1:B:231:ILE:HD12	1.87	0.57
1:D:470:GLY:HA2	1:D:489:TYR:HB2	1.85	0.57
1:C:114:PHE:CD2	1:C:178:PRO:HG3	2.40	0.56
1:C:109:SER:HA	1:C:114:PHE:HD2	1.70	0.56
1:B:534:ASN:H	1:B:534:ASN:ND2	2.02	0.56
1:D:397:ASP:OD2	1:D:398:ARG:NH2	2.28	0.56
1:B:207:ARG:HD2	1:B:275:PHE:CE2	2.40	0.56
1:B:160:THR:OG1	1:B:171:HIS:NE2	2.35	0.55
1:C:272:HIS:O	1:C:309:GLY:HA2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:PRO:HB3	1:C:427:PRO:HG2	1.88	0.55
1:A:282:ARG:HG3	1:A:294:SER:HB2	1.87	0.55
1:C:7:GLU:HB2	1:C:10:LYS:HG3	1.88	0.55
1:B:40:LEU:HD22	1:B:96:LEU:HD12	1.89	0.55
1:B:196:ARG:HG3	1:B:238:MET:CE	2.36	0.55
1:A:415:PHE:HE2	1:A:423:CYS:HB3	1.72	0.55
1:D:404:PRO:HB3	1:D:415:PHE:CG	2.42	0.54
1:A:137:TRP:HB3	1:A:167:LYS:HE2	1.89	0.54
1:B:91:ALA:O	1:B:96:LEU:HB2	2.08	0.54
1:D:328:ASP:OD1	1:D:331:ARG:NH2	2.41	0.54
1:B:106:HIS:CD2	1:B:177:GLN:HB3	2.43	0.54
1:B:136:VAL:CG2	1:B:170:TRP:HB3	2.38	0.54
1:A:428:ILE:HG22	1:A:434:GLY:HA2	1.90	0.54
1:D:57:PHE:HB2	1:D:68:VAL:HG13	1.90	0.54
1:B:10:LYS:HD3	1:B:310:GLN:HB2	1.90	0.53
1:B:136:VAL:HG23	1:B:170:TRP:HB3	1.90	0.53
1:A:244:PRO:O	1:A:246:ARG:NH1	2.41	0.53
1:D:517:ARG:HB3	1:D:552:ASN:O	2.08	0.53
1:A:272:HIS:O	1:A:309:GLY:HA2	2.08	0.53
1:C:408:ASN:HD21	1:C:414:GLY:HA3	1.74	0.53
1:D:52:TRP:CZ2	1:D:207:ARG:HD3	2.43	0.53
1:B:260:VAL:CG2	1:B:303:PRO:HD2	2.35	0.53
1:D:304:LYS:H	1:D:304:LYS:CE	2.17	0.53
1:D:255:TRP:HE3	1:D:256:PRO:HD3	1.73	0.53
1:D:207:ARG:HH21	1:D:209:ASP:HB2	1.72	0.52
1:A:339:ALA:HB2	1:A:350:ILE:HG12	1.92	0.52
1:B:306:PRO:HB2	1:B:308:PHE:CE1	2.44	0.52
1:C:519:PRO:HA	1:C:550:ARG:O	2.09	0.52
1:C:366:GLU:O	1:C:370:THR:HG23	2.09	0.52
1:B:229:HIS:HA	1:B:232:LEU:HD12	1.92	0.52
1:B:327:THR:HG23	1:B:330:GLU:OE1	2.08	0.52
1:B:463:ALA:HB3	1:B:464:HIS:CD2	2.44	0.52
1:D:236:ARG:HD3	1:D:270:GLU:O	2.09	0.52
1:D:107:THR:HG23	1:D:180:LEU:HD21	1.91	0.52
1:D:522:LEU:HD22	1:D:548:TRP:HB3	1.90	0.52
1:A:163:GLU:H	1:A:163:GLU:CD	2.16	0.52
1:B:109:SER:O	1:B:115:GLN:NE2	2.43	0.52
1:B:170:TRP:O	1:B:179:ASP:HB2	2.10	0.52
1:C:408:ASN:ND2	1:C:414:GLY:HA3	2.24	0.52
1:D:211:VAL:HG23	1:D:212:PRO:HD3	1.91	0.52
1:D:249:LEU:CD1	1:D:273:MET:HG3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TRP:CZ2	1:B:172:ARG:HD3	2.45	0.52
1:C:71:TYR:OH	1:C:107:THR:HG22	2.09	0.52
1:C:369:ASN:O	1:C:373:LEU:HG	2.10	0.52
1:D:161:LEU:HB2	1:D:168:TYR:CE1	2.45	0.52
1:B:255:TRP:HE3	1:B:256:PRO:HD3	1.74	0.51
1:B:363:ARG:NH2	1:D:363:ARG:HE	2.08	0.51
1:B:369:ASN:O	1:B:373:LEU:HG	2.10	0.51
1:B:519:PRO:HB2	1:B:528:LEU:HD12	1.92	0.51
1:A:250:ALA:HB2	1:A:271:PHE:CG	2.45	0.51
1:A:288:LYS:HD3	1:A:337:ALA:HB1	1.92	0.51
1:B:283:LEU:HA	1:B:295:ILE:HD11	1.91	0.51
1:D:183:ASP:OD2	1:D:217:ARG:NH1	2.31	0.51
1:D:327:THR:HG23	1:D:330:GLU:OE1	2.10	0.51
1:A:52:TRP:CD1	1:A:52:TRP:C	2.88	0.51
1:D:493:THR:HG21	1:D:514:PHE:HE2	1.75	0.51
1:A:13:VAL:H	1:A:49:ASP:HB2	1.75	0.51
1:B:477:THR:HG21	1:B:482:ILE:HG22	1.93	0.51
1:B:283:LEU:HD23	1:B:295:ILE:HD11	1.91	0.51
1:B:324:ASP:OD1	1:B:325:MET:HG2	2.11	0.51
1:D:260:VAL:HG11	1:D:303:PRO:HB2	1.91	0.51
1:D:395:LEU:HD11	1:D:426:PRO:HD2	1.92	0.51
1:A:18:SER:HB2	1:A:54:LEU:HD22	1.91	0.50
1:D:18:SER:HB2	1:D:54:LEU:HD22	1.92	0.50
1:B:153:ASP:OD1	1:B:153:ASP:N	2.42	0.50
1:B:339:ALA:HB2	1:B:350:ILE:HG12	1.93	0.50
1:B:406:GLN:HE22	1:B:428:ILE:HB	1.76	0.50
1:C:229:HIS:O	1:C:233:LYS:HG3	2.11	0.50
1:C:344:MET:SD	1:C:352:ARG:HD2	2.51	0.50
1:B:148:ARG:HH21	1:B:223:GLU:CD	2.18	0.50
1:B:236:ARG:HH12	1:B:308:PHE:HE2	1.58	0.50
1:C:196:ARG:HE	1:C:242:GLU:CD	2.19	0.50
1:C:52:TRP:CZ2	1:C:207:ARG:HD3	2.46	0.50
1:A:67:ASP:HB3	1:A:177:GLN:HG2	1.94	0.50
1:D:282:ARG:O	1:D:286:SER:HB3	2.11	0.50
1:A:71:TYR:OH	1:A:103:VAL:O	2.28	0.50
1:B:470:GLY:HA2	1:B:489:TYR:HB2	1.93	0.50
4:A:603:VDM:O2	4:A:603:VDM:H6'1	2.12	0.49
1:C:21:THR:HG23	1:C:404:PRO:HA	1.94	0.49
1:A:114:PHE:HB2	1:A:135:TYR:CZ	2.47	0.49
1:A:182:TYR:HB3	1:A:231:ILE:HD13	1.94	0.49
1:C:289:ARG:HG3	1:C:333:PHE:CZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:HB3	1:A:427:PRO:HG2	1.93	0.49
1:C:109:SER:HA	1:C:114:PHE:CD2	2.48	0.49
1:C:23:GLN:HE21	1:C:24:ASP:H	1.61	0.49
1:A:353:ARG:HG2	1:A:401:VAL:HG12	1.94	0.49
1:B:102:LEU:HB2	1:B:206:PHE:CD1	2.48	0.49
1:C:172:ARG:HD2	1:C:172:ARG:HA	1.49	0.49
1:B:282:ARG:HG3	1:B:294:SER:HB2	1.94	0.48
1:C:393:LEU:HD12	1:C:393:LEU:H	1.78	0.48
1:A:477:THR:HG21	1:A:482:ILE:HG22	1.94	0.48
1:A:496:ILE:HG23	1:A:548:TRP:CD1	2.47	0.48
1:C:10:LYS:NZ	1:C:307:SER:O	2.45	0.48
1:C:207:ARG:HD2	1:C:275:PHE:HE2	1.77	0.48
1:C:358:LEU:HD13	1:C:364:ARG:HB3	1.94	0.48
1:C:316:ARG:HH11	1:C:316:ARG:HA	1.77	0.48
1:A:439:ASN:O	1:A:443:GLN:HG3	2.13	0.48
1:B:217:ARG:O	1:B:220:THR:OG1	2.31	0.48
1:A:503:ASN:ND2	1:C:524:GLY:HA3	2.28	0.48
1:B:534:ASN:OD1	1:B:536:GLN:HG2	2.13	0.48
1:A:379:PRO:HD3	1:A:461:ARG:NH2	2.28	0.48
1:B:171:HIS:ND1	1:B:171:HIS:O	2.47	0.48
1:D:253:ASN:ND2	1:D:322:THR:HG21	2.29	0.48
1:A:148:ARG:NH2	1:A:324:ASP:OD2	2.46	0.48
1:A:467:PHE:O	1:A:487:ARG:NH2	2.44	0.48
1:B:233:LYS:HD2	1:B:268:GLU:HB3	1.95	0.48
1:B:236:ARG:NH1	1:B:270:GLU:O	2.37	0.48
1:C:253:ASN:HD22	4:C:603:VDM:H7C2	1.79	0.48
1:D:366:GLU:O	1:D:370:THR:HG23	2.14	0.47
1:A:58:PRO:HG2	1:A:70:ASP:HB3	1.96	0.47
1:A:340:PRO:HD2	1:A:344:MET:SD	2.54	0.47
1:B:247:LEU:HD11	1:B:273:MET:CG	2.44	0.47
1:C:282:ARG:O	1:C:286:SER:HB3	2.14	0.47
1:B:518:ALA:HB3	1:B:552:ASN:ND2	2.28	0.47
1:C:446:ASP:HB3	1:C:449:SER:HB3	1.95	0.47
1:C:482:ILE:HG23	1:C:541:MET:HE2	1.97	0.47
1:B:428:ILE:O	1:B:434:GLY:HA2	2.14	0.47
1:D:52:TRP:CE2	1:D:207:ARG:HD3	2.49	0.47
1:C:133:ASP:HB3	1:C:184:ASN:ND2	2.30	0.47
1:C:171:HIS:CD2	1:C:175:ALA:HA	2.49	0.47
1:C:432:VAL:HA	1:C:437:ARG:HH11	1.79	0.47
1:D:23:GLN:NE2	1:D:415:PHE:O	2.47	0.47
1:D:82:ASP:O	1:D:86:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:HH12	1:A:389:MET:CB	2.28	0.47
1:C:23:GLN:HE21	1:C:24:ASP:N	2.13	0.47
1:D:12:ALA:O	1:D:378:SER:HB3	2.14	0.47
1:B:52:TRP:CD1	1:B:52:TRP:C	2.92	0.47
1:B:233:LYS:CD	1:B:268:GLU:HB3	2.45	0.47
1:B:363:ARG:HH21	1:D:363:ARG:HE	1.64	0.47
1:D:291:ASP:OD1	1:D:293:SER:OG	2.24	0.47
1:C:432:VAL:HG13	1:C:437:ARG:HH12	1.80	0.46
1:A:147:THR:HG21	1:A:170:TRP:HH2	1.79	0.46
1:A:161:LEU:HD12	1:A:167:LYS:O	2.15	0.46
1:D:432:VAL:O	1:D:437:ARG:HD3	2.15	0.46
1:B:445:GLN:HE22	1:D:431:PRO:HG2	1.80	0.46
1:C:318:HIS:HD1	1:C:318:HIS:H	1.63	0.46
1:D:233:LYS:NZ	1:D:268:GLU:O	2.49	0.46
1:B:474:PHE:CE1	1:B:483:LEU:HD11	2.50	0.46
1:A:64:ASP:OD2	1:A:402:ARG:NH1	2.49	0.46
1:B:133:ASP:N	1:B:133:ASP:OD1	2.48	0.46
1:D:238:MET:HA	1:D:241:ARG:NH2	2.30	0.46
1:A:186:LYS:HD2	1:A:186:LYS:HA	1.64	0.46
1:A:316:ARG:NH1	1:A:317:ASN:H	2.13	0.46
1:C:373:LEU:HB3	1:C:461:ARG:HD2	1.98	0.46
1:A:159:TRP:CZ3	1:A:170:TRP:HB2	2.50	0.46
1:B:285:MET:HB2	1:B:334:MET:SD	2.56	0.46
1:D:30:LYS:HD3	1:D:77:ASP:CG	2.41	0.46
1:A:161:LEU:HB2	1:A:168:TYR:CE1	2.51	0.46
1:A:479:ASN:ND2	1:A:505:GLN:HB3	2.31	0.46
1:B:323:LEU:O	1:B:331:ARG:HD3	2.15	0.46
1:D:32:ASP:OD2	1:D:34:PRO:HD2	2.15	0.46
1:D:49:ASP:O	1:D:97:TRP:HE3	1.99	0.46
1:C:133:ASP:HB3	1:C:184:ASN:HD22	1.81	0.46
1:C:215:ILE:HG22	1:C:225:LEU:HD12	1.97	0.46
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.80	0.46
1:D:135:TYR:CD2	1:D:178:PRO:HB2	2.51	0.46
1:B:20:ARG:HD3	1:B:424:PHE:CZ	2.51	0.45
1:B:299:MET:HE2	1:B:375:LEU:HD22	1.98	0.45
1:A:488:GLN:CG	1:A:493:THR:HG23	2.47	0.45
1:B:20:ARG:HD3	1:B:424:PHE:CE1	2.51	0.45
1:C:118:ARG:NH2	1:C:164:GLN:HB3	2.30	0.45
1:A:18:SER:HB3	1:A:21:THR:HG22	1.98	0.45
1:A:52:TRP:CZ2	1:A:207:ARG:HD3	2.50	0.45
1:C:287:LEU:HD21	1:C:364:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:PRO:HG3	1:C:472:LEU:HB2	1.98	0.45
1:A:363:ARG:HH21	1:C:363:ARG:HH11	1.64	0.45
1:B:488:GLN:HG2	1:B:493:THR:HG23	1.98	0.45
1:C:131:TYR:HA	1:C:134:TYR:CD1	2.51	0.45
1:A:353:ARG:HG3	1:A:390:GLY:O	2.15	0.45
1:C:14:PHE:HB2	1:C:380:VAL:HB	1.99	0.45
1:D:306:PRO:HB2	1:D:308:PHE:CE1	2.52	0.45
1:A:276:ASN:HD21	1:A:299:MET:HE1	1.81	0.45
1:B:253:ASN:HD21	1:B:322:THR:HG21	1.81	0.45
1:C:358:LEU:HD11	1:C:368:LEU:HD12	1.99	0.45
1:D:24:ASP:HB3	1:D:416:SER:HB2	1.99	0.45
1:D:542:GLY:O	1:D:545:ASP:HB2	2.15	0.45
1:B:207:ARG:HG3	1:B:249:LEU:HD23	1.99	0.45
1:B:350:ILE:HG22	1:B:352:ARG:HG3	1.98	0.45
1:B:512:ALA:O	1:B:515:VAL:HG23	2.17	0.45
1:A:429:GLN:HG2	1:A:435:PHE:CE2	2.51	0.45
1:C:14:PHE:O	1:C:380:VAL:HA	2.16	0.45
1:C:207:ARG:HB2	1:C:249:LEU:HD23	1.99	0.45
1:A:182:TYR:HB3	1:A:231:ILE:CD1	2.46	0.45
1:A:530:VAL:O	1:A:532:THR:HG23	2.16	0.45
1:B:358:LEU:HD11	1:B:368:LEU:HD12	1.99	0.45
1:C:170:TRP:O	1:C:179:ASP:HB2	2.17	0.45
1:C:250:ALA:HB2	1:C:271:PHE:CD2	2.51	0.45
1:C:320:GLU:HG3	1:C:349:GLY:HA3	1.98	0.45
1:A:448:SER:OG	1:C:359:ASP:O	2.35	0.44
1:A:459:GLU:OE1	1:B:343:ARG:NH2	2.50	0.44
1:A:504:ALA:O	1:A:505:GLN:NE2	2.51	0.44
1:B:250:ALA:HB2	1:B:271:PHE:CG	2.51	0.44
1:D:233:LYS:HE2	1:D:270:GLU:OE2	2.17	0.44
4:D:603:VDM:H6'1	4:D:603:VDM:O2	2.18	0.44
1:B:162:ASP:HB3	1:B:165:ALA:HB3	2.00	0.44
1:C:162:ASP:OD2	1:C:165:ALA:N	2.40	0.44
1:C:52:TRP:CD1	1:C:52:TRP:C	2.94	0.44
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.88	0.44
1:D:10:LYS:NZ	1:D:307:SER:O	2.42	0.44
1:D:517:ARG:H	1:D:517:ARG:HG2	1.59	0.44
1:B:249:LEU:HD13	1:B:273:MET:HG3	2.00	0.44
1:B:428:ILE:HG22	1:B:434:GLY:HA2	1.99	0.44
1:B:503:ASN:O	1:B:505:GLN:HG2	2.18	0.44
1:C:429:GLN:HG2	1:C:435:PHE:CE2	2.53	0.44
1:C:522:LEU:HD23	1:C:522:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:GLU:HB2	1:D:52:TRP:CE3	2.52	0.44
1:A:52:TRP:CE2	1:A:207:ARG:HD3	2.53	0.44
1:A:164:GLN:O	1:A:166:GLY:N	2.51	0.44
1:B:235:PHE:O	1:B:239:VAL:HG23	2.17	0.44
1:D:376:PRO:HB3	1:D:487:ARG:NH2	2.33	0.44
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.86	0.44
1:A:334:MET:HE3	1:A:334:MET:HB3	1.82	0.44
1:D:217:ARG:HG2	1:D:225:LEU:HD13	1.99	0.44
1:D:106:HIS:HD2	1:D:177:GLN:HG2	1.83	0.43
1:D:235:PHE:O	1:D:239:VAL:HG23	2.19	0.43
1:D:272:HIS:O	1:D:309:GLY:HA2	2.18	0.43
1:A:172:ARG:HA	1:A:172:ARG:HD2	1.54	0.43
1:A:512:ALA:C	1:A:514:PHE:H	2.26	0.43
1:C:182:TYR:HB3	1:C:231:ILE:CD1	2.48	0.43
1:D:172:ARG:HA	1:D:172:ARG:HD2	1.68	0.43
1:A:280:MET:HB3	1:A:281:PRO:HD3	2.00	0.43
1:B:50:CYS:HA	1:B:97:TRP:O	2.18	0.43
1:D:170:TRP:CZ2	1:D:172:ARG:HD3	2.53	0.43
1:D:171:HIS:HA	1:D:179:ASP:OD1	2.18	0.43
1:A:437:ARG:HA	1:C:437:ARG:HG3	1.99	0.43
1:B:138:SER:O	1:B:167:LYS:HB3	2.18	0.43
1:B:479:ASN:ND2	1:B:506:ALA:O	2.41	0.43
1:C:211:VAL:HG11	1:C:271:PHE:CZ	2.52	0.43
1:C:20:ARG:NH1	1:C:20:ARG:HB2	2.33	0.43
1:D:198:TRP:HB2	1:D:206:PHE:HZ	1.83	0.43
1:D:7:GLU:OE1	1:D:10:LYS:HE3	2.18	0.43
1:D:375:LEU:HD23	1:D:375:LEU:HA	1.80	0.43
1:B:138:SER:OG	1:B:141:GLY:N	2.48	0.43
1:B:459:GLU:HA	1:B:462:ARG:NH2	2.33	0.43
1:C:328:ASP:OD1	1:C:331:ARG:NH1	2.51	0.43
1:C:482:ILE:HG23	1:C:541:MET:CE	2.49	0.43
1:D:471:ASP:OD1	1:D:488:GLN:HB2	2.19	0.43
1:B:323:LEU:HD22	1:B:334:MET:HG3	1.99	0.43
1:C:109:SER:N	1:C:176:SER:O	2.48	0.43
1:C:360:ASN:HB2	1:C:433:TYR:OH	2.18	0.43
1:C:504:ALA:HA	1:C:541:MET:O	2.19	0.43
1:D:118:ARG:HA	1:D:165:ALA:HB2	2.01	0.43
1:B:138:SER:HB3	1:B:159:TRP:CZ3	2.54	0.42
1:B:272:HIS:O	1:B:309:GLY:HA2	2.19	0.42
1:C:111:HIS:CE1	1:C:113:TRP:CD2	3.07	0.42
1:C:135:TYR:CD2	1:C:178:PRO:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ARG:HH21	1:D:124:PRO:HD3	1.84	0.42
1:D:236:ARG:NH1	1:D:269:PRO:HB2	2.34	0.42
1:B:74:ILE:O	1:B:75:HIS:C	2.62	0.42
1:B:288:LYS:HD3	1:B:338:TYR:CZ	2.54	0.42
1:C:304:LYS:HD2	1:C:304:LYS:HA	1.76	0.42
1:B:19:VAL:HG22	1:B:36:LEU:HD22	2.00	0.42
1:B:213:TYR:CE1	1:B:223:GLU:HG2	2.53	0.42
1:D:496:ILE:HD12	1:D:548:TRP:CD1	2.54	0.42
1:C:275:PHE:HE1	1:C:312:CYS:HG	1.64	0.42
1:C:470:GLY:HA2	1:C:489:TYR:HB2	2.01	0.42
1:A:119:ARG:HH11	1:A:123:LEU:HD22	1.84	0.42
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.77	0.42
1:B:361:ASP:HB3	1:B:364:ARG:HB2	2.01	0.42
1:B:503:ASN:ND2	1:D:526:SER:HB3	2.34	0.42
1:C:248:LEU:HD23	1:C:248:LEU:HA	1.81	0.42
1:C:283:LEU:HD23	1:C:283:LEU:HA	1.85	0.42
1:C:379:PRO:HD3	1:C:461:ARG:NH2	2.34	0.42
1:A:280:MET:CE	1:A:321:LEU:HG	2.43	0.42
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.92	0.42
1:B:253:ASN:ND2	1:B:322:THR:HG21	2.35	0.42
1:B:429:GLN:HG2	1:B:435:PHE:CE2	2.55	0.42
1:C:170:TRP:CZ2	1:C:172:ARG:HD3	2.54	0.42
1:D:387:ILE:HG22	1:D:451:LEU:HB2	2.00	0.42
1:A:181:ASN:C	1:A:181:ASN:ND2	2.76	0.42
1:A:355:ALA:HB3	1:A:356:PRO:HD3	2.00	0.42
1:C:217:ARG:O	1:C:220:THR:OG1	2.37	0.42
1:C:534:ASN:OD1	1:C:536:GLN:HG2	2.20	0.42
1:A:119:ARG:NH1	1:A:123:LEU:HD22	2.34	0.42
1:A:456:ARG:HG3	1:B:343:ARG:NH1	2.35	0.42
1:C:19:VAL:HG22	1:C:36:LEU:HD22	2.00	0.42
1:C:276:ASN:HD21	1:C:299:MET:CE	2.33	0.42
1:A:288:LYS:CD	1:A:337:ALA:HB1	2.48	0.42
1:A:360:ASN:HB2	1:A:433:TYR:OH	2.19	0.42
1:B:114:PHE:HA	1:B:117:ALA:HB3	2.02	0.42
1:B:257:GLU:H	1:B:257:GLU:CD	2.28	0.42
1:B:283:LEU:HD23	1:B:295:ILE:CD1	2.50	0.42
1:C:39:ARG:O	1:C:42:TYR:HB3	2.20	0.42
1:C:114:PHE:CE2	1:C:178:PRO:HG3	2.55	0.42
1:C:458:LEU:HD23	1:C:458:LEU:HA	1.89	0.42
1:D:429:GLN:HG2	1:D:435:PHE:CE2	2.54	0.42
1:A:286:SER:HB2	1:A:292:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LYS:HG2	1:B:270:GLU:HG3	2.01	0.41
1:B:450:LEU:O	1:B:454:THR:OG1	2.36	0.41
1:B:264:GLY:N	1:B:270:GLU:HB2	2.35	0.41
1:B:386:GLU:HG2	1:B:387:ILE:HG23	2.00	0.41
1:D:278:PRO:O	1:D:282:ARG:HD3	2.20	0.41
1:D:488:GLN:CG	1:D:493:THR:HG23	2.50	0.41
1:A:412:SER:HB3	1:A:427:PRO:HG3	2.02	0.41
1:B:32:ASP:OD1	1:B:32:ASP:N	2.53	0.41
1:C:277:PHE:N	1:C:278:PRO:CD	2.84	0.41
1:A:253:ASN:HB2	1:A:277:PHE:CD2	2.55	0.41
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.83	0.41
1:C:102:LEU:HD13	1:C:206:PHE:CE1	2.56	0.41
1:C:387:ILE:O	1:C:443:GLN:NE2	2.53	0.41
1:D:282:ARG:HG2	1:D:294:SER:O	2.21	0.41
1:D:441:GLN:O	1:D:445:GLN:HG3	2.21	0.41
1:D:495:LEU:N	1:D:549:LEU:O	2.47	0.41
1:B:67:ASP:HB2	1:B:108:SER:HB2	2.03	0.41
1:B:136:VAL:HG12	1:B:181:ASN:HB2	2.02	0.41
1:B:445:GLN:NE2	1:D:431:PRO:HG2	2.35	0.41
1:B:460:LEU:O	1:B:464:HIS:HD2	2.04	0.41
1:C:404:PRO:HB3	1:C:415:PHE:CG	2.56	0.41
1:D:296:ARG:HE	1:D:296:ARG:HB2	1.69	0.41
1:A:150:ILE:HG21	1:A:173:PHE:HE1	1.85	0.41
1:A:263:PHE:HE1	1:A:273:MET:HA	1.85	0.41
1:D:7:GLU:OE1	1:D:7:GLU:N	2.54	0.41
1:D:104:THR:OG1	1:D:214:LEU:HD21	2.21	0.41
1:A:471:ASP:OD1	1:A:488:GLN:HB2	2.20	0.41
1:B:182:TYR:HB3	1:B:231:ILE:CD1	2.50	0.41
1:C:150:ILE:HG22	1:C:151:PHE:CD1	2.56	0.41
1:D:123:LEU:HB3	1:D:124:PRO:HD2	2.03	0.41
1:A:81:LEU:O	1:A:85:LYS:HG3	2.20	0.41
1:A:299:MET:CE	1:A:302:LEU:HD12	2.51	0.41
1:B:316:ARG:HH11	1:B:316:ARG:HA	1.85	0.41
1:C:341:ASP:OD2	1:D:456:ARG:HD2	2.21	0.41
1:D:162:ASP:HB3	1:D:165:ALA:HB3	2.02	0.41
1:A:384:GLY:HA2	1:A:405:MET:HE1	2.02	0.40
1:B:75:HIS:ND1	1:B:77:ASP:HB2	2.36	0.40
1:C:488:GLN:HE21	1:C:488:GLN:HB2	1.62	0.40
1:D:280:MET:HE1	1:D:321:LEU:HA	2.02	0.40
1:D:420:PRO:HB3	1:D:427:PRO:HG2	2.03	0.40
1:B:51:LEU:N	1:B:97:TRP:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:TYR:HB3	4:B:603:VDM:O7'	2.21	0.40
1:B:405:MET:HG3	1:B:407:TRP:CE2	2.56	0.40
1:C:144:TYR:O	1:C:147:THR:HB	2.22	0.40
1:A:426:PRO:HA	1:A:427:PRO:HD2	1.96	0.40
1:B:209:ASP:OD1	4:B:603:VDM:HD	2.22	0.40
1:B:260:VAL:HG21	1:B:303:PRO:CD	2.41	0.40
1:B:288:LYS:HB3	1:B:333:PHE:HZ	1.86	0.40
1:C:185:PRO:O	1:C:189:GLU:HG2	2.20	0.40
1:A:552:ASN:HB2	1:A:553:SER:H	1.76	0.40
1:B:250:ALA:HB2	1:B:271:PHE:CD2	2.57	0.40
1:D:144:TYR:H	1:D:218:GLU:CD	2.29	0.40
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.69	0.40
1:B:186:LYS:HD2	1:B:186:LYS:HA	1.94	0.40
1:C:250:ALA:HB2	1:C:271:PHE:CD1	2.56	0.40
1:C:264:GLY:N	1:C:270:GLU:HB2	2.37	0.40
1:D:148:ARG:HG2	1:D:149:ILE:N	2.35	0.40
1:D:474:PHE:CD1	1:D:485:PHE:HB3	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	546/571 (96%)	517 (95%)	27 (5%)	2 (0%)	30	59
1	B	546/571 (96%)	516 (94%)	28 (5%)	2 (0%)	30	59
1	C	546/571 (96%)	511 (94%)	33 (6%)	2 (0%)	30	59
1	D	546/571 (96%)	514 (94%)	30 (6%)	2 (0%)	30	59
All	All	2184/2284 (96%)	2058 (94%)	118 (5%)	8 (0%)	30	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	552	ASN
1	A	165	ALA
1	B	552	ASN
1	C	70	ASP
1	D	125	ASP
1	B	211	VAL
1	D	346	ILE
1	C	348	VAL

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	465/484 (96%)	442 (95%)	23 (5%)	22	54
1	B	465/484 (96%)	436 (94%)	29 (6%)	16	46
1	C	465/484 (96%)	440 (95%)	25 (5%)	20	51
1	D	465/484 (96%)	447 (96%)	18 (4%)	28	63
All	All	1860/1936 (96%)	1765 (95%)	95 (5%)	21	53

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	17	LEU
1	A	52	TRP
1	A	103	VAL
1	A	136	VAL
1	A	148	ARG
1	A	160	THR
1	A	181	ASN
1	A	186	LYS
1	A	221	SER
1	A	279	VAL
1	A	322	THR
1	A	369	ASN
1	A	372	LEU

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Mol	Chain	Res	Type
1	A	411	THR
1	A	423	CYS
1	A	448	SER
1	A	460	LEU
1	A	473	THR
1	A	498	SER
1	A	551	LEU
1	A	552	ASN
1	A	553	SER
1	B	21	THR
1	B	64	ASP
1	B	130	GLU
1	B	133	ASP
1	B	138	SER
1	B	147	THR
1	B	150	ILE
1	B	152	THR
1	B	154	THR
1	B	160	THR
1	B	170	TRP
1	B	179	ASP
1	B	189	GLU
1	B	196	ARG
1	B	231	ILE
1	B	248	LEU
1	B	286	SER
1	B	289	ARG
1	B	310	GLN
1	B	322	THR
1	B	331	ARG
1	B	403	THR
1	B	419	GLN
1	B	421	SER
1	B	442	SER
1	B	448	SER
1	B	520	VAL
1	B	522	LEU
1	B	530	VAL
1	C	11	SER
1	C	64	ASP
1	C	101	ASP
1	C	136	VAL

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Mol	Chain	Res	Type
1	C	147	THR
1	C	148	ARG
1	C	152	THR
1	C	154	THR
1	C	179	ASP
1	C	196	ARG
1	C	209	ASP
1	C	211	VAL
1	C	228	THR
1	C	294	SER
1	C	304	LYS
1	C	310	GLN
1	C	313	ILE
1	C	327	THR
1	C	367	LEU
1	C	380	VAL
1	C	419	GLN
1	C	421	SER
1	C	473	THR
1	C	488	GLN
1	C	497	VAL
1	D	21	THR
1	D	54	LEU
1	D	64	ASP
1	D	101	ASP
1	D	147	THR
1	D	176	SER
1	D	181	ASN
1	D	211	VAL
1	D	268	GLU
1	D	286	SER
1	D	393	LEU
1	D	442	SER
1	D	472	LEU
1	D	498	SER
1	D	515	VAL
1	D	522	LEU
1	D	526	SER
1	D	539	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	164	GLN
1	A	181	ASN
1	A	441	GLN
1	A	464	HIS
1	A	479	ASN
1	A	488	GLN
1	A	505	GLN
1	B	192	HIS
1	B	253	ASN
1	B	310	GLN
1	B	406	GLN
1	B	429	GLN
1	B	445	GLN
1	B	464	HIS
1	B	503	ASN
1	C	45	ASN
1	C	158	ASN
1	C	310	GLN
1	C	441	GLN
1	C	488	GLN
1	D	115	GLN
1	D	158	ASN
1	D	164	GLN
1	D	177	GLN
1	D	253	ASN
1	D	276	ASN
1	D	399	ASN
1	D	441	GLN
1	D	445	GLN
1	D	503	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - 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	$\# Z > 2$
4	VDM	A	603	-	24,24,24	0.78	2 (8%)	26,35,35	1.24	2 (7%)
4	VDM	D	603	-	24,24,24	0.82	2 (8%)	26,35,35	1.72	5 (19%)
4	VDM	C	603	-	24,24,24	0.79	2 (8%)	26,35,35	1.52	5 (19%)
4	VDM	B	603	-	24,24,24	0.79	2 (8%)	26,35,35	1.68	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VDM	A	603	-	-	1/8/48/48	0/2/2/2
4	VDM	D	603	-	-	5/8/48/48	0/2/2/2
4	VDM	C	603	-	-	3/8/48/48	0/2/2/2
4	VDM	B	603	-	-	1/8/48/48	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	VDM	C1'-N1'	2.61	1.52	1.47
4	A	603	VDM	C1'-N1'	2.51	1.51	1.47
4	D	603	VDM	C1'-N1'	2.47	1.51	1.47
4	B	603	VDM	C1'-N1'	2.47	1.51	1.47
4	A	603	VDM	C1'-N1'	2.45	1.52	1.47
4	C	603	VDM	C1'-N1'	2.44	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	VDM	C1'-N1'	2.36	1.51	1.47
4	C	603	VDM	C1'-N1'	2.33	1.51	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	VDM	C5'-C6'-C1'	5.07	115.07	108.53
4	C	603	VDM	C5'-C6'-C1'	4.64	114.52	108.53
4	B	603	VDM	C5'-C6'-C1'	4.63	114.51	108.53
4	D	603	VDM	C3'-C2'-C1'	-4.44	104.51	111.02
4	A	603	VDM	C5'-C6'-C1'	4.27	114.05	108.53
4	B	603	VDM	C3'-C2'-C1'	-3.89	105.32	111.02
4	B	603	VDM	C6'-C5'-C7'	3.15	117.58	111.86
4	C	603	VDM	C6'-C5'-C7'	3.07	117.43	111.86
4	C	603	VDM	C3'-C2'-C1'	-3.02	106.58	111.02
4	B	603	VDM	C6'-C1'-C2'	2.89	115.85	109.89
4	D	603	VDM	C6'-C1'-C2'	2.71	115.47	109.89
4	D	603	VDM	C6-C1-N1'	2.48	114.34	110.68
4	A	603	VDM	C3'-C2'-C1'	-2.38	107.53	111.02
4	C	603	VDM	C6'-C1'-C2'	2.33	114.68	109.89
4	D	603	VDM	C6'-C1'-N1'	-2.15	107.56	112.33
4	C	603	VDM	C6'-C1'-N1'	-2.06	107.76	112.33

There are no chirality outliers.

All (10) torsion outliers are listed below:

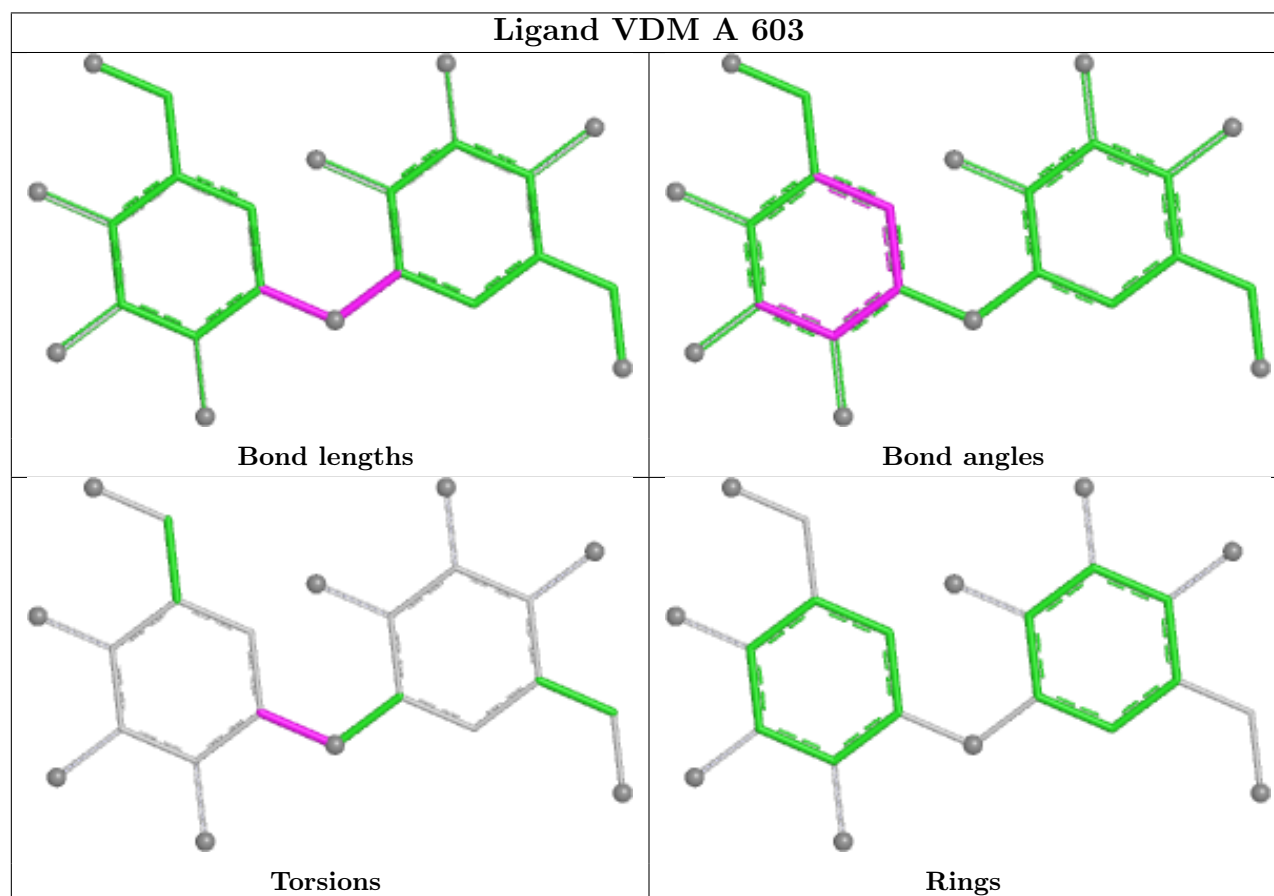
Mol	Chain	Res	Type	Atoms
4	A	603	VDM	C6'-C1'-N1'-C1
4	B	603	VDM	C6'-C1'-N1'-C1
4	C	603	VDM	C2-C1-N1'-C1'
4	C	603	VDM	C6'-C1'-N1'-C1
4	D	603	VDM	C6-C5-C7-O7
4	D	603	VDM	C2-C1-N1'-C1'
4	C	603	VDM	C6'-C5'-C7'-O7'
4	D	603	VDM	C6'-C5'-C7'-O7'
4	D	603	VDM	C6'-C1'-N1'-C1
4	D	603	VDM	C4-C5-C7-O7

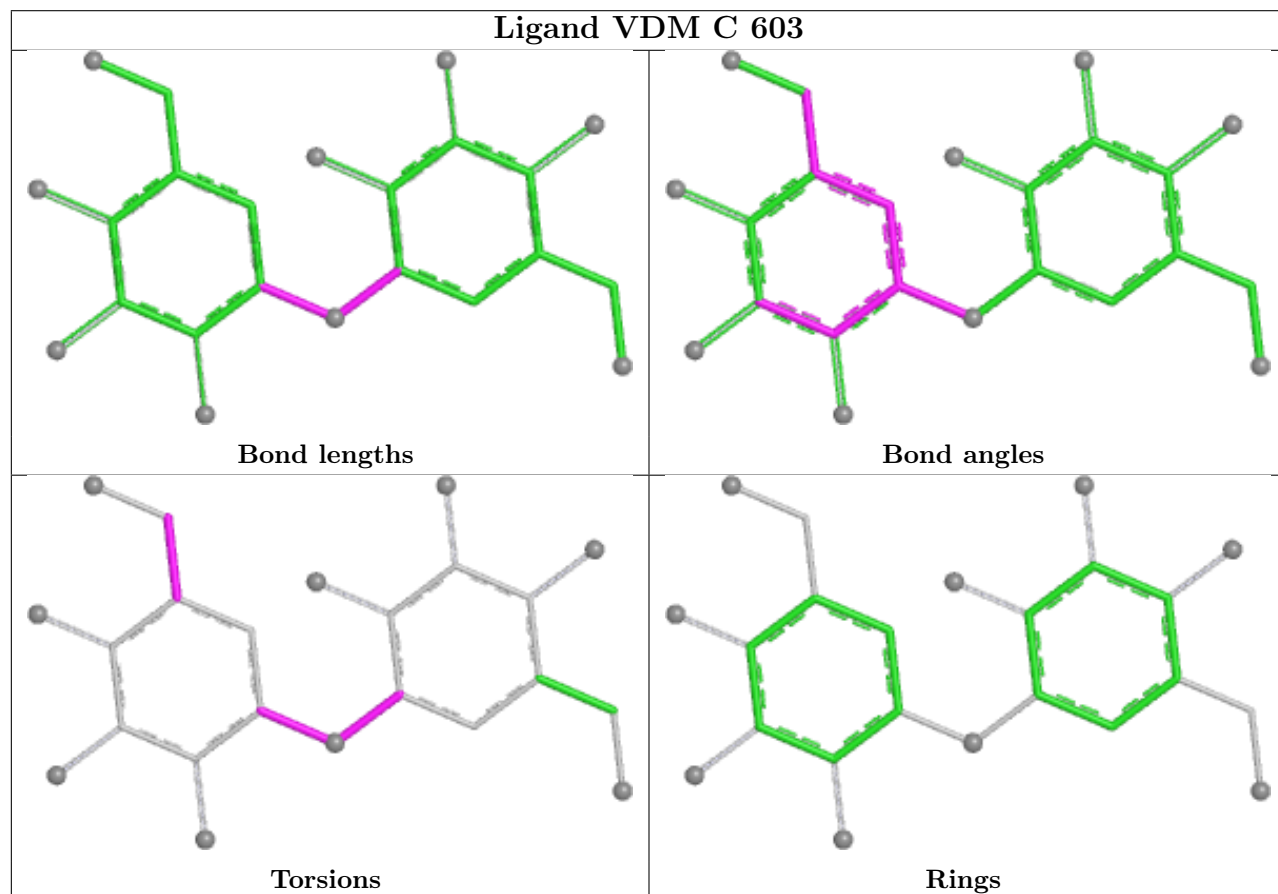
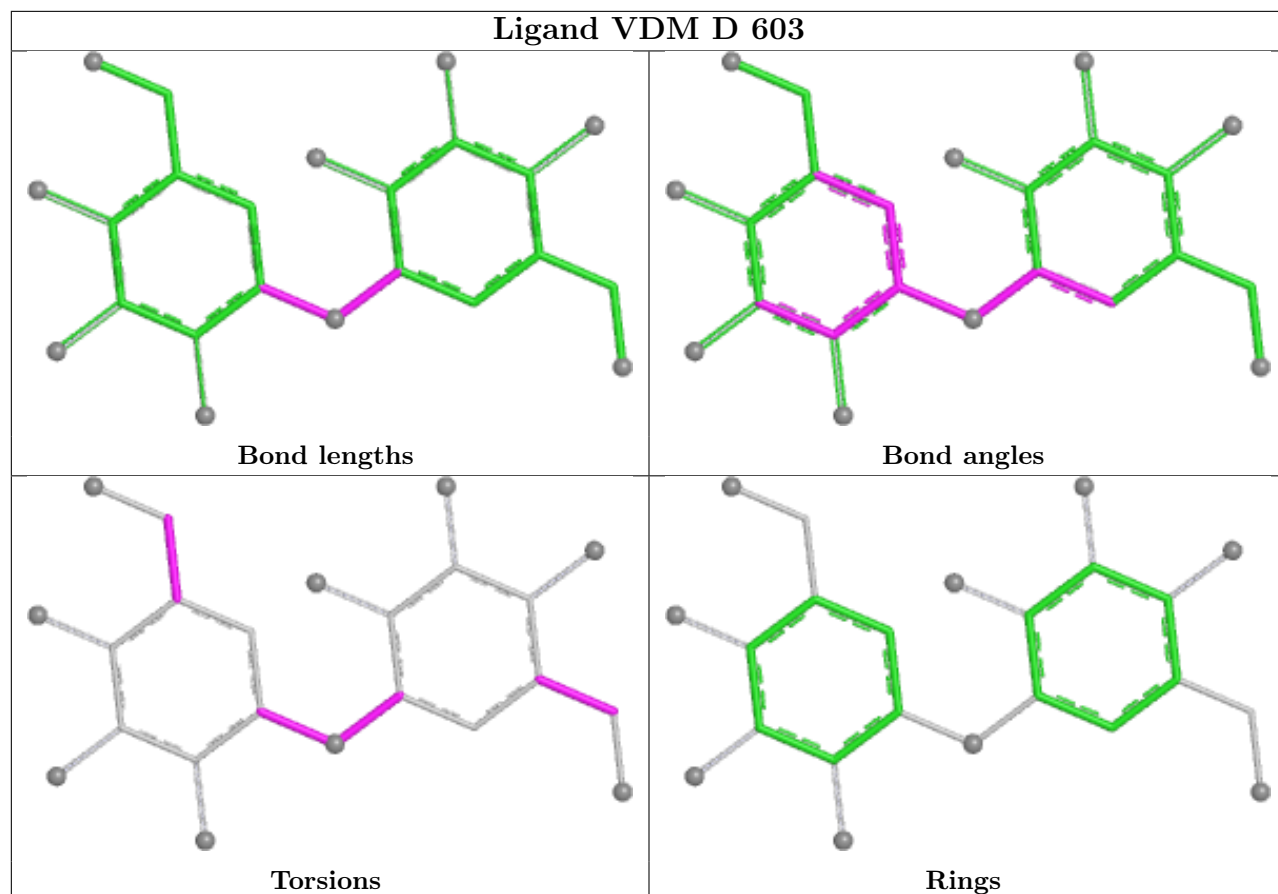
There are no ring outliers.

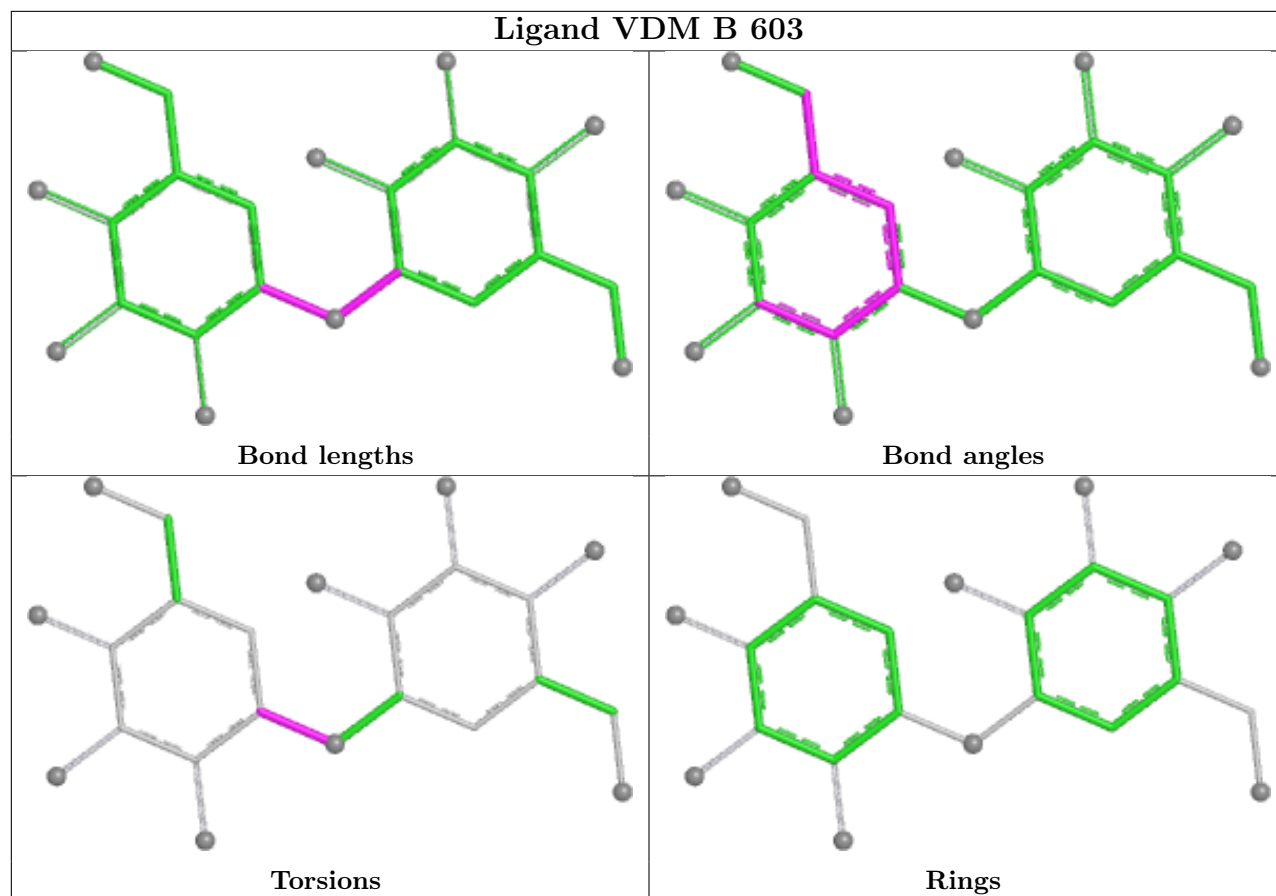
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	VDM	1	0
4	D	603	VDM	1	0
4	C	603	VDM	1	0
4	B	603	VDM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	548/571 (95%)	-1.91	0 100 100	9, 20, 34, 53	0
1	B	548/571 (95%)	-1.91	0 100 100	8, 21, 35, 49	0
1	C	548/571 (95%)	-1.85	0 100 100	9, 27, 56, 85	0
1	D	548/571 (95%)	-1.88	0 100 100	7, 25, 46, 75	0
All	All	2192/2284 (95%)	-1.89	0 100 100	7, 22, 45, 85	0

There are no RSRZ outliers to report.

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
2	CA	A	601	1/1	1.00	0.01	28,28,28,28	0
2	CA	B	601	1/1	1.00	0.03	32,32,32,32	0
2	CA	C	601	1/1	1.00	0.01	41,41,41,41	0
2	CA	D	601	1/1	1.00	0.01	28,28,28,28	0

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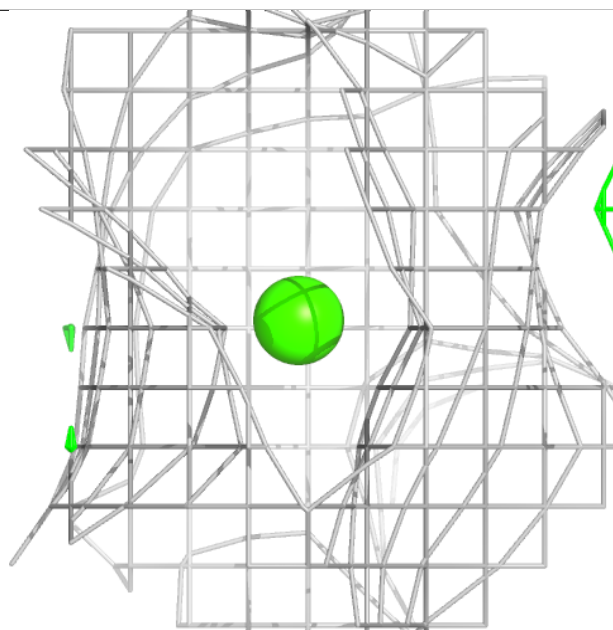
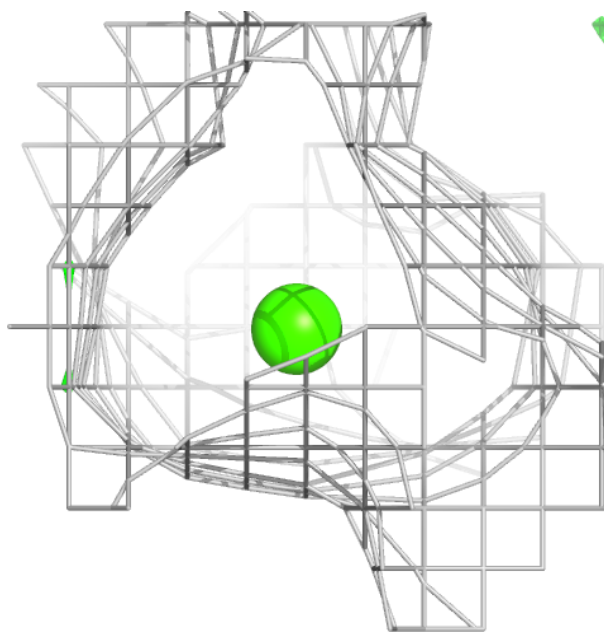
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	602	1/1	1.00	0.02	18,18,18,18	0
3	MG	B	602	1/1	1.00	0.02	27,27,27,27	0
3	MG	C	602	1/1	1.00	0.01	23,23,23,23	0
3	MG	D	602	1/1	1.00	0.01	20,20,20,20	0
4	VDM	A	603	23/23	1.00	0.02	20,29,38,41	0
4	VDM	B	603	23/23	1.00	0.02	20,26,33,42	0
4	VDM	C	603	23/23	1.00	0.03	26,39,48,58	0
4	VDM	D	603	23/23	1.00	0.03	25,31,37,40	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.

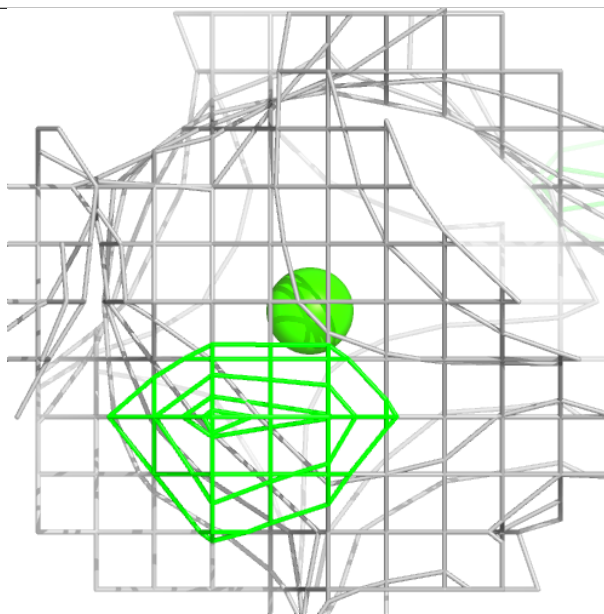
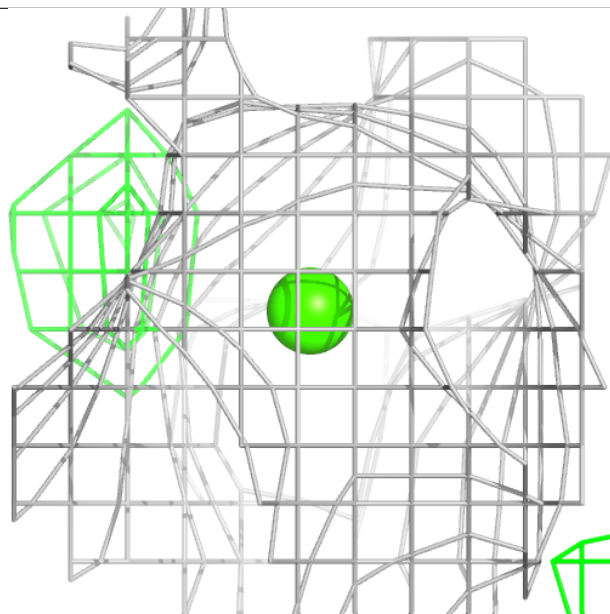
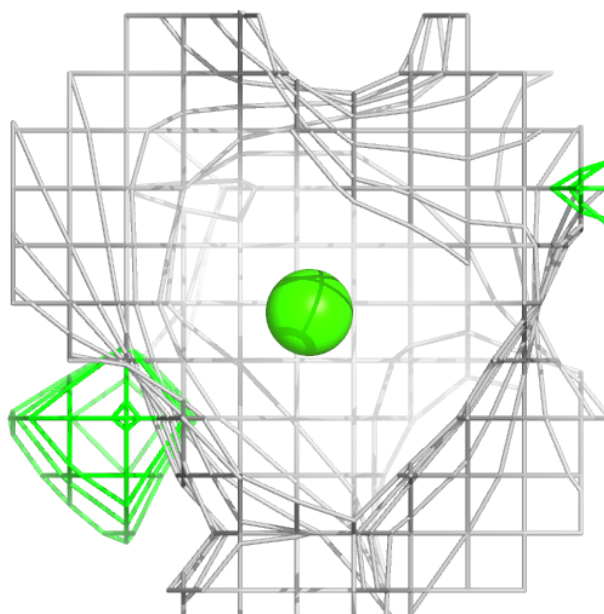
Electron density around CA A 601:

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



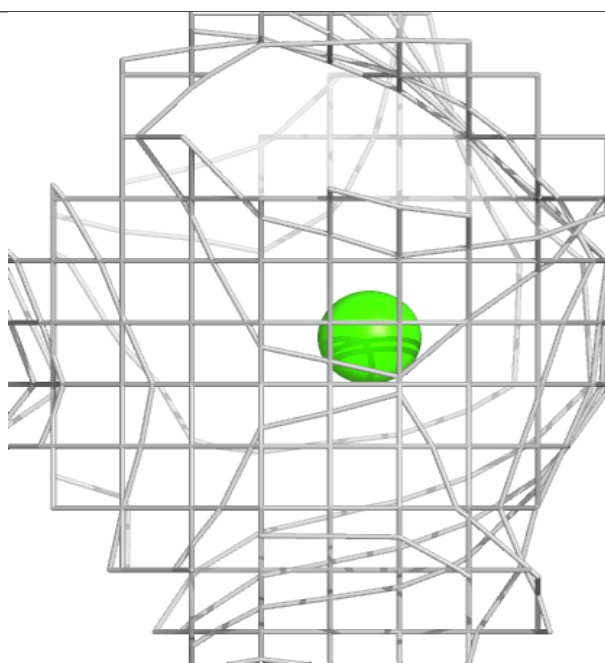
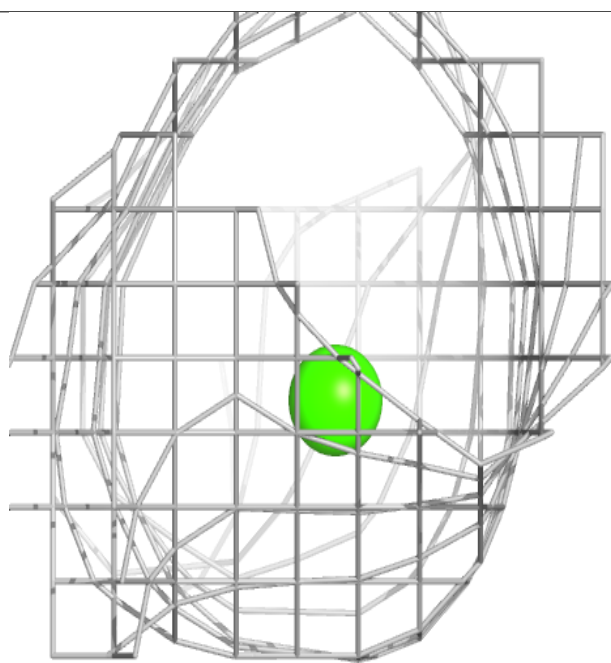
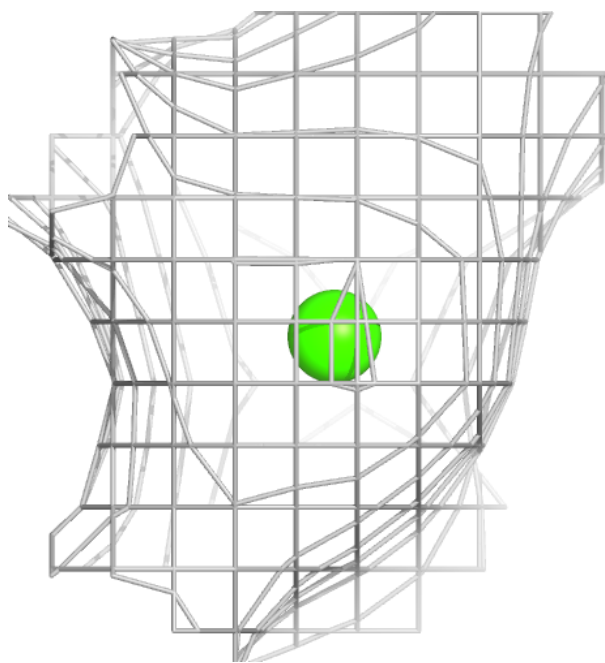
Electron density around CA B 601:

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



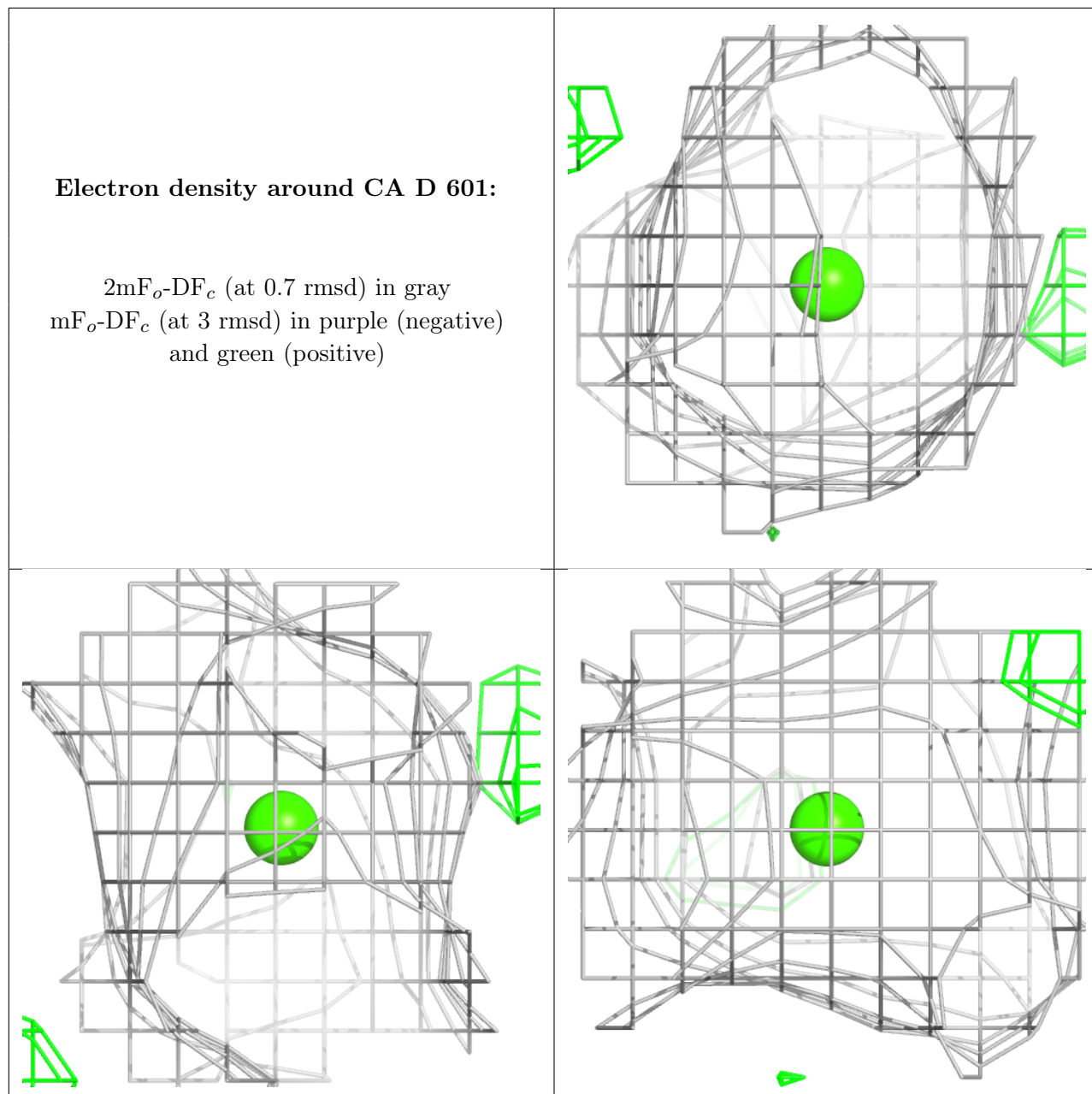
Electron density around CA C 601:

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



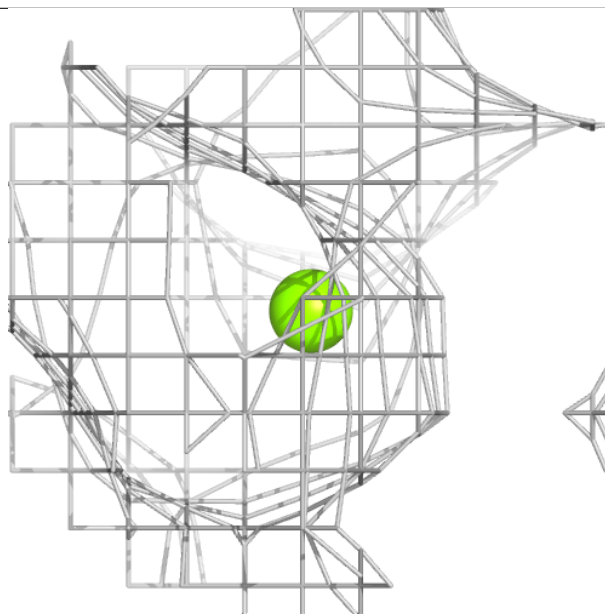
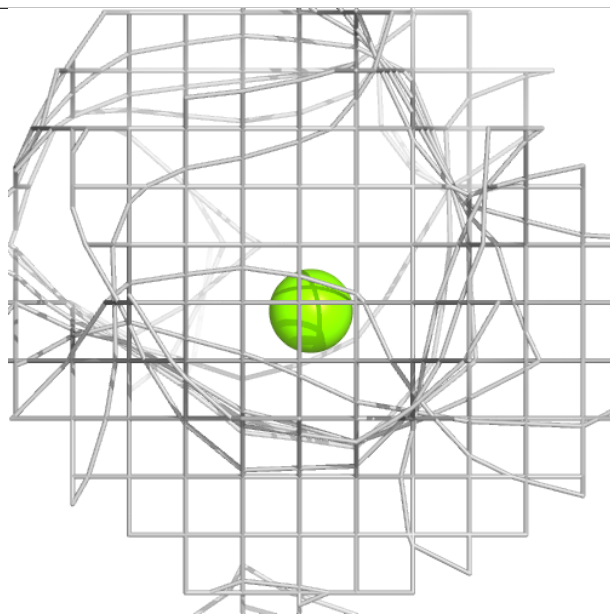
Electron density around CA D 601:

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



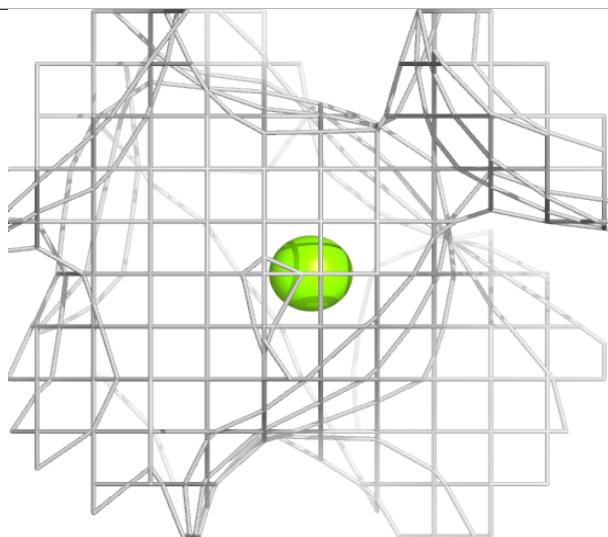
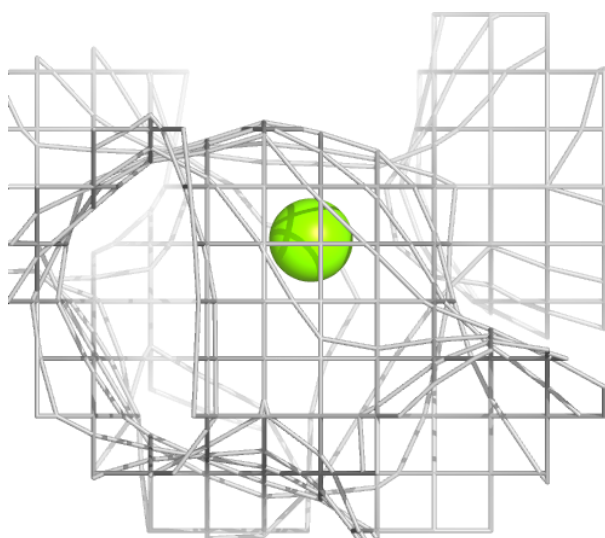
Electron density around MG A 602:

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



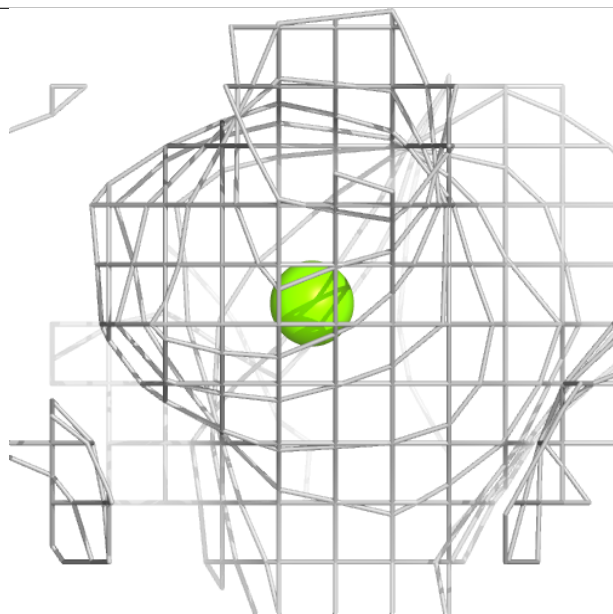
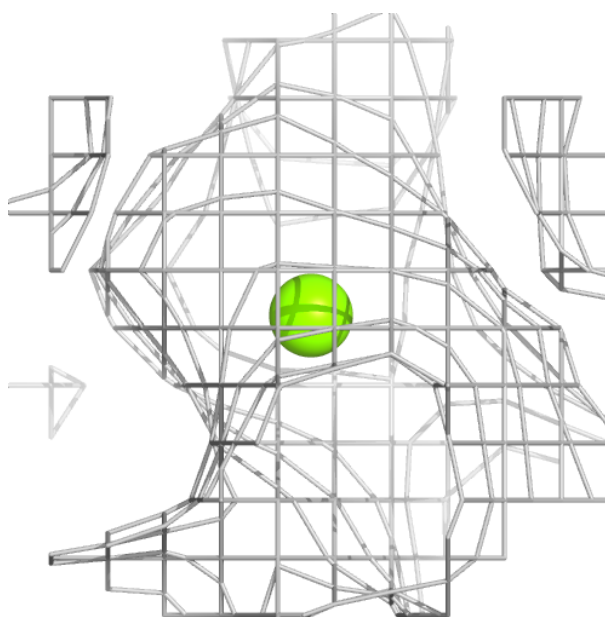
Electron density around MG B 602:

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and green (positive)



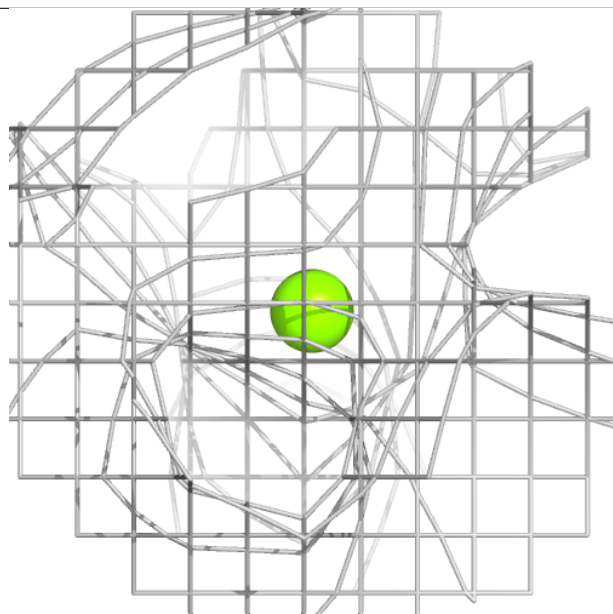
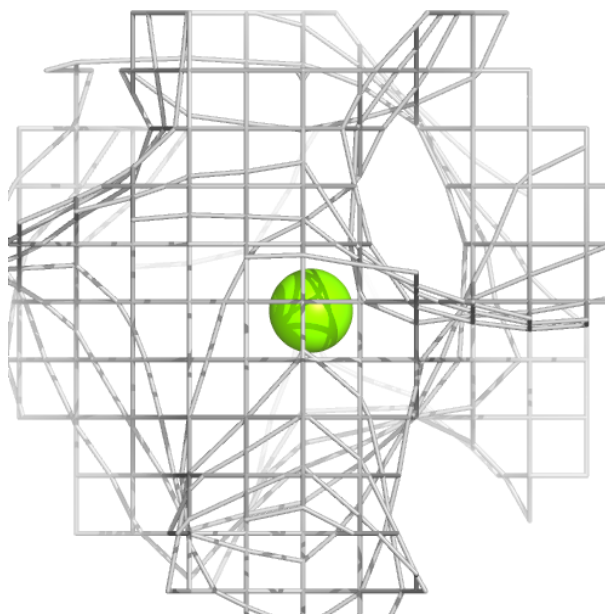
Electron density around MG C 602:

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and green (positive)



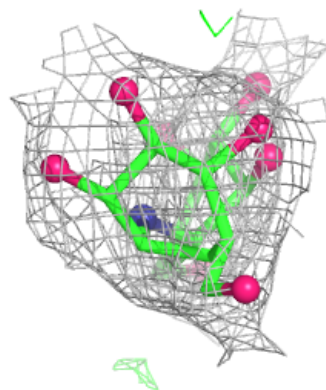
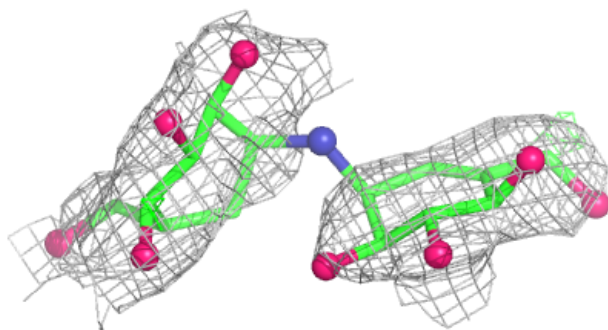
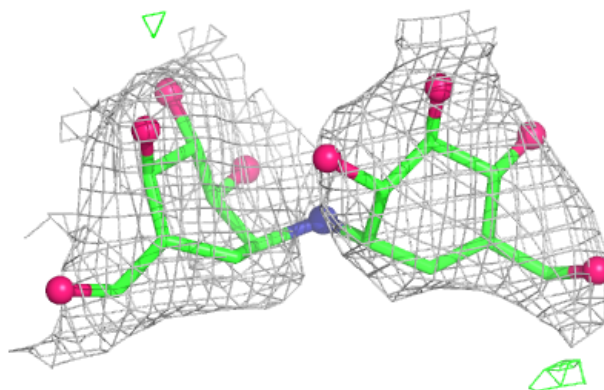
Electron density around MG D 602:

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and green (positive)

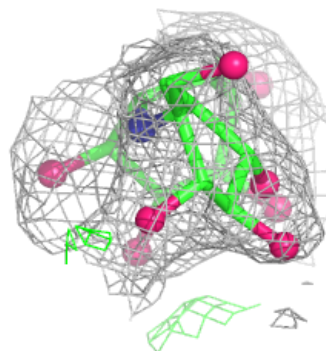
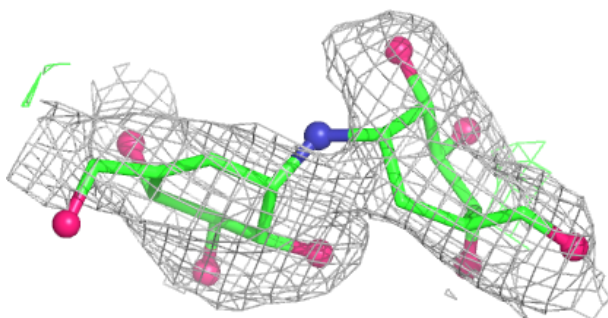
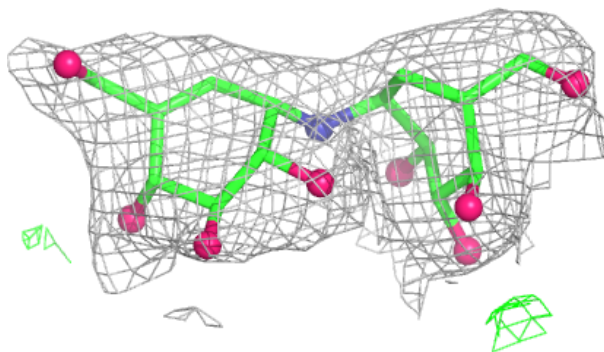


Electron density around VDM A 603:

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

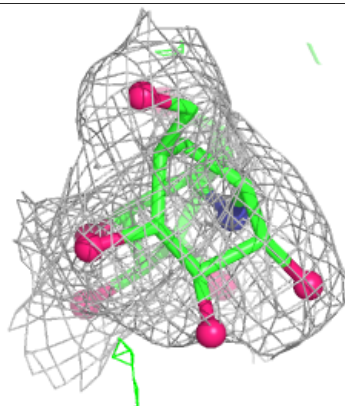
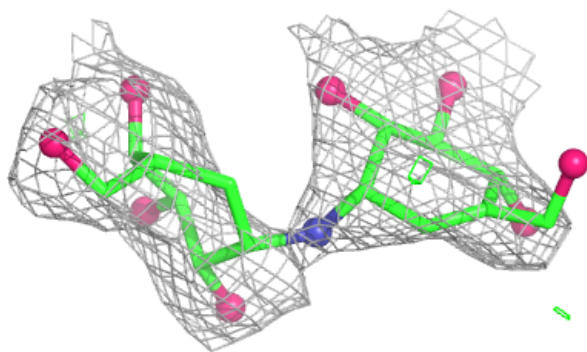
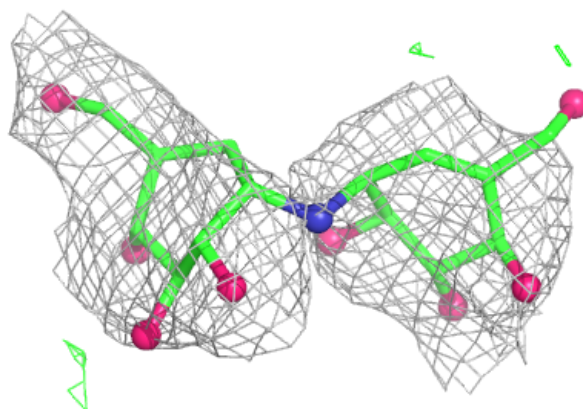
**Electron density around VDM B 603:**

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

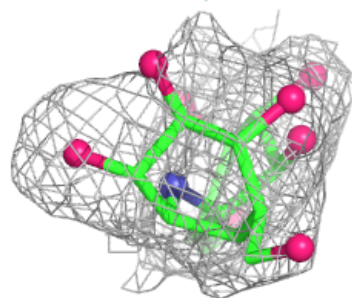
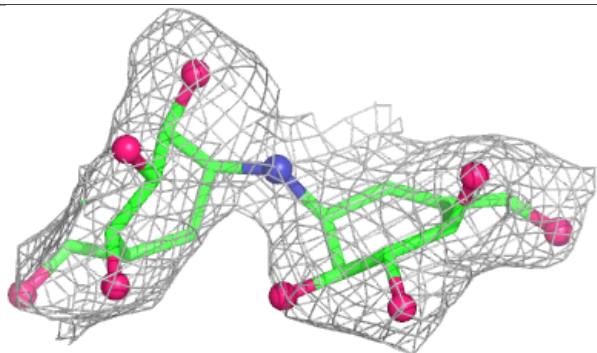
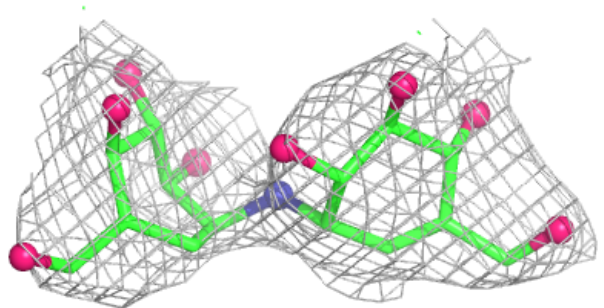


Electron density around VDM C 603:

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

**Electron density around VDM D 603:**

$2mF_o-DF_c$ (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.