



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:08 PM UTC

PDB ID : 5EJM / pdb_00005ejm
Title : ThDP-Mn²⁺ complex of R413A variant of EcMenD soaked with 2-ketoglutarate for 35 min
Authors : Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.
Deposited on : 2015-11-02
Resolution : 1.72 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

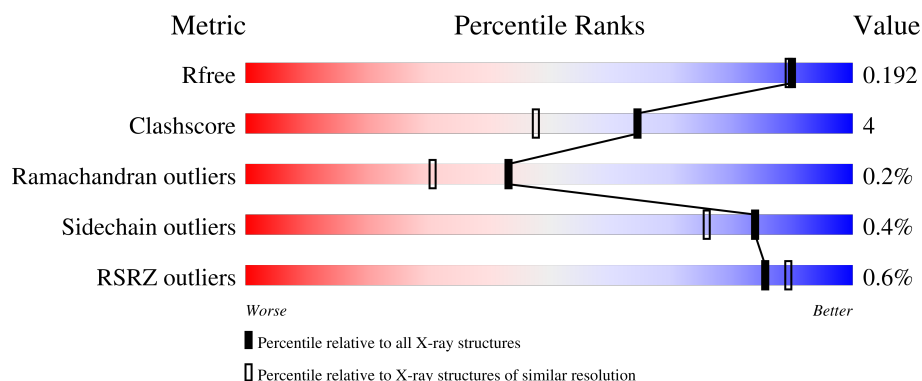
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	556	91% 9%
1	B	556	93% 7%
1	C	556	91% 9%
1	D	556	93% 7%
1	E	556	93% 7%

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Mol	Chain	Length	Quality of chain
1	F	556	% 91% 9%
1	G	556	% 92% 8%
1	H	556	% 92% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40337 atoms, of which 272 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	12	0
			4410	2794	799	802	15			
1	B	556	Total	C	N	O	S	0	8	0
			4378	2779	790	795	14			
1	C	556	Total	C	N	O	S	0	10	0
			4396	2783	798	800	15			
1	D	556	Total	C	N	O	S	0	10	0
			4388	2781	793	799	15			
1	E	556	Total	C	N	O	S	0	8	0
			4380	2775	794	796	15			
1	F	556	Total	C	N	O	S	0	8	0
			4379	2775	793	797	14			
1	G	556	Total	C	N	O	S	0	8	0
			4377	2773	791	798	15			
1	H	556	Total	C	N	O	S	0	6	0
			4355	2760	785	795	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	ALA	ARG	engineered mutation	UNP P17109
B	413	ALA	ARG	engineered mutation	UNP P17109
C	413	ALA	ARG	engineered mutation	UNP P17109
D	413	ALA	ARG	engineered mutation	UNP P17109
E	413	ALA	ARG	engineered mutation	UNP P17109
F	413	ALA	ARG	engineered mutation	UNP P17109
G	413	ALA	ARG	engineered mutation	UNP P17109
H	413	ALA	ARG	engineered mutation	UNP P17109

- Molecule 2 is (4 {R})-4-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-5-[2-[oxidanyl(phosphonooxy)phosphoryl]oxyethyl]-1,3-thiazol-3-ium-2-yl]-4-oxidanyl-butanoic acid (CCD ID: TD5) (formula: C₁₆H₂₅N₄O₁₀P₂S).



- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	F	1	Total	C	H	O	0	0
			10	2	6	2		
5	G	1	Total	C	H	O	0	0
			10	2	6	2		
5	H	1	Total	C	H	O	0	0
			10	2	6	2		

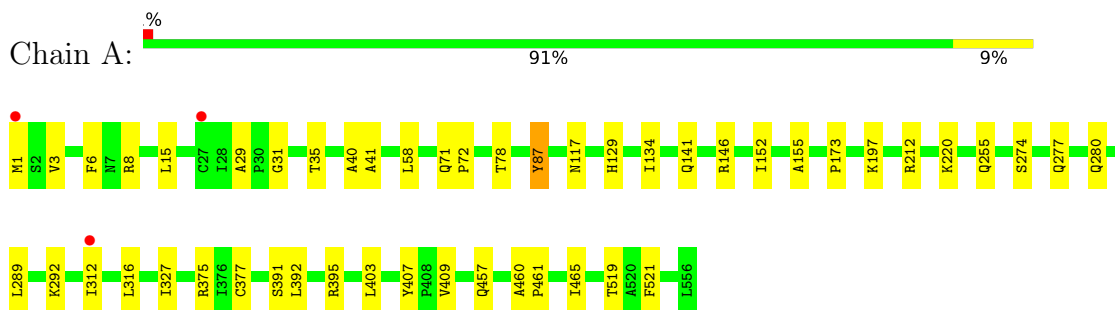
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	630	Total 630	O 630	0	0
6	B	611	Total 611	O 611	0	0
6	C	472	Total 472	O 472	0	0
6	D	579	Total 579	O 579	0	0
6	E	653	Total 653	O 653	0	0
6	F	622	Total 622	O 622	0	0
6	G	603	Total 603	O 603	0	0
6	H	480	Total 480	O 480	0	0

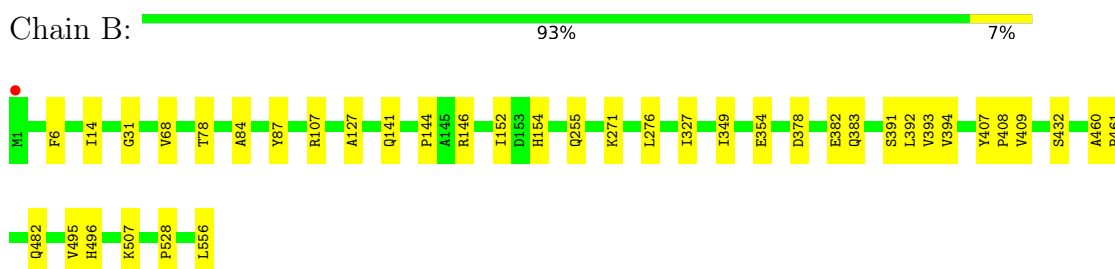
3 Residue-property plots

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.

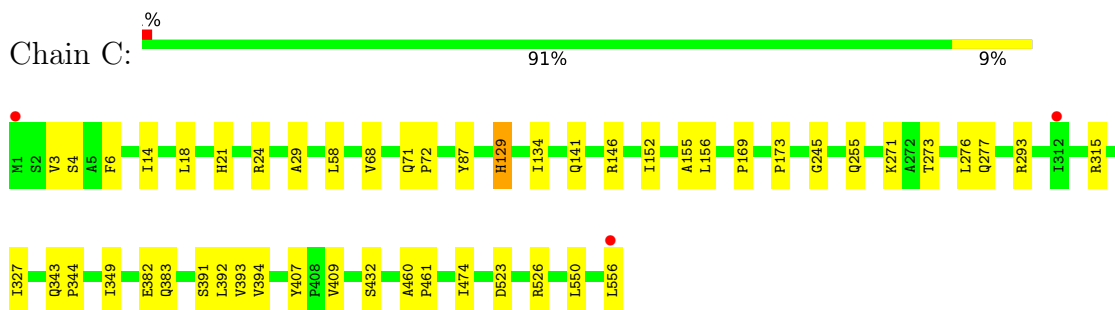
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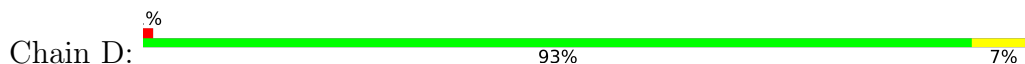
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

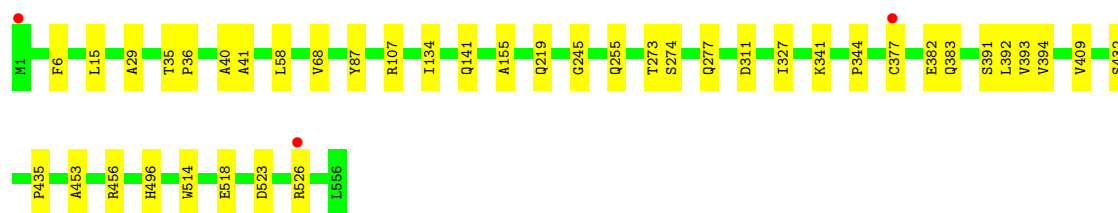


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

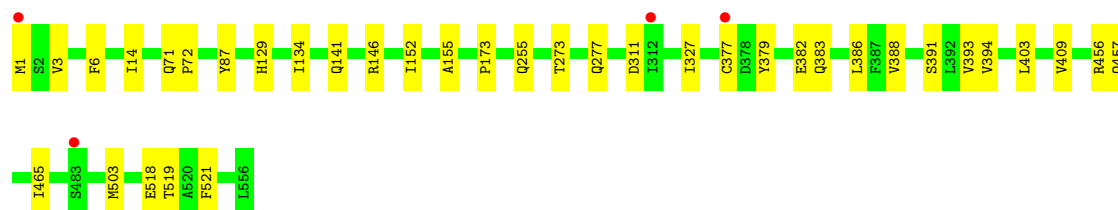
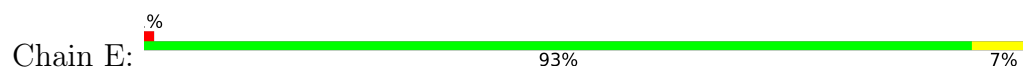


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

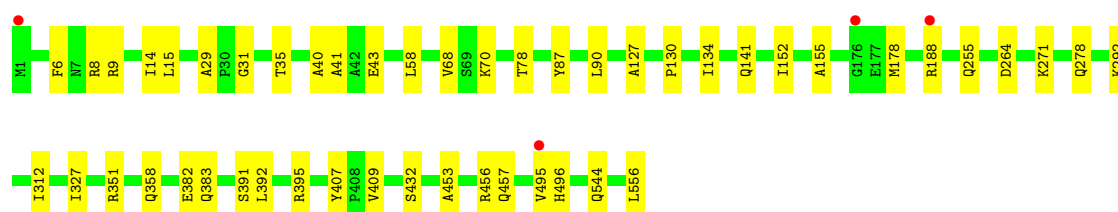




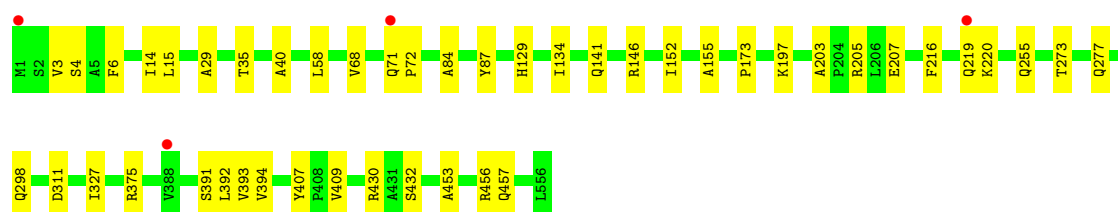
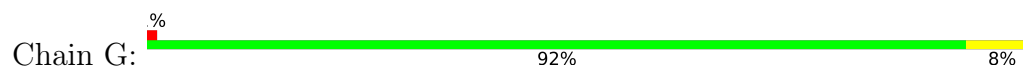
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



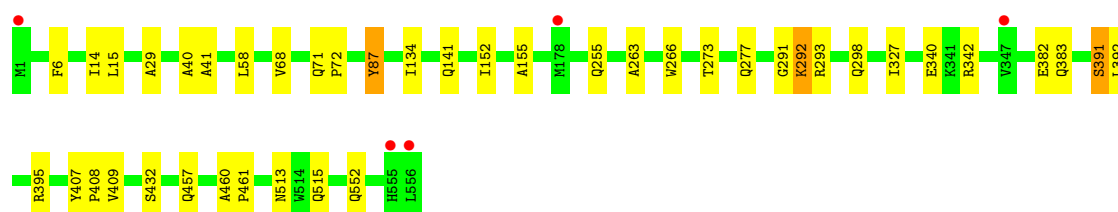
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.66Å 90.67Å 169.37Å 76.07° 83.29° 64.32°	Depositor
Resolution (Å)	31.48 – 1.72 31.48 – 1.72	Depositor EDS
% Data completeness (in resolution range)	95.8 (31.48-1.72) 92.6 (31.48-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.164 , 0.192 0.165 , 0.192	Depositor DCC
R_{free} test set	24074 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	40337	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.16% 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: GOL, EDO, TD5, MN

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	0.47	1/4519 (0.0%)	0.74	0/6166
1	B	0.47	1/4487 (0.0%)	0.73	1/6121 (0.0%)
1	C	0.41	1/4506 (0.0%)	0.72	2/6148 (0.0%)
1	D	0.44	1/4498 (0.0%)	0.73	0/6137
1	E	0.44	0/4489	0.75	0/6124
1	F	0.45	0/4488	0.73	1/6122 (0.0%)
1	G	0.44	0/4487	0.73	0/6123
1	H	0.41	0/4464	0.72	0/6091
All	All	0.44	4/35938 (0.0%)	0.73	4/49032 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	ARG	C-O	-6.52	1.15	1.23
1	C	474	ILE	C-O	-5.86	1.17	1.24
1	A	152	ILE	C-O	-5.40	1.17	1.24
1	D	107	ARG	C-O	-5.02	1.17	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ALA	CB-CA-C	-5.35	110.38	116.54
1	F	127	ALA	CB-CA-C	-5.04	110.74	116.54
1	C	129	HIS	CA-C-N	-5.04	114.76	119.85
1	C	129	HIS	C-N-CA	-5.04	114.76	119.85

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	4410	0	4360	46	1
1	B	4378	0	4333	29	1
1	C	4396	0	4335	32	0
1	D	4388	0	4327	37	0
1	E	4380	0	4330	27	0
1	F	4379	0	4321	36	0
1	G	4377	0	4320	36	0
1	H	4355	0	4294	34	0
2	A	33	20	0	1	0
2	B	33	20	0	1	0
2	C	33	20	0	1	0
2	D	33	20	0	2	0
2	E	33	20	0	0	0
2	F	33	20	0	1	0
2	G	33	20	0	2	0
2	H	33	20	0	1	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0
4	C	6	8	8	0	0
4	D	6	8	8	0	0
4	E	6	8	8	0	0
4	F	6	8	8	0	0
4	G	6	8	8	1	0
4	H	6	8	8	0	0
5	A	4	6	6	0	0
5	B	4	6	6	1	0
5	C	4	6	6	0	0
5	D	4	6	6	0	0
5	E	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	4	6	6	0	0
5	G	4	6	6	0	0
5	H	4	6	6	0	0
6	A	630	0	0	10	0
6	B	611	0	0	2	2
6	C	472	0	0	4	0
6	D	579	0	0	8	2
6	E	653	0	0	8	0
6	F	622	0	0	8	2
6	G	603	0	0	10	2
6	H	480	0	0	5	0
All	All	40065	272	34732	273	5

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 4.

All (273) 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:H:340:GLU:OE2	6:H:701:HOH:O	1.76	1.02
1:H:255:GLN:HE21	1:H:409:VAL:H	1.20	0.90
1:D:377[A]:CYS:SG	6:D:713:HOH:O	2.32	0.88
1:A:255:GLN:HE21	1:A:409:VAL:H	1.21	0.87
1:B:255:GLN:HE21	1:B:409:VAL:H	1.23	0.85
1:F:255:GLN:HE21	1:F:409:VAL:H	1.24	0.84
1:G:203:ALA:O	1:G:205:ARG:NH1	2.11	0.82
1:E:255:GLN:HE21	1:E:409:VAL:H	1.28	0.81
1:C:255:GLN:HE21	1:C:409:VAL:H	1.28	0.81
1:A:15[A]:LEU:HD12	1:A:40:ALA:HB3	1.62	0.80
1:G:255:GLN:HE21	1:G:409:VAL:H	1.25	0.80
1:A:146[B]:ARG:HG2	1:A:146[B]:ARG:HH21	1.47	0.78
1:F:271:LYS:NZ	1:F:556:LEU:OXT	2.18	0.76
1:H:291:GLY:HA2	1:H:395[A]:ARG:HH11	1.50	0.76
1:D:255:GLN:HE21	1:D:409:VAL:H	1.32	0.76
1:B:271:LYS:NZ	1:B:556:LEU:OXT	2.20	0.74
1:H:291:GLY:HA2	1:H:395[A]:ARG:NH1	2.02	0.74
1:E:146[B]:ARG:HG2	6:E:869:HOH:O	1.86	0.74
1:C:271:LYS:NZ	1:C:556:LEU:O	2.21	0.74
1:C:293:ARG:NH1	1:C:550:LEU:HD11	2.01	0.73
1:D:453:ALA:HA	1:D:456:ARG:HD2	1.69	0.73
1:C:523:ASP:OD1	1:C:526:ARG:NH2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:SER:HA	1:A:277:GLN:HE21	1.55	0.70
1:H:15:LEU:HD12	1:H:40:ALA:HB3	1.72	0.70
1:A:312:ILE:HD11	1:A:316:LEU:HD21	1.73	0.69
1:D:523:ASP:HA	1:D:526:ARG:HE	1.57	0.68
1:H:391:SER:O	1:H:395[B]:ARG:HD2	1.94	0.68
1:D:15[A]:LEU:HD12	1:D:40:ALA:HB3	1.76	0.68
1:G:216:PHE:CZ	1:G:220:LYS:HE3	2.30	0.66
1:D:382:GLU:HG3	1:D:383:GLN:HG2	1.76	0.66
1:A:220:LYS:HE3	1:A:280:GLN:NE2	2.10	0.66
1:F:70:LYS:NZ	6:F:702:HOH:O	2.27	0.66
1:F:188[A]:ARG:NH1	6:F:706:HOH:O	2.29	0.66
1:B:528:PRO:O	6:B:701:HOH:O	2.14	0.65
1:G:453:ALA:HA	1:G:456:ARG:HD2	1.77	0.65
1:D:311[B]:ASP:OD2	6:D:701:HOH:O	2.15	0.64
1:A:6:PHE:CE1	1:A:141:GLN:HG2	2.33	0.64
1:F:453:ALA:HA	1:F:456:ARG:HD2	1.77	0.64
1:F:495[B]:VAL:HG12	1:F:496:HIS:O	1.97	0.64
1:C:6:PHE:CE1	1:C:141:GLN:HG2	2.34	0.63
1:E:6:PHE:CE1	1:E:141:GLN:HG2	2.34	0.63
1:A:15[A]:LEU:HD12	1:A:40:ALA:CB	2.29	0.63
2:G:601:TD5:OL1	6:G:701:HOH:O	2.16	0.61
1:B:495[B]:VAL:HG12	1:B:496:HIS:O	2.01	0.61
1:D:341:LYS:NZ	6:D:708:HOH:O	2.30	0.61
1:F:15:LEU:HD12	1:F:40:ALA:HB3	1.82	0.60
1:H:255:GLN:NE2	1:H:409:VAL:H	1.94	0.60
1:A:375:ARG:HD3	6:A:812:HOH:O	2.02	0.60
1:E:382:GLU:HG3	1:E:383:GLN:HG2	1.84	0.60
1:H:382:GLU:HG3	1:H:383:GLN:HG2	1.84	0.59
1:F:544:GLN:HG2	6:F:709:HOH:O	2.01	0.59
1:B:495[B]:VAL:HG12	1:B:496:HIS:N	2.17	0.59
1:A:146[B]:ARG:HG2	6:A:953:HOH:O	2.01	0.59
1:B:255:GLN:NE2	1:B:409:VAL:H	1.98	0.59
1:A:255:GLN:NE2	1:A:409:VAL:H	1.98	0.59
1:A:465:ILE:HD11	1:A:521:PHE:HZ	1.68	0.58
1:E:457:GLN:HG3	6:E:900:HOH:O	2.03	0.58
1:C:146[B]:ARG:HG2	6:C:850:HOH:O	2.04	0.57
1:D:523:ASP:HA	1:D:526:ARG:NE	2.18	0.57
1:H:513:ASN:OD1	1:H:515:GLN:HG3	2.04	0.57
1:D:6:PHE:CE1	1:D:141:GLN:HG2	2.40	0.57
1:F:495[B]:VAL:HG12	1:F:496:HIS:N	2.19	0.57
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:TYR:OH	6:E:701:HOH:O	2.16	0.56
1:F:351:ARG:NE	6:F:714:HOH:O	2.38	0.56
1:D:273:THR:O	1:D:277:GLN:HG3	2.05	0.56
1:E:134:ILE:HD11	1:E:155:ALA:HB2	1.87	0.56
2:D:601:TD5:OL1	6:D:702:HOH:O	2.17	0.56
1:F:8:ARG:NH2	1:F:43:GLU:OE2	2.39	0.56
1:F:358:GLN:OE1	6:F:701:HOH:O	2.18	0.56
1:E:255:GLN:NE2	1:E:409:VAL:H	2.01	0.55
1:H:6:PHE:CE1	1:H:141:GLN:HG2	2.41	0.55
1:D:514:TRP:O	1:D:518:GLU:HG3	2.05	0.55
1:F:6:PHE:CE1	1:F:141:GLN:HG2	2.41	0.55
1:C:523:ASP:HA	1:C:526:ARG:HE	1.70	0.55
1:H:14:ILE:HG12	1:H:152:ILE:HD11	1.88	0.55
1:A:8:ARG:HB3	6:A:1146:HOH:O	2.06	0.55
1:F:382:GLU:HG3	1:F:383:GLN:HG2	1.88	0.55
1:G:15:LEU:HD12	1:G:40:ALA:HB3	1.89	0.55
1:C:21:HIS:HB2	1:C:156:LEU:HD23	1.89	0.55
1:D:435:PRO:HG3	6:D:1238:HOH:O	2.06	0.55
1:D:29:ALA:HB2	1:D:58:LEU:HD22	1.89	0.54
1:D:15[A]:LEU:HD12	1:D:40:ALA:CB	2.38	0.54
1:D:496:HIS:NE2	6:D:712:HOH:O	2.34	0.54
1:D:327:ILE:N	1:D:327:ILE:HD12	2.23	0.54
1:G:68:VAL:HG11	1:G:432:SER:HB3	1.89	0.54
1:H:15:LEU:HD12	1:H:40:ALA:CB	2.37	0.53
1:D:15[B]:LEU:HD22	1:D:40:ALA:HB3	1.89	0.53
1:E:14:ILE:HG12	1:E:152:ILE:HD11	1.91	0.53
1:H:273:THR:O	1:H:277:GLN:HG3	2.08	0.53
1:A:3:VAL:HB	1:A:173:PRO:HD2	1.90	0.52
1:G:298:GLN:OE1	6:G:702:HOH:O	2.19	0.52
1:G:457:GLN:HG3	6:G:844:HOH:O	2.08	0.52
1:A:197:LYS:NZ	6:A:716:HOH:O	2.41	0.52
1:A:117:ASN:ND2	6:A:718:HOH:O	2.43	0.52
1:C:3:VAL:HB	1:C:173:PRO:HD2	1.92	0.52
1:E:3:VAL:HB	1:E:173:PRO:HD2	1.91	0.52
1:H:342:ARG:HD3	6:H:717:HOH:O	2.09	0.52
1:D:68:VAL:HG11	1:D:432:SER:HB3	1.92	0.52
1:E:465:ILE:HD11	1:E:521:PHE:HZ	1.75	0.52
1:G:129:HIS:HD2	6:G:1114:HOH:O	1.92	0.52
1:H:457:GLN:HG3	6:H:946:HOH:O	2.09	0.52
1:H:327:ILE:N	1:H:327:ILE:HD12	2.24	0.52
1:A:15[A]:LEU:HD13	1:A:41:ALA:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LEU:HB2	2:B:601:TD5:O2B	2.09	0.52
1:D:392:LEU:HB2	2:D:601:TD5:O2B	2.10	0.52
1:C:255:GLN:NE2	1:C:409:VAL:H	2.01	0.51
1:G:71[B]:GLN:HB3	1:G:72:PRO:HD2	1.92	0.51
1:E:377[A]:CYS:SG	1:E:403:LEU:HD23	2.49	0.51
1:D:518:GLU:HB3	6:D:733:HOH:O	2.10	0.51
1:G:6:PHE:CE1	1:G:141:GLN:HG2	2.46	0.51
1:E:311:ASP:HB3	6:E:1211:HOH:O	2.09	0.51
1:H:392:LEU:HB2	2:H:601:TD5:O2B	2.11	0.51
1:F:15:LEU:HD12	1:F:40:ALA:CB	2.41	0.50
1:C:71[B]:GLN:HB3	1:C:72:PRO:HD2	1.92	0.50
1:G:71[B]:GLN:HE21	1:G:72:PRO:HD2	1.76	0.50
1:B:378:ASP:OD2	5:B:604:EDO:O1	2.29	0.50
1:A:312:ILE:CD1	1:A:316:LEU:HD21	2.40	0.50
1:F:457:GLN:HG3	6:F:848:HOH:O	2.11	0.50
1:H:68:VAL:HG11	1:H:432:SER:HB3	1.92	0.50
1:B:68:VAL:HG11	1:B:432:SER:HB3	1.93	0.50
1:A:292:LYS:HB3	1:A:395[B]:ARG:NH1	2.27	0.49
1:D:523:ASP:CG	1:D:526:ARG:HH11	2.19	0.49
1:B:482:GLN:HG2	6:B:852:HOH:O	2.13	0.49
1:B:382:GLU:HG2	1:B:383:GLN:HG2	1.93	0.49
1:F:255:GLN:NE2	1:F:409:VAL:H	2.02	0.49
1:F:292:LYS:NZ	6:F:708:HOH:O	2.31	0.49
1:A:519:THR:HG21	1:G:219:GLN:OE1	2.13	0.49
1:A:15[B]:LEU:CD2	1:A:41:ALA:HB2	2.42	0.49
1:A:395[B]:ARG:NH2	6:A:707:HOH:O	2.46	0.49
1:E:71[B]:GLN:HB3	1:E:72:PRO:HD2	1.95	0.48
1:A:15[A]:LEU:CD1	1:A:40:ALA:HB3	2.39	0.48
1:B:14:ILE:HG12	1:B:152[A]:ILE:HD11	1.96	0.48
1:E:327:ILE:HD12	1:E:327:ILE:N	2.28	0.48
1:A:220:LYS:HE3	1:A:280:GLN:CD	2.39	0.48
1:C:24:ARG:HD3	6:C:743:HOH:O	2.14	0.48
1:H:134:ILE:HD11	1:H:155:ALA:HB2	1.95	0.48
1:H:292:LYS:HE3	1:H:293:ARG:NH1	2.29	0.48
1:G:29:ALA:HB2	1:G:58:LEU:HD22	1.96	0.47
1:G:207:GLU:OE2	6:G:703:HOH:O	2.20	0.47
1:A:134:ILE:HD11	1:A:155:ALA:HB2	1.96	0.47
1:A:457:GLN:HG3	6:A:819:HOH:O	2.15	0.47
1:D:523:ASP:OD1	1:D:526:ARG:NH1	2.44	0.47
1:A:29:ALA:HB2	1:A:58:LEU:HD22	1.97	0.47
1:A:327:ILE:N	1:A:327:ILE:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:THR:O	1:C:277:GLN:HG3	2.15	0.47
1:G:3:VAL:HB	1:G:173:PRO:HD2	1.96	0.47
1:A:129:HIS:HD2	6:A:1101:HOH:O	1.98	0.47
1:E:518:GLU:HG3	6:E:701:HOH:O	2.14	0.47
1:E:273:THR:O	1:E:277:GLN:HG3	2.15	0.47
1:E:386:LEU:HG	1:E:388[B]:VAL:HG23	1.97	0.47
1:G:430:ARG:NH2	4:G:603:GOL:O3	2.47	0.47
1:G:273:THR:O	1:G:277:GLN:HG3	2.15	0.46
1:B:144:PRO:HB2	1:B:146:ARG:HG2	1.98	0.46
1:B:255:GLN:HG2	1:B:407:TYR:O	2.15	0.46
1:E:129:HIS:HD2	6:E:1116:HOH:O	1.98	0.46
1:F:264:ASP:OD2	1:F:395[B]:ARG:NH2	2.47	0.46
1:G:146[B]:ARG:HG2	6:G:1038:HOH:O	2.15	0.46
1:B:327:ILE:HD12	1:B:327:ILE:N	2.31	0.46
1:C:327:ILE:N	1:C:327:ILE:HD12	2.29	0.46
1:F:14:ILE:HG12	1:F:152:ILE:HD11	1.98	0.46
1:F:134:ILE:HD11	1:F:155:ALA:HB2	1.98	0.46
1:B:271:LYS:HZ1	1:B:556:LEU:C	2.24	0.46
1:B:393:VAL:HG13	1:B:394:VAL:N	2.31	0.46
1:C:392:LEU:HB2	2:C:601:TD5:O2B	2.16	0.46
1:E:1:MET:N	6:E:723:HOH:O	2.44	0.46
1:H:263:ALA:HA	1:H:266:TRP:NE1	2.30	0.46
1:C:382:GLU:HG3	1:C:383:GLN:HG2	1.98	0.45
1:D:15[B]:LEU:HD23	1:D:41:ALA:CA	2.46	0.45
1:D:219:GLN:HB2	6:D:1042:HOH:O	2.14	0.45
1:F:15:LEU:HD13	1:F:41:ALA:CA	2.47	0.45
1:A:146[B]:ARG:HG2	1:A:146[B]:ARG:NH2	2.24	0.45
1:C:129:HIS:HD2	6:C:1042:HOH:O	1.99	0.45
1:A:289:LEU:HD12	6:A:733:HOH:O	2.16	0.45
1:B:14:ILE:HA	1:B:152[A]:ILE:CD1	2.47	0.45
1:A:377[A]:CYS:SG	1:A:403:LEU:HD23	2.56	0.45
1:D:393:VAL:HG13	1:D:394:VAL:N	2.32	0.45
1:G:375:ARG:HD3	6:G:935:HOH:O	2.17	0.45
1:A:15[B]:LEU:HD23	1:A:41:ALA:CA	2.47	0.45
1:A:392:LEU:HB2	2:A:601:TD5:O2B	2.16	0.45
1:G:393:VAL:HB	6:G:1203:HOH:O	2.16	0.45
1:D:523:ASP:HA	1:D:526:ARG:HH11	1.82	0.44
1:A:15[B]:LEU:HD23	1:A:41:ALA:HA	1.98	0.44
1:F:327:ILE:N	1:F:327:ILE:HD12	2.32	0.44
1:H:255:GLN:HG2	1:H:407:TYR:O	2.18	0.44
1:H:292:LYS:NZ	1:H:293:ARG:HH12	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:GLY:O	1:D:344:PRO:HA	2.17	0.44
1:H:71:GLN:HB3	1:H:72:PRO:HD2	1.98	0.44
1:G:327:ILE:HD12	1:G:327:ILE:N	2.32	0.44
1:F:29:ALA:HB2	1:F:58:LEU:HD22	1.99	0.44
1:H:460:ALA:HB1	1:H:461:PRO:HD2	2.00	0.44
1:C:343:GLN:OE1	1:C:344:PRO:HD2	2.18	0.44
1:C:393:VAL:HG13	1:C:394:VAL:N	2.32	0.44
1:G:134:ILE:HD11	1:G:155:ALA:HB2	2.00	0.44
1:G:255:GLN:HG2	1:G:407:TYR:O	2.18	0.44
1:G:311:ASP:OD2	6:G:704:HOH:O	2.21	0.44
1:A:146[B]:ARG:HH21	1:A:146[B]:ARG:CG	2.24	0.44
1:D:15[A]:LEU:HD13	1:D:41:ALA:N	2.33	0.44
1:A:15[B]:LEU:HD21	1:A:41:ALA:HB2	1.99	0.44
1:C:18:LEU:HD22	1:C:156:LEU:HD21	2.00	0.44
1:H:29:ALA:HB2	1:H:58:LEU:HD22	1.99	0.44
1:C:68:VAL:HG11	1:C:432:SER:HB3	1.99	0.43
1:G:4[A]:SER:OG	1:G:173:PRO:HB2	2.17	0.43
1:E:456:ARG:NH1	6:E:707:HOH:O	2.31	0.43
1:A:87:TYR:HB3	1:B:84:ALA:HB1	2.01	0.43
1:D:15[B]:LEU:N	1:D:15[B]:LEU:HD12	2.33	0.43
1:E:14:ILE:HA	1:E:152:ILE:HD13	2.00	0.43
1:E:503:MET:CE	1:F:495[B]:VAL:HG11	2.48	0.43
1:H:15:LEU:HD13	1:H:41:ALA:N	2.33	0.43
1:C:169:PRO:HD2	6:C:966:HOH:O	2.18	0.43
1:F:68:VAL:HG11	1:F:432:SER:HB3	2.00	0.43
1:B:495[B]:VAL:CG1	1:B:496:HIS:N	2.82	0.43
1:D:15[B]:LEU:HD23	1:D:41:ALA:HA	2.00	0.43
1:F:392:LEU:HB2	2:F:601:TD5:O2B	2.19	0.43
1:H:255:GLN:HE21	1:H:409:VAL:N	2.02	0.43
1:A:31:GLY:HA3	1:A:78:THR:HB	2.01	0.42
1:B:14:ILE:HA	1:B:152[A]:ILE:HD13	2.00	0.42
1:F:495[B]:VAL:CG1	1:F:496:HIS:N	2.81	0.42
1:G:392:LEU:HB2	2:G:601:TD5:O2B	2.19	0.42
1:B:276:LEU:HG	1:B:349:ILE:HD11	2.02	0.42
1:H:298:GLN:NE2	6:H:702:HOH:O	2.16	0.42
1:B:154:HIS:HB2	1:C:315[B]:ARG:HD3	2.01	0.42
1:E:134:ILE:HD11	1:E:155:ALA:CB	2.50	0.42
1:H:552:GLN:NE2	6:H:727:HOH:O	2.50	0.42
1:C:14:ILE:HG12	1:C:152:ILE:HD11	2.01	0.42
1:F:31:GLY:HA3	1:F:78:THR:HB	2.01	0.42
1:G:15:LEU:HD12	1:G:40:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:ILE:HA	1:H:152:ILE:HD13	2.01	0.42
1:H:292:LYS:HE3	1:H:292:LYS:HB3	1.79	0.42
1:A:312:ILE:HD11	1:A:316:LEU:CD2	2.46	0.42
1:C:134:ILE:HD11	1:C:155:ALA:HB2	2.01	0.42
1:F:255:GLN:HG2	1:F:407:TYR:O	2.19	0.42
1:G:84:ALA:HB1	1:H:87:TYR:HB3	2.01	0.42
1:G:220:LYS:HD3	1:G:220:LYS:HA	1.83	0.42
1:C:4[A]:SER:OG	1:C:173:PRO:HB2	2.19	0.42
1:F:15:LEU:HD13	1:F:41:ALA:N	2.34	0.42
1:H:407:TYR:HA	1:H:408:PRO:HD3	1.93	0.42
1:F:271:LYS:HZ1	1:F:556:LEU:C	2.26	0.41
1:G:393:VAL:HG13	1:G:394:VAL:N	2.35	0.41
1:A:1:MET:N	6:A:741:HOH:O	2.54	0.41
1:C:276:LEU:HG	1:C:349:ILE:HD11	2.02	0.41
1:D:219:GLN:OE1	1:E:519:THR:HG21	2.20	0.41
1:B:460:ALA:HB1	1:B:461:PRO:HD2	2.02	0.41
1:C:29:ALA:HB2	1:C:58:LEU:HD22	2.02	0.41
1:D:15[B]:LEU:HD22	1:D:40:ALA:CB	2.50	0.41
1:D:35:THR:HB	1:D:36:PRO:HD3	2.00	0.41
1:D:134:ILE:HD11	1:D:155:ALA:HB2	2.01	0.41
1:D:274[A]:SER:HA	1:D:277:GLN:NE2	2.36	0.41
1:E:393:VAL:HG13	1:E:394:VAL:N	2.34	0.41
1:A:312:ILE:HD11	1:A:316:LEU:HD11	2.02	0.41
1:A:460:ALA:HB1	1:A:461:PRO:HD2	2.02	0.41
1:F:278:GLN:HG2	6:F:1210:HOH:O	2.20	0.41
1:G:255:GLN:NE2	1:G:409:VAL:H	2.03	0.41
1:C:245:GLY:O	1:C:344:PRO:HA	2.21	0.41
1:F:9:ARG:HG2	1:F:178:MET:HE1	2.03	0.41
1:F:14:ILE:HA	1:F:152:ILE:CD1	2.51	0.41
1:G:14:ILE:HG12	1:G:152:ILE:HD11	2.01	0.41
1:G:456:ARG:NH2	6:G:718:HOH:O	2.41	0.41
1:A:292:LYS:CB	1:A:395[B]:ARG:NH1	2.84	0.41
1:B:407:TYR:HA	1:B:408:PRO:HD3	1.95	0.41
1:G:14:ILE:HA	1:G:152:ILE:HD13	2.01	0.41
1:G:197:LYS:HB2	1:G:197:LYS:HE2	1.83	0.41
1:B:31:GLY:HA3	1:B:78:THR:HB	2.03	0.41
1:A:255:GLN:HG2	1:A:407:TYR:O	2.21	0.40
1:D:523:ASP:HA	1:D:526:ARG:NH1	2.36	0.40
1:F:90:LEU:HD21	1:F:130:PRO:HG3	2.03	0.40
1:A:71[B]:GLN:HB3	1:A:72:PRO:HD2	2.03	0.40
1:C:21:HIS:CB	1:C:156:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLN:HG2	1:C:407:TYR:O	2.22	0.40
1:E:14:ILE:HA	1:E:152:ILE:CD1	2.52	0.40
1:C:460:ALA:HB1	1:C:461:PRO:HD2	2.03	0.40

All (5) 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)
6:F:825:HOH:O	6:G:1205:HOH:O[1_465]	2.05	0.15
6:B:1226:HOH:O	6:D:727:HOH:O[1_645]	2.09	0.11
6:F:753:HOH:O	6:G:1205:HOH:O[1_465]	2.11	0.09
1:A:212:ARG:NH2	1:B:354:GLU:OE2[1_565]	2.12	0.08
6:B:1226:HOH:O	6:D:722:HOH:O[1_645]	2.17	0.03

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	566/556 (102%)	555 (98%)	10 (2%)	1 (0%)	43	31
1	B	562/556 (101%)	551 (98%)	10 (2%)	1 (0%)	43	31
1	C	564/556 (101%)	553 (98%)	10 (2%)	1 (0%)	43	31
1	D	564/556 (101%)	553 (98%)	10 (2%)	1 (0%)	43	31
1	E	562/556 (101%)	550 (98%)	11 (2%)	1 (0%)	43	31
1	F	562/556 (101%)	551 (98%)	10 (2%)	1 (0%)	43	31
1	G	562/556 (101%)	550 (98%)	11 (2%)	1 (0%)	43	31
1	H	560/556 (101%)	549 (98%)	10 (2%)	1 (0%)	43	31
All	All	4502/4448 (101%)	4412 (98%)	82 (2%)	8 (0%)	43	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	391	SER
1	G	391	SER
1	A	391	SER
1	B	391	SER
1	C	391	SER
1	E	391	SER
1	F	391	SER
1	H	391	SER

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	459/451 (102%)	457 (100%)	2 (0%)	84	76
1	B	454/451 (101%)	453 (100%)	1 (0%)	87	81
1	C	457/451 (101%)	456 (100%)	1 (0%)	87	81
1	D	456/451 (101%)	455 (100%)	1 (0%)	87	81
1	E	455/451 (101%)	454 (100%)	1 (0%)	87	81
1	F	453/451 (100%)	450 (99%)	3 (1%)	76	64
1	G	456/451 (101%)	454 (100%)	2 (0%)	84	76
1	H	452/451 (100%)	450 (100%)	2 (0%)	84	76
All	All	3642/3608 (101%)	3629 (100%)	13 (0%)	84	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	87	TYR
1	B	87	TYR
1	C	87	TYR
1	D	87	TYR
1	E	87	TYR
1	F	35	THR
1	F	87	TYR

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Mol	Chain	Res	Type
1	F	312	ILE
1	G	35	THR
1	G	87	TYR
1	H	87	TYR
1	H	292	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	129	HIS
1	A	219	GLN
1	A	255	GLN
1	A	277	GLN
1	A	355	GLN
1	A	493	GLN
1	A	538	ASN
1	A	552	GLN
1	B	117	ASN
1	B	255	GLN
1	B	277	GLN
1	B	298	GLN
1	B	358	GLN
1	B	493	GLN
1	B	544	GLN
1	C	117	ASN
1	C	129	HIS
1	C	255	GLN
1	C	296	GLN
1	C	482	GLN
1	C	493	GLN
1	D	255	GLN
1	D	277	GLN
1	D	358	GLN
1	D	493	GLN
1	D	538	ASN
1	D	544	GLN
1	D	552	GLN
1	E	129	HIS
1	E	141	GLN
1	E	219	GLN
1	E	255	GLN

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Mol	Chain	Res	Type
1	E	355	GLN
1	E	493	GLN
1	F	255	GLN
1	F	277	GLN
1	F	493	GLN
1	F	544	GLN
1	F	552	GLN
1	G	129	HIS
1	G	255	GLN
1	G	355	GLN
1	G	482	GLN
1	G	493	GLN
1	G	538	ASN
1	G	552	GLN
1	H	255	GLN
1	H	493	GLN
1	H	538	ASN
1	H	544	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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	GOL	B	603	-	5,5,5	0.39	0	5,5,5	0.46	0
4	GOL	E	603	-	5,5,5	0.41	0	5,5,5	0.47	0
4	GOL	G	603	-	5,5,5	0.47	0	5,5,5	0.30	0
2	TD5	A	601	3	31,34,34	1.58	7 (22%)	38,50,50	1.71	8 (21%)
4	GOL	C	603	-	5,5,5	0.47	0	5,5,5	0.35	0
2	TD5	C	601	3	31,34,34	1.60	7 (22%)	38,50,50	1.81	8 (21%)
4	GOL	D	603	-	5,5,5	0.40	0	5,5,5	0.31	0
5	EDO	A	604	-	3,3,3	0.45	0	2,2,2	0.27	0
5	EDO	H	604	-	3,3,3	0.43	0	2,2,2	0.31	0
2	TD5	B	601	3	31,34,34	1.76	7 (22%)	38,50,50	1.83	8 (21%)
4	GOL	H	603	-	5,5,5	0.34	0	5,5,5	0.34	0
5	EDO	F	604	-	3,3,3	0.43	0	2,2,2	0.41	0
4	GOL	F	603	-	5,5,5	0.45	0	5,5,5	0.68	0
2	TD5	D	601	3	31,34,34	1.74	9 (29%)	38,50,50	1.79	7 (18%)
2	TD5	F	601	3	31,34,34	1.73	7 (22%)	38,50,50	1.90	9 (23%)
2	TD5	H	601	3	31,34,34	1.71	8 (25%)	38,50,50	1.91	9 (23%)
5	EDO	G	604	-	3,3,3	0.50	0	2,2,2	0.12	0
2	TD5	E	601	3	31,34,34	1.65	7 (22%)	38,50,50	1.57	7 (18%)
4	GOL	A	603	-	5,5,5	0.44	0	5,5,5	0.36	0
2	TD5	G	601	3	31,34,34	1.67	7 (22%)	38,50,50	1.86	12 (31%)
5	EDO	D	604	-	3,3,3	0.44	0	2,2,2	0.27	0
5	EDO	B	604	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	C	604	-	3,3,3	0.44	0	2,2,2	0.34	0
5	EDO	E	604	-	3,3,3	0.45	0	2,2,2	0.28	0

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	GOL	B	603	-	-	2/4/4/4	-
4	GOL	E	603	-	-	2/4/4/4	-
4	GOL	G	603	-	-	1/4/4/4	-
2	TD5	A	601	3	-	3/25/26/26	0/2/2/2
4	GOL	C	603	-	-	2/4/4/4	-
2	TD5	C	601	3	-	1/25/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	603	-	-	2/4/4/4	-
5	EDO	A	604	-	-	0/1/1/1	-
5	EDO	H	604	-	-	0/1/1/1	-
2	TD5	B	601	3	-	2/25/26/26	0/2/2/2
4	GOL	H	603	-	-	2/4/4/4	-
5	EDO	F	604	-	-	0/1/1/1	-
4	GOL	F	603	-	-	2/4/4/4	-
2	TD5	D	601	3	-	1/25/26/26	0/2/2/2
2	TD5	F	601	3	-	3/25/26/26	0/2/2/2
2	TD5	H	601	3	-	2/25/26/26	0/2/2/2
5	EDO	G	604	-	-	0/1/1/1	-
2	TD5	E	601	3	-	1/25/26/26	0/2/2/2
4	GOL	A	603	-	-	1/4/4/4	-
2	TD5	G	601	3	-	1/25/26/26	0/2/2/2
5	EDO	D	604	-	-	0/1/1/1	-
5	EDO	B	604	-	-	0/1/1/1	-
5	EDO	C	604	-	-	0/1/1/1	-
5	EDO	E	604	-	-	0/1/1/1	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	TD5	C4-N3	-4.09	1.34	1.40
2	G	601	TD5	C4-N3	-4.00	1.35	1.40
2	B	601	TD5	C4-N3	-3.75	1.35	1.40
2	F	601	TD5	C4-N3	-3.63	1.35	1.40
2	D	601	TD5	CM4-C4	3.54	1.57	1.49
2	H	601	TD5	C4-N3	-3.52	1.35	1.40
2	G	601	TD5	CM4-C4	3.49	1.56	1.49
2	A	601	TD5	C4-N3	-3.49	1.35	1.40
2	F	601	TD5	CM4-C4	3.41	1.56	1.49
2	B	601	TD5	C7'-C5'	3.39	1.57	1.51
2	E	601	TD5	CM4-C4	3.39	1.56	1.49
2	B	601	TD5	CM4-C4	3.37	1.56	1.49
2	E	601	TD5	C4-N3	-3.33	1.35	1.40
2	H	601	TD5	CM4-C4	3.29	1.56	1.49
2	C	601	TD5	C4-N3	-3.27	1.36	1.40
2	A	601	TD5	CM4-C4	3.16	1.56	1.49
2	C	601	TD5	CM4-C4	3.01	1.55	1.49
2	A	601	TD5	CM2-C2'	3.01	1.58	1.49
2	H	601	TD5	C6-C5	3.00	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	TD5	CM2-C2'	2.97	1.57	1.49
2	F	601	TD5	C7'-C5'	2.91	1.56	1.51
2	G	601	TD5	CM2-C2'	2.91	1.57	1.49
2	D	601	TD5	CM2-C2'	2.90	1.57	1.49
2	H	601	TD5	CM2-C2'	2.87	1.57	1.49
2	H	601	TD5	C7'-C5'	2.87	1.56	1.51
2	C	601	TD5	CM2-C2'	2.87	1.57	1.49
2	B	601	TD5	C5-C4	2.86	1.41	1.35
2	F	601	TD5	C6-C5	2.82	1.56	1.50
2	F	601	TD5	CLB-C11	2.78	1.57	1.53
2	E	601	TD5	C7'-C5'	2.77	1.56	1.51
2	D	601	TD5	C7'-C5'	2.76	1.56	1.51
2	B	601	TD5	CM2-C2'	2.75	1.57	1.49
2	B	601	TD5	C6-C5	2.73	1.56	1.50
2	D	601	TD5	C5-C4	2.71	1.40	1.35
2	E	601	TD5	C5-C4	2.71	1.40	1.35
2	C	601	TD5	C6-C5	2.68	1.56	1.50
2	A	601	TD5	C5-C4	2.67	1.40	1.35
2	D	601	TD5	C6-C5	2.65	1.56	1.50
2	G	601	TD5	C6-C5	2.64	1.56	1.50
2	E	601	TD5	CM2-C2'	2.64	1.56	1.49
2	A	601	TD5	C6-C5	2.63	1.56	1.50
2	G	601	TD5	CLB-C11	2.62	1.57	1.53
2	E	601	TD5	C6-C5	2.61	1.56	1.50
2	E	601	TD5	CLB-C11	2.57	1.57	1.53
2	G	601	TD5	C5-C4	2.55	1.40	1.35
2	A	601	TD5	C7'-C5'	2.54	1.55	1.51
2	C	601	TD5	CLB-C11	2.52	1.57	1.53
2	F	601	TD5	C5-C4	2.51	1.40	1.35
2	H	601	TD5	C5-C4	2.51	1.40	1.35
2	H	601	TD5	CLB-C11	2.47	1.57	1.53
2	C	601	TD5	C7'-C5'	2.46	1.55	1.51
2	B	601	TD5	CLB-C11	2.43	1.57	1.53
2	D	601	TD5	C7'-N3	2.43	1.50	1.47
2	C	601	TD5	C5-C4	2.29	1.40	1.35
2	G	601	TD5	C7'-C5'	2.26	1.55	1.51
2	H	601	TD5	C4'-N3'	2.17	1.37	1.35
2	D	601	TD5	CLB-C11	2.17	1.56	1.53
2	A	601	TD5	CLB-C11	2.10	1.56	1.53
2	D	601	TD5	C4'-N3'	2.06	1.37	1.35

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	TD5	C4-C5-S1	-5.05	105.33	110.56
2	C	601	TD5	C4-C5-S1	-4.79	105.60	110.56
2	F	601	TD5	C4-C5-S1	-4.58	105.81	110.56
2	H	601	TD5	C6-C5-S1	4.50	128.95	119.29
2	D	601	TD5	C4-C5-S1	-4.43	105.97	110.56
2	F	601	TD5	C6-C5-S1	4.41	128.75	119.29
2	G	601	TD5	C4-C5-S1	-4.35	106.06	110.56
2	B	601	TD5	C6-C5-S1	4.24	128.39	119.29
2	B	601	TD5	C4-C5-S1	-4.23	106.18	110.56
2	D	601	TD5	C6-C5-S1	4.21	128.32	119.29
2	F	601	TD5	C6'-N1'-C2'	4.15	122.89	116.07
2	A	601	TD5	C4-C5-S1	-4.08	106.33	110.56
2	H	601	TD5	C6'-N1'-C2'	4.05	122.72	116.07
2	B	601	TD5	C6'-N1'-C2'	3.98	122.61	116.07
2	C	601	TD5	C6-C5-S1	3.98	127.83	119.29
2	D	601	TD5	C6'-N1'-C2'	3.95	122.56	116.07
2	G	601	TD5	C6'-N1'-C2'	3.93	122.53	116.07
2	G	601	TD5	C6-C5-S1	3.93	127.73	119.29
2	C	601	TD5	C6'-N1'-C2'	3.92	122.51	116.07
2	F	601	TD5	N1'-C2'-N3'	-3.72	119.34	125.53
2	E	601	TD5	C4-C5-S1	-3.62	106.82	110.56
2	D	601	TD5	N1'-C2'-N3'	-3.59	119.56	125.53
2	A	601	TD5	C6'-N1'-C2'	3.56	121.92	116.07
2	G	601	TD5	N1'-C2'-N3'	-3.52	119.68	125.53
2	A	601	TD5	N1'-C2'-N3'	-3.49	119.73	125.53
2	C	601	TD5	N1'-C2'-N3'	-3.44	119.80	125.53
2	E	601	TD5	C6'-N1'-C2'	3.29	121.48	116.07
2	H	601	TD5	N1'-C2'-N3'	-3.28	120.08	125.53
2	E	601	TD5	N1'-C2'-N3'	-3.26	120.10	125.53
2	B	601	TD5	N1'-C2'-N3'	-3.25	120.12	125.53
2	G	601	TD5	C5'-C6'-N1'	-3.23	118.58	123.83
2	H	601	TD5	C5'-C6'-N1'	-3.17	118.68	123.83
2	A	601	TD5	CM2-C2'-N1'	3.15	120.56	117.20
2	B	601	TD5	C5'-C6'-N1'	-3.12	118.75	123.83
2	F	601	TD5	CM2-C2'-N1'	3.08	120.48	117.20
2	H	601	TD5	CM2-C2'-N1'	3.04	120.44	117.20
2	C	601	TD5	C5'-C6'-N1'	-3.03	118.90	123.83
2	E	601	TD5	CM2-C2'-N1'	2.98	120.37	117.20
2	A	601	TD5	C6-C5-S1	2.95	125.62	119.29
2	D	601	TD5	C5'-C6'-N1'	-2.94	119.05	123.83
2	F	601	TD5	C5'-C6'-N1'	-2.90	119.12	123.83
2	G	601	TD5	C13-CLB-C11	2.73	118.71	114.48
2	B	601	TD5	CM2-C2'-N1'	2.72	120.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	TD5	CM2-C2'-N3'	2.68	121.14	117.13
2	E	601	TD5	C6-C5-S1	2.67	125.02	119.29
2	A	601	TD5	O1B-PB-O3A	2.65	113.52	104.64
2	D	601	TD5	CM4-C4-C5	-2.60	121.09	127.75
2	C	601	TD5	CM2-C2'-N1'	2.55	119.92	117.20
2	A	601	TD5	C5'-C6'-N1'	-2.52	119.74	123.83
2	F	601	TD5	O1B-PB-O3A	2.48	112.96	104.64
2	E	601	TD5	C5'-C6'-N1'	-2.45	119.85	123.83
2	G	601	TD5	CM2-C2'-N3'	2.43	120.76	117.13
2	B	601	TD5	CM4-C4-C5	-2.38	121.65	127.75
2	H	601	TD5	CM4-C4-C5	-2.38	121.66	127.75
2	E	601	TD5	CM4-C4-C5	-2.33	121.77	127.75
2	C	601	TD5	CM4-C4-C5	-2.32	121.81	127.75
2	G	601	TD5	C6'-C5'-C4'	2.24	118.30	115.55
2	F	601	TD5	CM4-C4-C5	-2.22	122.05	127.75
2	G	601	TD5	CM2-C2'-N1'	2.21	119.56	117.20
2	H	601	TD5	C13-CLB-C11	2.17	117.84	114.48
2	G	601	TD5	CM4-C4-C5	-2.16	122.21	127.75
2	G	601	TD5	O3B-PB-O3A	2.15	111.85	104.64
2	A	601	TD5	CM4-C4-C5	-2.14	122.28	127.75
2	C	601	TD5	CM2-C2'-N3'	2.11	120.28	117.13
2	F	601	TD5	CM2-C2'-N3'	2.04	120.18	117.13
2	B	601	TD5	C13-CLB-C11	2.04	117.64	114.48
2	H	601	TD5	O1B-PB-O3A	2.04	111.47	104.64
2	G	601	TD5	O1B-PB-O3A	2.03	111.44	104.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TD5	CLC-C13-CLB-C11
2	B	601	TD5	CLC-C13-CLB-C11
2	C	601	TD5	CLC-C13-CLB-C11
2	D	601	TD5	CLC-C13-CLB-C11
2	E	601	TD5	CLC-C13-CLB-C11
2	F	601	TD5	CLC-C13-CLB-C11
2	H	601	TD5	CLC-C13-CLB-C11
4	A	603	GOL	C1-C2-C3-O3
4	B	603	GOL	C1-C2-C3-O3
4	C	603	GOL	C1-C2-C3-O3
4	D	603	GOL	C1-C2-C3-O3
4	E	603	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	F	603	GOL	C1-C2-C3-O3
4	H	603	GOL	C1-C2-C3-O3
4	H	603	GOL	O2-C2-C3-O3
4	B	603	GOL	O2-C2-C3-O3
4	D	603	GOL	O2-C2-C3-O3
4	E	603	GOL	O2-C2-C3-O3
4	F	603	GOL	O2-C2-C3-O3
4	C	603	GOL	O2-C2-C3-O3
2	A	601	TD5	C4'-C5'-C7'-N3
2	F	601	TD5	C4'-C5'-C7'-N3
2	G	601	TD5	C4'-C5'-C7'-N3
2	B	601	TD5	C4'-C5'-C7'-N3
2	F	601	TD5	C6'-C5'-C7'-N3
2	H	601	TD5	C4'-C5'-C7'-N3
4	G	603	GOL	C1-C2-C3-O3
2	A	601	TD5	C6'-C5'-C7'-N3

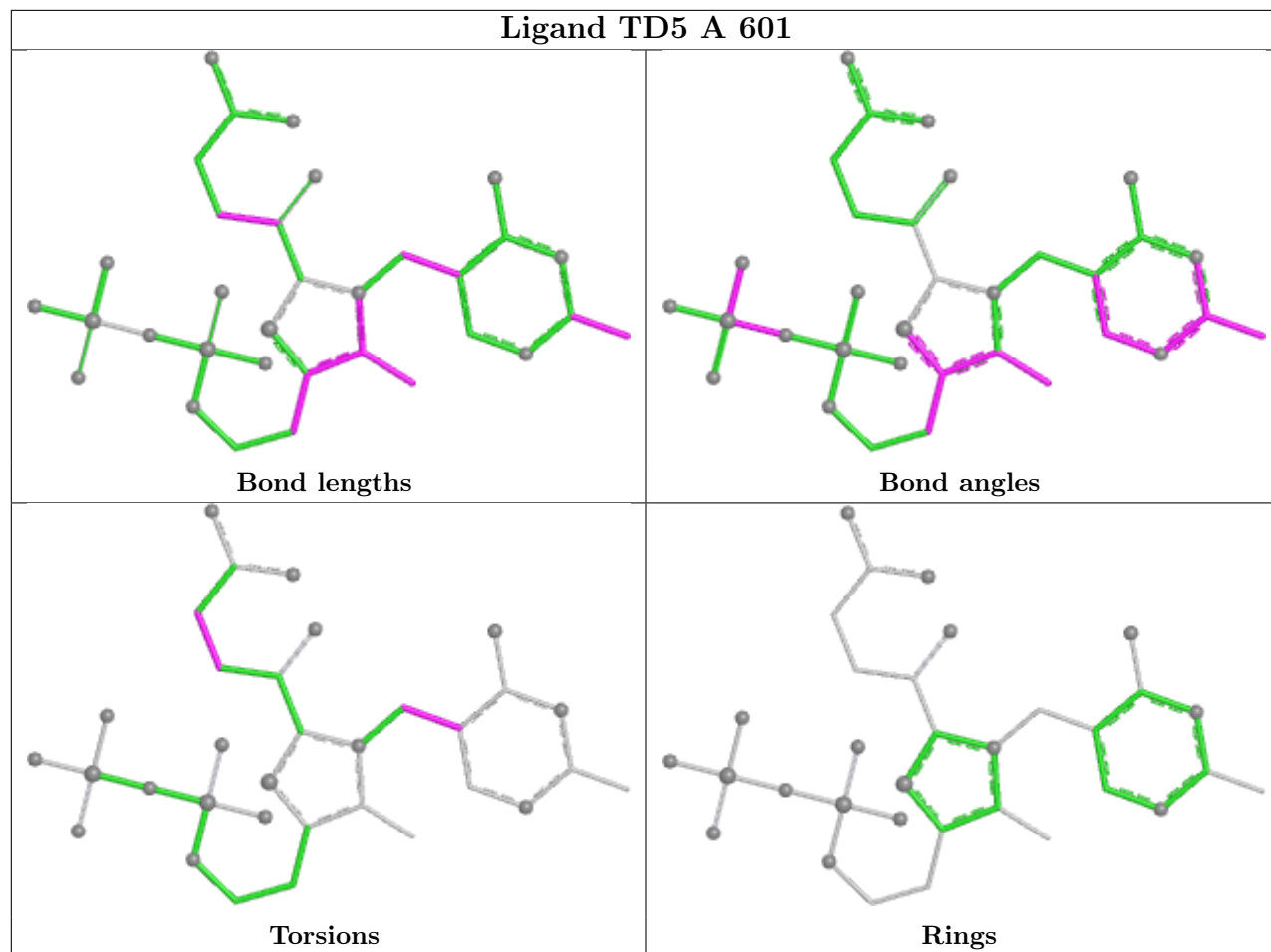
There are no ring outliers.

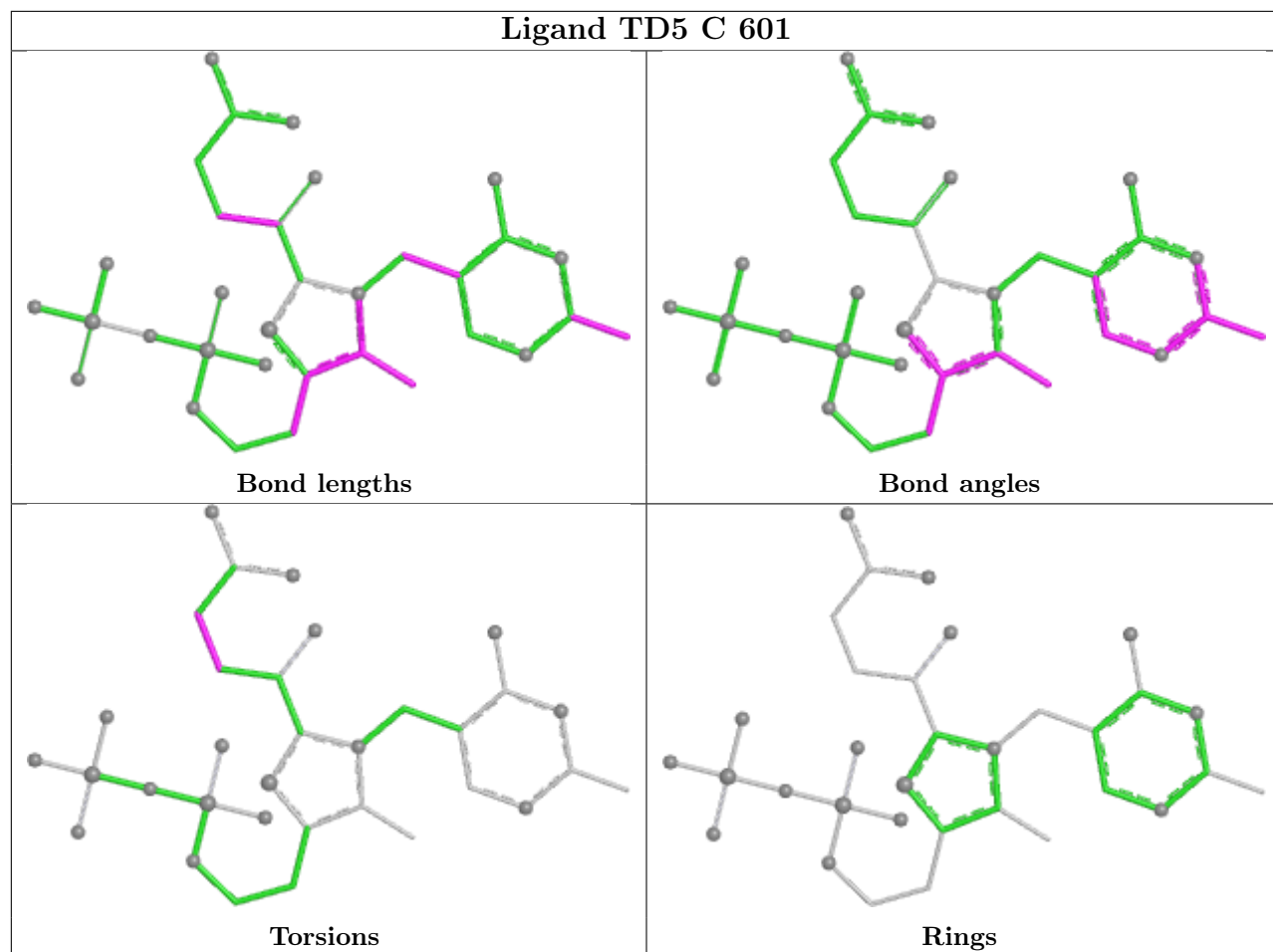
9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	603	GOL	1	0
2	A	601	TD5	1	0
2	C	601	TD5	1	0
2	B	601	TD5	1	0
2	D	601	TD5	2	0
2	F	601	TD5	1	0
2	H	601	TD5	1	0
2	G	601	TD5	2	0
5	B	604	EDO	1	0

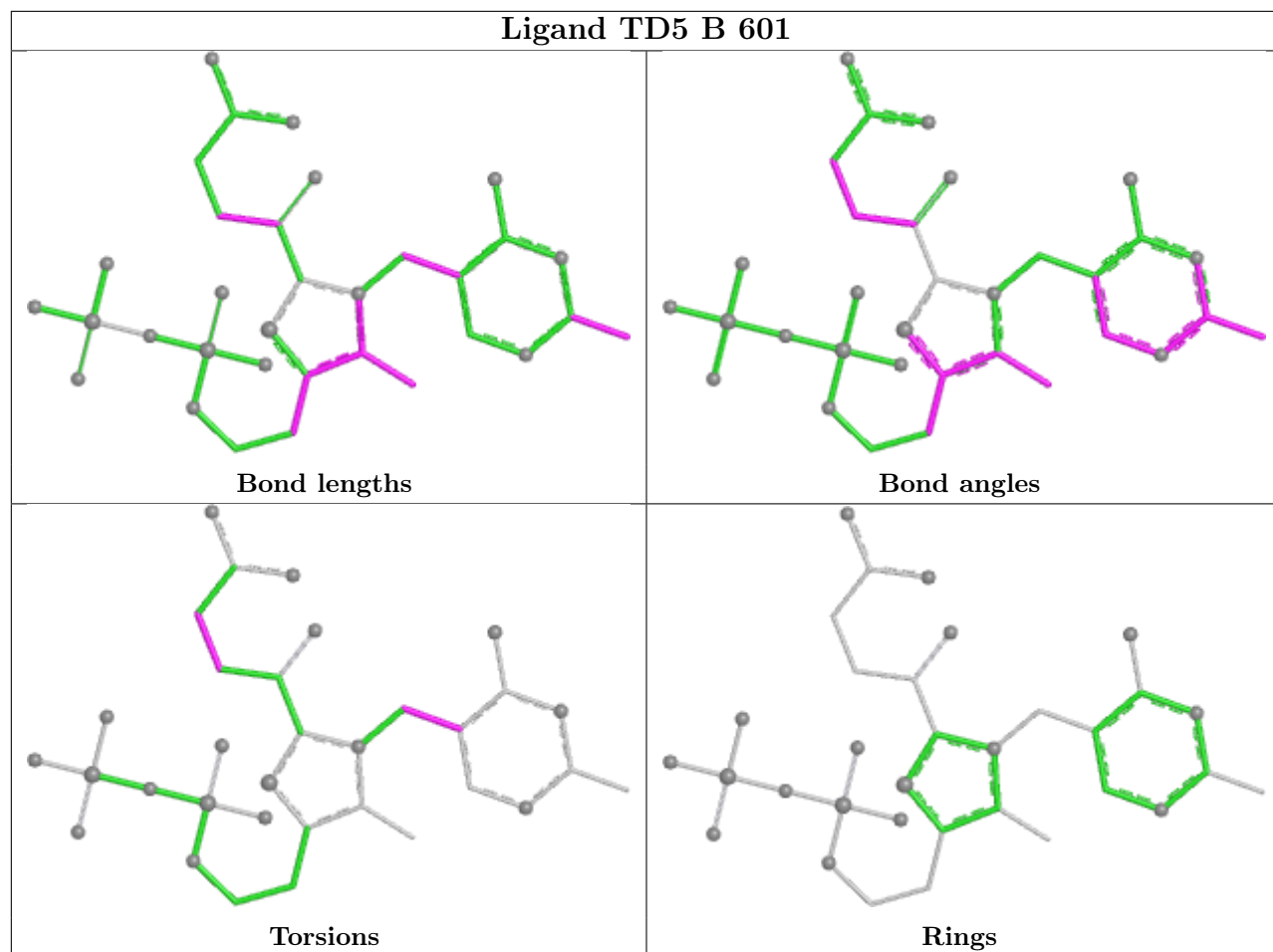
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

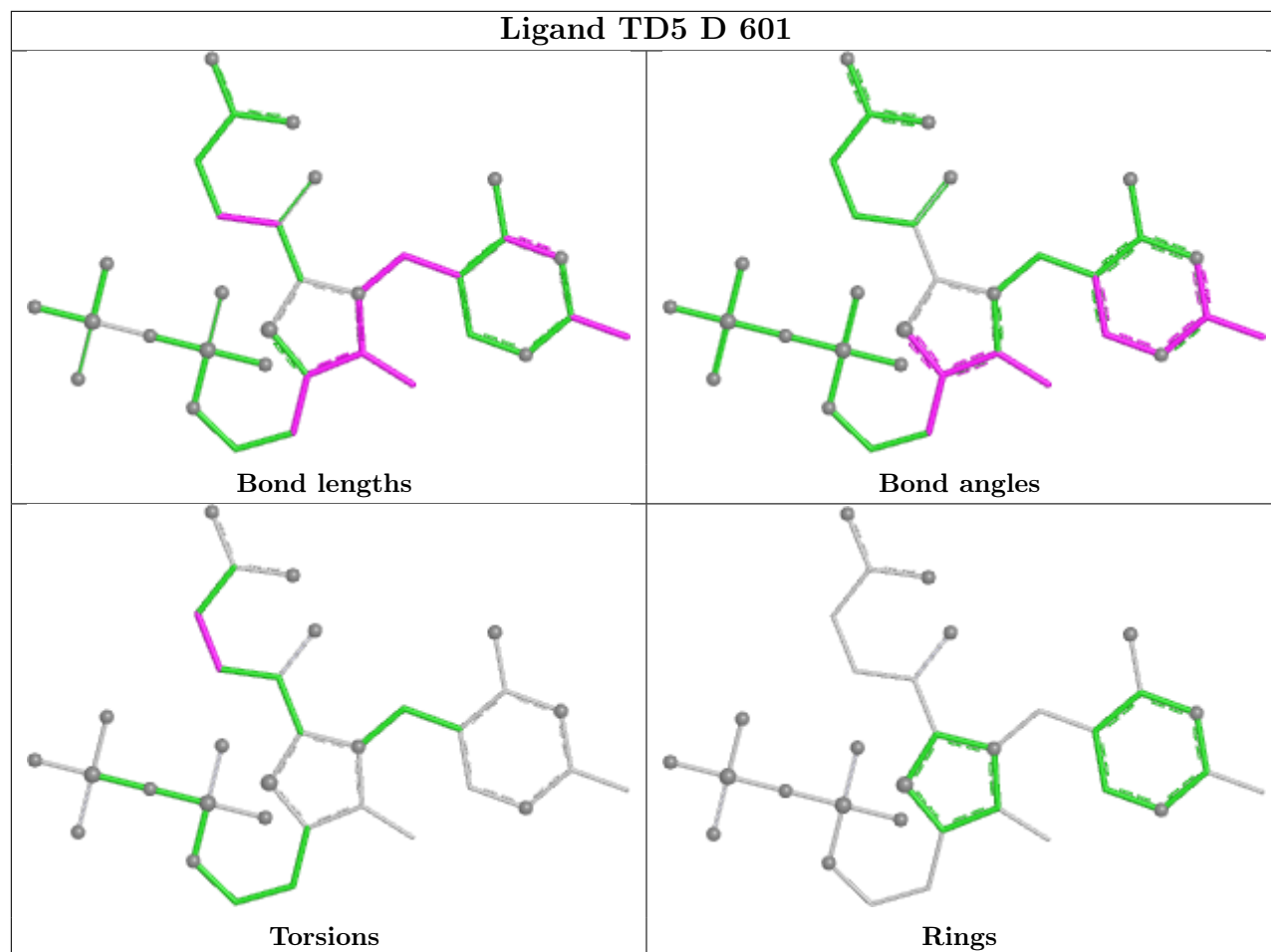




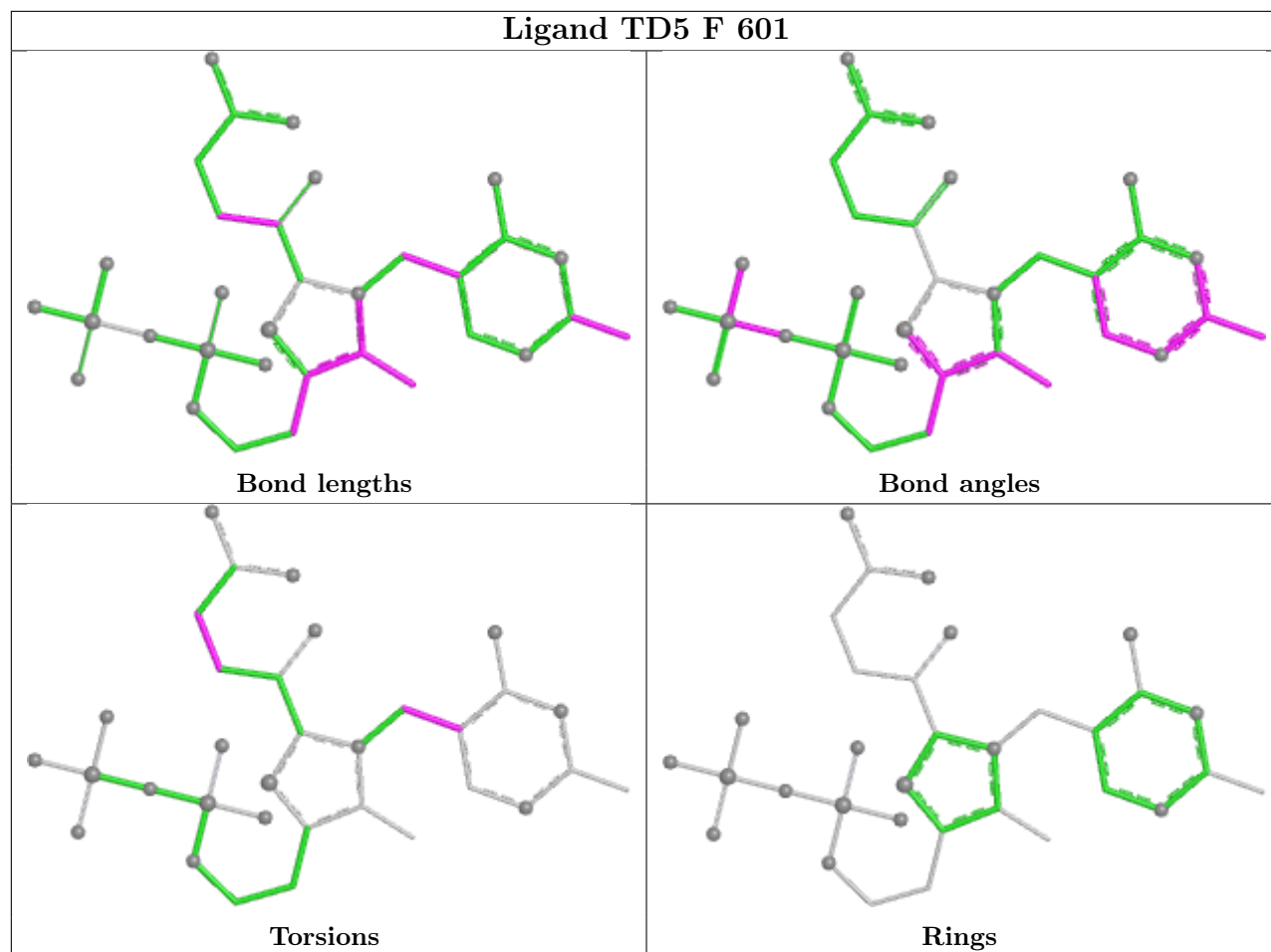
Ligand TD5 B 601



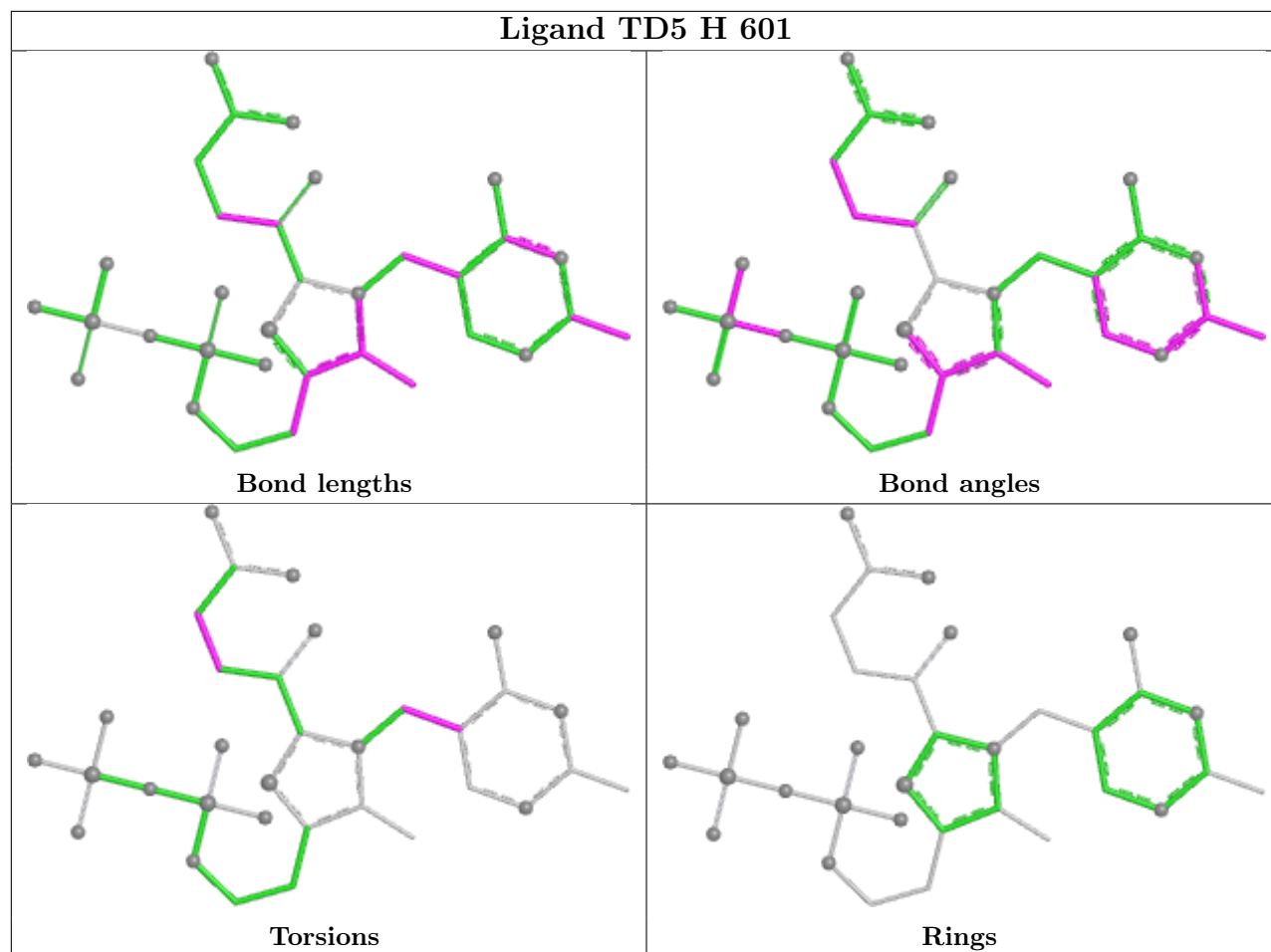
Ligand TD5 D 601



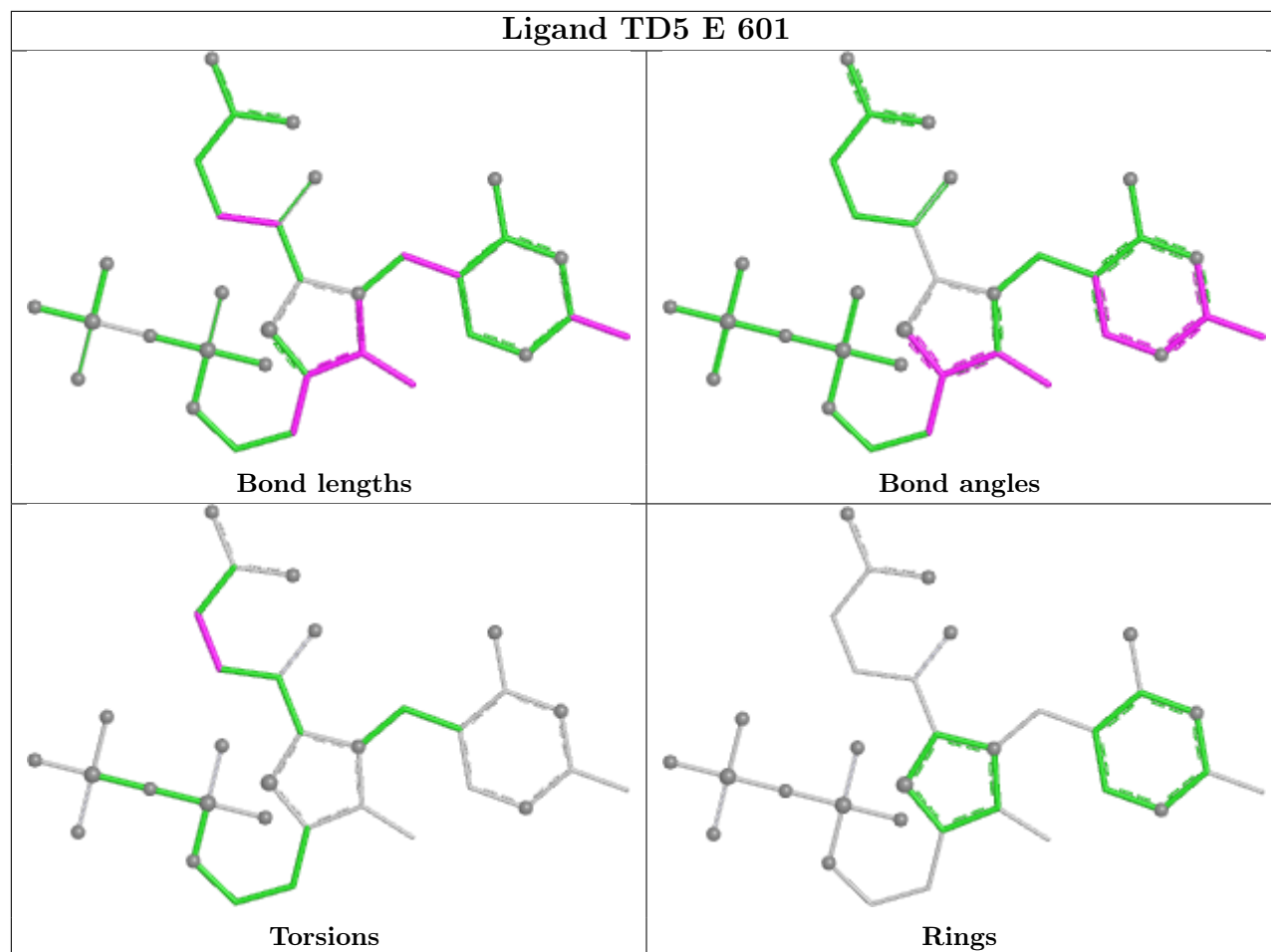
Ligand TD5 F 601

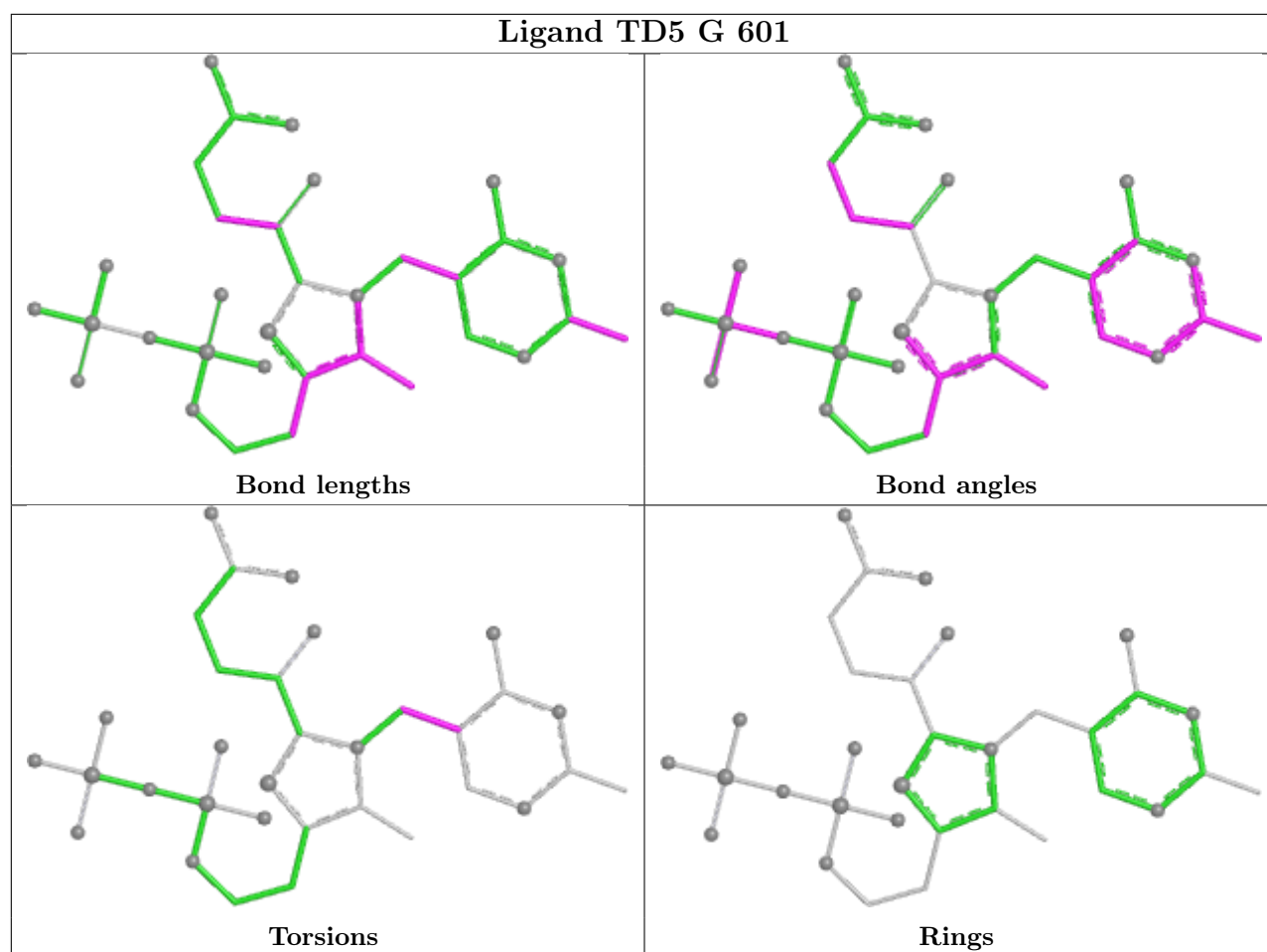


Ligand TD5 H 601



Ligand TD5 E 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	556/556 (100%)	-0.28	3 (0%) 87 90	8, 17, 30, 47	15 (2%)
1	B	556/556 (100%)	-0.25	1 (0%) 91 93	8, 18, 29, 47	11 (1%)
1	C	556/556 (100%)	0.01	3 (0%) 87 90	8, 23, 42, 63	14 (2%)
1	D	556/556 (100%)	-0.19	3 (0%) 87 90	7, 19, 32, 49	11 (1%)
1	E	556/556 (100%)	-0.26	4 (0%) 84 88	7, 17, 30, 44	11 (1%)
1	F	556/556 (100%)	-0.27	4 (0%) 84 88	9, 18, 28, 43	10 (1%)
1	G	556/556 (100%)	-0.16	4 (0%) 84 88	8, 18, 31, 46	9 (1%)
1	H	556/556 (100%)	-0.08	5 (0%) 81 85	8, 22, 38, 60	8 (1%)
All	All	4448/4448 (100%)	-0.19	27 (0%) 85 89	7, 18, 34, 63	89 (2%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	71[A]	GLN	9.7
1	E	377[A]	CYS	3.7
1	C	556	LEU	3.3
1	E	1	MET	3.3
1	C	1	MET	3.2
1	A	27	CYS	3.2
1	D	377[A]	CYS	3.0
1	D	1	MET	2.9
1	H	555	HIS	2.9
1	B	1	MET	2.7
1	G	388[A]	VAL	2.7
1	G	1	MET	2.6
1	F	495[A]	VAL	2.6
1	E	312	ILE	2.6
1	A	312	ILE	2.4
1	F	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	178	MET	2.4
1	G	219	GLN	2.4
1	C	312	ILE	2.3
1	H	347	VAL	2.3
1	A	1	MET	2.2
1	H	556	LEU	2.2
1	H	1	MET	2.2
1	F	176	GLY	2.2
1	E	483	SER	2.2
1	F	188[A]	ARG	2.1
1	D	526	ARG	2.1

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
5	EDO	C	604	4/4	0.77	0.15	47,57,61,62	0
5	EDO	F	604	4/4	0.79	0.17	28,35,39,42	0
5	EDO	H	604	4/4	0.88	0.10	27,33,38,40	0
5	EDO	B	604	4/4	0.90	0.15	23,29,35,35	0
5	EDO	D	604	4/4	0.90	0.12	29,35,37,37	0
4	GOL	C	603	6/6	0.91	0.15	26,32,38,38	0
5	EDO	G	604	4/4	0.92	0.09	26,32,38,39	0
5	EDO	E	604	4/4	0.93	0.07	26,31,33,34	0
4	GOL	G	603	6/6	0.93	0.10	21,30,34,36	0
4	GOL	H	603	6/6	0.93	0.11	19,32,37,38	0
5	EDO	A	604	4/4	0.93	0.07	27,32,35,35	0
4	GOL	E	603	6/6	0.94	0.08	17,26,31,31	0

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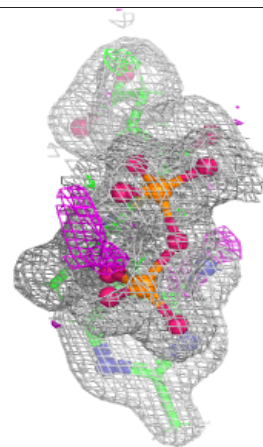
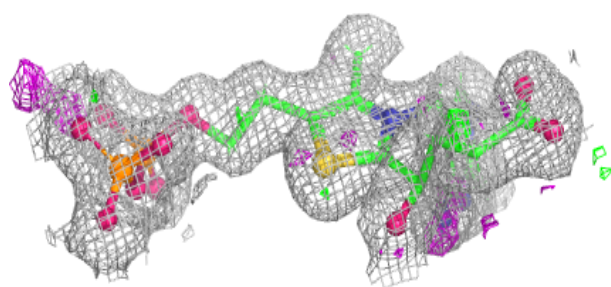
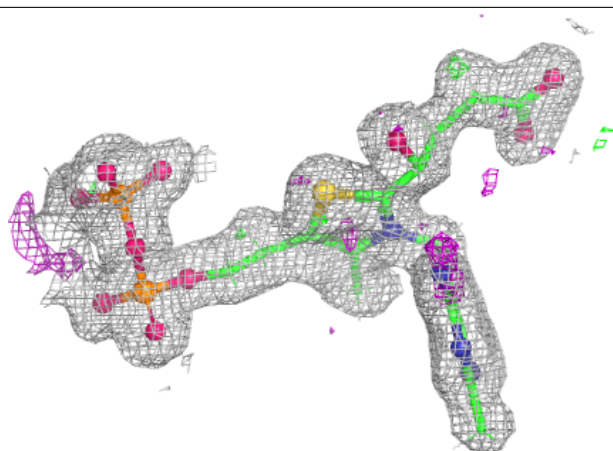
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	F	603	6/6	0.94	0.07	19,24,29,29	0
4	GOL	D	603	6/6	0.94	0.09	20,33,38,40	0
4	GOL	A	603	6/6	0.95	0.08	16,25,33,33	0
2	TD5	H	601	33/33	0.96	0.07	16,23,36,52	0
2	TD5	C	601	33/33	0.96	0.07	13,23,38,49	0
2	TD5	D	601	33/33	0.97	0.06	13,19,32,36	0
2	TD5	E	601	33/33	0.97	0.07	12,19,33,54	0
2	TD5	F	601	33/33	0.97	0.06	12,20,33,33	0
2	TD5	G	601	33/33	0.97	0.06	14,20,31,37	0
2	TD5	B	601	33/33	0.97	0.07	11,19,35,42	0
2	TD5	A	601	33/33	0.97	0.06	11,18,35,46	0
4	GOL	B	603	6/6	0.97	0.06	19,25,30,30	0
3	MN	C	602	1/1	0.98	0.06	28,28,28,28	0
3	MN	G	602	1/1	0.99	0.07	23,23,23,23	0
3	MN	H	602	1/1	0.99	0.06	23,23,23,23	0
3	MN	B	602	1/1	0.99	0.06	22,22,22,22	0
3	MN	D	602	1/1	0.99	0.10	23,23,23,23	0
3	MN	E	602	1/1	0.99	0.10	21,21,21,21	0
3	MN	F	602	1/1	0.99	0.09	20,20,20,20	0
3	MN	A	602	1/1	1.00	0.09	22,22,22,22	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.

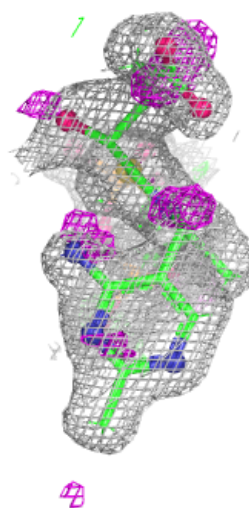
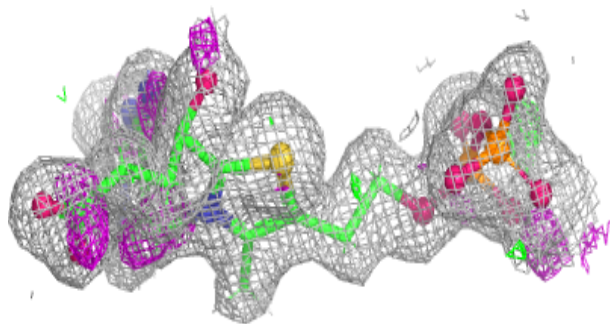
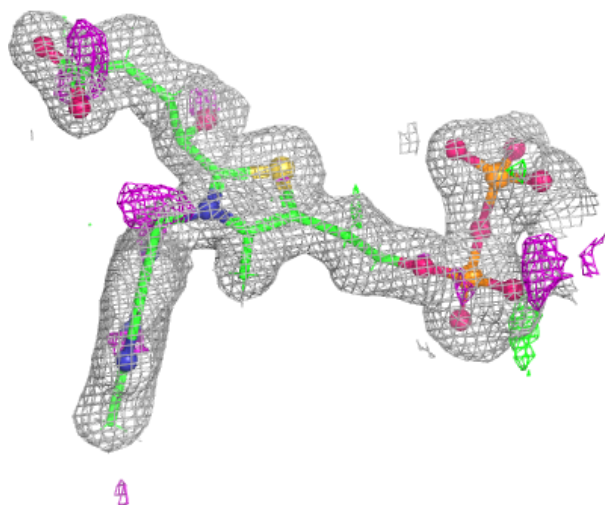
Electron density around TD5 H 601:

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



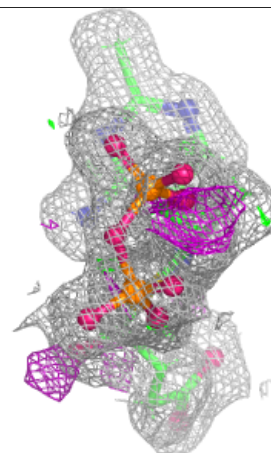
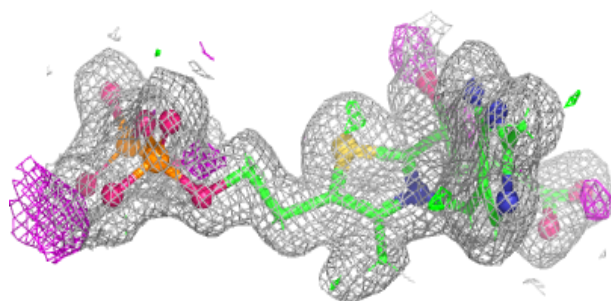
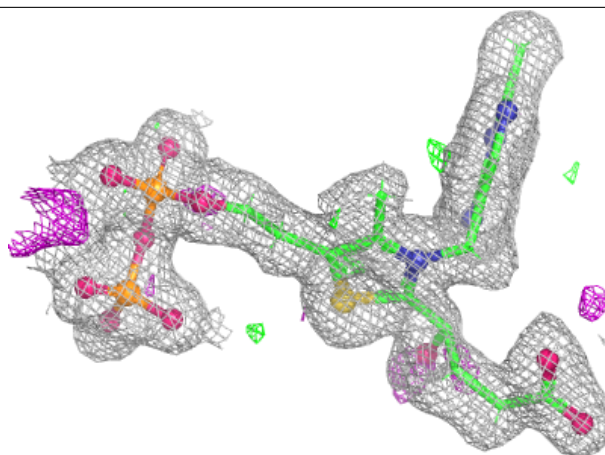
Electron density around TD5 C 601:

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



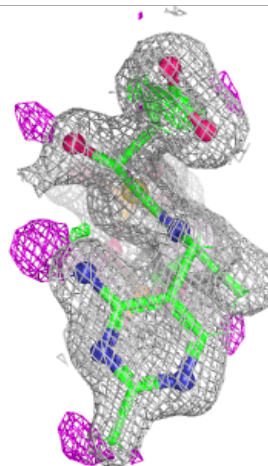
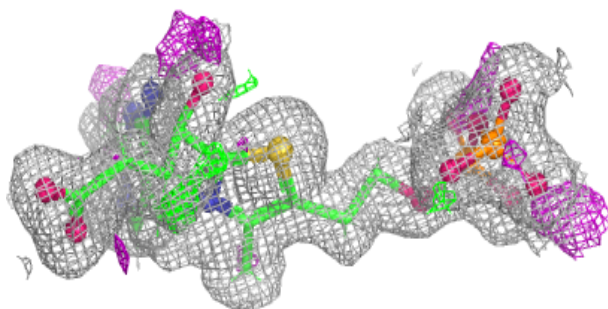
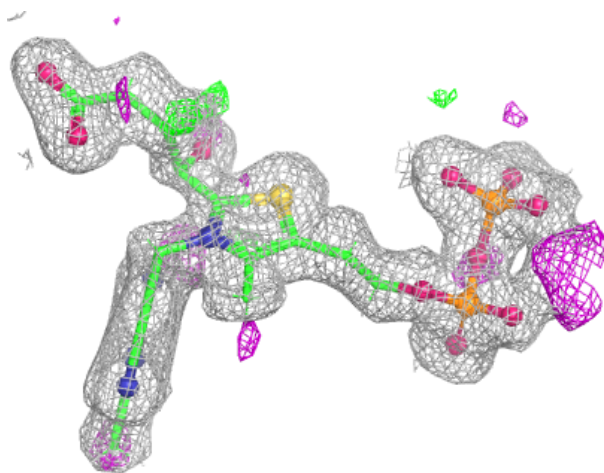
Electron density around TD5 D 601:

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



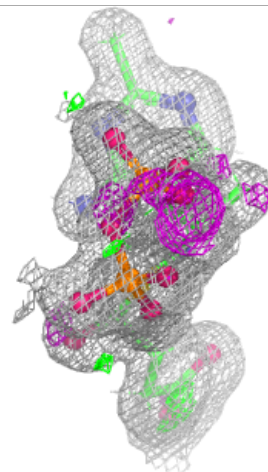
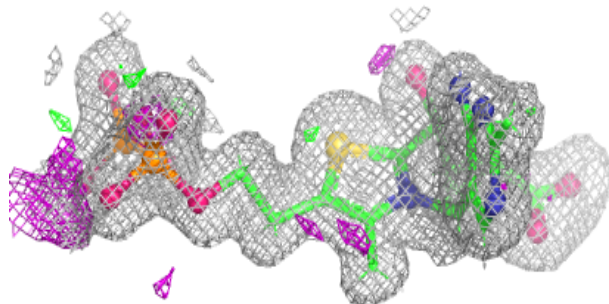
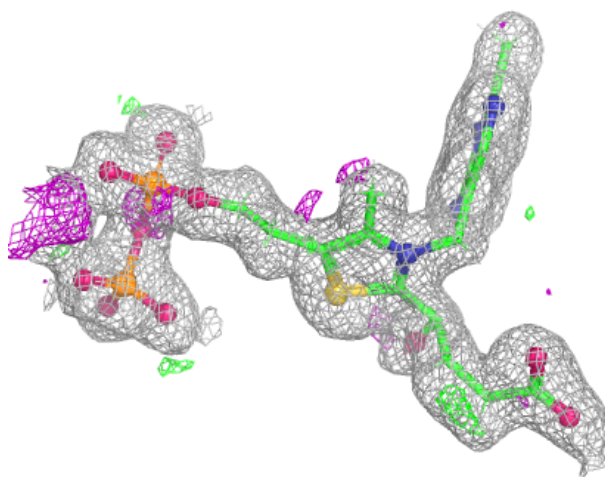
Electron density around TD5 E 601:

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



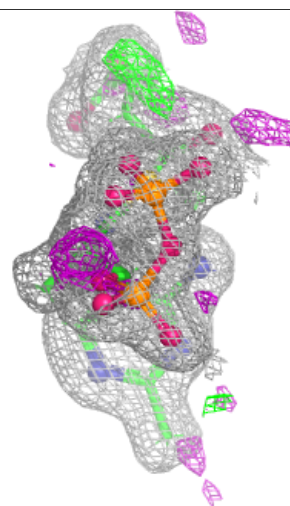
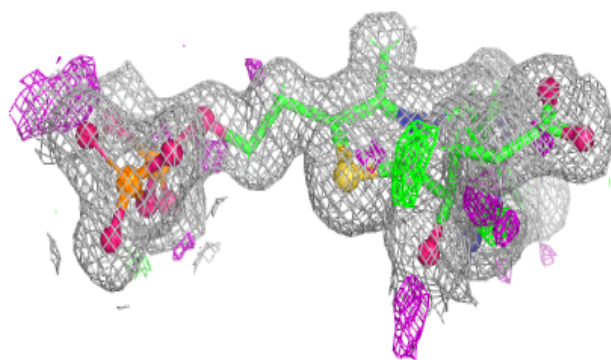
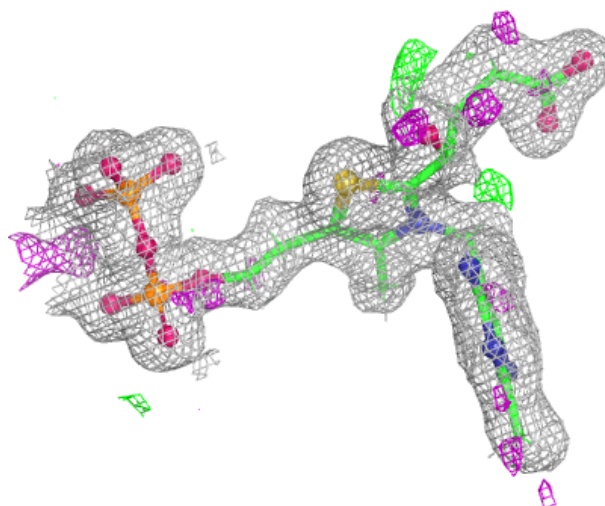
Electron density around TD5 F 601:

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



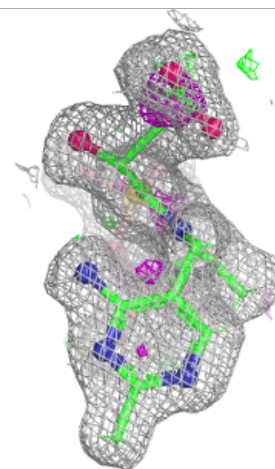
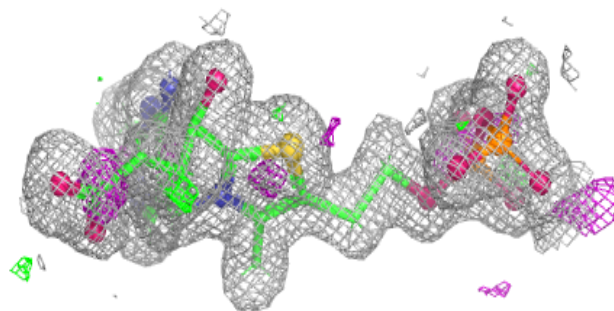
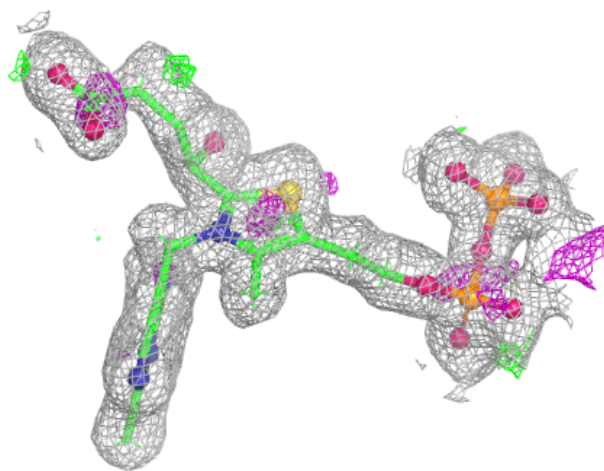
Electron density around TD5 G 601:

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



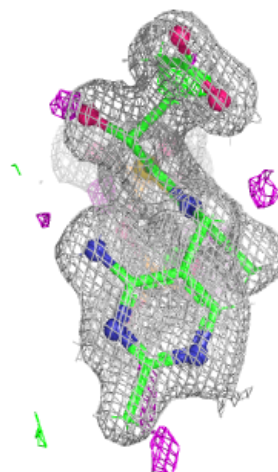
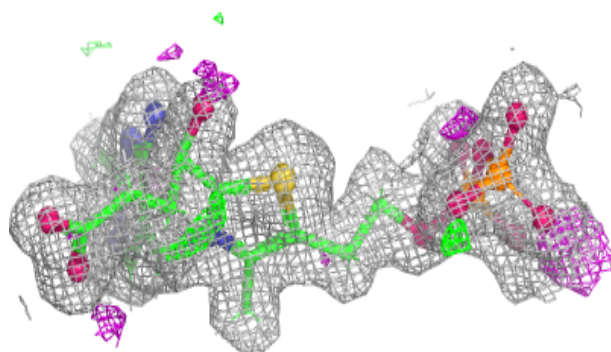
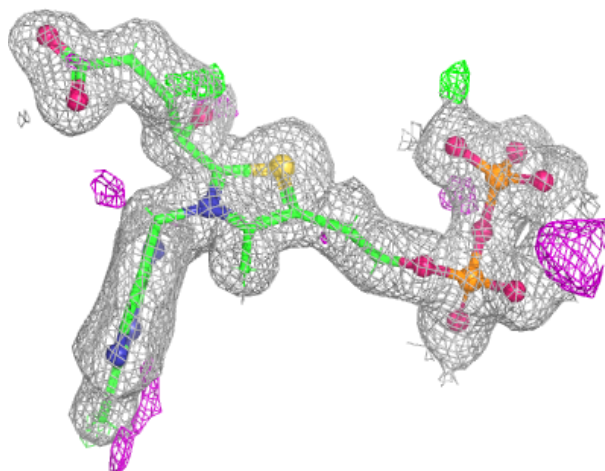
Electron density around TD5 B 601:

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



Electron density around TD5 A 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.