



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 AM UTC

PDB ID : 4EJX / pdb_00004ejx
Title : Structure of ceruloplasmin-myeloperoxidase complex
Authors : Samygina, V.R.; Sokolov, A.V.; Bourenkov, G.; Vasilyev, V.B.; Bartunik, H.
Deposited on : 2012-04-07
Resolution : 4.69 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

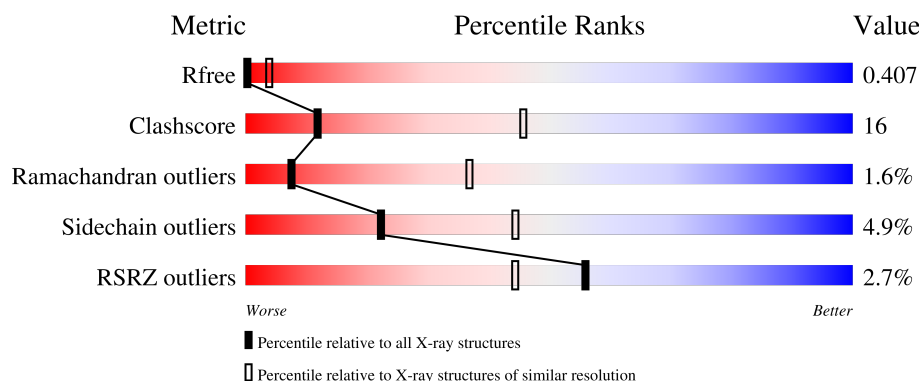
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

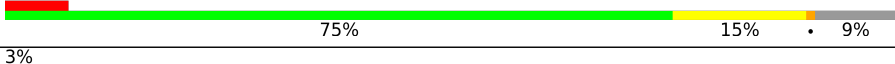
The reported resolution of this entry is 4.69 Å.

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	1020 (5.48-3.92)
Clashscore	190562	1005 (5.40-3.96)
Ramachandran outliers	187476	1095 (5.50-3.90)
Sidechain outliers	187428	1077 (5.50-3.90)
RSRZ outliers	180081	1015 (5.48-3.92)

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	1065	
2	B	114	
3	D	467	
4	C	3	

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
5	CU	A	1101	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13093 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 Ceruloplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1034	Total	C	N	O	S	0	0	0
			8380	5339	1400	1603	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	GLN	GLU	conflict	UNP P00450
A	252	SER	PRO	conflict	UNP P00450

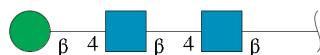
- Molecule 2 is a protein called Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			837	529	148	155	5			

- Molecule 3 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	466	Total	C	N	O	S	0	0	0
			3731	2351	687	666	27			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

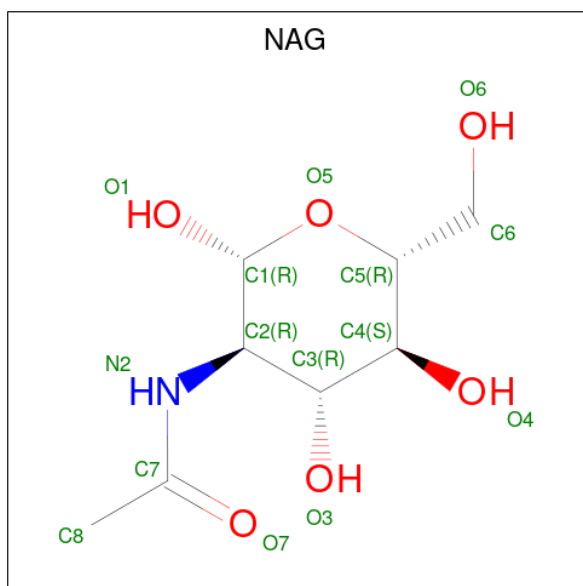


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

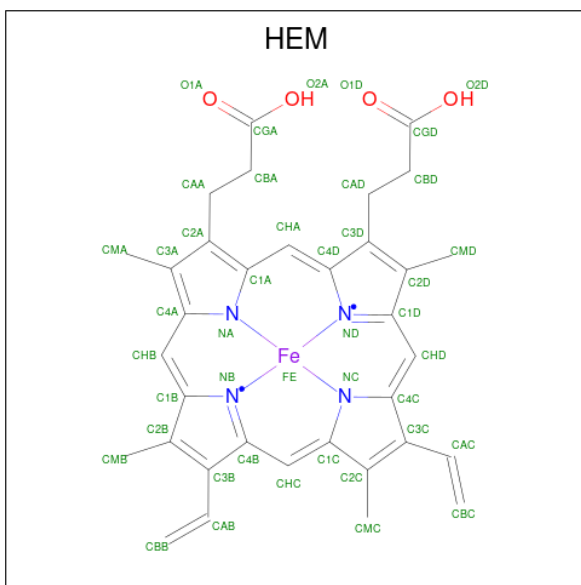
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	Cu	0	0
			7	7		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

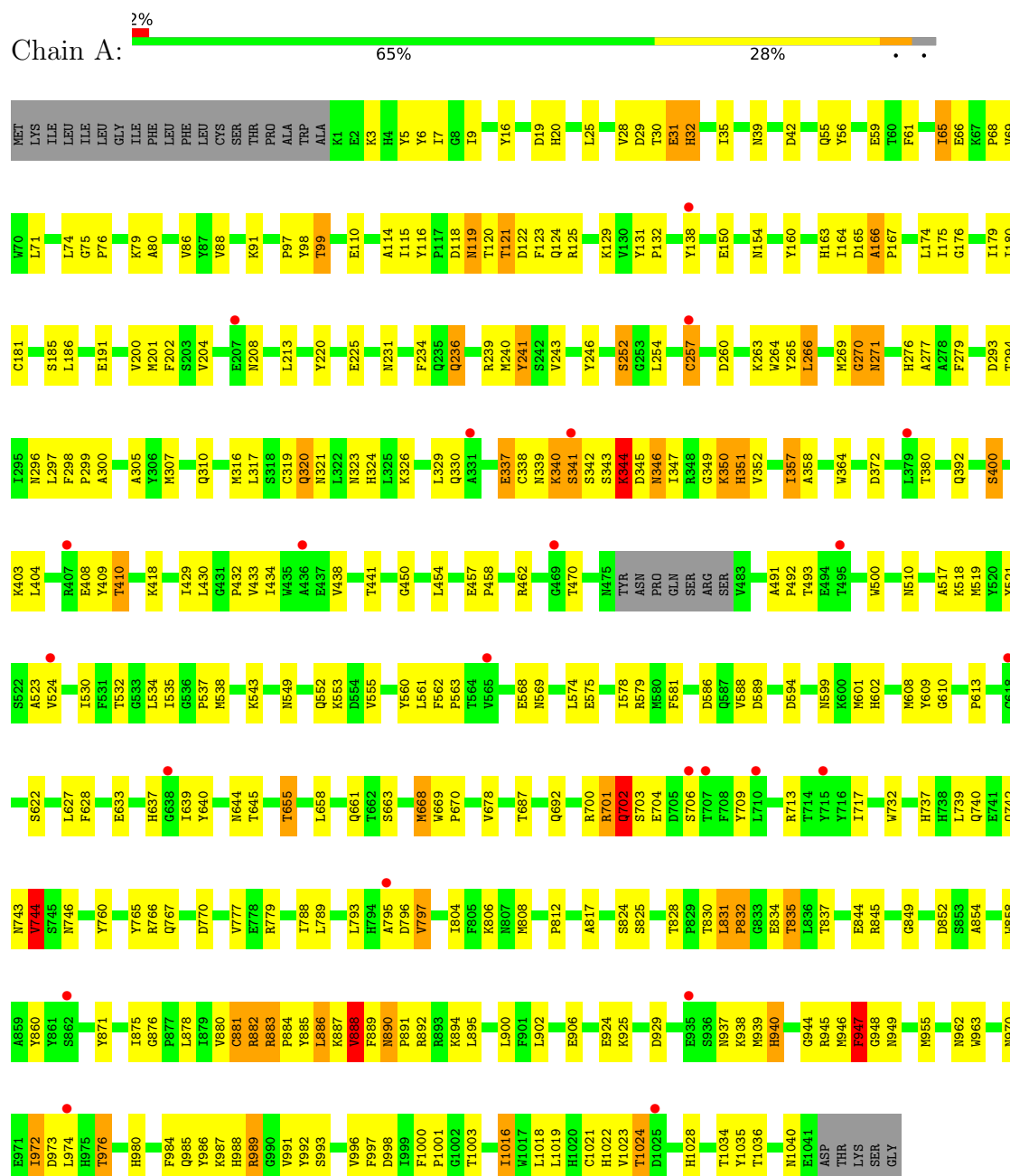


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

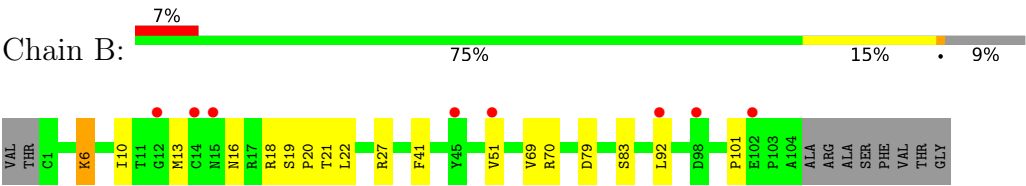
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

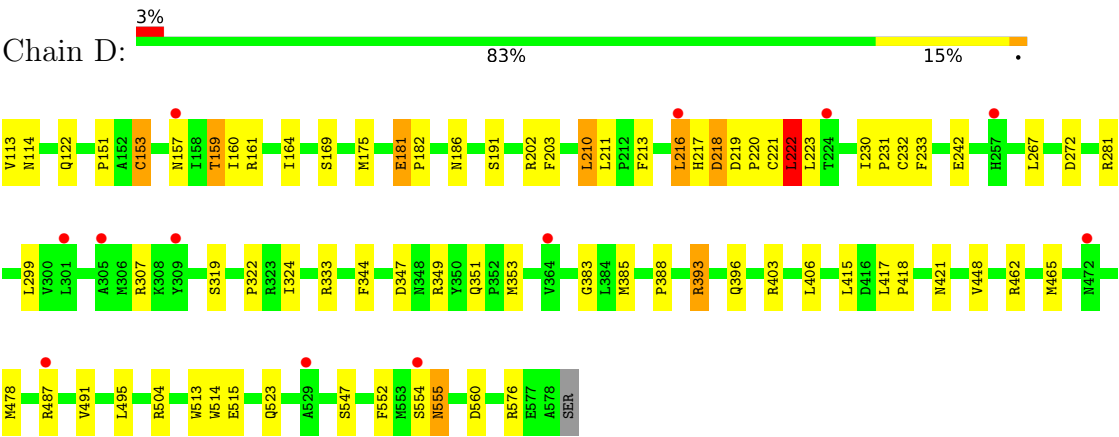
• Molecule 1: Ceruloplasmin



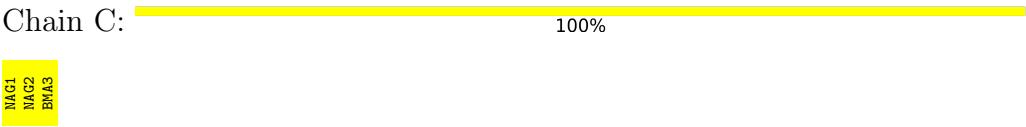
● Molecule 2: Myeloperoxidase light chain



● Molecule 3: Myeloperoxidase heavy chain



● Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	106.25Å 106.25Å 834.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 4.69 15.00 – 4.69	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-4.69) 95.1 (15.00-4.69)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 4.64Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.366 , 0.401 0.360 , 0.407	Depositor DCC
R_{free} test set	752 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	13093	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: CU, BMA, NAG, 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	0.60	10/8615 (0.1%)	0.82	17/11689 (0.1%)
2	B	0.59	0/862	0.88	0/1174
3	D	0.61	1/3817 (0.0%)	0.86	1/5180 (0.0%)
All	All	0.60	11/13294 (0.1%)	0.83	18/18043 (0.1%)

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	2
3	D	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	LYS	CA-C	16.57	1.60	1.52
1	A	940	HIS	C-N	12.48	1.49	1.33
1	A	66	GLU	C-N	11.57	1.57	1.33
1	A	945	ARG	C-N	10.39	1.47	1.33
1	A	271	ASN	C-N	-8.98	1.22	1.33
1	A	770	ASP	C-N	8.78	1.46	1.33
1	A	939	MET	C-N	7.52	1.43	1.33
1	A	270	GLY	C-N	6.61	1.40	1.33
3	D	210	LEU	C-N	6.44	1.46	1.33
1	A	32	HIS	C-N	-6.23	1.25	1.33
1	A	947	PHE	C-N	-5.60	1.25	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ILE	CA-C-N	-14.31	100.55	120.87
1	A	65	ILE	C-N-CA	-14.31	100.55	120.87
1	A	66	GLU	O-C-N	13.42	139.26	122.89
1	A	65	ILE	O-C-N	10.01	135.16	122.94
3	D	210	LEU	O-C-N	-8.93	110.72	122.59
1	A	939	MET	CA-C-N	7.85	134.81	122.26
1	A	939	MET	C-N-CA	7.85	134.81	122.26
1	A	340	LYS	N-CA-C	6.77	118.86	108.30
1	A	75	GLY	CA-C-N	6.27	126.28	119.89
1	A	75	GLY	C-N-CA	6.27	126.28	119.89
1	A	491	ALA	CA-C-N	5.98	127.32	119.84
1	A	491	ALA	C-N-CA	5.98	127.32	119.84
1	A	524	VAL	N-CA-C	-5.70	107.28	111.90
1	A	270	GLY	O-C-N	-5.60	115.42	122.70
1	A	770	ASP	O-C-N	5.53	129.59	122.68
1	A	271	ASN	O-C-N	5.33	129.01	122.88
1	A	1040	ASN	N-CA-C	5.26	117.32	110.43
1	A	252	SER	N-CA-CB	-5.05	103.02	111.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	GLY	Mainchain
1	A	947	PHE	Mainchain
3	D	210	LEU	Mainchain

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	8380	0	7954	326	8
2	B	837	0	798	16	6
3	D	3731	0	3729	115	7
4	C	39	0	34	0	0
5	A	7	0	0	2	0
6	A	28	0	26	0	0
6	D	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	43	0	30	4	0
All	All	13093	0	12597	404	13

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 16.

All (404) 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:345:ASP:HA	1:A:346:ASN:CB	1.36	1.45
1:A:345:ASP:CA	1:A:346:ASN:HB2	1.55	1.30
1:A:340:LYS:CB	1:A:341:SER:HA	1.41	1.27
1:A:989:ARG:HG3	3:D:202:ARG:NE	1.49	1.27
3:D:216:LEU:HB2	3:D:222:LEU:CD1	1.66	1.26
1:A:989:ARG:HG3	3:D:202:ARG:CZ	1.65	1.25
1:A:743:ASN:CA	1:A:744:VAL:HB	1.62	1.23
1:A:743:ASN:HA	1:A:744:VAL:CB	1.63	1.23
1:A:885:TYR:HA	3:D:218:ASP:OD1	1.38	1.20
3:D:216:LEU:CB	3:D:222:LEU:HD11	1.71	1.19
1:A:150:GLU:OE1	3:D:202:ARG:HD2	1.42	1.18
1:A:338:CYS:N	1:A:339:ASN:HA	1.47	1.16
1:A:19:ASP:CB	1:A:20:HIS:HA	1.72	1.15
1:A:277:ALA:HB3	1:A:320:GLN:HB2	1.16	1.13
1:A:166:ALA:HB3	1:A:167:PRO:HD3	1.25	1.12
1:A:340:LYS:CB	1:A:341:SER:CA	2.27	1.11
1:A:987:LYS:CG	1:A:992:TYR:CD2	2.33	1.11
3:D:216:LEU:HB2	3:D:222:LEU:HD11	1.19	1.11
1:A:987:LYS:HG3	1:A:992:TYR:CE2	1.86	1.10
1:A:987:LYS:HG2	1:A:992:TYR:HD2	1.15	1.07
1:A:987:LYS:HG2	1:A:992:TYR:CD2	1.89	1.06
1:A:150:GLU:OE1	3:D:202:ARG:CD	2.03	1.06
1:A:986:TYR:CZ	1:A:992:TYR:HB3	1.91	1.06
1:A:340:LYS:HB2	1:A:341:SER:HA	1.12	1.06
1:A:19:ASP:HB3	1:A:20:HIS:HA	1.10	1.04
1:A:989:ARG:HE	3:D:202:ARG:CZ	1.71	1.02
1:A:277:ALA:CB	1:A:320:GLN:HB2	1.89	1.02
1:A:340:LYS:HB3	1:A:341:SER:HA	1.41	1.01
1:A:987:LYS:HB3	1:A:991:VAL:HG22	1.39	1.01
1:A:890:ASN:HB3	1:A:891:PRO:CD	1.92	0.99
1:A:987:LYS:HB3	1:A:991:VAL:CG2	1.91	0.99
1:A:989:ARG:NE	3:D:202:ARG:NH2	2.11	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:HB3	1:A:341:SER:CA	1.91	0.98
1:A:989:ARG:CG	3:D:202:ARG:NH2	2.26	0.98
1:A:277:ALA:HB3	1:A:320:GLN:CB	1.94	0.97
1:A:987:LYS:HG3	1:A:992:TYR:CD2	1.98	0.96
1:A:118:ASP:O	1:A:120:THR:HG23	1.63	0.96
1:A:319:CYS:SG	5:A:1101:CU:CU	1.57	0.94
1:A:19:ASP:HB3	1:A:20:HIS:CA	1.98	0.94
1:A:986:TYR:CZ	1:A:992:TYR:CB	2.52	0.93
1:A:986:TYR:CE2	1:A:992:TYR:CD2	2.56	0.93
1:A:345:ASP:CA	1:A:346:ASN:CB	2.23	0.92
1:A:890:ASN:HB3	1:A:891:PRO:HD3	1.51	0.91
1:A:340:LYS:HD3	1:A:342:SER:O	1.70	0.91
1:A:338:CYS:H	1:A:339:ASN:HA	1.09	0.91
3:D:216:LEU:HB2	3:D:222:LEU:HD13	1.53	0.91
1:A:236:GLN:NE2	1:A:239:ARG:NH1	2.18	0.90
1:A:989:ARG:CG	3:D:202:ARG:CZ	2.48	0.90
1:A:319:CYS:HG	5:A:1101:CU:CU	0.82	0.89
1:A:338:CYS:N	1:A:339:ASN:CA	2.36	0.88
1:A:989:ARG:HG3	3:D:202:ARG:NH2	1.88	0.88
1:A:338:CYS:H	1:A:339:ASN:CA	1.87	0.88
1:A:279:PHE:HB3	1:A:320:GLN:HE22	1.38	0.87
1:A:321:ASN:HB3	1:A:324:HIS:HB2	1.56	0.87
2:B:6:LYS:H	2:B:6:LYS:HE3	1.40	0.86
1:A:32:HIS:CE1	1:A:35:ILE:CD1	2.59	0.86
1:A:340:LYS:CD	1:A:342:SER:O	2.23	0.85
1:A:989:ARG:HG3	3:D:202:ARG:HE	1.40	0.85
1:A:884:PRO:HD2	3:D:217:HIS:CE1	2.12	0.84
1:A:989:ARG:HE	3:D:202:ARG:NH1	1.75	0.84
1:A:989:ARG:NE	3:D:202:ARG:CZ	2.40	0.84
1:A:236:GLN:NE2	1:A:239:ARG:HH11	1.76	0.83
1:A:987:LYS:CG	1:A:992:TYR:CE2	2.59	0.82
1:A:340:LYS:HB3	1:A:342:SER:N	1.93	0.82
3:D:211:LEU:HD12	3:D:233:PHE:HB3	1.58	0.82
1:A:883:ARG:HB2	1:A:884:PRO:HD3	1.59	0.82
3:D:211:LEU:HD12	3:D:233:PHE:CB	2.10	0.81
1:A:320:GLN:HG3	1:A:661:GLN:HB2	1.62	0.81
1:A:986:TYR:CE2	1:A:992:TYR:CB	2.63	0.80
1:A:946:MET:O	1:A:949:ASN:ND2	2.14	0.80
1:A:989:ARG:CD	3:D:202:ARG:NH2	2.45	0.80
1:A:885:TYR:HA	3:D:218:ASP:CG	2.09	0.78
3:D:211:LEU:CD1	3:D:233:PHE:HB3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:221:CYS:C	3:D:223:LEU:H	1.93	0.76
1:A:299:PRO:HB2	1:A:976:THR:HG21	1.66	0.76
1:A:166:ALA:HB3	1:A:167:PRO:CD	2.11	0.76
1:A:340:LYS:HB3	1:A:341:SER:C	2.10	0.76
1:A:713:ARG:HH22	1:A:886:LEU:HG	1.51	0.75
1:A:553:LYS:HD3	3:D:272:ASP:HB3	1.68	0.75
1:A:166:ALA:CB	1:A:167:PRO:HD3	2.10	0.75
1:A:989:ARG:CG	3:D:202:ARG:HH21	1.96	0.75
3:D:221:CYS:SG	3:D:232:CYS:HA	2.28	0.74
1:A:433:VAL:HG22	1:A:537:PRO:HG2	1.69	0.74
1:A:150:GLU:CD	3:D:202:ARG:CD	2.61	0.73
3:D:211:LEU:HB2	3:D:233:PHE:CD1	2.22	0.73
3:D:221:CYS:SG	3:D:232:CYS:CA	2.76	0.73
1:A:32:HIS:CE1	1:A:35:ILE:HD12	2.22	0.72
1:A:150:GLU:OE2	3:D:202:ARG:HG2	1.89	0.72
1:A:884:PRO:HD2	3:D:217:HIS:HE1	1.51	0.72
1:A:987:LYS:CB	1:A:991:VAL:CG2	2.65	0.72
1:A:987:LYS:CB	1:A:991:VAL:HG22	2.19	0.72
1:A:887:LYS:O	1:A:888:VAL:HG12	1.90	0.71
1:A:29:ASP:OD1	1:A:32:HIS:HB2	1.90	0.71
1:A:323:ASN:HA	1:A:326:LYS:HE2	1.73	0.71
1:A:110:GLU:HG2	1:A:123:PHE:CE2	2.26	0.71
1:A:150:GLU:CD	3:D:202:ARG:HD2	2.16	0.71
1:A:578:ILE:HG23	1:A:588:VAL:HG21	1.72	0.71
1:A:150:GLU:OE1	3:D:202:ARG:HD3	1.89	0.71
1:A:236:GLN:HE21	1:A:239:ARG:NH1	1.89	0.71
3:D:216:LEU:HB3	3:D:222:LEU:HD21	1.73	0.70
1:A:279:PHE:HB3	1:A:320:GLN:NE2	2.07	0.70
1:A:986:TYR:CE2	1:A:992:TYR:HB2	2.25	0.70
1:A:32:HIS:ND1	1:A:35:ILE:HD11	2.06	0.69
1:A:986:TYR:CE2	1:A:992:TYR:CG	2.80	0.69
3:D:211:LEU:HB2	3:D:233:PHE:HD1	1.55	0.69
3:D:388:PRO:HA	3:D:555:ASN:HD22	1.57	0.69
1:A:986:TYR:CE1	1:A:992:TYR:HB3	2.27	0.69
1:A:888:VAL:HG21	3:D:114:ASN:OD1	1.93	0.69
3:D:216:LEU:CB	3:D:222:LEU:CD1	2.44	0.69
1:A:343:SER:O	1:A:344:LYS:HB2	1.92	0.68
1:A:55:GLN:HB2	1:A:76:PRO:HB3	1.75	0.68
1:A:610:GLY:HA2	1:A:692:GLN:HA	1.76	0.67
1:A:118:ASP:O	1:A:119:ASN:C	2.36	0.67
1:A:989:ARG:HG2	3:D:202:ARG:HH21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:O	1:A:266:LEU:HA	1.96	0.66
1:A:890:ASN:CB	1:A:891:PRO:CD	2.68	0.66
2:B:83:SER:HB3	3:D:555:ASN:HB3	1.76	0.66
1:A:887:LYS:HB2	1:A:892:ARG:HH21	1.61	0.66
2:B:101:PRO:HD2	3:D:164:ILE:O	1.95	0.66
1:A:986:TYR:HE2	1:A:992:TYR:CD2	2.11	0.65
3:D:216:LEU:CA	3:D:222:LEU:HD11	2.25	0.65
1:A:79:LYS:HG2	1:A:179:ILE:HB	1.78	0.65
1:A:885:TYR:CA	3:D:218:ASP:OD1	2.30	0.65
1:A:986:TYR:CD2	1:A:992:TYR:HB2	2.31	0.65
3:D:216:LEU:HB3	3:D:222:LEU:HD11	1.72	0.65
1:A:310:GLN:HB2	1:A:462:ARG:HH12	1.61	0.65
1:A:340:LYS:HB2	1:A:341:SER:CA	2.06	0.65
1:A:320:GLN:HG3	1:A:661:GLN:CB	2.26	0.65
2:B:41:PHE:HD1	3:D:160:ILE:HG12	1.62	0.65
1:A:32:HIS:ND1	1:A:35:ILE:CD1	2.59	0.64
1:A:347:ILE:HB	1:A:350:LYS:HG3	1.79	0.64
3:D:221:CYS:O	3:D:223:LEU:N	2.30	0.64
1:A:25:LEU:HB2	1:A:28:VAL:HB	1.79	0.64
1:A:888:VAL:CG2	3:D:114:ASN:OD1	2.46	0.64
1:A:888:VAL:O	3:D:114:ASN:ND2	2.31	0.63
1:A:1016:ILE:HG22	1:A:1034:THR:HB	1.80	0.63
1:A:25:LEU:HB3	1:A:330:GLN:HE22	1.63	0.62
1:A:231:ASN:HB3	1:A:234:PHE:HB3	1.82	0.62
1:A:986:TYR:CE2	1:A:992:TYR:HD2	2.13	0.62
1:A:989:ARG:NE	3:D:202:ARG:HH22	1.96	0.62
3:D:221:CYS:SG	3:D:232:CYS:N	2.73	0.62
1:A:470:THR:HB	1:A:523:ALA:HB1	1.81	0.61
1:A:16:TYR:O	1:A:246:TYR:HA	2.01	0.61
1:A:989:ARG:CG	3:D:202:ARG:NE	2.43	0.61
1:A:553:LYS:HD3	3:D:272:ASP:CB	2.30	0.61
3:D:221:CYS:HB3	3:D:230:ILE:O	2.01	0.60
3:D:554:SER:HB3	3:D:560:ASP:HB3	1.83	0.60
1:A:986:TYR:O	1:A:987:LYS:HB2	2.01	0.60
3:D:219:ASP:HB2	3:D:220:PRO:HD2	1.83	0.60
1:A:887:LYS:HD3	1:A:892:ARG:NH2	2.17	0.60
3:D:203:PHE:CD2	3:D:213:PHE:HE1	2.20	0.59
1:A:299:PRO:HG2	1:A:1023:VAL:HG22	1.85	0.59
1:A:320:GLN:HG2	1:A:661:GLN:HB3	1.85	0.59
3:D:203:PHE:HD2	3:D:213:PHE:HE1	1.49	0.59
1:A:430:LEU:HD11	1:A:562:PHE:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:VAL:HG23	1:A:881:CYS:O	2.02	0.59
1:A:264:TRP:HB2	1:A:305:ALA:HB3	1.84	0.59
1:A:279:PHE:CB	1:A:320:GLN:NE2	2.65	0.59
1:A:938:LYS:O	1:A:940:HIS:ND1	2.36	0.58
1:A:404:LEU:HD23	1:A:454:LEU:HD11	1.85	0.58
1:A:340:LYS:HB3	1:A:342:SER:H	1.64	0.58
1:A:887:LYS:HB2	1:A:892:ARG:NH2	2.18	0.58
1:A:320:GLN:CG	1:A:661:GLN:CB	2.82	0.57
1:A:906:GLU:HB3	1:A:937:ASN:HB3	1.87	0.57
1:A:29:ASP:O	1:A:31:GLU:N	2.38	0.57
1:A:404:LEU:HB3	1:A:534:LEU:HD21	1.86	0.57
1:A:408:GLU:HB2	1:A:432:PRO:CG	2.34	0.57
1:A:510:ASN:O	3:D:191:SER:HB3	2.04	0.57
1:A:408:GLU:HB2	1:A:432:PRO:HG3	1.86	0.57
1:A:737:HIS:HA	1:A:740:GLN:HE21	1.69	0.56
1:A:88:VAL:HB	1:A:138:TYR:HB2	1.86	0.56
1:A:1023:VAL:O	1:A:1024:THR:C	2.49	0.56
1:A:890:ASN:HB3	1:A:891:PRO:HD2	1.84	0.56
3:D:554:SER:HB3	3:D:560:ASP:CB	2.35	0.56
1:A:154:ASN:HB3	1:A:185:SER:HB3	1.87	0.56
1:A:858:TRP:HB2	1:A:878:LEU:HD23	1.87	0.56
1:A:345:ASP:HA	1:A:346:ASN:HB3	1.68	0.56
1:A:364:TRP:HB3	1:A:403:LYS:HD3	1.87	0.56
1:A:279:PHE:CB	1:A:320:GLN:HE22	2.15	0.56
1:A:343:SER:O	1:A:344:LYS:CB	2.53	0.55
1:A:860:TYR:CZ	1:A:876:GLY:HA3	2.41	0.55
1:A:795:ALA:O	1:A:880:VAL:HA	2.06	0.55
1:A:32:HIS:CE1	1:A:35:ILE:HD11	2.40	0.55
1:A:110:GLU:HG3	1:A:124:GLN:HG2	1.88	0.55
3:D:153:CYS:SG	3:D:159:THR:HG21	2.47	0.55
1:A:79:LYS:HD3	1:A:186:LEU:HD21	1.88	0.55
1:A:519:MET:HE2	1:A:628:PHE:HB2	1.89	0.55
2:B:92:LEU:HG	3:D:175:MET:HE3	1.90	0.54
1:A:871:TYR:HE1	1:A:902:LEU:HD11	1.72	0.54
1:A:458:PRO:HG3	1:A:500:TRP:CE2	2.42	0.54
1:A:3:LYS:HB2	1:A:86:VAL:HG13	1.90	0.54
3:D:478:MET:HE3	3:D:478:MET:HA	1.90	0.54
1:A:535:ILE:HG21	1:A:562:PHE:CE2	2.43	0.54
1:A:789:LEU:HD11	1:A:900:LEU:HB3	1.89	0.54
3:D:221:CYS:C	3:D:223:LEU:N	2.60	0.54
1:A:32:HIS:O	1:A:35:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HD2	1:A:71:LEU:HD12	1.89	0.54
1:A:154:ASN:HB2	1:A:191:GLU:OE2	2.08	0.54
1:A:320:GLN:O	1:A:321:ASN:C	2.49	0.54
1:A:296:ASN:HB3	1:A:298:PHE:CE1	2.44	0.54
1:A:766:ARG:CZ	1:A:779:ARG:HH22	2.21	0.54
1:A:987:LYS:CB	1:A:991:VAL:HG23	2.38	0.54
2:B:69:VAL:HG11	3:D:418:PRO:HG2	1.90	0.54
1:A:150:GLU:OE2	3:D:202:ARG:CG	2.56	0.53
1:A:345:ASP:HA	1:A:346:ASN:HB2	0.59	0.53
3:D:169:SER:HB2	3:D:324:ILE:HG12	1.90	0.53
1:A:263:LYS:HG2	1:A:265:TYR:CZ	2.44	0.53
1:A:765:TYR:O	1:A:766:ARG:NH1	2.41	0.53
1:A:150:GLU:OE2	3:D:202:ARG:CD	2.56	0.53
1:A:561:LEU:HB2	1:A:627:LEU:HD22	1.90	0.53
1:A:115:ILE:HG22	1:A:164:ILE:HA	1.91	0.53
1:A:986:TYR:CZ	1:A:992:TYR:HB2	2.43	0.53
1:A:806:LYS:HD3	1:A:808:MET:HG3	1.91	0.52
3:D:242:GLU:OE1	7:D:601:HEM:HBB2	2.09	0.52
1:A:19:ASP:CB	1:A:20:HIS:CA	2.60	0.52
1:A:167:PRO:HG2	1:A:1028:HIS:CE1	2.44	0.52
1:A:241:TYR:HE2	1:A:324:HIS:CD2	2.28	0.52
3:D:203:PHE:HD2	3:D:213:PHE:CE1	2.27	0.52
1:A:114:ALA:HA	1:A:163:HIS:HB3	1.90	0.52
1:A:316:MET:SD	1:A:330:GLN:HB3	2.49	0.52
2:B:79:ASP:O	3:D:388:PRO:HB3	2.09	0.52
1:A:831:LEU:HB3	1:A:832:PRO:HD2	1.91	0.52
1:A:989:ARG:HD2	1:A:989:ARG:O	2.10	0.52
3:D:417:LEU:HB3	3:D:418:PRO:HD3	1.92	0.52
1:A:357:ILE:HD11	1:A:434:ILE:HD11	1.91	0.52
1:A:989:ARG:CG	3:D:202:ARG:HE	2.14	0.51
3:D:203:PHE:CD2	3:D:213:PHE:CE1	2.98	0.51
1:A:29:ASP:O	1:A:29:ASP:CG	2.52	0.51
1:A:310:GLN:CB	1:A:462:ARG:HH12	2.23	0.51
1:A:894:LYS:O	1:A:895:LEU:C	2.52	0.51
1:A:645:THR:HG23	1:A:845:ARG:HH11	1.75	0.51
1:A:998:ASP:HB3	1:A:1000:PHE:CZ	2.45	0.51
1:A:277:ALA:CB	1:A:320:GLN:CB	2.71	0.51
1:A:433:VAL:HG22	1:A:537:PRO:CG	2.40	0.51
1:A:150:GLU:CD	3:D:202:ARG:HD3	2.33	0.51
1:A:410:THR:HG23	1:A:418:LYS:HB2	1.92	0.51
2:B:19:SER:HB3	2:B:22:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:349:ARG:HG3	3:D:351:GLN:HG2	1.92	0.51
1:A:563:PRO:HG2	1:A:639:ILE:HG13	1.93	0.50
1:A:433:VAL:HG11	1:A:560:TYR:CZ	2.47	0.50
1:A:986:TYR:CE1	1:A:992:TYR:CB	2.91	0.50
1:A:340:LYS:HD2	1:A:342:SER:C	2.36	0.50
1:A:19:ASP:HB2	1:A:20:HIS:HA	1.79	0.50
3:D:333:ARG:NH2	7:D:601:HEM:HAD1	2.26	0.50
1:A:470:THR:HA	1:A:523:ALA:O	2.12	0.50
1:A:732:TRP:CD2	1:A:948:GLY:HA3	2.46	0.50
1:A:575:GLU:O	1:A:579:ARG:HG2	2.12	0.50
1:A:888:VAL:C	3:D:114:ASN:ND2	2.68	0.50
1:A:349:GLY:O	1:A:350:LYS:O	2.30	0.50
1:A:743:ASN:HA	1:A:744:VAL:HB	0.70	0.49
3:D:388:PRO:HA	3:D:555:ASN:ND2	2.25	0.49
3:D:211:LEU:HD12	3:D:233:PHE:CG	2.46	0.49
1:A:55:GLN:HB3	1:A:65:ILE:HB	1.93	0.49
1:A:602:HIS:O	1:A:608:MET:HG2	2.12	0.49
3:D:385:MET:O	3:D:555:ASN:HA	2.12	0.49
1:A:700:ARG:O	1:A:701:ARG:C	2.53	0.49
3:D:406:LEU:HB3	3:D:415:LEU:HB2	1.93	0.49
1:A:404:LEU:HD21	1:A:450:GLY:HA3	1.93	0.49
1:A:438:VAL:O	1:A:543:LYS:HD3	2.12	0.49
1:A:970:ASN:H	1:A:973:ASP:HB2	1.77	0.49
1:A:165:ASP:O	1:A:166:ALA:C	2.55	0.49
1:A:955:MET:HE1	1:A:963:TRP:CZ2	2.48	0.49
1:A:854:ALA:O	1:A:881:CYS:HA	2.13	0.49
1:A:68:PRO:O	1:A:71:LEU:HB2	2.13	0.49
3:D:220:PRO:HG2	3:D:232:CYS:SG	2.53	0.48
1:A:457:GLU:HB2	1:A:523:ALA:HB2	1.95	0.48
1:A:337:GLU:HG2	1:A:339:ASN:OD1	2.13	0.48
1:A:552:GLN:HB2	1:A:555:VAL:HB	1.94	0.48
1:A:131:TYR:HB3	1:A:132:PRO:HD2	1.95	0.48
1:A:1019:LEU:HD12	1:A:1035:TYR:HD1	1.79	0.48
1:A:760:TYR:CE2	1:A:906:GLU:HG2	2.49	0.48
2:B:10:ILE:HD13	3:D:281:ARG:NH2	2.28	0.48
1:A:118:ASP:O	1:A:120:THR:N	2.47	0.48
1:A:351:HIS:O	1:A:441:THR:N	2.47	0.47
1:A:955:MET:HE1	1:A:963:TRP:HZ2	1.78	0.47
1:A:984:PHE:CZ	1:A:997:PHE:HB2	2.49	0.47
1:A:569:ASN:HA	1:A:574:LEU:HD13	1.95	0.47
1:A:796:ASP:O	1:A:797:VAL:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:393:ARG:HB2	3:D:396:GLN:HB2	1.96	0.47
3:D:181:GLU:N	3:D:182:PRO:HD2	2.30	0.47
1:A:300:ALA:O	1:A:996:VAL:HG11	2.14	0.47
1:A:1016:ILE:HG12	1:A:1036:THR:HG23	1.97	0.47
1:A:938:LYS:O	1:A:940:HIS:CE1	2.68	0.47
1:A:201:MET:O	1:A:243:VAL:HA	2.14	0.47
1:A:294:THR:HG21	1:A:661:GLN:HB3	1.97	0.47
1:A:817:ALA:HA	1:A:860:TYR:HA	1.97	0.47
1:A:987:LYS:HE3	1:A:992:TYR:HE2	1.79	0.46
1:A:457:GLU:HB3	1:A:521:TYR:O	2.16	0.46
1:A:202:PHE:HD1	1:A:297:LEU:HD12	1.81	0.46
1:A:279:PHE:CE1	1:A:293:ASP:HB2	2.51	0.46
1:A:644:ASN:HB3	1:A:668:MET:SD	2.56	0.46
1:A:888:VAL:CG2	3:D:114:ASN:CG	2.86	0.46
2:B:22:LEU:HB3	3:D:322:PRO:HD2	1.97	0.46
3:D:333:ARG:HH21	7:D:601:HEM:HAD1	1.80	0.46
1:A:204:VAL:HA	1:A:240:MET:O	2.15	0.46
1:A:744:VAL:O	1:A:744:VAL:HG13	2.16	0.46
1:A:849:GLY:N	1:A:852:ASP:HB2	2.30	0.46
2:B:41:PHE:HD1	3:D:160:ILE:CG1	2.29	0.46
3:D:299:LEU:HD22	3:D:552:PHE:HB2	1.98	0.46
1:A:347:ILE:CB	1:A:350:LYS:HG3	2.46	0.46
1:A:986:TYR:CD2	1:A:992:TYR:HD2	2.33	0.46
1:A:849:GLY:H	1:A:852:ASP:HB2	1.81	0.46
1:A:269:MET:HE1	1:A:1022:HIS:CE1	2.50	0.46
1:A:345:ASP:CA	1:A:346:ASN:HB3	2.32	0.46
1:A:80:ALA:HB3	1:A:180:ILE:HD13	1.98	0.45
1:A:988:HIS:HE1	3:D:213:PHE:HB2	1.81	0.45
3:D:267:LEU:HD12	3:D:576:ARG:HB2	1.99	0.45
3:D:514:TRP:CE2	3:D:515:GLU:HG3	2.51	0.45
1:A:578:ILE:HG12	1:A:588:VAL:HG11	1.98	0.45
1:A:844:GLU:OE1	3:D:186:ASN:ND2	2.50	0.45
3:D:333:ARG:HH11	3:D:421:ASN:HD22	1.64	0.45
1:A:116:TYR:O	1:A:125:ARG:NH2	2.50	0.45
1:A:854:ALA:HB1	1:A:882:ARG:HB2	1.99	0.45
1:A:202:PHE:CD1	1:A:297:LEU:HD12	2.52	0.45
1:A:320:GLN:CG	1:A:661:GLN:HB3	2.46	0.44
1:A:257:CYS:O	1:A:260:ASP:HB2	2.17	0.44
1:A:340:LYS:HZ2	1:A:343:SER:HB2	1.82	0.44
1:A:883:ARG:HB2	1:A:884:PRO:CD	2.37	0.44
1:A:179:ILE:HG22	1:A:181:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASN:OD1	1:A:744:VAL:CG1	2.66	0.44
1:A:884:PRO:O	3:D:218:ASP:OD1	2.35	0.44
1:A:812:PRO:HG3	1:A:831:LEU:HD22	1.99	0.44
3:D:347:ASP:HB3	3:D:353:MET:HG3	1.99	0.44
1:A:568:GLU:HB2	1:A:599:ASN:HB3	1.99	0.44
1:A:622:SER:HA	1:A:669:TRP:CD1	2.52	0.44
1:A:824:SER:OG	1:A:825:SER:N	2.51	0.43
1:A:985:GLN:HA	1:A:992:TYR:O	2.18	0.43
1:A:1019:LEU:HD12	1:A:1035:TYR:CD1	2.52	0.43
3:D:220:PRO:O	3:D:223:LEU:HB2	2.17	0.43
1:A:5:TYR:HD2	1:A:55:GLN:NE2	2.15	0.43
1:A:555:VAL:HA	1:A:622:SER:HB3	2.00	0.43
1:A:834:GLU:HG2	1:A:835:THR:N	2.33	0.43
1:A:300:ALA:CB	1:A:996:VAL:HG11	2.48	0.43
1:A:637:HIS:HB2	1:A:658:LEU:HB2	2.00	0.43
1:A:9:ILE:HG23	1:A:174:LEU:HD21	1.99	0.43
1:A:358:ALA:HB3	1:A:409:TYR:CE1	2.52	0.43
1:A:989:ARG:CD	3:D:202:ARG:CZ	2.92	0.43
2:B:16:ASN:O	2:B:20:PRO:HA	2.17	0.43
1:A:804:ILE:HD13	1:A:837:THR:HG23	1.99	0.43
1:A:208:ASN:HA	1:A:213:LEU:HD22	2.01	0.43
1:A:350:LYS:O	1:A:352:VAL:HG23	2.18	0.43
1:A:561:LEU:HB2	1:A:627:LEU:CD2	2.48	0.43
3:D:216:LEU:HD13	3:D:216:LEU:H	1.84	0.43
3:D:344:PHE:O	3:D:383:GLY:HA3	2.18	0.43
1:A:6:TYR:CE1	1:A:59:GLU:HG3	2.53	0.43
1:A:98:TYR:O	1:A:99:THR:HG23	2.19	0.43
1:A:154:ASN:HB3	1:A:185:SER:CB	2.48	0.43
1:A:74:LEU:HD21	1:A:201:MET:SD	2.59	0.43
1:A:392:GLN:NE2	1:A:581:PHE:HD1	2.16	0.43
1:A:976:THR:CG2	1:A:1023:VAL:HG23	2.49	0.43
3:D:347:ASP:OD1	3:D:349:ARG:HG2	2.19	0.43
1:A:767:GLN:HE21	1:A:777:VAL:HG21	1.83	0.43
1:A:400:SER:HB2	1:A:581:PHE:CZ	2.54	0.42
1:A:160:TYR:N	1:A:176:GLY:O	2.47	0.42
1:A:517:ALA:O	1:A:663:SER:HB2	2.19	0.42
1:A:788:ILE:HB	1:A:944:GLY:HA3	2.01	0.42
3:D:213:PHE:HB3	3:D:231:PRO:HG2	2.01	0.42
1:A:39:ASN:HD21	1:A:220:TYR:HB3	1.85	0.42
1:A:266:LEU:HD12	1:A:266:LEU:H	1.84	0.42
1:A:269:MET:HA	1:A:299:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:GLN:HE21	1:A:702:GLN:HB2	1.67	0.42
1:A:987:LYS:HA	1:A:987:LYS:HD3	1.67	0.42
3:D:221:CYS:SG	3:D:232:CYS:CB	3.08	0.42
1:A:321:ASN:HB3	1:A:324:HIS:CB	2.38	0.42
3:D:217:HIS:CD2	3:D:217:HIS:H	2.36	0.42
3:D:491:VAL:HB	3:D:495:LEU:HB2	2.01	0.42
1:A:129:LYS:HG2	1:A:131:TYR:CE2	2.54	0.42
1:A:345:ASP:CB	1:A:346:ASN:HB3	2.50	0.42
1:A:669:TRP:HA	1:A:670:PRO:HD3	1.90	0.42
7:D:601:HEM:HMC1	7:D:601:HEM:HBC2	2.02	0.42
1:A:271:ASN:HA	1:A:1023:VAL:HG13	2.01	0.41
1:A:345:ASP:CB	1:A:346:ASN:CB	2.96	0.41
1:A:7:ILE:HD12	1:A:76:PRO:HG2	2.01	0.41
1:A:640:TYR:HB2	1:A:655:THR:HG23	2.02	0.41
1:A:987:LYS:O	1:A:988:HIS:C	2.62	0.41
3:D:216:LEU:CB	3:D:222:LEU:HD21	2.47	0.41
1:A:25:LEU:HB3	1:A:330:GLN:NE2	2.33	0.41
1:A:702:GLN:O	1:A:703:SER:OG	2.31	0.41
1:A:875:ILE:HG21	1:A:900:LEU:HD22	2.03	0.41
1:A:372:ASP:OD1	1:A:609:TYR:HB3	2.20	0.41
1:A:889:PHE:CG	1:A:890:ASN:N	2.89	0.41
2:B:18:ARG:NH2	3:D:319:SER:OG	2.53	0.41
3:D:113:VAL:HG21	3:D:122:GLN:HB2	2.03	0.41
3:D:151:PRO:HG3	3:D:161:ARG:NH2	2.36	0.41
1:A:888:VAL:O	1:A:888:VAL:HG13	2.09	0.41
1:A:97:PRO:HG3	1:A:131:TYR:CD1	2.55	0.41
1:A:276:HIS:HB2	1:A:297:LEU:HB2	2.03	0.41
1:A:601:MET:HB3	1:A:608:MET:SD	2.61	0.41
2:B:70:ARG:HB2	3:D:403:ARG:CZ	2.51	0.41
1:A:56:TYR:CG	1:A:61:PHE:HD2	2.39	0.41
1:A:518:LYS:HB2	1:A:538:MET:HB3	2.03	0.41
1:A:521:TYR:HB2	1:A:530:ILE:HG12	2.03	0.41
1:A:890:ASN:HD22	1:A:891:PRO:HD3	1.86	0.41
3:D:448:VAL:HB	3:D:465:MET:HG3	2.03	0.41
1:A:980:HIS:CG	1:A:1018:LEU:HB3	2.55	0.41
3:D:513:TRP:CD1	3:D:515:GLU:HB2	2.56	0.41
1:A:344:LYS:HB3	1:A:345:ASP:H	1.66	0.40
1:A:717:ILE:CG2	1:A:765:TYR:HB3	2.52	0.40
1:A:972:ILE:H	1:A:972:ILE:HG13	1.65	0.40
1:A:976:THR:O	1:A:1021:CYS:HA	2.21	0.40
1:A:98:TYR:CD1	1:A:174:LEU:HD12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LEU:HG	1:A:860:TYR:CE2	2.57	0.40
2:B:13:MET:HA	2:B:20:PRO:O	2.21	0.40
2:B:41:PHE:CD1	3:D:160:ILE:HG12	2.49	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:LYS:CB	3:D:462:ARG:NH2[1_455]	1.50	0.70
1:A:706:SER:CB	3:D:157:ASN:ND2[10_555]	1.71	0.49
2:B:27:ARG:NH2	2:B:41:PHE:CE2[10_555]	1.83	0.37
1:A:925:LYS:CA	3:D:462:ARG:NH2[1_455]	1.91	0.29
2:B:27:ARG:CZ	2:B:41:PHE:CZ[10_555]	1.98	0.22
2:B:27:ARG:NE	2:B:41:PHE:CZ[10_555]	2.01	0.19
1:A:589:ASP:OD1	3:D:487:ARG:CD[1_455]	2.02	0.18
1:A:586:ASP:O	3:D:307:ARG:NE[1_455]	2.03	0.17
1:A:706:SER:OG	3:D:157:ASN:ND2[10_555]	2.08	0.12
1:A:706:SER:O	3:D:157:ASN:OD1[10_555]	2.09	0.11
2:B:21:THR:CG2	2:B:41:PHE:CZ[10_555]	2.09	0.11
2:B:27:ARG:CZ	2:B:41:PHE:CE2[10_555]	2.12	0.08
1:A:701:ARG:NH2	2:B:51:VAL:CG1[10_555]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1030/1065 (97%)	897 (87%)	110 (11%)	23 (2%)	5	28
2	B	102/114 (90%)	98 (96%)	4 (4%)	0	100	100
3	D	464/467 (99%)	446 (96%)	15 (3%)	3 (1%)	21	59
All	All	1596/1646 (97%)	1441 (90%)	129 (8%)	26 (2%)	7	37

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	166	ALA
1	A	350	LYS
1	A	744	VAL
1	A	890	ASN
1	A	1024	THR
3	D	218	ASP
3	D	222	LEU
1	A	30	THR
1	A	344	LYS
1	A	346	ASN
1	A	797	VAL
1	A	883	ARG
1	A	888	VAL
3	D	555	ASN
1	A	254	LEU
1	A	701	ARG
1	A	702	GLN
1	A	832	PRO
1	A	882	ARG
1	A	492	PRO
1	A	947	PHE
1	A	121	THR
1	A	241	TYR
1	A	613	PRO
1	A	1001	PRO

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	909/937 (97%)	850 (94%)	59 (6%)	15	38
2	B	90/97 (93%)	89 (99%)	1 (1%)	65	74
3	D	411/412 (100%)	402 (98%)	9 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1410/1446 (98%)	1341 (95%)	69 (5%)	22	44

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	42	ASP
1	A	69	VAL
1	A	91	LYS
1	A	99	THR
1	A	121	THR
1	A	122	ASP
1	A	175	ILE
1	A	225	GLU
1	A	236	GLN
1	A	252	SER
1	A	257	CYS
1	A	266	LEU
1	A	307	MET
1	A	317	LEU
1	A	320	GLN
1	A	329	LEU
1	A	337	GLU
1	A	341	SER
1	A	344	LYS
1	A	351	HIS
1	A	357	ILE
1	A	380	THR
1	A	400	SER
1	A	410	THR
1	A	429	ILE
1	A	493	THR
1	A	532	THR
1	A	549	ASN
1	A	594	ASP
1	A	633	GLU
1	A	655	THR
1	A	668	MET
1	A	678	VAL
1	A	687	THR
1	A	702	GLN
1	A	704	GLU

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Mol	Chain	Res	Type
1	A	709	TYR
1	A	739	LEU
1	A	742	GLN
1	A	744	VAL
1	A	746	ASN
1	A	828	THR
1	A	830	THR
1	A	831	LEU
1	A	835	THR
1	A	881	CYS
1	A	886	LEU
1	A	888	VAL
1	A	924	GLU
1	A	929	ASP
1	A	962	ASN
1	A	972	ILE
1	A	974	LEU
1	A	976	THR
1	A	989	ARG
1	A	993	SER
1	A	1003	THR
1	A	1016	ILE
2	B	6	LYS
3	D	153	CYS
3	D	159	THR
3	D	181	GLU
3	D	216	LEU
3	D	222	LEU
3	D	393	ARG
3	D	504	ARG
3	D	523	GLN
3	D	547	SER

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	55	GLN
1	A	111	HIS
1	A	135	GLN
1	A	236	GLN
1	A	283	GLN
1	A	324	HIS

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Mol	Chain	Res	Type
1	A	330	GLN
1	A	336	GLN
1	A	351	HIS
1	A	365	ASN
1	A	467	ASN
1	A	549	ASN
1	A	569	ASN
1	A	599	ASN
1	A	657	ASN
1	A	702	GLN
1	A	740	GLN
1	A	746	ASN
1	A	807	ASN
1	A	890	ASN
1	A	937	ASN
1	A	951	GLN
1	A	988	HIS
1	A	1005	GLN
1	A	1026	HIS
3	D	121	GLN
3	D	215	ASN
3	D	348	ASN
3	D	421	ASN
3	D	516	ASN
3	D	523	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

3 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
4	NAG	C	1	4,3	14,14,15	0.53	0	17,19,21	2.06	3 (17%)
4	NAG	C	2	4	14,14,15	0.53	0	17,19,21	1.11	1 (5%)
4	BMA	C	3	4	11,11,12	0.74	0	15,15,17	1.68	3 (20%)

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	NAG	C	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C1-O5-C5	7.04	121.61	112.19
4	C	3	BMA	O3-C3-C2	-3.60	102.72	110.05
4	C	3	BMA	C1-C2-C3	3.58	114.86	109.64
4	C	2	NAG	C1-O5-C5	3.36	116.68	112.19
4	C	1	NAG	C3-C4-C5	-2.57	105.58	110.23
4	C	3	BMA	C2-C3-C4	2.12	114.59	110.86
4	C	1	NAG	O3-C3-C2	2.03	113.62	109.40

There are no chirality outliers.

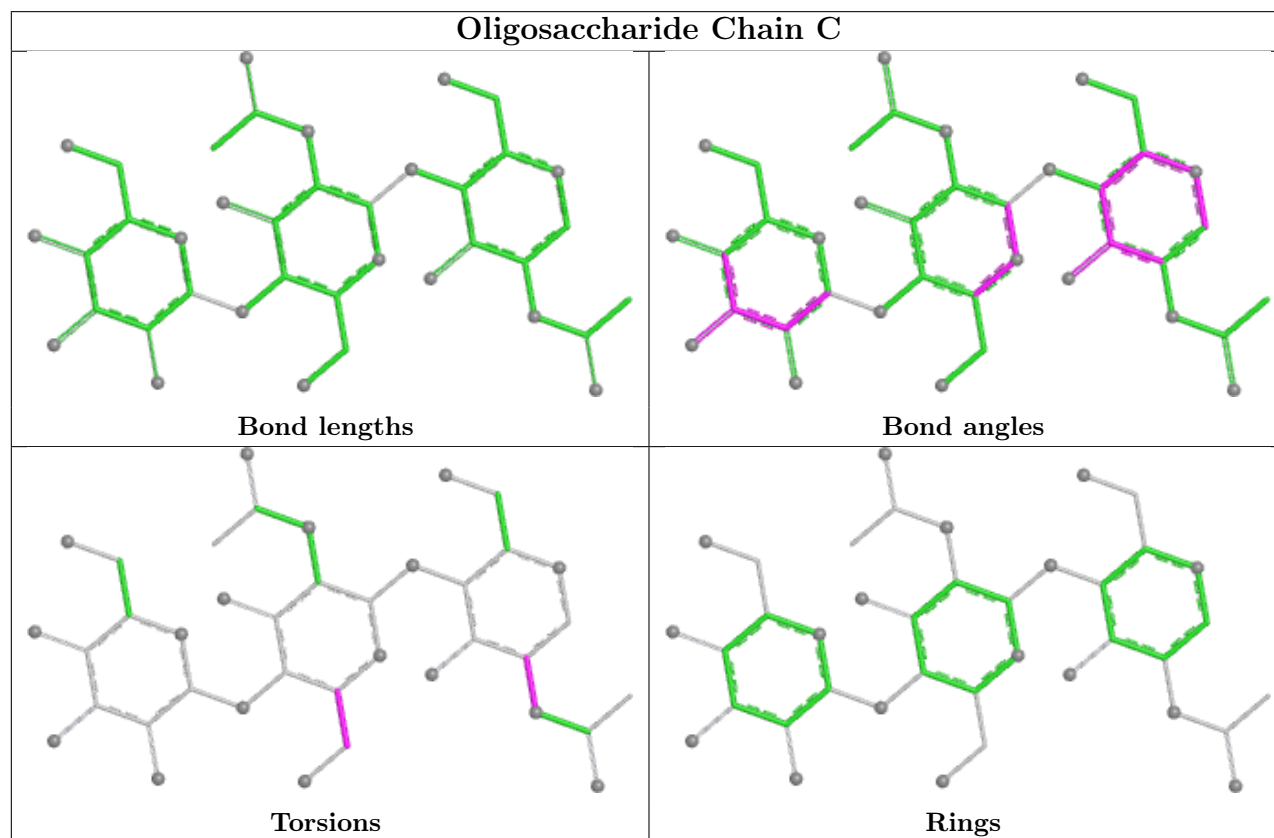
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	C	1	NAG	C1-C2-N2-C7

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 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\# Z > 2$
7	HEM	D	601	3	50,50,50	2.63	24 (48%)	67,82,82	1.64	10 (14%)
6	NAG	D	606	3	14,14,15	0.54	0	17,19,21	0.99	0
6	NAG	D	605	3	14,14,15	0.54	0	17,19,21	1.11	1 (5%)
6	NAG	A	1108	1	14,14,15	0.64	0	17,19,21	1.54	2 (11%)
6	NAG	A	1109	1	14,14,15	0.56	0	17,19,21	0.93	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEM	D	601	3	-	6/14/54/54	-
6	NAG	D	606	3	-	0/6/23/26	0/1/1/1
6	NAG	D	605	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1108	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1109	1	-	2/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	601	HEM	FE-NB	4.83	2.09	1.94
7	D	601	HEM	FE-NA	4.78	2.10	1.95
7	D	601	HEM	FE-NC	4.68	2.10	1.95
7	D	601	HEM	CHA-C4D	4.60	1.47	1.38
7	D	601	HEM	FE-ND	4.59	2.09	1.94
7	D	601	HEM	CBC-CAC	4.02	1.49	1.30
7	D	601	HEM	CHC-C1C	4.02	1.46	1.38
7	D	601	HEM	CBB-CAB	3.88	1.49	1.30
7	D	601	HEM	C4D-ND	-3.87	1.33	1.40
7	D	601	HEM	C4A-NA	-3.62	1.32	1.39
7	D	601	HEM	CHB-C1B	3.51	1.45	1.38
7	D	601	HEM	C4C-NC	-3.43	1.33	1.39
7	D	601	HEM	CHD-C4C	3.41	1.45	1.38
7	D	601	HEM	CHA-C1A	3.32	1.46	1.39
7	D	601	HEM	C1A-NA	-3.31	1.33	1.39
7	D	601	HEM	C1C-NC	-3.30	1.33	1.39
7	D	601	HEM	CHD-C1D	3.28	1.46	1.39
7	D	601	HEM	C1B-NB	-3.19	1.34	1.40
7	D	601	HEM	CHC-C4B	3.00	1.46	1.39
7	D	601	HEM	C1A-C2A	-2.79	1.39	1.44
7	D	601	HEM	C1D-ND	-2.63	1.33	1.38
7	D	601	HEM	C4B-NB	-2.62	1.33	1.38
7	D	601	HEM	CHB-C4A	2.53	1.45	1.39
7	D	601	HEM	C4A-C3A	-2.21	1.37	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	601	HEM	C3B-C2B-C1B	-5.44	102.33	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	601	HEM	CBD-CAD-C3D	-4.76	99.37	112.53
6	A	1108	NAG	C4-C3-C2	4.35	117.39	111.02
7	D	601	HEM	CHD-C1D-C2D	-3.94	118.80	125.03
7	D	601	HEM	C3C-C2C-C1C	-3.93	103.33	107.05
7	D	601	HEM	C2B-C1B-NB	3.70	114.09	109.84
6	A	1108	NAG	C3-C4-C5	3.67	116.89	110.23
6	D	605	NAG	C1-O5-C5	3.17	116.44	112.19
7	D	601	HEM	C1D-C2D-C3D	-2.78	104.06	106.98
7	D	601	HEM	CHB-C1B-C2B	-2.74	119.15	126.95
6	A	1109	NAG	C4-C3-C2	2.58	114.80	111.02
7	D	601	HEM	C2D-C1D-ND	2.10	112.33	109.90
7	D	601	HEM	CAD-CBD-CGD	2.02	119.01	113.67
7	D	601	HEM	CBA-CAA-C2A	-2.00	107.00	112.53

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1108	NAG	C8-C7-N2-C2
6	A	1108	NAG	O7-C7-N2-C2
6	A	1109	NAG	C8-C7-N2-C2
6	A	1109	NAG	O7-C7-N2-C2
7	D	601	HEM	C2B-C3B-CAB-CBB
7	D	601	HEM	CAD-CBD-CGD-O2D
7	D	601	HEM	CAD-CBD-CGD-O1D
7	D	601	HEM	CAA-CBA-CGA-O2A
7	D	601	HEM	CAA-CBA-CGA-O1A
7	D	601	HEM	C4B-C3B-CAB-CBB

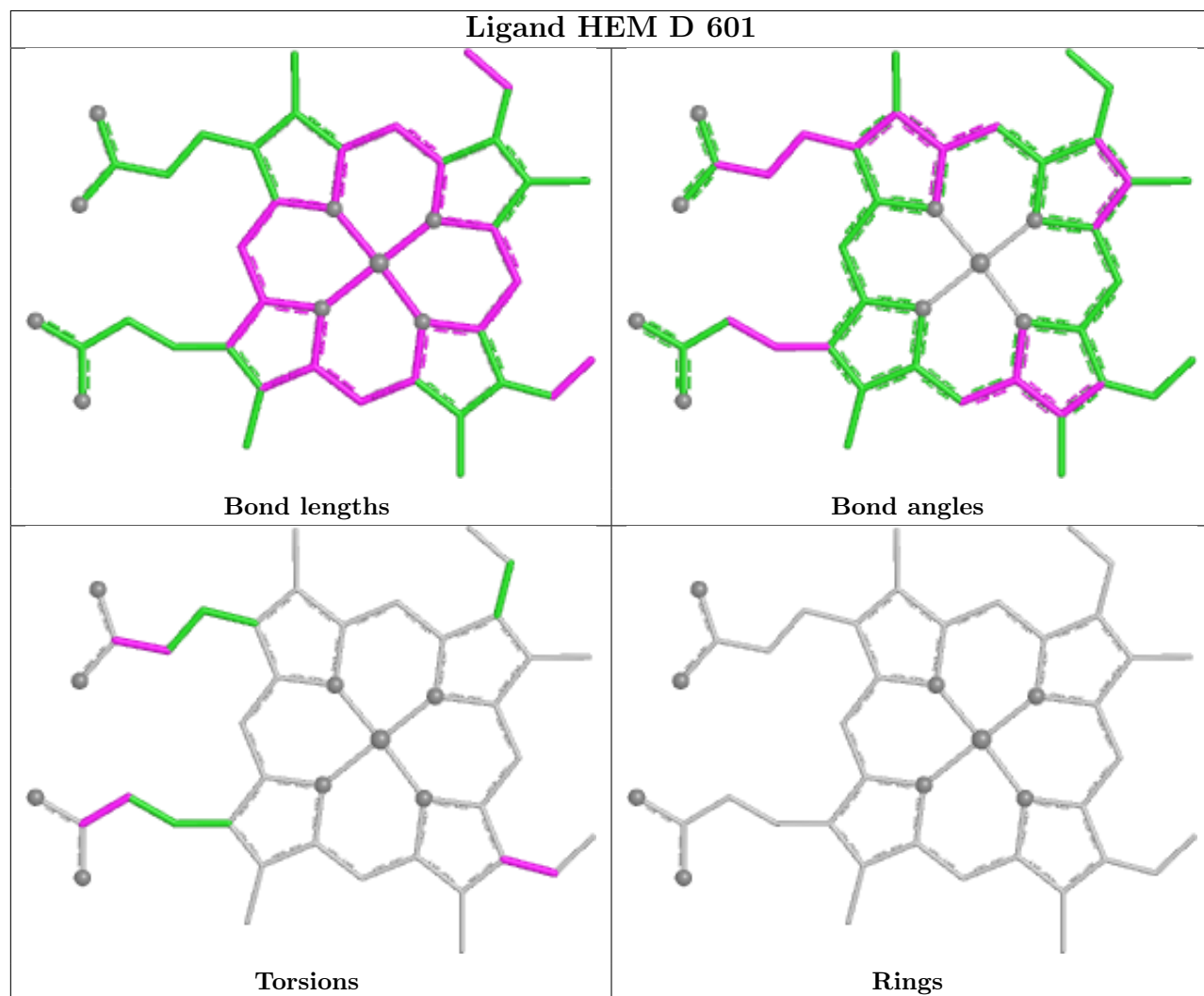
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	601	HEM	4	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

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	1034/1065 (97%)	-0.02	23 (2%) 62 49	13, 20, 20, 20	7 (0%)
2	B	104/114 (91%)	0.40	8 (7%) 19 22	20, 20, 20, 20	0
3	D	466/467 (99%)	0.27	12 (2%) 57 45	20, 20, 20, 20	0
All	All	1604/1646 (97%)	0.09	43 (2%) 56 44	13, 20, 20, 20	7 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	554	SER	5.0
1	A	706	SER	4.5
3	D	216	LEU	4.1
1	A	618	CYS	4.0
1	A	638	GLY	3.9
1	A	707	THR	3.9
1	A	715	TYR	3.3
2	B	15	ASN	3.2
1	A	257	CYS	3.1
2	B	12	GLY	3.1
1	A	207	GLU	3.1
1	A	935	GLU	3.0
1	A	436	ALA	2.9
3	D	301	LEU	2.9
3	D	364	VAL	2.8
1	A	341	SER	2.8
3	D	309	TYR	2.7
1	A	495	THR	2.6
3	D	157	ASN	2.5
1	A	565	VAL	2.5
1	A	862	SER	2.5
1	A	1025	ASP	2.5
3	D	224	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	487	ARG	2.4
2	B	92	LEU	2.4
1	A	524	VAL	2.4
3	D	257	HIS	2.4
1	A	795	ALA	2.3
1	A	138	TYR	2.3
2	B	51	VAL	2.3
3	D	529	ALA	2.2
1	A	407	ARG	2.2
1	A	974	LEU	2.2
2	B	14	CYS	2.2
1	A	469	GLY	2.2
2	B	102	GLU	2.2
1	A	331	ALA	2.1
2	B	98	ASP	2.1
3	D	305	ALA	2.1
2	B	45	TYR	2.1
1	A	710	LEU	2.1
3	D	472	ASN	2.0
1	A	379	LEU	2.0

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

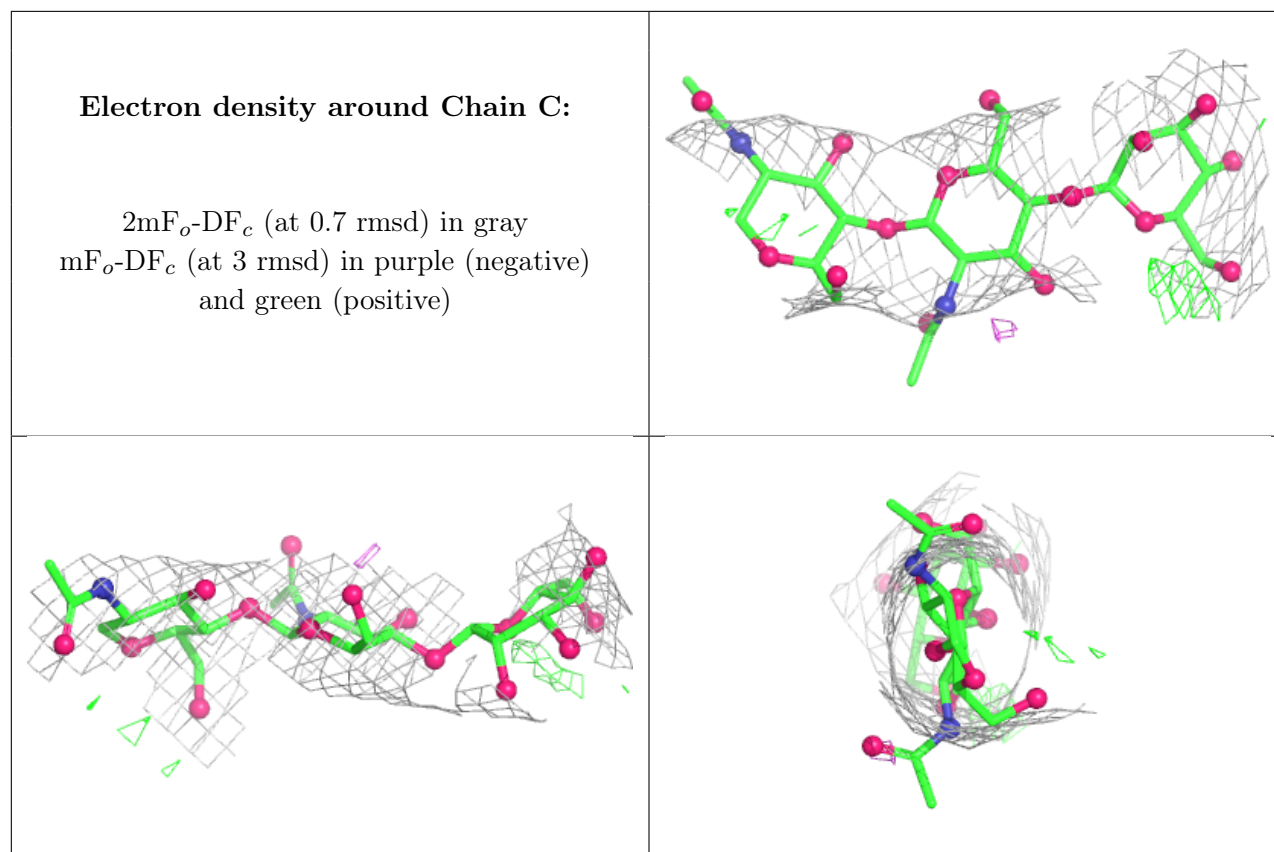
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	C	1	14/15	-	-	20,20,20,20	0
4	NAG	C	2	14/15	-	-	20,20,20,20	0
4	BMA	C	3	11/12	-	-	20,20,20,20	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.



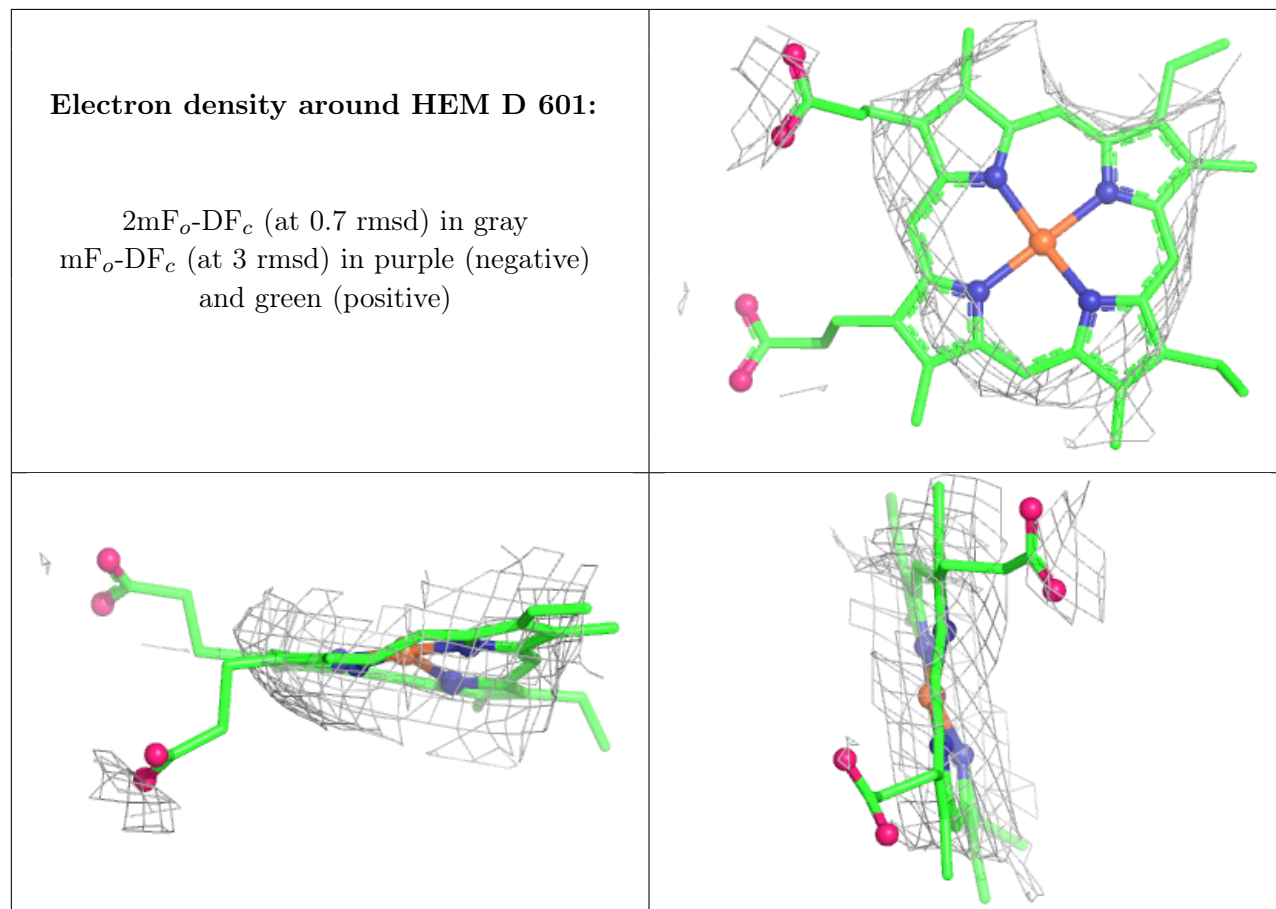
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	D	605	14/15	0.70	0.15	20,20,20,20	0
6	NAG	D	606	14/15	0.71	0.12	20,20,20,20	0
6	NAG	A	1108	14/15	0.80	0.10	20,20,20,20	0
5	CU	A	1107	1/1	0.81	0.26	20,20,20,20	1
6	NAG	A	1109	14/15	0.88	0.08	20,20,20,20	0
7	HEM	D	601	43/43	0.91	0.12	20,20,20,20	0
5	CU	A	1102	1/1	0.93	0.09	20,20,20,20	0
5	CU	A	1103	1/1	0.94	0.12	20,20,20,20	0
5	CU	A	1104	1/1	0.96	0.20	20,20,20,20	0
5	CU	A	1101	1/1	0.98	0.02	20,20,20,20	0
5	CU	A	1106	1/1	0.98	0.08	20,20,20,20	0
5	CU	A	1105	1/1	0.99	0.03	20,20,20,20	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.