



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:21 PM UTC

PDB ID : 4B7Q / pdb_00004b7q
Title : H1N1 2009 Pandemic Influenza Virus: Resistance of the I223R Neuraminidase Mutant Explained by Kinetic and Structural Analysis
Authors : Liu, J.; van der Vries, E.; Vachieri, S.G.; Xiong, X.; Collins, P.J.; Walker, P.A.; Haire, L.F.; Hay, A.J.; Schutten, M.; Osterhaus, A.D.M.E.; Martin, S.R.; Boucher, C.A.B.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2012-08-21
Resolution : 2.73 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](#) ①) 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

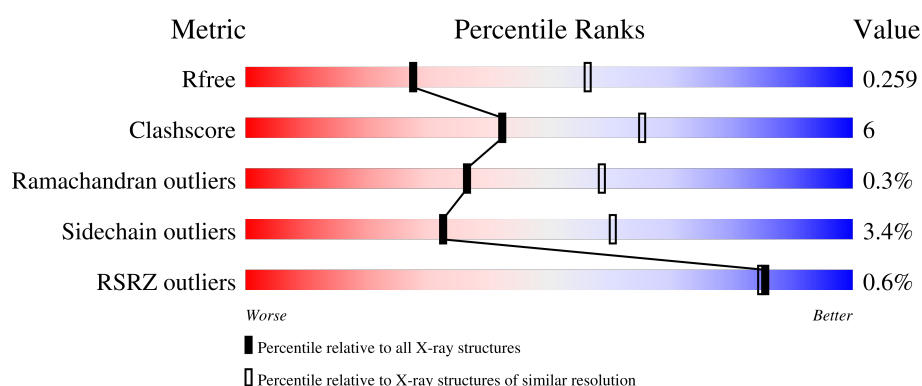
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	469	
1	B	469	
1	C	469	
1	D	469	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12571 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	B	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	C	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			
1	D	387	Total	C	N	O	S	0	0	0
			2994	1880	517	576	21			

There are 4 discrepancies between the modelled and reference sequences:

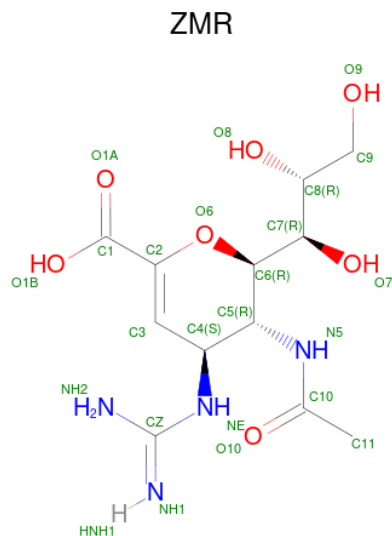
Chain	Residue	Modelled	Actual	Comment	Reference
A	351	PHE	TYR	conflict	UNP C7FH46
B	351	PHE	TYR	conflict	UNP C7FH46
C	351	PHE	TYR	conflict	UNP C7FH46
D	351	PHE	TYR	conflict	UNP C7FH46

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



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

- Molecule 3 is ZANAMIVIR (CCD ID: ZMR) (formula: $C_{12}H_{20}N_4O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 23	C 12	N 4	O 7	0	0
3	B	1	Total 23	C 12	N 4	O 7	0	0
3	C	1	Total 23	C 12	N 4	O 7	0	0
3	D	1	Total 23	C 12	N 4	O 7	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	86	Total O 86 86	0	0

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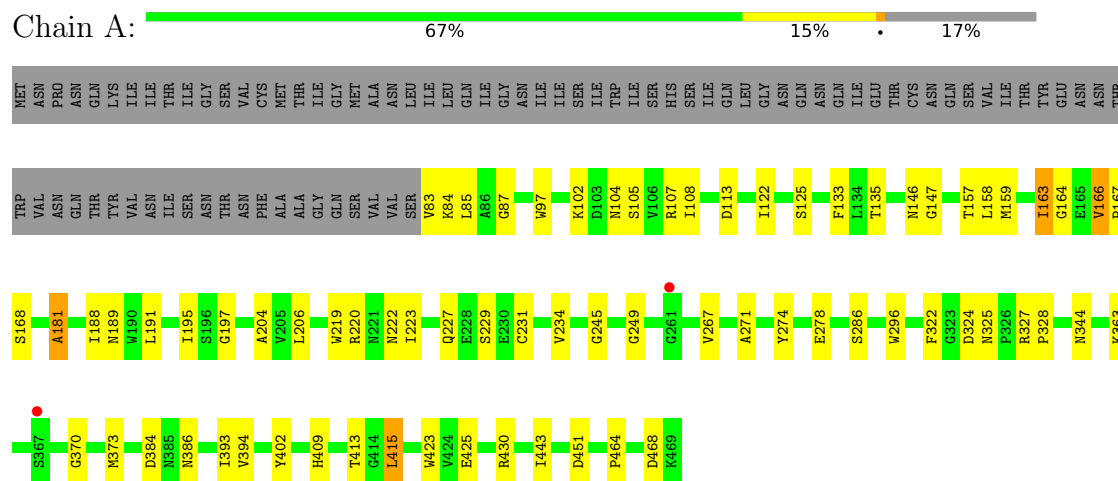
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	94	Total 94	O 94	0	0
5	C	120	Total 120	O 120	0	0
5	D	86	Total 86	O 86	0	0

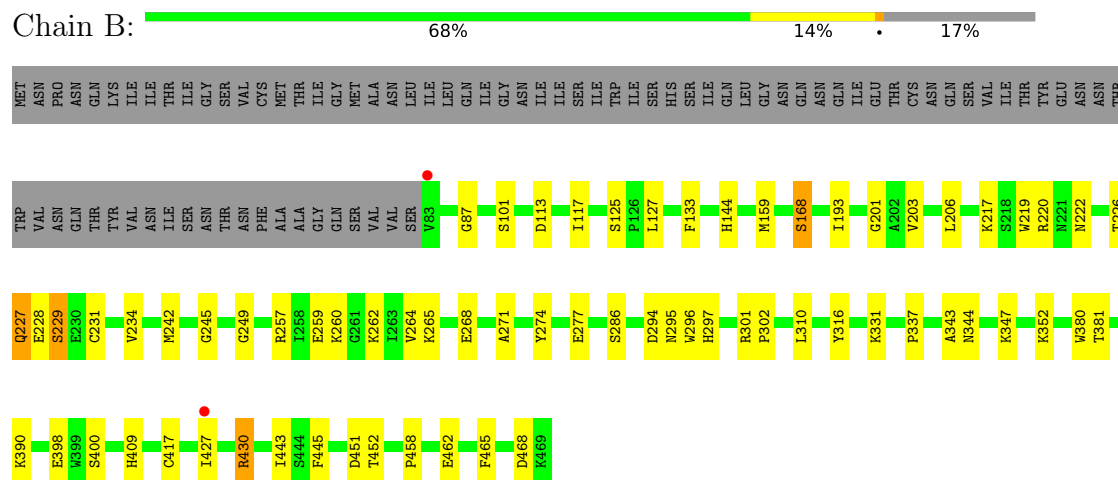
3 Residue-property plots

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.

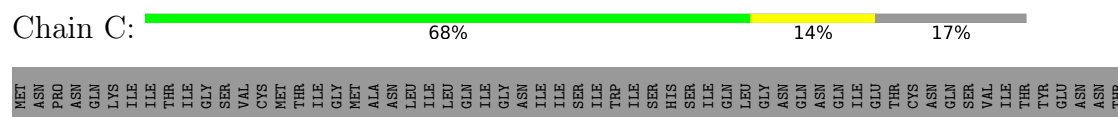
• Molecule 1: NEURAMINIDASE

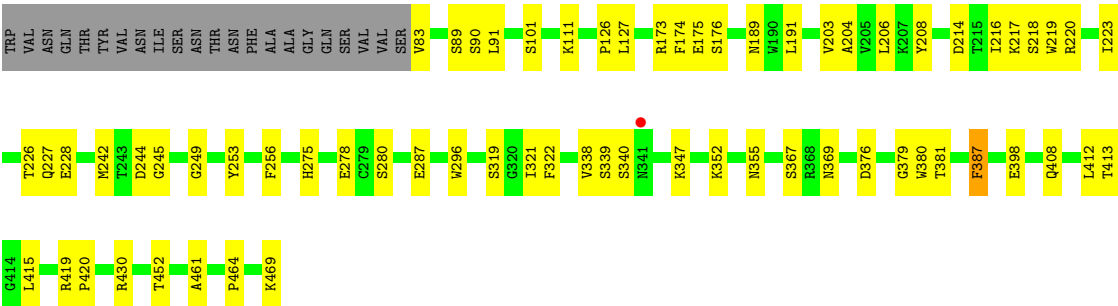


• Molecule 1: NEURAMINIDASE

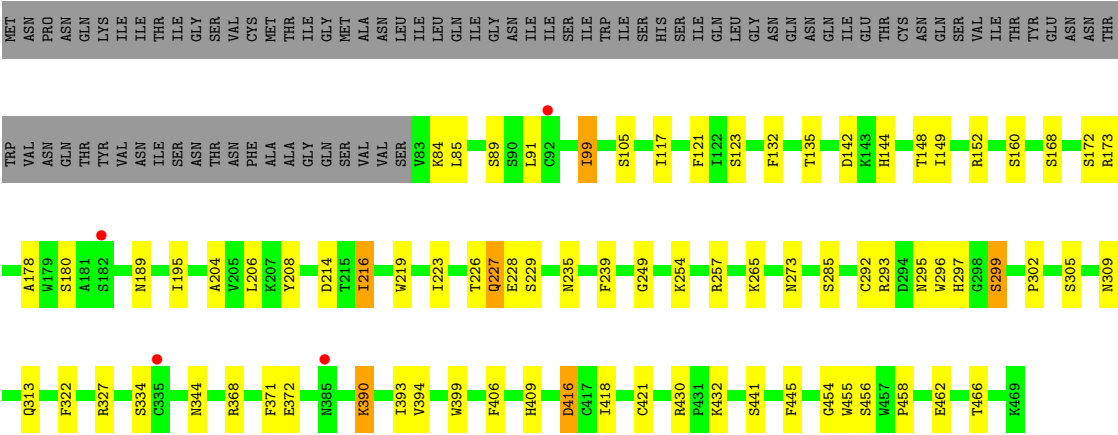


• Molecule 1: NEURAMINIDASE





● Molecule 1: NEURAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.65Å 148.82Å 166.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.49 – 2.73 55.49 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.0 (55.49-2.73) 99.0 (55.49-2.73)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.174 , 0.258 0.178 , 0.259	Depositor DCC
R_{free} test set	2790 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12571	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: ZMR, CA, NAG

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	0.48	0/3076	0.84	5/4180 (0.1%)
1	B	0.50	0/3076	0.89	5/4180 (0.1%)
1	C	0.54	0/3076	0.87	5/4180 (0.1%)
1	D	0.51	0/3076	0.84	2/4180 (0.0%)
All	All	0.51	0/12304	0.86	17/16720 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	GLN	N-CA-C	6.34	118.19	111.28
1	A	125	SER	CA-C-N	-6.06	113.39	120.12
1	A	125	SER	C-N-CA	-6.06	113.39	120.12
1	A	227	GLN	N-CA-C	5.94	117.76	111.28
1	B	227	GLN	N-CA-C	5.94	117.76	111.28
1	C	101	SER	N-CA-C	5.94	118.10	109.07
1	B	409	HIS	CA-C-N	5.36	125.43	119.32
1	B	409	HIS	C-N-CA	5.36	125.43	119.32
1	C	245	GLY	CA-C-N	5.26	125.26	119.89
1	C	245	GLY	C-N-CA	5.26	125.26	119.89
1	D	105	SER	N-CA-C	5.11	117.24	111.11
1	D	227	GLN	N-CA-C	5.08	116.51	111.07
1	A	84	LYS	N-CA-C	5.07	117.38	110.24
1	C	387	PHE	N-CA-C	5.02	116.82	109.24
1	A	181	ALA	N-CA-C	5.01	116.42	108.96
1	B	125	SER	CA-C-N	-5.00	114.57	120.12
1	B	125	SER	C-N-CA	-5.00	114.57	120.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2994	0	2829	44	0
1	B	2994	0	2827	41	0
1	C	2994	0	2827	35	0
1	D	2994	0	2828	37	0
2	A	14	0	13	1	0
2	B	28	0	26	0	0
2	C	42	0	39	0	0
2	D	28	0	26	0	0
3	A	23	0	19	0	0
3	B	23	0	19	0	0
3	C	23	0	19	0	0
3	D	23	0	19	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	86	0	0	6	0
5	B	94	0	0	6	0
5	C	120	0	0	4	0
5	D	86	0	0	4	0
All	All	12571	0	11491	148	0

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

All (148) 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:C:355:ASN:OD1	1:C:381:THR:OG1	2.03	0.76
1:D:265:LYS:NZ	1:D:309:ASN:O	2.22	0.72
1:C:91:LEU:HD22	1:C:420:PRO:HG3	1.72	0.72
1:A:87:GLY:HA3	1:A:234:VAL:HG13	1.71	0.71
1:B:265:LYS:HG2	1:B:310:LEU:HD12	1.72	0.70
1:A:157:THR:O	5:A:2018:HOH:O	2.09	0.70
1:D:173:ARG:NH1	5:D:2018:HOH:O	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LEU:HD13	1:D:214:ASP:HB3	1.75	0.69
1:D:285:SER:O	5:D:2052:HOH:O	2.11	0.68
1:B:398:GLU:HG2	1:B:458:PRO:CB	2.24	0.68
1:D:416:ASP:N	1:D:416:ASP:OD1	2.25	0.67
1:C:204:ALA:HB3	1:C:216:ILE:HG23	1.75	0.67
1:B:257:ARG:NH2	1:B:259:GLU:OE2	2.27	0.66
1:B:443:ILE:HD12	1:B:445:PHE:HE1	1.60	0.66
1:B:398:GLU:HG2	1:B:458:PRO:HB3	1.77	0.65
1:C:206:LEU:HD13	1:C:214:ASP:HB3	1.78	0.65
1:A:133:PHE:O	5:A:2018:HOH:O	2.12	0.65
1:D:204:ALA:HB3	1:D:216:ILE:HG23	1.79	0.65
1:A:393:ILE:HG22	1:A:394:VAL:HG23	1.81	0.63
1:D:121:PHE:CG	1:D:229:SER:HA	2.34	0.62
1:A:271:ALA:HB1	1:A:274:TYR:HB2	1.82	0.61
1:A:105:SER:HA	1:A:166:VAL:HG22	1.82	0.61
1:A:107:ARG:HG2	1:B:144:HIS:HD2	1.64	0.61
1:C:376:ASP:OD1	5:C:2089:HOH:O	2.16	0.60
1:A:113:ASP:O	1:A:168:SER:HB2	2.01	0.60
1:C:242:MET:HB2	1:C:256:PHE:HE1	1.67	0.59
1:D:219:TRP:CE2	1:D:254:LYS:HE3	2.37	0.58
1:B:430:ARG:NH2	5:B:2088:HOH:O	2.37	0.58
1:C:398:GLU:OE1	5:C:2097:HOH:O	2.17	0.57
1:D:372:GLU:OE1	1:D:390:LYS:NZ	2.30	0.57
1:A:146:ASN:HD22	2:A:511:NAG:H83	1.68	0.57
1:A:324:ASP:OD1	1:A:325:ASN:N	2.37	0.57
1:D:117:ILE:HG22	1:D:135:THR:HA	1.85	0.57
1:D:152:ARG:NH1	3:D:601:ZMR:O10	2.38	0.56
1:A:344:ASN:HB3	5:A:2071:HOH:O	2.06	0.56
1:B:113:ASP:O	1:B:168:SER:HB2	2.06	0.56
1:C:367:SER:OG	1:C:369:ASN:OD1	2.24	0.56
1:C:464:PRO:HG2	1:C:469:LYS:HE3	1.88	0.55
1:D:91:LEU:HD12	1:D:418:ILE:O	2.07	0.55
1:A:402:TYR:HB2	1:A:425:GLU:OE1	2.05	0.55
1:A:102:LYS:HG3	1:A:443:ILE:HG22	1.88	0.55
1:A:322:PHE:HB2	1:A:327:ARG:HD2	1.89	0.55
1:D:84:LYS:NZ	1:D:235:ASN:OD1	2.39	0.54
1:C:278:GLU:OE1	1:C:347:LYS:HB2	2.08	0.54
1:C:218:SER:OG	1:C:244:ASP:OD2	2.21	0.53
1:B:226:THR:HB	1:B:242:MET:HG2	1.91	0.53
1:A:107:ARG:HG2	1:B:144:HIS:CD2	2.42	0.53
1:A:122:ILE:HD12	1:A:423:TRP:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:SER:OG	1:D:228:GLU:OE2	2.25	0.53
1:B:398:GLU:HG2	1:B:458:PRO:HB2	1.91	0.53
1:A:249:GLY:HA2	1:A:296:TRP:CD1	2.43	0.52
1:B:226:THR:OG1	1:B:227:GLN:N	2.41	0.52
1:C:203:VAL:HG22	1:C:217:LYS:HG3	1.92	0.52
1:B:193:ILE:HG12	1:B:206:LEU:HG	1.91	0.52
1:B:451:ASP:HB3	1:C:217:LYS:HB2	1.90	0.52
1:B:465:PHE:N	1:B:468:ASP:OD2	2.39	0.52
1:A:384:ASP:OD2	1:A:386:ASN:HB2	2.10	0.51
1:C:321:ILE:HD11	1:C:387:PHE:HB3	1.92	0.51
1:D:456:SER:O	1:D:458:PRO:HD3	2.11	0.51
1:A:278:GLU:OE2	1:A:402:TYR:OH	2.25	0.51
1:B:234:VAL:HG11	1:B:286:SER:HA	1.93	0.51
1:D:313:GLN:NE2	5:D:2057:HOH:O	2.32	0.51
1:B:87:GLY:HA3	1:B:234:VAL:HG22	1.92	0.51
1:B:101:SER:HA	1:C:174:PHE:CZ	2.47	0.50
1:A:135:THR:HG23	5:A:2018:HOH:O	2.13	0.48
1:A:195:ILE:HG12	1:A:204:ALA:HB2	1.94	0.48
1:C:219:TRP:CD1	1:C:220:ARG:HG2	2.48	0.48
1:D:168:SER:O	1:D:172:SER:HB3	2.12	0.48
1:B:381:THR:OG1	5:B:2072:HOH:O	2.20	0.48
1:D:393:ILE:HG22	1:D:394:VAL:HG23	1.96	0.48
1:B:260:LYS:NZ	5:B:2045:HOH:O	2.47	0.47
1:C:220:ARG:HB2	1:C:244:ASP:CG	2.39	0.47
1:D:189:ASN:HB2	1:D:208:TYR:CZ	2.49	0.47
1:B:331:LYS:NZ	5:B:2063:HOH:O	2.47	0.47
1:A:133:PHE:CE2	1:A:159:MET:HB2	2.50	0.47
1:A:133:PHE:CZ	1:A:167:PRO:HB3	2.50	0.47
1:A:464:PRO:HB2	1:A:468:ASP:HB2	1.96	0.47
1:C:111:LYS:HB2	1:D:142:ASP:HB2	1.97	0.47
1:C:189:ASN:HB2	1:C:208:TYR:CZ	2.49	0.47
1:D:371:PHE:O	1:D:393:ILE:HB	2.15	0.47
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.51	0.46
1:B:271:ALA:HB1	1:B:274:TYR:HB2	1.97	0.46
1:D:239:PHE:CE2	1:D:257:ARG:HG3	2.51	0.46
1:B:133:PHE:CE1	1:B:159:MET:HB2	2.51	0.45
1:A:158:LEU:HD22	1:A:181:ALA:HB1	1.99	0.45
1:B:400:SER:O	1:B:427:ILE:HG12	2.17	0.45
1:D:226:THR:OG1	1:D:227:GLN:N	2.50	0.45
1:D:293:ARG:NH2	1:D:295:ASN:OD1	2.42	0.45
1:D:454:GLY:HA3	5:D:2070:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:LYS:HD2	1:C:380:TRP:CE2	2.52	0.45
1:D:299:SER:OG	1:D:327:ARG:HA	2.17	0.45
1:A:85:LEU:HD13	1:A:409:HIS:CE1	2.51	0.44
1:B:228:GLU:O	1:B:347:LYS:HE2	2.17	0.44
1:C:249:GLY:HA2	1:C:296:TRP:CE2	2.52	0.44
1:D:99:ILE:HD12	1:D:445:PHE:CZ	2.53	0.44
1:D:292:CYS:HB2	1:D:302:PRO:HG2	1.98	0.44
1:A:220:ARG:NE	5:A:2047:HOH:O	2.46	0.44
1:A:222:ASN:ND2	1:A:245:GLY:O	2.49	0.44
1:D:399:TRP:CH2	1:D:432:LYS:HB3	2.52	0.44
1:A:147:GLY:CA	1:A:430:ARG:HH22	2.31	0.44
1:A:363:LYS:HB2	1:A:370:GLY:HA3	2.00	0.44
1:A:197:GLY:HA2	1:D:455:TRP:CE3	2.53	0.44
1:C:322:PHE:CE1	1:C:338:VAL:HG21	2.52	0.44
1:D:132:PHE:CD2	1:D:160:SER:HB3	2.53	0.43
1:C:430:ARG:NE	5:C:2108:HOH:O	2.40	0.43
1:C:408:GLN:HB3	1:C:412:LEU:HD23	2.01	0.43
1:C:352:LYS:HB2	1:C:380:TRP:CZ3	2.53	0.43
1:A:327:ARG:O	5:A:2065:HOH:O	2.21	0.43
1:B:316:TYR:CE1	1:B:337:PRO:HG3	2.53	0.43
1:C:253:TYR:OH	1:C:275:HIS:HA	2.19	0.43
1:A:219:TRP:CD1	1:A:220:ARG:HG2	2.54	0.43
1:A:249:GLY:HA2	1:A:296:TRP:CG	2.54	0.43
1:B:222:ASN:HB3	1:B:245:GLY:HA2	2.01	0.43
1:B:343:ALA:O	1:B:344:ASN:HB2	2.19	0.43
1:C:173:ARG:HD2	1:C:175:GLU:OE2	2.19	0.43
1:C:461:ALA:HA	1:D:144:HIS:NE2	2.33	0.42
1:C:419:ARG:HA	1:C:420:PRO:HD3	1.87	0.42
1:A:413:THR:OG1	1:A:415:LEU:HB2	2.20	0.42
1:B:249:GLY:HA2	1:B:296:TRP:CE2	2.55	0.42
1:A:104:ASN:O	1:A:108:ILE:HG12	2.19	0.42
1:A:234:VAL:HG11	1:A:286:SER:HA	2.01	0.42
1:C:413:THR:HG23	1:C:415:LEU:HB2	2.00	0.42
1:B:227:GLN:HB3	1:B:229:SER:HB2	2.01	0.42
1:A:191:LEU:HD11	1:A:206:LEU:HD23	2.01	0.42
1:A:163:ILE:HG13	1:A:164:GLY:N	2.35	0.42
1:C:126:PRO:O	1:C:127:LEU:HD23	2.19	0.42
1:A:451:ASP:HB3	1:B:217:LYS:HB2	2.02	0.41
1:B:294:ASP:OD1	1:B:297:HIS:N	2.49	0.41
1:B:301:ARG:HA	1:B:302:PRO:HD2	1.93	0.41
1:B:398:GLU:HG3	5:B:2081:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:THR:HB	1:C:242:MET:HG2	2.03	0.41
1:B:451:ASP:CB	1:C:217:LYS:HB2	2.51	0.41
1:D:85:LEU:HD13	1:D:409:HIS:CG	2.55	0.41
1:D:322:PHE:HB2	1:D:327:ARG:HD2	2.02	0.41
1:A:430:ARG:HE	1:A:430:ARG:HB2	1.56	0.41
1:B:219:TRP:CD1	1:B:220:ARG:HG2	2.56	0.41
1:A:97:TRP:CE2	1:A:373:MET:HE2	2.56	0.41
1:A:322:PHE:CD2	1:A:328:PRO:HD2	2.56	0.41
1:B:277:GLU:OE1	1:B:295:ASN:HB2	2.21	0.41
1:B:352:LYS:HB2	1:B:380:TRP:CE3	2.56	0.41
1:B:427:ILE:O	1:B:427:ILE:HG13	2.20	0.41
1:D:178:ALA:HA	1:D:195:ILE:O	2.20	0.41
1:D:249:GLY:HA2	1:D:296:TRP:CE2	2.56	0.40
1:B:262:LYS:O	1:B:264:VAL:HG13	2.22	0.40
1:B:390:LYS:NZ	5:B:2075:HOH:O	2.46	0.40
1:C:319:SER:HB2	1:C:379:GLY:CA	2.52	0.40
1:A:188:ILE:HG22	1:A:189:ASN:ND2	2.36	0.40
1:C:339:SER:O	5:C:2081:HOH:O	2.22	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	385/469 (82%)	358 (93%)	26 (7%)	1 (0%)	36	59
1	B	385/469 (82%)	365 (95%)	19 (5%)	1 (0%)	36	59
1	C	385/469 (82%)	365 (95%)	19 (5%)	1 (0%)	36	59
1	D	385/469 (82%)	363 (94%)	20 (5%)	2 (0%)	24	46
All	All	1540/1876 (82%)	1451 (94%)	84 (6%)	5 (0%)	36	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	223	ILE
1	D	148	THR
1	B	201	GLY
1	C	223	ILE
1	A	223	ILE

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	334/408 (82%)	327 (98%)	7 (2%)	47	73
1	B	334/408 (82%)	323 (97%)	11 (3%)	33	61
1	C	334/408 (82%)	324 (97%)	10 (3%)	36	64
1	D	334/408 (82%)	316 (95%)	18 (5%)	20	43
All	All	1336/1632 (82%)	1290 (97%)	46 (3%)	32	60

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	163	ILE
1	A	166	VAL
1	A	229	SER
1	A	231	CYS
1	A	267	VAL
1	A	415	LEU
1	B	117	ILE
1	B	127	LEU
1	B	168	SER
1	B	203	VAL
1	B	229	SER
1	B	231	CYS
1	B	268	GLU
1	B	417	CYS
1	B	430	ARG
1	B	452	THR

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Mol	Chain	Res	Type
1	B	462	GLU
1	C	83	VAL
1	C	89	SER
1	C	90	SER
1	C	176	SER
1	C	191	LEU
1	C	228	GLU
1	C	280	SER
1	C	287	GLU
1	C	340	SER
1	C	452	THR
1	D	89	SER
1	D	99	ILE
1	D	123	SER
1	D	149	ILE
1	D	216	ILE
1	D	273	ASN
1	D	297	HIS
1	D	299	SER
1	D	305	SER
1	D	334	SER
1	D	344	ASN
1	D	368	ARG
1	D	390	LYS
1	D	416	ASP
1	D	430	ARG
1	D	441	SER
1	D	462	GLU
1	D	466	THR

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

Mol	Chain	Res	Type
1	A	189	ASN
1	A	308	GLN
1	A	449	ASN
1	B	275	HIS
1	C	104	ASN
1	C	325	ASN
1	C	344	ASN
1	D	273	ASN
1	D	344	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	$\# Z > 2$
2	NAG	B	511	1	14,14,15	0.52	0	17,19,21	0.69	0
2	NAG	C	511	1	14,14,15	0.51	0	17,19,21	1.49	1 (5%)
2	NAG	B	501	1	14,14,15	0.53	0	17,19,21	1.41	1 (5%)
2	NAG	C	521	1	14,14,15	0.50	0	17,19,21	1.85	2 (11%)
3	ZMR	A	601	-	22,23,23	4.24	10 (45%)	24,32,32	3.67	6 (25%)
2	NAG	C	501	1	14,14,15	0.61	0	17,19,21	1.38	2 (11%)
2	NAG	D	501	1	14,14,15	0.40	0	17,19,21	1.32	2 (11%)
3	ZMR	C	601	-	22,23,23	4.20	10 (45%)	24,32,32	3.78	8 (33%)
3	ZMR	D	601	-	22,23,23	4.14	10 (45%)	24,32,32	3.59	7 (29%)
3	ZMR	B	601	-	22,23,23	4.24	10 (45%)	24,32,32	3.48	6 (25%)
2	NAG	D	511	1	14,14,15	0.54	0	17,19,21	2.51	2 (11%)
2	NAG	A	511	1	14,14,15	0.55	0	17,19,21	1.81	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
2	NAG	B	511	1	-	2/6/23/26	0/1/1/1
2	NAG	C	511	1	-	2/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	521	1	-	4/6/23/26	0/1/1/1
3	ZMR	A	601	-	-	4/22/38/38	0/1/1/1
2	NAG	C	501	1	-	3/6/23/26	0/1/1/1
2	NAG	D	501	1	-	2/6/23/26	0/1/1/1
3	ZMR	C	601	-	-	6/22/38/38	0/1/1/1
3	ZMR	D	601	-	-	4/22/38/38	0/1/1/1
3	ZMR	B	601	-	-	4/22/38/38	0/1/1/1
2	NAG	D	511	1	-	2/6/23/26	0/1/1/1
2	NAG	A	511	1	-	2/6/23/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	ZMR	C3-C2	12.62	1.55	1.33
3	A	601	ZMR	C3-C2	12.13	1.54	1.33
3	D	601	ZMR	C3-C2	11.92	1.54	1.33
3	C	601	ZMR	C3-C2	11.86	1.54	1.33
3	A	601	ZMR	CZ-NE	8.36	1.47	1.33
3	B	601	ZMR	CZ-NE	8.15	1.47	1.33
3	C	601	ZMR	CZ-NE	8.02	1.47	1.33
3	D	601	ZMR	CZ-NE	8.01	1.47	1.33
3	D	601	ZMR	C4-NE	7.00	1.55	1.46
3	C	601	ZMR	C4-NE	6.90	1.55	1.46
3	A	601	ZMR	C4-NE	6.64	1.55	1.46
3	A	601	ZMR	C5-N5	6.41	1.55	1.45
3	B	601	ZMR	C4-NE	6.22	1.54	1.46
3	B	601	ZMR	C5-N5	5.99	1.55	1.45
3	B	601	ZMR	C2-C1	-5.81	1.35	1.48
3	C	601	ZMR	C5-N5	5.69	1.54	1.45
3	D	601	ZMR	C2-C1	-5.57	1.36	1.48
3	D	601	ZMR	C5-N5	5.45	1.54	1.45
3	C	601	ZMR	C2-C1	-5.39	1.36	1.48
3	A	601	ZMR	C2-C1	-5.22	1.37	1.48
3	C	601	ZMR	C6-C5	-4.74	1.45	1.53
3	A	601	ZMR	C6-C5	-4.52	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	ZMR	C6-C5	-4.21	1.46	1.53
3	D	601	ZMR	C6-C5	-4.16	1.46	1.53
3	A	601	ZMR	O6-C2	3.49	1.49	1.37
3	D	601	ZMR	O6-C2	3.40	1.49	1.37
3	B	601	ZMR	C10-N5	3.40	1.45	1.34
3	B	601	ZMR	O6-C2	3.37	1.49	1.37
3	A	601	ZMR	C10-N5	3.36	1.45	1.34
3	C	601	ZMR	C4-C3	-3.31	1.45	1.50
3	C	601	ZMR	O6-C2	3.25	1.49	1.37
3	D	601	ZMR	C10-N5	3.18	1.44	1.34
3	D	601	ZMR	C4-C3	-2.99	1.46	1.50
3	C	601	ZMR	C10-N5	2.91	1.43	1.34
3	A	601	ZMR	C4-C3	-2.83	1.46	1.50
3	A	601	ZMR	O8-C8	-2.51	1.38	1.43
3	C	601	ZMR	O8-C8	-2.48	1.38	1.43
3	B	601	ZMR	C4-C3	-2.46	1.47	1.50
3	B	601	ZMR	O8-C8	-2.34	1.38	1.43
3	D	601	ZMR	O8-C8	-2.17	1.38	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	ZMR	O6-C2-C3	-16.35	106.33	124.62
3	A	601	ZMR	O6-C2-C3	-16.12	106.59	124.62
3	D	601	ZMR	O6-C2-C3	-15.37	107.43	124.62
3	B	601	ZMR	O6-C2-C3	-15.10	107.73	124.62
2	D	511	NAG	C1-O5-C5	9.20	124.51	112.19
2	A	511	NAG	C1-O5-C5	6.11	120.38	112.19
2	C	521	NAG	C1-O5-C5	6.10	120.36	112.19
2	C	511	NAG	C1-O5-C5	5.25	119.23	112.19
3	D	601	ZMR	C3-C2-C1	-4.50	113.82	123.56
3	C	601	ZMR	C3-C2-C1	-4.38	114.08	123.56
3	B	601	ZMR	C3-C2-C1	-4.25	114.36	123.56
3	A	601	ZMR	C3-C2-C1	-4.23	114.39	123.56
2	B	501	NAG	C1-O5-C5	4.07	117.64	112.19
2	C	521	NAG	O5-C1-C2	4.02	117.51	111.29
2	D	501	NAG	C1-O5-C5	3.68	117.12	112.19
3	C	601	ZMR	C3-C4-NE	-3.63	105.92	110.98
3	D	601	ZMR	O9-C9-C8	3.42	118.34	111.16
3	A	601	ZMR	O9-C9-C8	3.40	118.30	111.16
2	C	501	NAG	C4-C3-C2	3.32	115.88	111.02
3	D	601	ZMR	C3-C4-NE	-3.14	106.60	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	ZMR	C11-C10-N5	2.99	121.08	116.12
2	C	501	NAG	C1-O5-C5	2.80	115.94	112.19
3	A	601	ZMR	C3-C4-NE	-2.76	107.13	110.98
3	B	601	ZMR	O1B-C1-C2	2.72	120.23	114.06
3	D	601	ZMR	C8-C7-C6	-2.69	108.01	113.05
3	D	601	ZMR	C6-C5-N5	-2.62	106.73	110.91
3	A	601	ZMR	O1B-C1-C2	2.60	119.96	114.06
3	C	601	ZMR	C11-C10-N5	2.46	120.20	116.12
2	D	511	NAG	O5-C1-C2	2.42	115.04	111.29
3	A	601	ZMR	C11-C10-N5	2.39	120.08	116.12
2	D	501	NAG	C4-C3-C2	-2.36	107.55	111.02
3	C	601	ZMR	O1B-C1-C2	2.17	118.99	114.06
3	C	601	ZMR	O9-C9-C8	2.16	115.68	111.16
3	B	601	ZMR	O9-C9-C8	2.14	115.65	111.16
3	C	601	ZMR	O10-C10-N5	-2.12	118.24	121.98
3	B	601	ZMR	C8-C7-C6	-2.11	109.09	113.05
3	C	601	ZMR	C5-N5-C10	-2.10	118.20	123.11
3	D	601	ZMR	O1B-C1-C2	2.06	118.73	114.06

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	511	NAG	C8-C7-N2-C2
2	C	501	NAG	C8-C7-N2-C2
2	C	501	NAG	O7-C7-N2-C2
2	C	521	NAG	C8-C7-N2-C2
2	C	521	NAG	O7-C7-N2-C2
2	D	501	NAG	C8-C7-N2-C2
2	D	501	NAG	O7-C7-N2-C2
3	B	601	ZMR	O1B-C1-C2-C3
3	C	601	ZMR	O1A-C1-C2-O6
3	C	601	ZMR	O1B-C1-C2-O6
3	D	601	ZMR	O1A-C1-C2-O6
3	D	601	ZMR	O1B-C1-C2-O6
2	A	511	NAG	O7-C7-N2-C2
2	C	511	NAG	O5-C5-C6-O6
2	B	511	NAG	C8-C7-N2-C2
2	B	511	NAG	O7-C7-N2-C2
2	D	511	NAG	C8-C7-N2-C2
2	C	521	NAG	O5-C5-C6-O6
2	C	511	NAG	C4-C5-C6-O6

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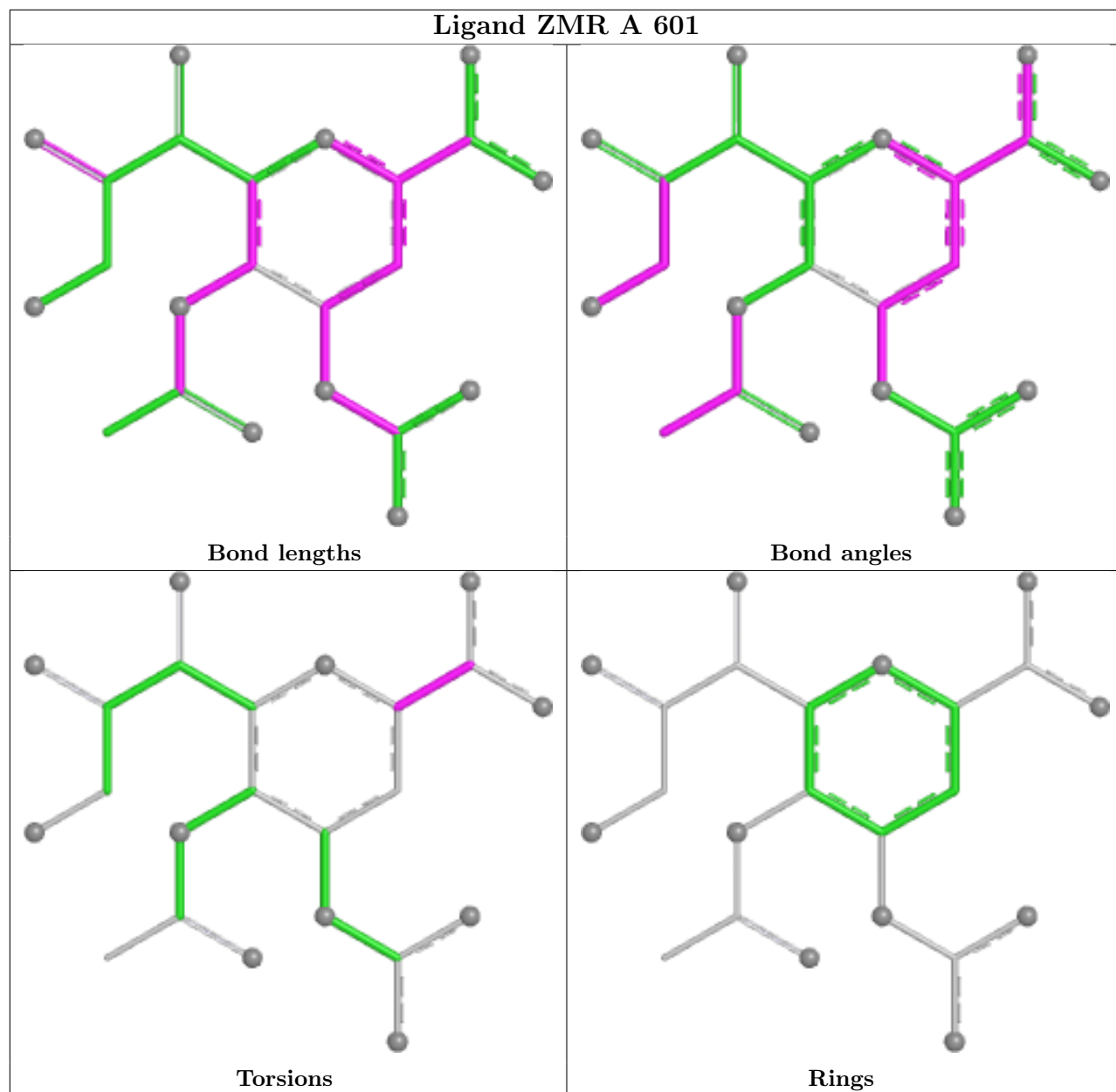
Mol	Chain	Res	Type	Atoms
2	D	511	NAG	O7-C7-N2-C2
3	B	601	ZMR	O1A-C1-C2-C3
3	B	601	ZMR	O1A-C1-C2-O6
3	B	601	ZMR	O1B-C1-C2-O6
3	C	601	ZMR	O1B-C1-C2-C3
3	C	601	ZMR	O8-C8-C9-O9
3	C	601	ZMR	NH2-CZ-NE-C4
3	D	601	ZMR	O8-C8-C9-O9
2	C	501	NAG	C1-C2-N2-C7
2	C	521	NAG	C1-C2-N2-C7
3	A	601	ZMR	O1A-C1-C2-C3
3	A	601	ZMR	O1A-C1-C2-O6
3	A	601	ZMR	O1B-C1-C2-C3
3	A	601	ZMR	O1B-C1-C2-O6
3	C	601	ZMR	C7-C8-C9-O9
3	D	601	ZMR	C7-C8-C9-O9

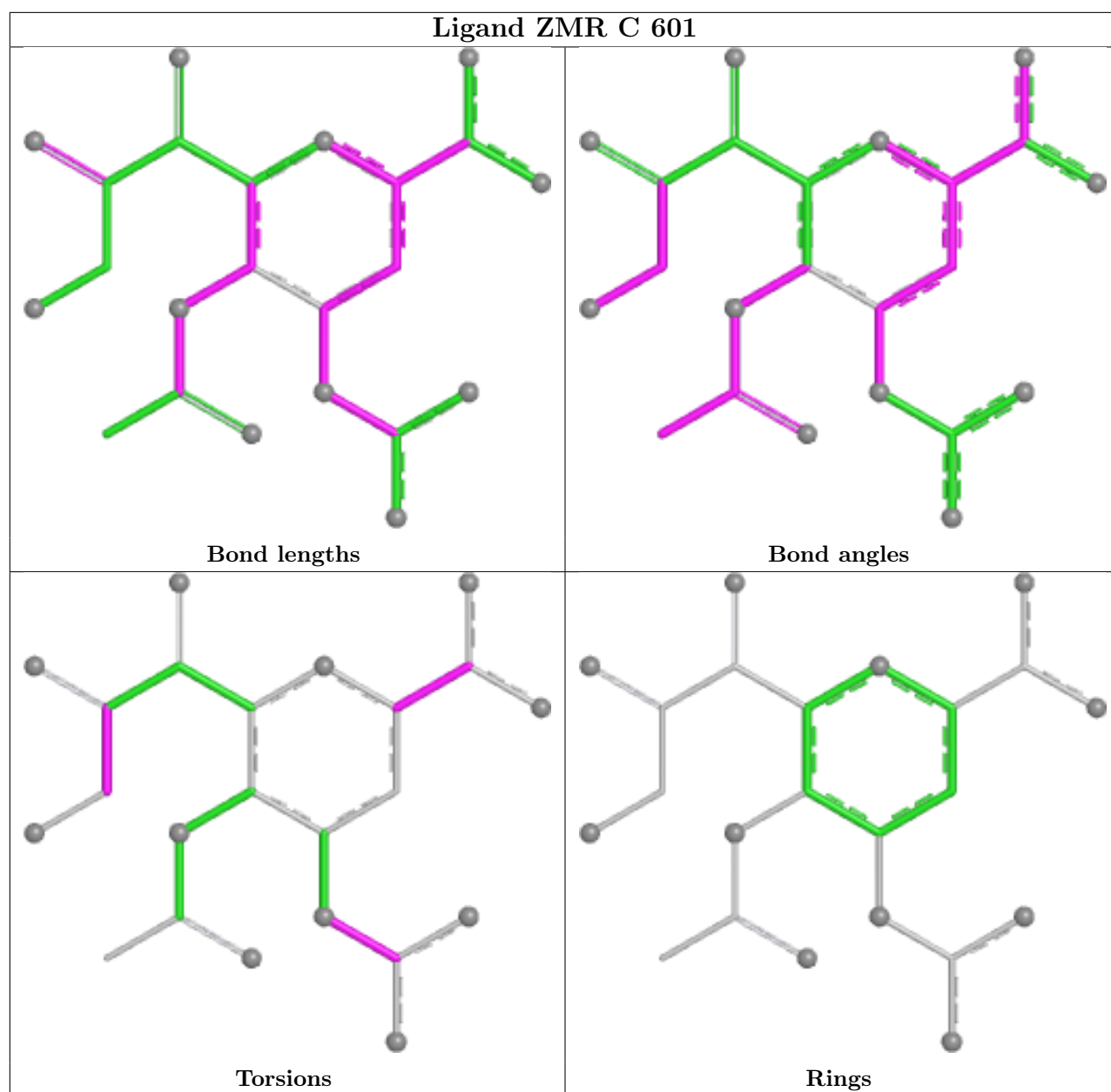
There are no ring outliers.

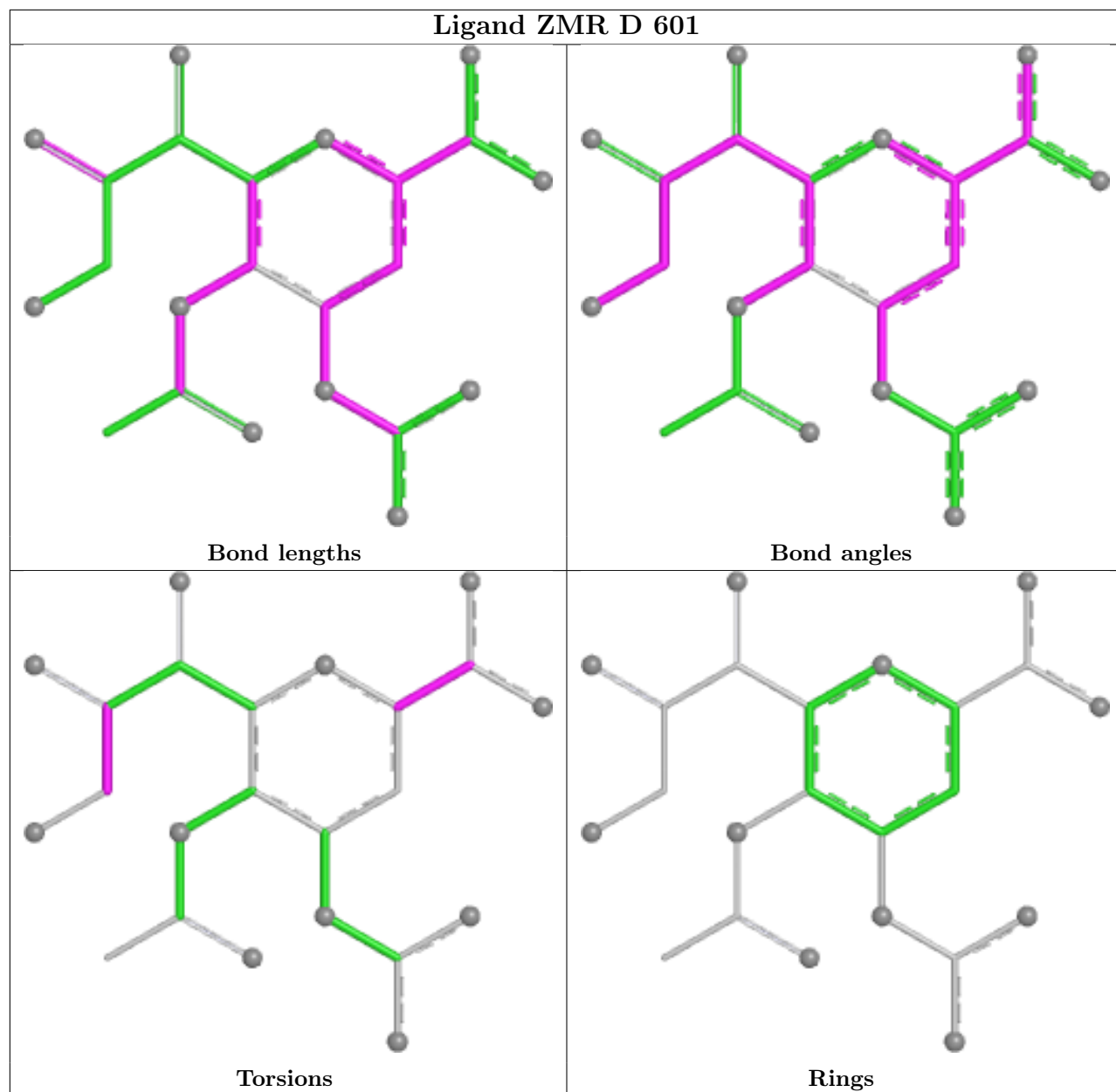
2 monomers are involved in 2 short contacts:

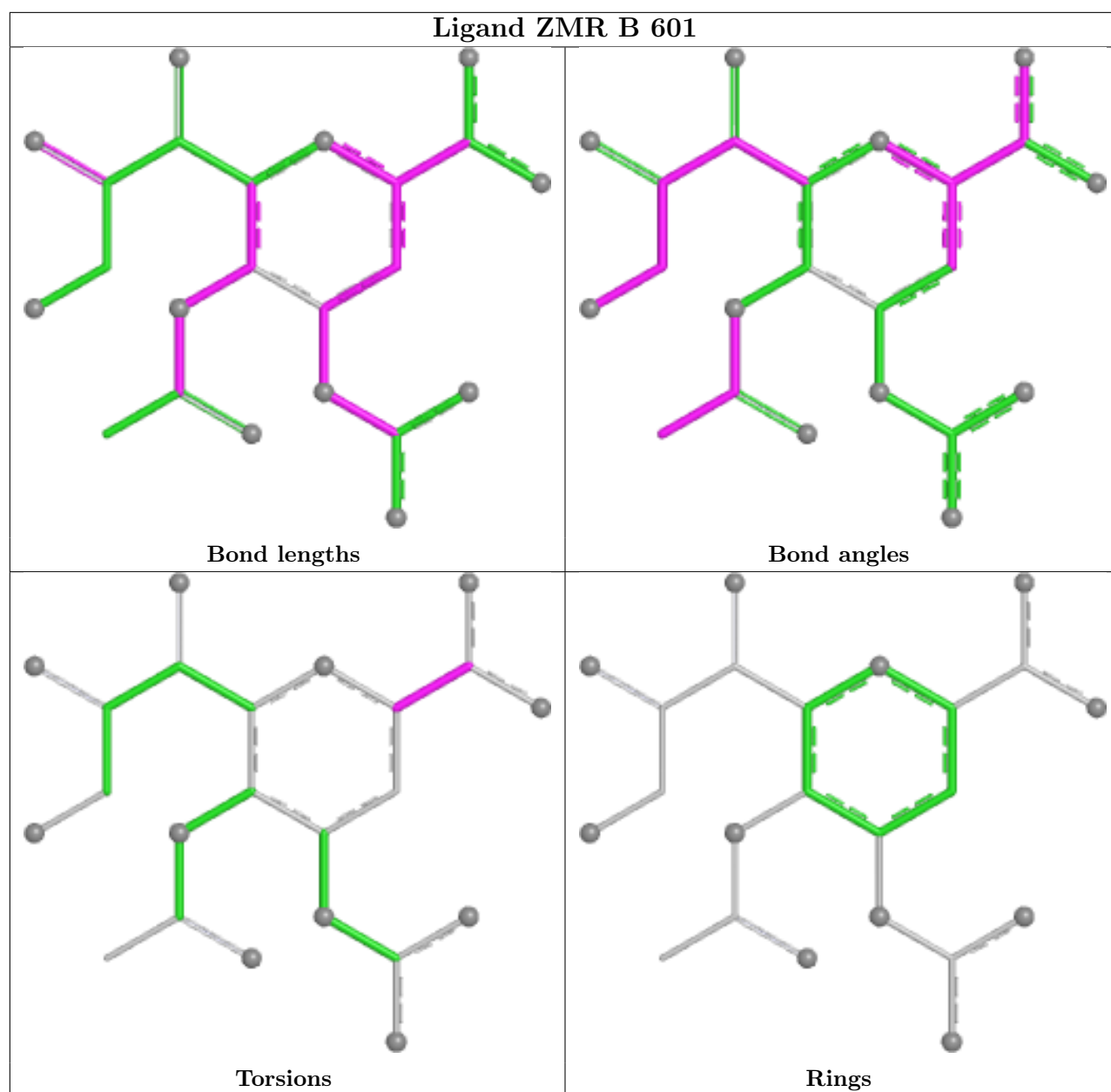
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	ZMR	1	0
2	A	511	NAG	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/469 (82%)	0.10	2 (0%) 87 86	21, 35, 52, 74	0
1	B	387/469 (82%)	-0.04	2 (0%) 87 86	20, 31, 44, 62	0
1	C	387/469 (82%)	-0.06	1 (0%) 90 89	19, 29, 44, 57	0
1	D	387/469 (82%)	-0.00	4 (1%) 79 78	18, 33, 49, 66	0
All	All	1548/1876 (82%)	0.00	9 (0%) 85 85	18, 32, 48, 74	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	GLY	3.6
1	B	427	ILE	2.7
1	B	83	VAL	2.7
1	D	182	SER	2.3
1	C	341	ASN	2.3
1	D	92	CYS	2.2
1	D	335	CYS	2.2
1	D	385	ASN	2.2
1	A	367	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

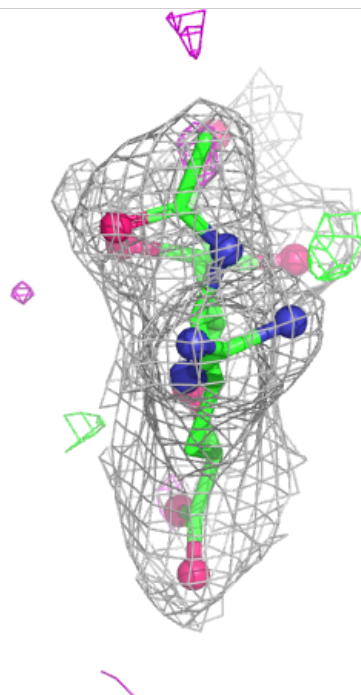
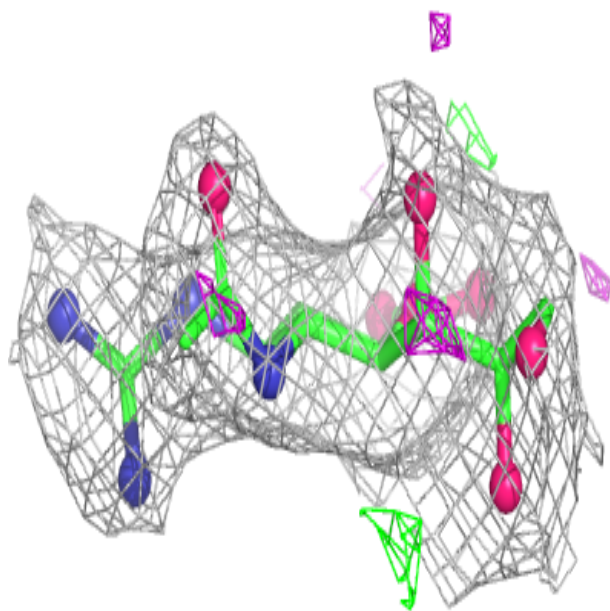
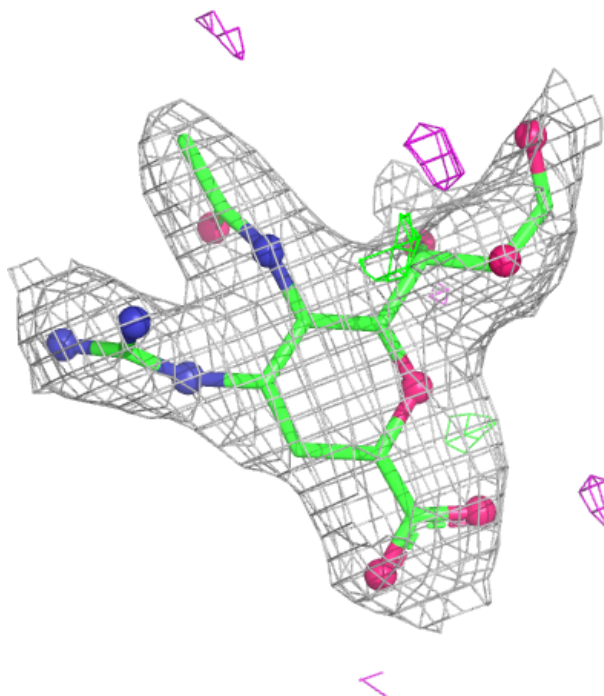
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	C	521	14/15	0.51	0.17	57,74,87,89	0
2	NAG	D	501	14/15	0.60	0.15	67,71,76,77	0
2	NAG	B	501	14/15	0.67	0.22	63,79,101,105	0
2	NAG	D	511	14/15	0.79	0.13	46,59,68,70	0
2	NAG	C	501	14/15	0.80	0.12	40,58,65,66	0
2	NAG	A	511	14/15	0.82	0.11	35,43,51,55	0
2	NAG	B	511	14/15	0.86	0.13	50,67,76,80	0
2	NAG	C	511	14/15	0.87	0.09	25,54,63,63	0
3	ZMR	B	601	23/23	0.93	0.08	5,31,38,39	0
4	CA	A	702	1/1	0.94	0.11	77,77,77,77	0
3	ZMR	D	601	23/23	0.95	0.07	23,29,39,44	0
4	CA	A	701	1/1	0.95	0.08	42,42,42,42	0
3	ZMR	A	601	23/23	0.95	0.07	12,30,37,39	0
4	CA	D	701	1/1	0.96	0.04	41,41,41,41	0
3	ZMR	C	601	23/23	0.97	0.07	3,21,35,38	0
4	CA	C	701	1/1	0.98	0.05	26,26,26,26	0
4	CA	B	701	1/1	0.98	0.02	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.

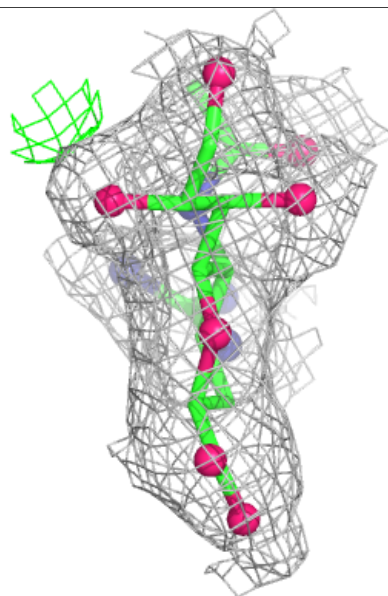
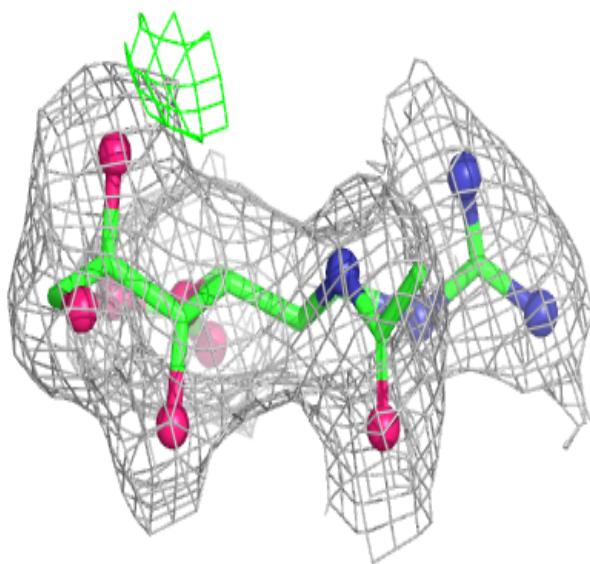
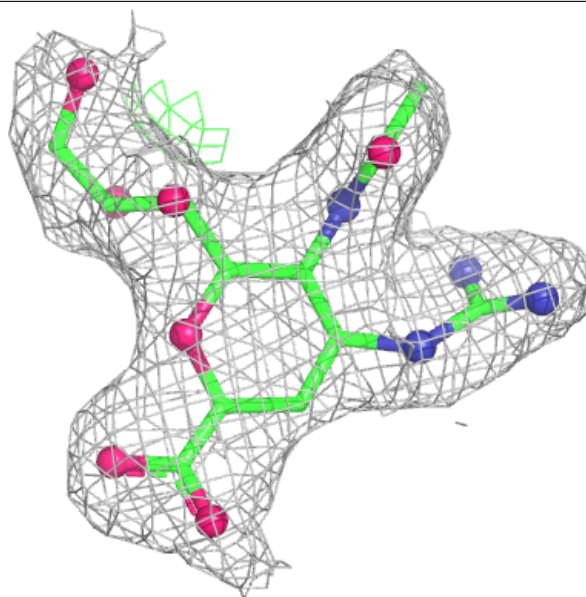
Electron density around ZMR B 601:

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



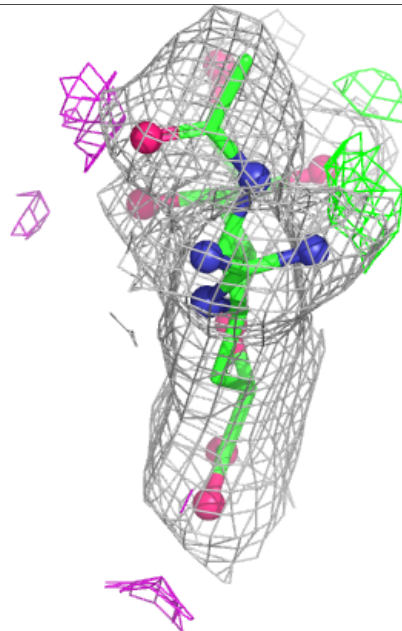
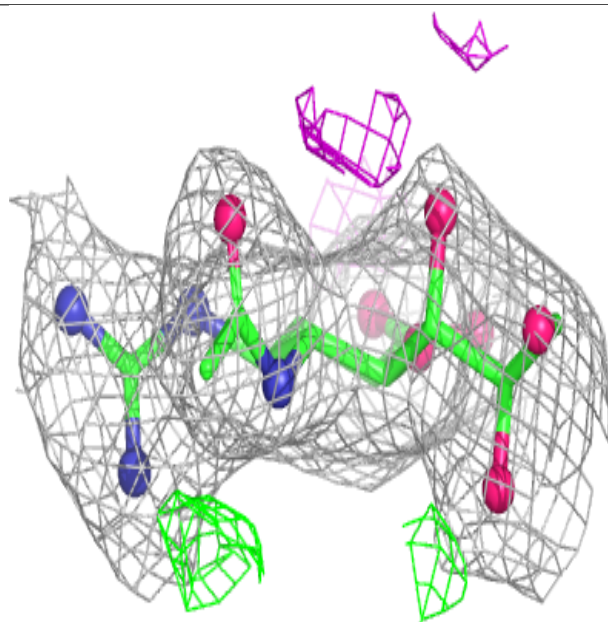
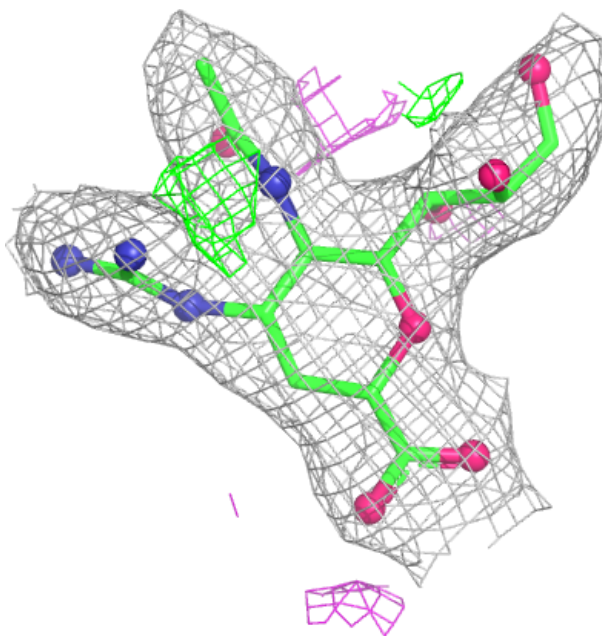
Electron density around ZMR D 601:

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



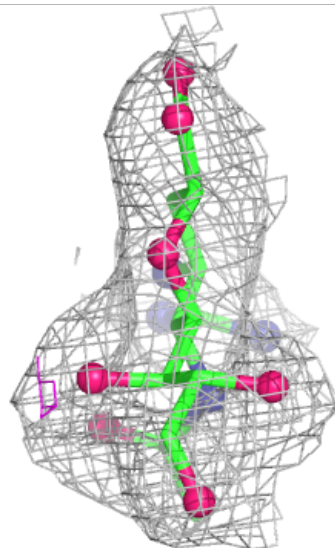
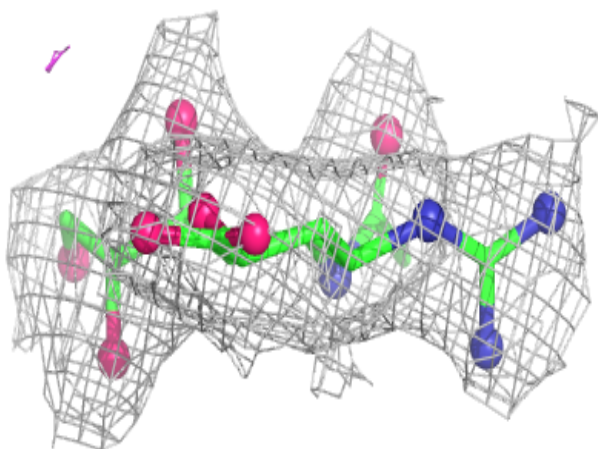
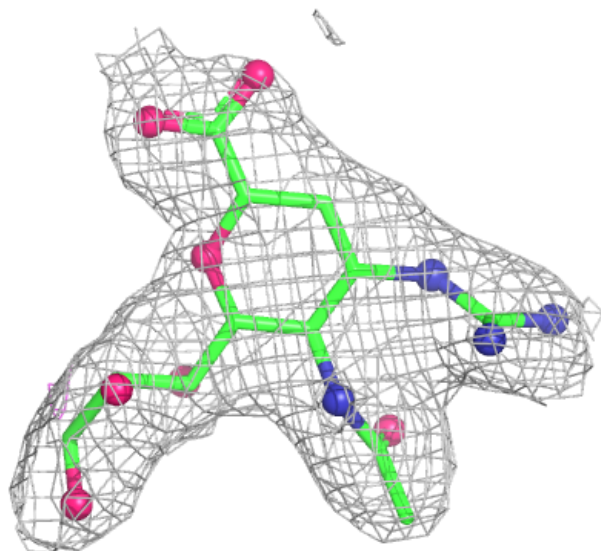
Electron density around ZMR A 601:

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



Electron density around ZMR C 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.