



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:27 AM UTC

PDB ID : 2Y0D / pdb_00002y0d
Title : BceC mutation Y10K
Authors : Rocha, J.; Popescu, A.O.; Borges, P.; Mil-Homens, D.; Sa-Correia, I.; Fialho, A.M.; Frazao, C.
Deposited on : 2010-12-02
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

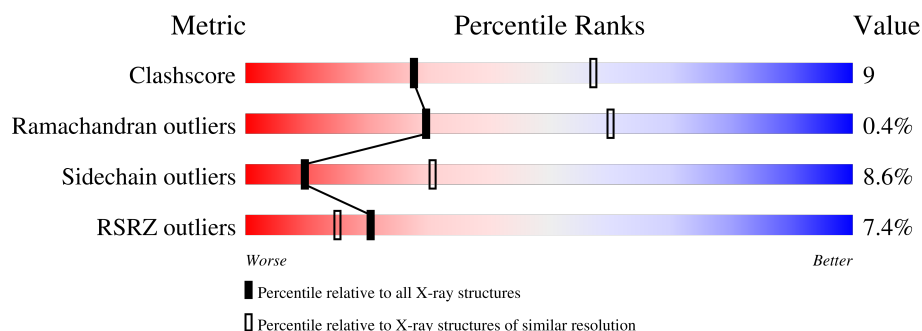
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	478	6% 74% 18% • 5%
1	B	478	6% 73% 18% • 6%
1	C	478	9% 73% 18% • 6%
1	D	478	7% 71% 21% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	1455	-	-	X	-
3	SO4	C	1456	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14125 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 UDP-GLUCOSE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3513	2206	629	664	14			
1	B	448	Total	C	N	O	S	0	0	0
			3455	2174	618	649	14			
1	C	451	Total	C	N	O	S	0	0	0
			3478	2187	621	656	14			
1	D	453	Total	C	N	O	S	0	0	0
			3491	2194	626	657	14			

There are 36 discrepancies between the modelled and reference sequences:

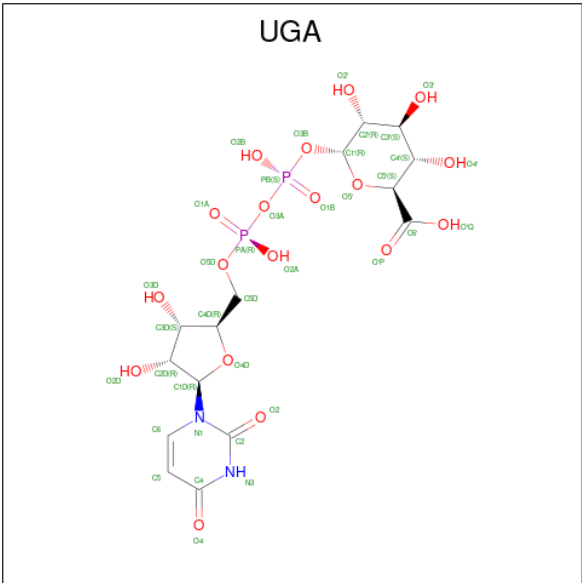
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP C9E261
A	-6	HIS	-	expression tag	UNP C9E261
A	-5	HIS	-	expression tag	UNP C9E261
A	-4	HIS	-	expression tag	UNP C9E261
A	-3	HIS	-	expression tag	UNP C9E261
A	-2	HIS	-	expression tag	UNP C9E261
A	-1	GLY	-	expression tag	UNP C9E261
A	0	SER	-	expression tag	UNP C9E261
A	10	LYS	TYR	engineered mutation	UNP C9E261
B	-7	HIS	-	expression tag	UNP C9E261
B	-6	HIS	-	expression tag	UNP C9E261
B	-5	HIS	-	expression tag	UNP C9E261
B	-4	HIS	-	expression tag	UNP C9E261
B	-3	HIS	-	expression tag	UNP C9E261
B	-2	HIS	-	expression tag	UNP C9E261
B	-1	GLY	-	expression tag	UNP C9E261
B	0	SER	-	expression tag	UNP C9E261
B	10	LYS	TYR	engineered mutation	UNP C9E261
C	-7	HIS	-	expression tag	UNP C9E261
C	-6	HIS	-	expression tag	UNP C9E261
C	-5	HIS	-	expression tag	UNP C9E261

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP C9E261
C	-3	HIS	-	expression tag	UNP C9E261
C	-2	HIS	-	expression tag	UNP C9E261
C	-1	GLY	-	expression tag	UNP C9E261
C	0	SER	-	expression tag	UNP C9E261
C	10	LYS	TYR	engineered mutation	UNP C9E261
D	-7	HIS	-	expression tag	UNP C9E261
D	-6	HIS	-	expression tag	UNP C9E261
D	-5	HIS	-	expression tag	UNP C9E261
D	-4	HIS	-	expression tag	UNP C9E261
D	-3	HIS	-	expression tag	UNP C9E261
D	-2	HIS	-	expression tag	UNP C9E261
D	-1	GLY	-	expression tag	UNP C9E261
D	0	SER	-	expression tag	UNP C9E261
D	10	LYS	TYR	engineered mutation	UNP C9E261

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (CCD ID: UGA) (formula: C₁₅H₂₂N₂O₁₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

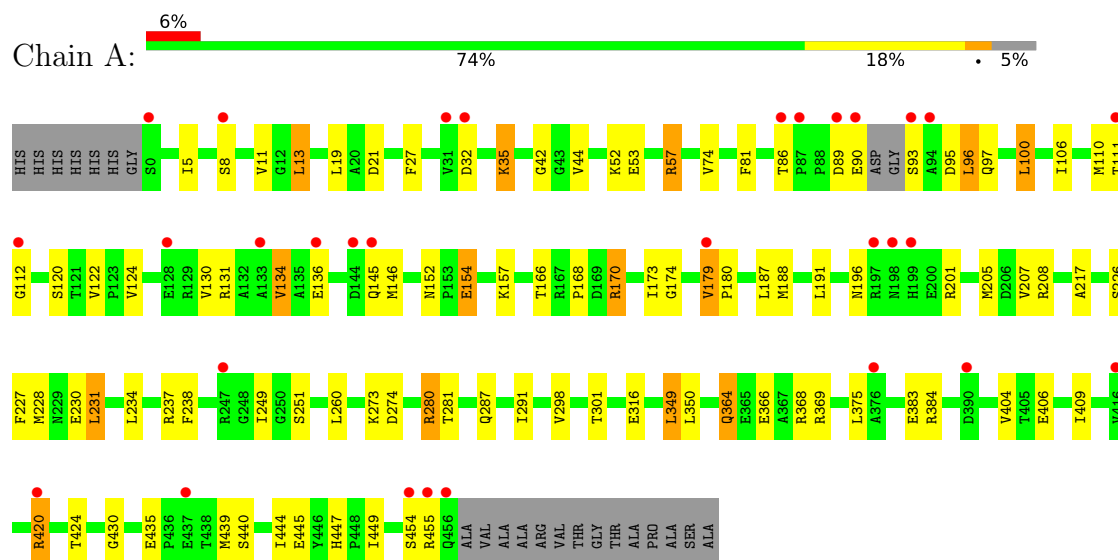


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

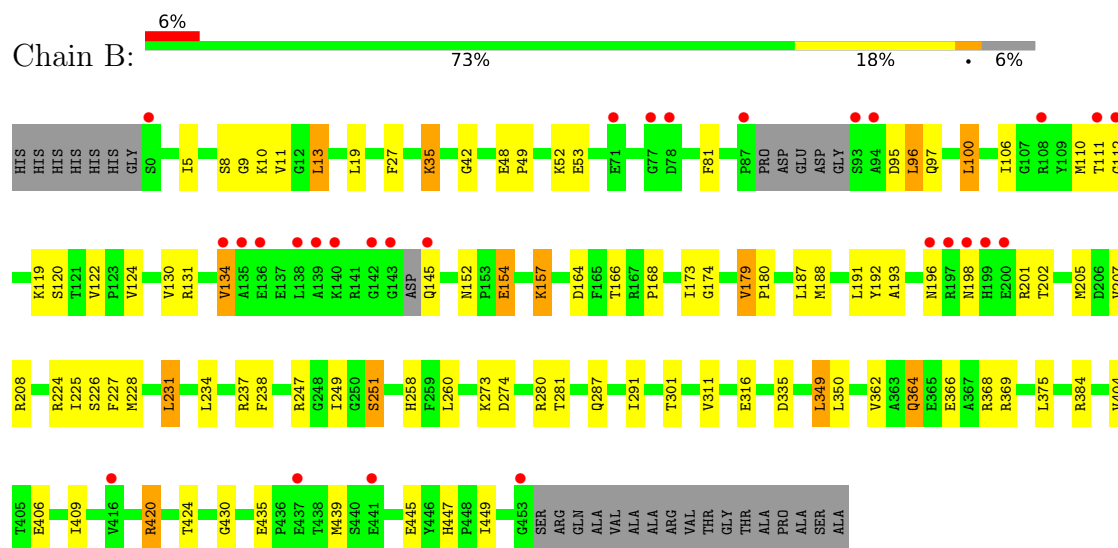
3 Residue-property plots [i](#)

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

• Molecule 1: UDP-GLUCOSE DEHYDROGENASE

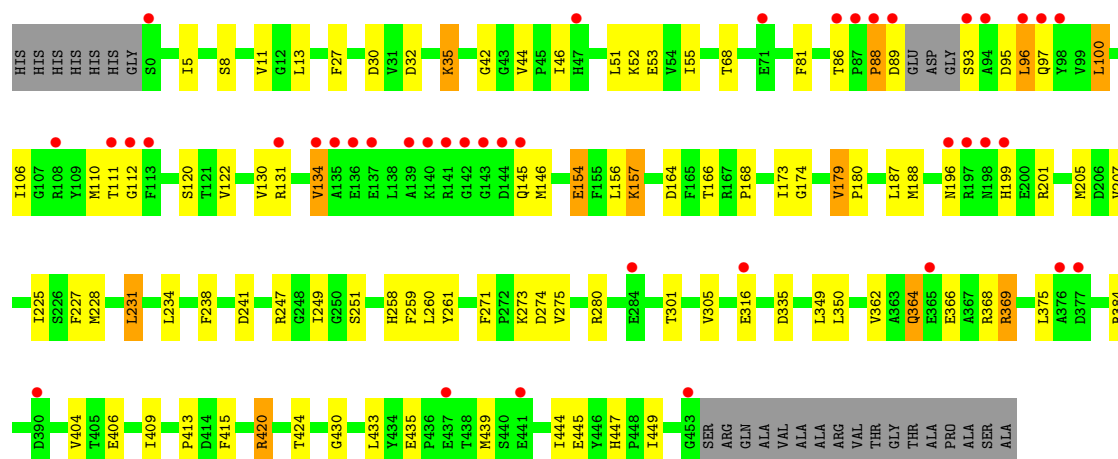


• Molecule 1: UDP-GLUCOSE DEHYDROGENASE

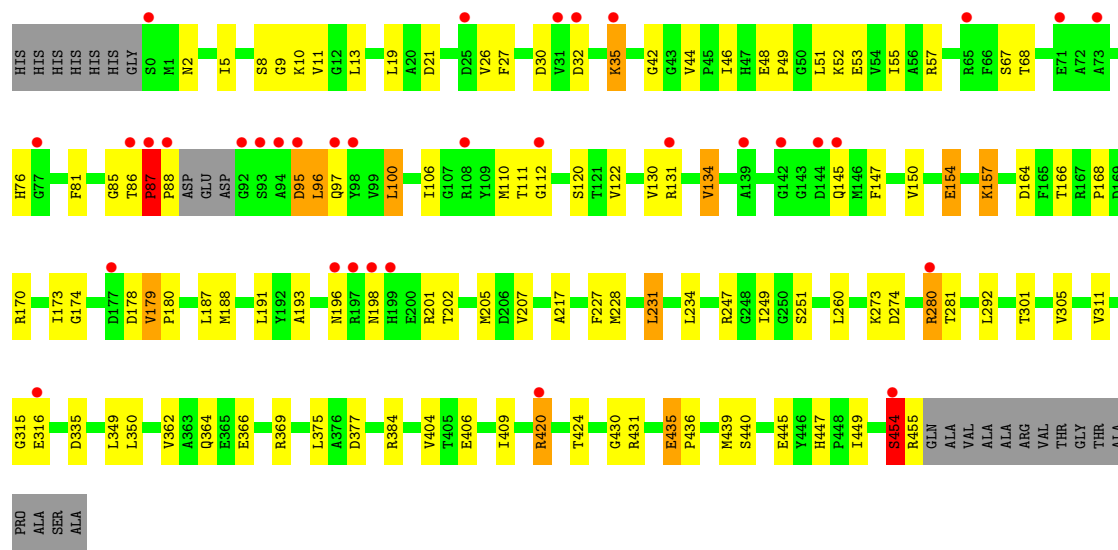


• Molecule 1: UDP-GLUCOSE DEHYDROGENASE





• Molecule 1: UDP-GLUCOSE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.62Å 109.25Å 183.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.63 – 2.80 54.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (54.63-2.80) 99.6 (54.63-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.212 , 0.264 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14125	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UGA, SO4

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	0.75	0/3578	1.01	10/4842 (0.2%)
1	B	0.78	1/3518 (0.0%)	0.99	3/4759 (0.1%)
1	C	0.76	0/3543	1.02	9/4796 (0.2%)
1	D	0.80	1/3556 (0.0%)	1.04	10/4812 (0.2%)
All	All	0.77	2/14195 (0.0%)	1.02	32/19209 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	ALA	CA-CB	-6.83	1.47	1.54
1	D	193	ALA	CA-CB	-5.13	1.49	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	THR	CA-C-N	11.82	132.56	120.38
1	D	86	THR	C-N-CA	11.82	132.56	120.38
1	C	247	ARG	NE-CZ-NH2	-10.21	110.01	119.20
1	C	86	THR	CA-C-N	9.99	130.67	120.38
1	C	86	THR	C-N-CA	9.99	130.67	120.38
1	A	86	THR	CA-C-N	9.03	129.68	120.38
1	A	86	THR	C-N-CA	9.03	129.68	120.38
1	C	247	ARG	CD-NE-CZ	8.79	136.71	124.40
1	C	247	ARG	NE-CZ-NH1	8.72	130.22	121.50
1	A	57	ARG	NE-CZ-NH2	-8.07	111.94	119.20
1	A	57	ARG	NE-CZ-NH1	6.90	128.40	121.50
1	D	122	VAL	CA-C-N	6.78	126.80	119.89
1	D	122	VAL	C-N-CA	6.78	126.80	119.89
1	A	57	ARG	CD-NE-CZ	6.60	133.63	124.40
1	C	122	VAL	CA-C-N	6.60	126.62	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	VAL	C-N-CA	6.60	126.62	119.89
1	D	315	GLY	N-CA-C	6.36	118.53	112.04
1	D	95	ASP	N-CA-C	6.33	118.59	108.41
1	A	122	VAL	CA-C-N	6.16	126.12	119.78
1	A	122	VAL	C-N-CA	6.16	126.12	119.78
1	D	26	VAL	N-CA-C	5.92	116.63	107.99
1	B	122	VAL	CA-C-N	5.81	125.77	119.78
1	B	122	VAL	C-N-CA	5.81	125.77	119.78
1	D	305	VAL	N-CA-C	5.72	115.92	110.42
1	D	87	PRO	CB-CA-C	-5.55	104.15	110.92
1	C	305	VAL	N-CA-C	5.42	115.63	110.42
1	C	444	ILE	N-CA-C	5.23	115.50	108.17
1	A	444	ILE	N-CA-C	5.21	115.47	108.17
1	A	152	ASN	CA-C-N	5.18	125.92	120.11
1	A	152	ASN	C-N-CA	5.18	125.92	120.11
1	B	225	ILE	N-CA-C	5.12	115.33	110.42
1	D	85	GLY	N-CA-C	5.09	119.05	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3513	0	3481	69	1
1	B	3455	0	3433	78	0
1	C	3478	0	3449	65	0
1	D	3491	0	3466	67	1
2	A	37	0	19	0	0
2	B	37	0	19	0	0
2	C	37	0	19	0	0
2	D	37	0	19	0	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
3	C	15	0	0	4	0
3	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14125	0	13905	251	1

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 9.

All (251) 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:D:228:MET:HE1	1:D:249:ILE:HD11	1.48	0.93
1:C:439:MET:HE2	1:C:439:MET:HA	1.52	0.90
1:C:228:MET:HE1	1:C:249:ILE:HD11	1.54	0.90
1:B:228:MET:HE1	1:B:249:ILE:HD11	1.54	0.90
1:B:130:VAL:O	1:B:134:VAL:HG12	1.76	0.85
1:A:439:MET:HE2	1:A:439:MET:HA	1.57	0.85
1:A:228:MET:HE1	1:A:249:ILE:HD11	1.58	0.85
1:A:130:VAL:O	1:A:134:VAL:HG12	1.78	0.84
1:B:439:MET:HA	1:B:439:MET:HE2	1.60	0.84
1:D:439:MET:HE2	1:D:439:MET:HA	1.61	0.82
1:D:228:MET:HE3	1:D:260:LEU:HD22	1.59	0.82
1:C:130:VAL:O	1:C:134:VAL:HG12	1.83	0.78
1:C:89:ASP:HB3	1:C:93:SER:N	1.97	0.78
1:B:247:ARG:HD3	1:D:198:ASN:OD1	1.84	0.78
1:C:228:MET:HE1	1:C:249:ILE:CD1	2.16	0.76
1:D:130:VAL:O	1:D:134:VAL:HG12	1.86	0.75
1:D:228:MET:CE	1:D:249:ILE:HD11	2.16	0.75
1:B:228:MET:CE	1:B:249:ILE:HD11	2.15	0.75
1:C:228:MET:CE	1:C:249:ILE:HD11	2.16	0.75
1:B:198:ASN:OD1	1:D:247:ARG:HD3	1.86	0.74
1:A:89:ASP:HB3	1:A:93:SER:N	2.03	0.74
1:D:196:ASN:HD22	1:D:201:ARG:H	1.35	0.74
1:B:247:ARG:HD3	1:D:198:ASN:CG	2.14	0.73
1:A:228:MET:HE3	1:A:260:LEU:HD22	1.71	0.72
1:A:228:MET:CE	1:A:249:ILE:HD11	2.19	0.72
1:C:228:MET:HE3	1:C:260:LEU:HD22	1.72	0.72
1:B:228:MET:HE3	1:B:260:LEU:HD22	1.70	0.72
1:D:228:MET:HE1	1:D:249:ILE:CD1	2.20	0.71
1:B:228:MET:HE1	1:B:249:ILE:CD1	2.20	0.70
1:C:227:PHE:CD1	1:C:228:MET:HE2	2.26	0.70
1:C:131:ARG:HG3	1:C:131:ARG:HH11	1.56	0.69
1:A:228:MET:HE1	1:A:249:ILE:CD1	2.23	0.69
1:B:106:ILE:O	1:B:110:MET:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:HD22	1:B:201:ARG:H	1.41	0.67
1:A:227:PHE:CD1	1:A:228:MET:HE2	2.30	0.66
1:A:8:SER:OG	1:A:35:LYS:HD3	1.95	0.66
1:B:8:SER:OG	1:B:35:LYS:HD3	1.94	0.66
1:C:196:ASN:HD22	1:C:201:ARG:H	1.41	0.66
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.59	0.65
1:C:106:ILE:O	1:C:110:MET:HG3	1.97	0.65
1:B:198:ASN:CG	1:D:247:ARG:HD3	2.22	0.65
1:A:226:SER:HB3	1:B:291:ILE:HD11	1.79	0.65
1:A:350:LEU:O	1:A:384:ARG:NH2	2.29	0.64
1:B:227:PHE:CD1	1:B:228:MET:HE2	2.33	0.64
1:D:131:ARG:HG3	1:D:131:ARG:HH11	1.62	0.64
1:D:227:PHE:CD1	1:D:228:MET:HE2	2.32	0.64
1:A:124:VAL:HG11	1:B:238:PHE:HB3	1.78	0.64
1:D:5:ILE:HD13	1:D:81:PHE:HB2	1.79	0.64
1:D:106:ILE:O	1:D:110:MET:HG3	1.98	0.64
1:A:196:ASN:HD22	1:A:201:ARG:H	1.45	0.64
1:B:350:LEU:O	1:B:384:ARG:NH2	2.31	0.64
1:C:179:VAL:HG13	1:C:180:PRO:HD3	1.80	0.64
1:C:8:SER:OG	1:C:35:LYS:HD3	1.98	0.63
1:A:238:PHE:O	1:B:208:ARG:HD3	1.98	0.63
1:C:350:LEU:O	1:C:384:ARG:NH2	2.33	0.61
1:D:350:LEU:O	1:D:384:ARG:NH2	2.32	0.61
1:A:5:ILE:HD13	1:A:81:PHE:HB2	1.81	0.61
1:A:445:GLU:OE2	1:A:447:HIS:HE1	1.83	0.61
1:A:208:ARG:HD3	1:B:238:PHE:O	2.01	0.61
1:C:196:ASN:ND2	1:C:201:ARG:H	1.98	0.60
1:C:5:ILE:HD13	1:C:81:PHE:HB2	1.84	0.60
1:D:430:GLY:HA2	1:D:449:ILE:HD12	1.82	0.60
1:C:273:LYS:HE3	1:C:274:ASP:OD1	2.03	0.59
1:D:8:SER:OG	1:D:35:LYS:HD3	2.02	0.59
1:D:196:ASN:ND2	1:D:201:ARG:H	1.99	0.59
1:A:106:ILE:O	1:A:110:MET:HG3	2.03	0.59
1:B:273:LYS:HE3	1:B:274:ASP:OD1	2.04	0.58
1:C:11:VAL:HG22	1:C:154:GLU:HG3	1.84	0.58
1:B:131:ARG:HH11	1:B:131:ARG:HG3	1.67	0.58
1:D:95:ASP:OD1	1:D:97:GLN:HG2	2.04	0.58
1:A:420:ARG:HH11	1:A:420:ARG:HB2	1.69	0.57
1:C:89:ASP:CB	1:C:93:SER:N	2.66	0.57
1:A:291:ILE:HD11	1:B:226:SER:HB3	1.87	0.57
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:LYS:HB2	1:C:164:ASP:OD2	2.05	0.56
1:A:406:GLU:O	1:A:406:GLU:HG2	2.05	0.56
1:B:179:VAL:HG13	1:B:180:PRO:HD3	1.88	0.56
1:B:366:GLU:OE2	1:B:369:ARG:NH1	2.39	0.55
1:D:445:GLU:OE2	1:D:447:HIS:HE1	1.90	0.55
1:B:95:ASP:OD1	1:B:97:GLN:HG2	2.06	0.55
1:A:95:ASP:OD1	1:A:97:GLN:HG2	2.06	0.55
1:B:196:ASN:ND2	1:B:201:ARG:H	2.04	0.55
1:C:131:ARG:HG3	1:C:131:ARG:NH1	2.21	0.55
1:A:366:GLU:OE2	1:A:369:ARG:NH1	2.39	0.55
1:A:273:LYS:HE3	1:A:274:ASP:OD1	2.06	0.54
1:B:420:ARG:HB2	1:B:420:ARG:HH11	1.72	0.54
1:C:227:PHE:HD1	1:C:228:MET:HE2	1.69	0.54
1:D:454:SER:C	1:D:455:ARG:HG2	2.32	0.54
1:A:281:THR:HG21	1:B:238:PHE:CZ	2.42	0.54
1:D:420:ARG:HB2	1:D:420:ARG:HH11	1.72	0.54
1:B:227:PHE:HD1	1:B:228:MET:HE2	1.72	0.54
1:B:430:GLY:HA2	1:B:449:ILE:HD12	1.90	0.54
1:C:95:ASP:OD1	1:C:97:GLN:HG2	2.08	0.54
1:D:42:GLY:O	1:D:52:LYS:HE3	2.08	0.54
1:B:247:ARG:NH1	1:D:198:ASN:OD1	2.39	0.53
1:A:227:PHE:HD1	1:A:228:MET:HE2	1.70	0.53
1:B:111:THR:HG22	1:B:112:GLY:N	2.24	0.53
1:C:439:MET:HE2	1:C:439:MET:CA	2.33	0.53
1:A:420:ARG:HH11	1:A:420:ARG:CB	2.21	0.53
1:B:247:ARG:CD	1:D:198:ASN:HA	2.39	0.53
1:A:430:GLY:HA2	1:A:449:ILE:HD12	1.89	0.53
1:D:174:GLY:HA2	1:D:205:MET:O	2.09	0.52
1:B:27:PHE:CD1	1:B:27:PHE:C	2.88	0.52
1:B:42:GLY:O	1:B:52:LYS:HE3	2.09	0.52
1:D:87:PRO:CB	1:D:88:PRO:CD	2.87	0.52
1:D:131:ARG:HG3	1:D:131:ARG:NH1	2.25	0.52
1:B:335:ASP:HB3	1:B:362:VAL:HG12	1.92	0.52
1:A:238:PHE:HB3	1:B:124:VAL:HG11	1.91	0.51
1:D:111:THR:HG22	1:D:112:GLY:N	2.24	0.51
1:D:420:ARG:HH11	1:D:420:ARG:CB	2.24	0.51
1:A:111:THR:HG22	1:A:112:GLY:N	2.25	0.51
1:B:5:ILE:HD13	1:B:81:PHE:HB2	1.91	0.51
1:D:273:LYS:HE3	1:D:274:ASP:OD1	2.10	0.51
1:A:445:GLU:HG3	1:A:455:ARG:HA	1.92	0.51
1:D:95:ASP:OD1	1:D:95:ASP:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:MET:HA	1:D:188:MET:HE2	1.93	0.51
1:D:227:PHE:HD1	1:D:228:MET:HE2	1.74	0.51
1:C:42:GLY:O	1:C:52:LYS:HE3	2.11	0.51
1:A:287:GLN:HB2	1:B:237:ARG:NH1	2.25	0.50
1:A:191:LEU:O	1:A:191:LEU:HD23	2.11	0.50
1:A:238:PHE:CD2	1:B:124:VAL:HG21	2.46	0.50
1:C:420:ARG:HH11	1:C:420:ARG:HB2	1.76	0.50
1:A:11:VAL:HG22	1:A:154:GLU:HG3	1.94	0.50
1:B:439:MET:HE2	1:B:439:MET:CA	2.39	0.50
1:C:366:GLU:OE2	1:C:369:ARG:NH1	2.44	0.49
1:A:196:ASN:ND2	1:A:201:ARG:H	2.11	0.49
1:A:455:ARG:CZ	1:A:455:ARG:HB2	2.42	0.49
1:D:157:LYS:HB2	1:D:164:ASP:OD2	2.12	0.49
1:D:227:PHE:CE1	1:D:231:LEU:HD22	2.47	0.49
1:B:166:THR:C	1:B:168:PRO:HD3	2.38	0.49
1:B:406:GLU:O	1:B:406:GLU:HG2	2.12	0.49
1:C:199:HIS:CE1	3:C:1456:SO4:O4	2.66	0.49
1:B:131:ARG:HG3	1:B:131:ARG:NH1	2.27	0.49
1:C:96:LEU:HB3	1:C:100:LEU:HD22	1.94	0.49
1:C:335:ASP:HB3	1:C:362:VAL:HG12	1.94	0.49
1:C:445:GLU:OE2	1:C:447:HIS:HE1	1.95	0.49
1:B:11:VAL:HG22	1:B:154:GLU:HG3	1.95	0.48
1:B:227:PHE:CE1	1:B:231:LEU:HD22	2.48	0.48
1:B:420:ARG:HH11	1:B:420:ARG:CB	2.26	0.48
1:B:445:GLU:OE2	1:B:447:HIS:HE1	1.95	0.48
1:C:27:PHE:CD1	1:C:27:PHE:C	2.91	0.48
1:B:48:GLU:O	1:B:49:PRO:C	2.57	0.48
1:C:111:THR:HG22	1:C:112:GLY:N	2.28	0.48
1:D:191:LEU:O	1:D:191:LEU:HD23	2.13	0.48
1:D:366:GLU:OE2	1:D:369:ARG:NH1	2.46	0.48
1:A:166:THR:C	1:A:168:PRO:HD3	2.39	0.48
1:C:238:PHE:CZ	1:D:281:THR:HG21	2.49	0.47
1:C:238:PHE:CZ	1:D:281:THR:CG2	2.98	0.47
1:B:335:ASP:HB3	1:B:362:VAL:CG1	2.45	0.47
1:A:191:LEU:HD23	1:A:191:LEU:C	2.40	0.47
1:A:238:PHE:CZ	1:B:281:THR:HG21	2.49	0.47
1:C:364:GLN:NE2	1:C:368:ARG:HH12	2.12	0.47
1:C:227:PHE:CE1	1:C:231:LEU:HD22	2.50	0.47
1:C:430:GLY:HA2	1:C:449:ILE:HD12	1.96	0.47
1:A:227:PHE:CE1	1:A:231:LEU:HD22	2.50	0.47
1:C:51:LEU:O	1:C:55:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:HD23	1:B:191:LEU:O	2.16	0.46
1:C:89:ASP:C	1:C:93:SER:N	2.73	0.46
1:A:124:VAL:HG21	1:B:238:PHE:CD2	2.51	0.46
1:A:281:THR:HG21	1:B:238:PHE:HZ	1.80	0.46
1:C:174:GLY:HA2	1:C:205:MET:O	2.15	0.46
1:C:251:SER:HB2	1:D:170:ARG:HD2	1.97	0.46
1:A:217:ALA:HB2	1:B:249:ILE:HG22	1.96	0.46
1:C:227:PHE:CE1	1:C:228:MET:HE2	2.51	0.46
1:D:9:GLY:O	1:D:10:LYS:C	2.59	0.46
1:A:188:MET:HE2	1:A:188:MET:HA	1.98	0.46
1:A:445:GLU:OE2	1:A:447:HIS:CE1	2.68	0.46
1:A:42:GLY:O	1:A:52:LYS:HE3	2.16	0.46
1:C:166:THR:C	1:C:168:PRO:HD3	2.41	0.46
1:A:27:PHE:CD1	1:A:27:PHE:C	2.94	0.46
1:B:174:GLY:HA2	1:B:205:MET:O	2.15	0.45
1:B:157:LYS:HB2	1:B:157:LYS:HE2	1.69	0.45
1:C:179:VAL:N	1:C:180:PRO:CD	2.79	0.45
1:C:261:TYR:HE2	3:C:1455:SO4:O4	1.99	0.45
1:C:271:PHE:O	1:C:275:VAL:HG23	2.15	0.45
1:C:406:GLU:HG2	1:C:406:GLU:O	2.17	0.45
1:A:237:ARG:NH1	1:B:287:GLN:HB2	2.32	0.45
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.72	0.45
1:A:90:GLU:OE2	1:A:280:ARG:HD2	2.17	0.45
1:A:21:ASP:CG	1:A:57:ARG:HH11	2.25	0.45
1:A:364:GLN:NE2	1:A:368:ARG:HH12	2.15	0.45
1:A:174:GLY:HA2	1:A:205:MET:O	2.17	0.44
1:D:179:VAL:N	1:D:180:PRO:CD	2.80	0.44
1:D:11:VAL:HG22	1:D:154:GLU:HG3	1.98	0.44
1:D:166:THR:C	1:D:168:PRO:HD3	2.42	0.44
1:C:146:MET:HE2	1:C:180:PRO:HG3	1.99	0.44
1:D:51:LEU:O	1:D:55:ILE:HG13	2.18	0.44
1:D:2:ASN:HB3	1:D:76:HIS:CE1	2.53	0.44
1:D:335:ASP:HB3	1:D:362:VAL:HG12	2.00	0.44
1:C:225:ILE:HD11	1:C:259:PHE:CD2	2.53	0.44
1:A:170:ARG:HD2	1:B:251:SER:HB2	1.99	0.44
1:A:238:PHE:HZ	1:B:281:THR:HG21	1.83	0.44
1:D:191:LEU:HD23	1:D:191:LEU:C	2.43	0.44
1:B:224:ARG:NH2	1:B:258:HIS:O	2.42	0.43
1:D:21:ASP:CG	1:D:57:ARG:HH21	2.26	0.43
1:B:119:LYS:NZ	1:B:152:ASN:ND2	2.66	0.43
1:C:249:ILE:HG22	1:D:217:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:PHE:CD1	1:D:27:PHE:C	2.96	0.43
1:B:179:VAL:N	1:B:180:PRO:CD	2.82	0.43
1:B:27:PHE:C	1:B:27:PHE:HD1	2.26	0.43
1:B:188:MET:HA	1:B:188:MET:HE2	1.99	0.43
1:D:406:GLU:O	1:D:406:GLU:HG2	2.19	0.43
1:A:281:THR:CG2	1:B:238:PHE:CZ	3.01	0.43
1:B:96:LEU:HB3	1:B:100:LEU:HD22	2.00	0.43
1:A:8:SER:O	1:A:13:LEU:HD22	2.19	0.43
1:A:146:MET:HE2	1:A:180:PRO:HG3	2.00	0.43
1:B:152:ASN:ND2	1:B:192:TYR:OH	2.52	0.43
1:C:30:ASP:O	1:C:68:THR:HG22	2.19	0.43
1:C:96:LEU:HB3	1:C:100:LEU:CD2	2.49	0.42
1:B:157:LYS:HB2	1:B:164:ASP:OD2	2.18	0.42
1:A:349:LEU:HD12	1:A:349:LEU:HA	1.84	0.42
1:B:196:ASN:ND2	1:B:202:THR:HG22	2.34	0.42
1:C:88:PRO:HG3	1:C:273:LYS:HG3	2.01	0.42
1:D:280:ARG:O	1:D:281:THR:C	2.61	0.42
1:D:435:GLU:O	1:D:436:PRO:C	2.62	0.42
1:C:439:MET:HA	1:C:439:MET:CE	2.38	0.42
1:A:179:VAL:N	1:A:180:PRO:CD	2.83	0.42
1:A:439:MET:HE2	1:A:439:MET:CA	2.39	0.42
1:C:406:GLU:CB	1:C:433:LEU:HD11	2.49	0.42
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.80	0.42
1:C:131:ARG:NH1	1:C:131:ARG:CG	2.82	0.41
1:C:413:PRO:HG2	1:C:415:PHE:CZ	2.55	0.41
1:A:96:LEU:HB3	1:A:100:LEU:HD22	2.01	0.41
1:B:364:GLN:NE2	1:B:368:ARG:HH12	2.19	0.41
1:C:199:HIS:ND1	3:C:1456:SO4:O2	2.45	0.41
1:C:258:HIS:ND1	3:C:1455:SO4:O2	2.48	0.41
1:B:191:LEU:HD23	1:B:191:LEU:C	2.45	0.41
1:D:292:LEU:HD12	1:D:292:LEU:HA	1.75	0.41
1:A:95:ASP:OD1	1:A:95:ASP:C	2.62	0.41
1:A:89:ASP:CB	1:A:93:SER:N	2.78	0.41
1:A:238:PHE:CG	1:B:124:VAL:HG11	2.56	0.41
1:B:13:LEU:HD12	1:B:13:LEU:HA	1.78	0.41
1:C:154:GLU:HG2	1:C:156:LEU:HG	2.02	0.41
1:C:188:MET:HE2	1:C:188:MET:HA	2.03	0.41
1:D:19:LEU:HA	1:D:19:LEU:HD23	1.82	0.41
1:D:134:VAL:HG13	1:D:147:PHE:CZ	2.56	0.41
1:D:178:ASP:CG	1:D:180:PRO:HD2	2.46	0.41
1:D:196:ASN:ND2	1:D:202:THR:HG22	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:GLU:OE2	1:D:447:HIS:CE1	2.74	0.41
1:A:230:GLU:HG3	1:A:298:VAL:HG21	2.03	0.41
1:D:431:ARG:HA	1:D:431:ARG:HD3	1.96	0.41
1:C:44:VAL:HG12	1:C:46:ILE:H	1.85	0.40
1:D:48:GLU:O	1:D:49:PRO:C	2.64	0.40
1:B:9:GLY:O	1:B:10:LYS:C	2.64	0.40
1:D:30:ASP:O	1:D:68:THR:HG22	2.21	0.40
1:D:96:LEU:HB3	1:D:100:LEU:HD22	2.03	0.40
1:B:95:ASP:OD1	1:B:95:ASP:C	2.64	0.40
1:C:241:ASP:OD1	1:C:241:ASP:C	2.63	0.40
1:C:406:GLU:HB2	1:C:433:LEU:HD11	2.03	0.40
1:D:44:VAL:HG12	1:D:46:ILE:H	1.84	0.40
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.82	0.40

All (1) 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:383:GLU:OE1	1:D:377:ASP:OD1[1_545]	2.02	0.18

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	451/478 (94%)	431 (96%)	18 (4%)	2 (0%)	30	60
1	B	442/478 (92%)	423 (96%)	19 (4%)	0	100	100
1	C	447/478 (94%)	428 (96%)	17 (4%)	2 (0%)	30	60
1	D	449/478 (94%)	432 (96%)	14 (3%)	3 (1%)	18	47
All	All	1789/1912 (94%)	1714 (96%)	68 (4%)	7 (0%)	30	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	C	32	ASP
1	C	88	PRO
1	D	32	ASP
1	A	454	SER
1	D	454	SER
1	D	87	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	363/377 (96%)	330 (91%)	33 (9%)	9	28
1	B	356/377 (94%)	327 (92%)	29 (8%)	11	33
1	C	359/377 (95%)	331 (92%)	28 (8%)	11	35
1	D	360/377 (96%)	327 (91%)	33 (9%)	8	27
All	All	1438/1508 (95%)	1315 (91%)	123 (9%)	10	31

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	35	LYS
1	A	44	VAL
1	A	53	GLU
1	A	74	VAL
1	A	96	LEU
1	A	100	LEU
1	A	120	SER
1	A	134	VAL
1	A	136	GLU
1	A	145	GLN
1	A	154	GLU
1	A	157	LYS
1	A	170	ARG
1	A	173	ILE

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	187	LEU
1	A	207	VAL
1	A	231	LEU
1	A	234	LEU
1	A	251	SER
1	A	280	ARG
1	A	301	THR
1	A	316	GLU
1	A	349	LEU
1	A	364	GLN
1	A	375	LEU
1	A	404	VAL
1	A	409	ILE
1	A	420	ARG
1	A	424	THR
1	A	435	GLU
1	A	440	SER
1	B	13	LEU
1	B	35	LYS
1	B	53	GLU
1	B	96	LEU
1	B	100	LEU
1	B	120	SER
1	B	134	VAL
1	B	145	GLN
1	B	154	GLU
1	B	157	LYS
1	B	173	ILE
1	B	179	VAL
1	B	187	LEU
1	B	207	VAL
1	B	231	LEU
1	B	234	LEU
1	B	251	SER
1	B	280	ARG
1	B	301	THR
1	B	311	VAL
1	B	316	GLU
1	B	349	LEU
1	B	364	GLN
1	B	375	LEU

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Mol	Chain	Res	Type
1	B	404	VAL
1	B	409	ILE
1	B	420	ARG
1	B	424	THR
1	B	435	GLU
1	C	13	LEU
1	C	35	LYS
1	C	53	GLU
1	C	96	LEU
1	C	100	LEU
1	C	120	SER
1	C	134	VAL
1	C	145	GLN
1	C	154	GLU
1	C	157	LYS
1	C	173	ILE
1	C	179	VAL
1	C	187	LEU
1	C	207	VAL
1	C	231	LEU
1	C	234	LEU
1	C	280	ARG
1	C	301	THR
1	C	316	GLU
1	C	349	LEU
1	C	364	GLN
1	C	369	ARG
1	C	375	LEU
1	C	404	VAL
1	C	409	ILE
1	C	420	ARG
1	C	424	THR
1	C	435	GLU
1	D	13	LEU
1	D	35	LYS
1	D	53	GLU
1	D	67	SER
1	D	96	LEU
1	D	100	LEU
1	D	120	SER
1	D	134	VAL
1	D	145	GLN

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Mol	Chain	Res	Type
1	D	150	VAL
1	D	154	GLU
1	D	157	LYS
1	D	173	ILE
1	D	179	VAL
1	D	187	LEU
1	D	207	VAL
1	D	231	LEU
1	D	234	LEU
1	D	251	SER
1	D	280	ARG
1	D	301	THR
1	D	311	VAL
1	D	316	GLU
1	D	349	LEU
1	D	364	GLN
1	D	375	LEU
1	D	404	VAL
1	D	409	ILE
1	D	420	ARG
1	D	424	THR
1	D	435	GLU
1	D	440	SER
1	D	454	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	47	HIS
1	A	152	ASN
1	A	196	ASN
1	A	233	ASN
1	A	364	GLN
1	A	378	HIS
1	A	447	HIS
1	B	33	GLN
1	B	97	GLN
1	B	152	ASN
1	B	196	ASN
1	B	233	ASN
1	B	364	GLN

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Mol	Chain	Res	Type
1	B	447	HIS
1	C	47	HIS
1	C	97	GLN
1	C	152	ASN
1	C	196	ASN
1	C	364	GLN
1	C	447	HIS
1	D	33	GLN
1	D	47	HIS
1	D	97	GLN
1	D	152	ASN
1	D	196	ASN
1	D	364	GLN
1	D	378	HIS
1	D	447	HIS

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](#)

12 ligands 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
3	SO4	C	1456	-	4,4,4	0.25	0	6,6,6	0.39	0
2	UGA	C	500	-	38,39,39	1.20	3 (7%)	56,60,60	1.56	7 (12%)
2	UGA	B	500	-	38,39,39	1.08	2 (5%)	56,60,60	1.98	15 (26%)
3	SO4	D	1456	-	4,4,4	0.41	0	6,6,6	0.38	0
3	SO4	B	1454	-	4,4,4	0.36	0	6,6,6	0.35	0
3	SO4	C	1454	-	4,4,4	0.21	0	6,6,6	0.38	0
2	UGA	A	500	-	38,39,39	1.17	5 (13%)	56,60,60	1.97	17 (30%)
3	SO4	A	1458	-	4,4,4	0.26	0	6,6,6	0.31	0
3	SO4	C	1455	-	4,4,4	0.34	0	6,6,6	0.44	0
3	SO4	A	1459	-	4,4,4	0.27	0	6,6,6	0.49	0
3	SO4	A	1457	-	4,4,4	0.27	0	6,6,6	0.51	0
2	UGA	D	500	-	38,39,39	1.47	4 (10%)	56,60,60	1.58	12 (21%)

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	UGA	D	500	-	-	3/25/61/61	0/3/3/3
2	UGA	A	500	-	-	9/25/61/61	0/3/3/3
2	UGA	C	500	-	-	4/25/61/61	0/3/3/3
2	UGA	B	500	-	-	6/25/61/61	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	UGA	PB-O3A	4.69	1.64	1.59
2	D	500	UGA	PA-O3A	4.25	1.64	1.59
2	C	500	UGA	C2-N1	-3.25	1.33	1.38
2	B	500	UGA	PA-O3A	3.05	1.62	1.59
2	A	500	UGA	PB-O3A	3.00	1.62	1.59
2	D	500	UGA	C2-N1	-2.92	1.33	1.38
2	A	500	UGA	C6-C5	2.56	1.41	1.35
2	A	500	UGA	O4-C4	2.53	1.29	1.24
2	D	500	UGA	C6-C5	2.40	1.40	1.35
2	C	500	UGA	C4-N3	-2.39	1.34	1.38
2	B	500	UGA	C6-C5	2.38	1.40	1.35
2	C	500	UGA	C2-N3	-2.27	1.34	1.38
2	A	500	UGA	O2-C2	2.15	1.26	1.23
2	A	500	UGA	PA-O3A	2.14	1.61	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	UGA	C4-N3-C2	-6.38	118.69	126.61
2	B	500	UGA	C4-N3-C2	-5.72	119.51	126.61
2	A	500	UGA	N3-C2-N1	5.65	122.25	114.89
2	D	500	UGA	N3-C2-N1	5.51	122.07	114.89
2	B	500	UGA	N3-C2-N1	5.48	122.02	114.89
2	C	500	UGA	C4-N3-C2	-4.99	120.42	126.61
2	B	500	UGA	C1'-O5'-C5'	4.91	120.29	112.23
2	D	500	UGA	C4-N3-C2	-4.52	121.00	126.61
2	C	500	UGA	N3-C2-N1	4.50	120.75	114.89
2	B	500	UGA	C5-C4-N3	4.24	120.75	114.80
2	A	500	UGA	O4-C4-C5	-4.01	118.24	125.16
2	B	500	UGA	O3A-PB-O1B	-3.79	99.30	110.70
2	A	500	UGA	O2-C2-N1	-3.61	118.10	122.80
2	C	500	UGA	C5-C4-N3	3.58	119.81	114.80
2	B	500	UGA	O2-C2-N3	-3.47	115.10	121.49
2	C	500	UGA	O3'-C3'-C2'	-3.44	102.27	110.38
2	A	500	UGA	O4-C4-N3	3.24	123.97	119.27
2	A	500	UGA	C5-C6-N1	-2.97	117.02	121.84
2	B	500	UGA	O5'-C5'-C6'	2.85	115.06	106.14
2	C	500	UGA	O2'-C2'-C3'	-2.82	103.73	110.38
2	A	500	UGA	C1'-O5'-C5'	2.78	116.79	112.23
2	A	500	UGA	O2B-PB-O3A	-2.73	99.90	107.27
2	D	500	UGA	C1'-O5'-C5'	2.73	116.70	112.23
2	A	500	UGA	O3A-PA-O1A	-2.72	102.51	110.70
2	B	500	UGA	O2A-PA-O1A	2.65	124.79	112.44
2	B	500	UGA	O5'-C1'-C2'	2.63	115.78	110.37
2	D	500	UGA	O3'-C3'-C4'	-2.54	104.38	110.38
2	C	500	UGA	O4-C4-C5	-2.54	120.78	125.16
2	C	500	UGA	O2B-PB-O3A	-2.50	100.50	107.27
2	D	500	UGA	O2'-C2'-C3'	-2.50	104.47	110.38
2	B	500	UGA	C3'-C4'-C5'	2.48	113.56	109.30
2	A	500	UGA	O4'-C4'-C5'	-2.39	104.30	109.76
2	B	500	UGA	O3B-C1'-C2'	-2.37	104.05	108.38
2	A	500	UGA	C6-C5-C4	2.32	122.49	119.53
2	D	500	UGA	O3D-C3D-C4D	-2.30	104.48	111.08
2	A	500	UGA	PB-O3B-C1'	2.28	130.49	121.21
2	D	500	UGA	C3'-C4'-C5'	2.25	113.18	109.30
2	A	500	UGA	O2A-PA-O3A	2.22	113.26	107.27
2	B	500	UGA	O'Q-C6'-C5'	2.22	121.64	113.64
2	A	500	UGA	C1D-N1-C2	2.21	121.56	117.59
2	D	500	UGA	C5-C4-N3	2.21	117.89	114.80
2	A	500	UGA	O3D-C3D-C4D	-2.19	104.78	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	UGA	O'Q-C6'-O'P	-2.17	119.16	124.08
2	D	500	UGA	O5'-C1'-O3B	2.14	114.17	111.36
2	A	500	UGA	C5-C4-N3	2.13	117.78	114.80
2	A	500	UGA	O2A-PA-O1A	2.10	122.24	112.44
2	D	500	UGA	O3'-C3'-C2'	-2.10	105.42	110.38
2	D	500	UGA	O2-C2-N3	-2.09	117.63	121.49
2	B	500	UGA	O5'-C1'-O3B	2.09	114.09	111.36
2	D	500	UGA	C1'-C2'-C3'	2.01	114.25	110.01
2	B	500	UGA	O4-C4-N3	-2.01	116.37	119.27

There are no chirality outliers.

All (22) torsion outliers are listed below:

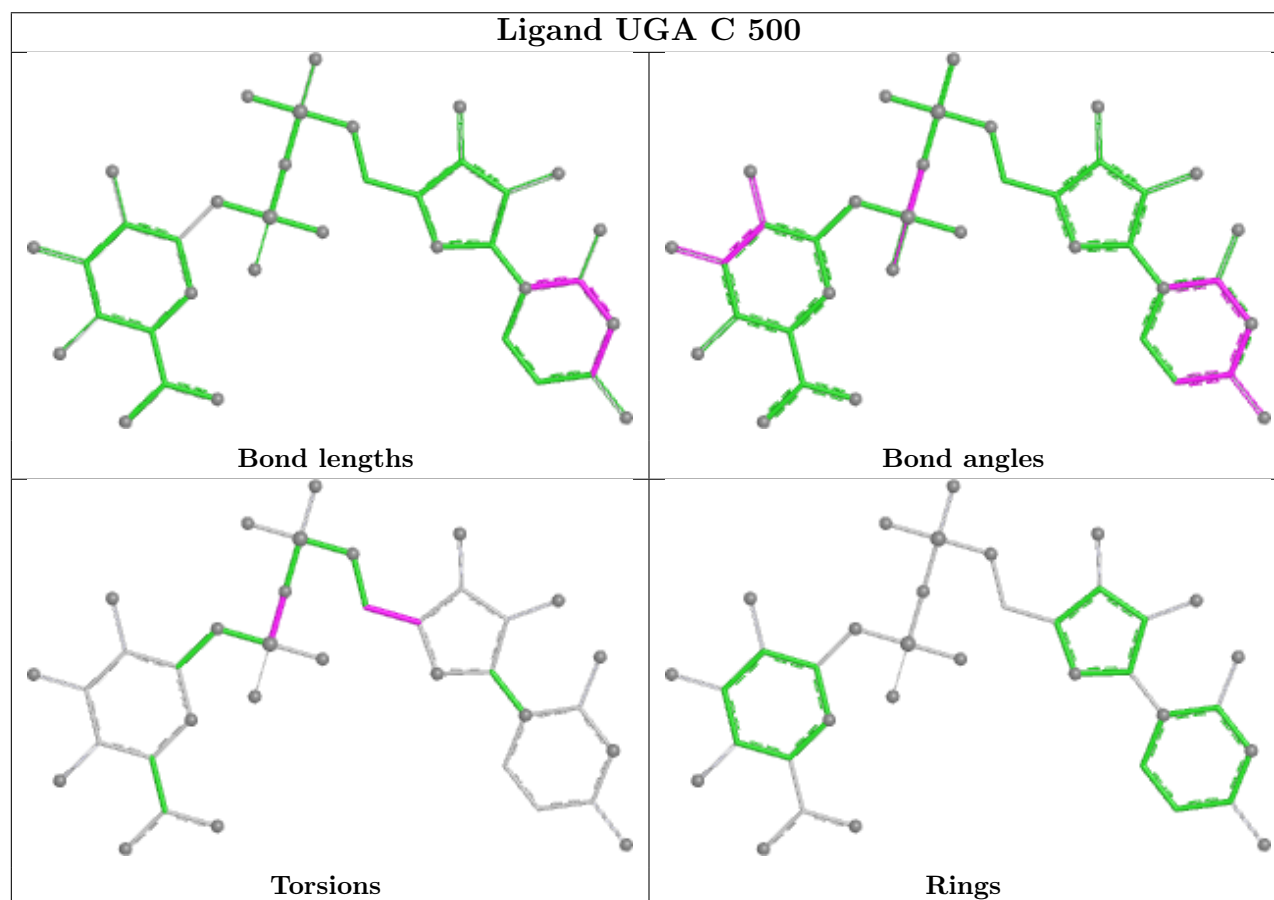
Mol	Chain	Res	Type	Atoms
2	A	500	UGA	C1'-O3B-PB-O3A
2	A	500	UGA	C5D-O5D-PA-O3A
2	A	500	UGA	C5D-O5D-PA-O2A
2	B	500	UGA	C1'-O3B-PB-O2B
2	B	500	UGA	C1'-O3B-PB-O3A
2	D	500	UGA	C5D-O5D-PA-O3A
2	A	500	UGA	C3D-C4D-C5D-O5D
2	A	500	UGA	O4D-C4D-C5D-O5D
2	B	500	UGA	C2'-C1'-O3B-PB
2	C	500	UGA	O4D-C4D-C5D-O5D
2	A	500	UGA	PA-O3A-PB-O3B
2	C	500	UGA	PA-O3A-PB-O3B
2	D	500	UGA	PA-O3A-PB-O3B
2	C	500	UGA	C3D-C4D-C5D-O5D
2	B	500	UGA	PA-O3A-PB-O1B
2	D	500	UGA	PA-O3A-PB-O1B
2	A	500	UGA	C5D-O5D-PA-O1A
2	A	500	UGA	PB-O3A-PA-O1A
2	A	500	UGA	PB-O3A-PA-O2A
2	B	500	UGA	PA-O3A-PB-O3B
2	C	500	UGA	PA-O3A-PB-O1B
2	B	500	UGA	PB-O3A-PA-O2A

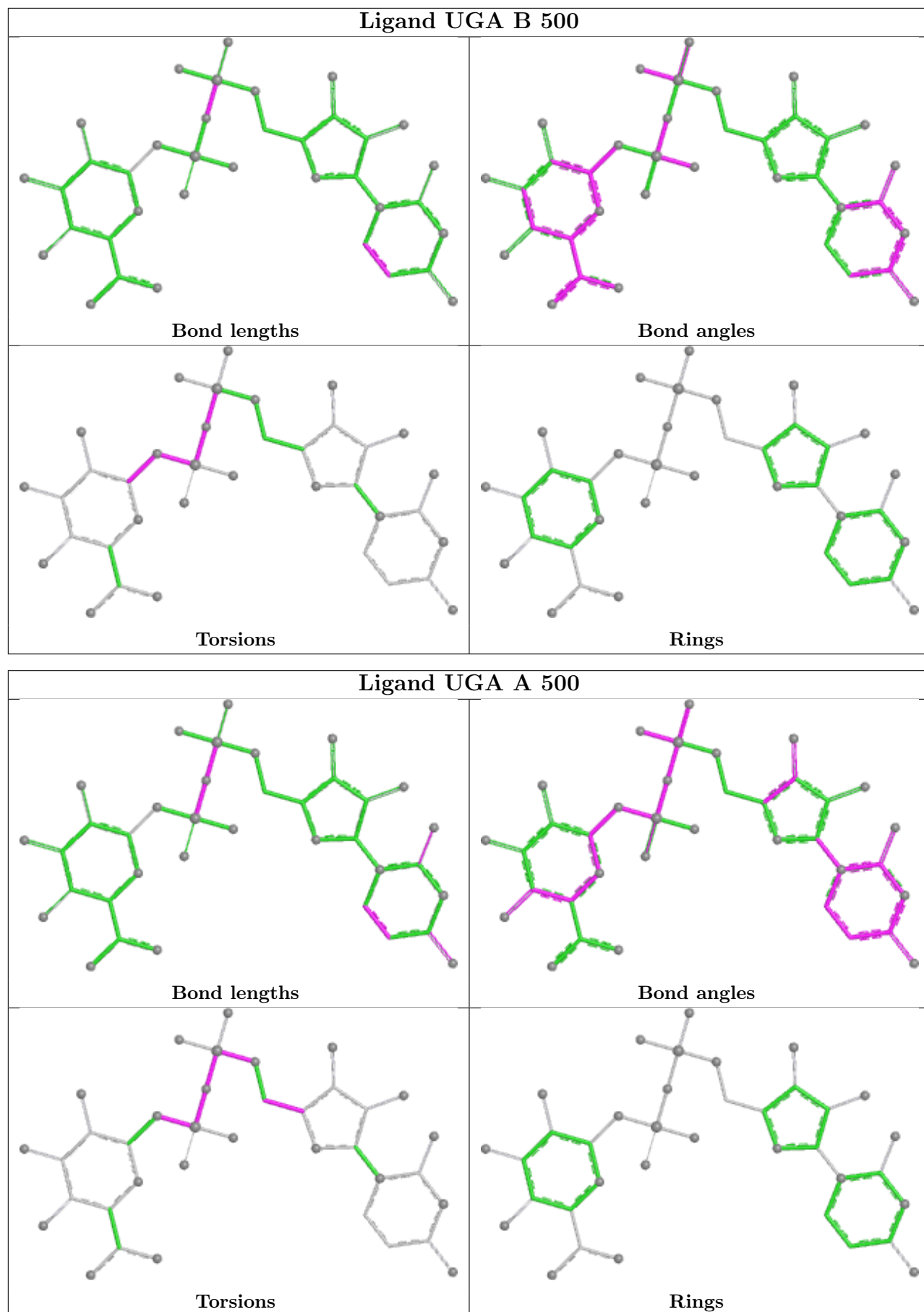
There are no ring outliers.

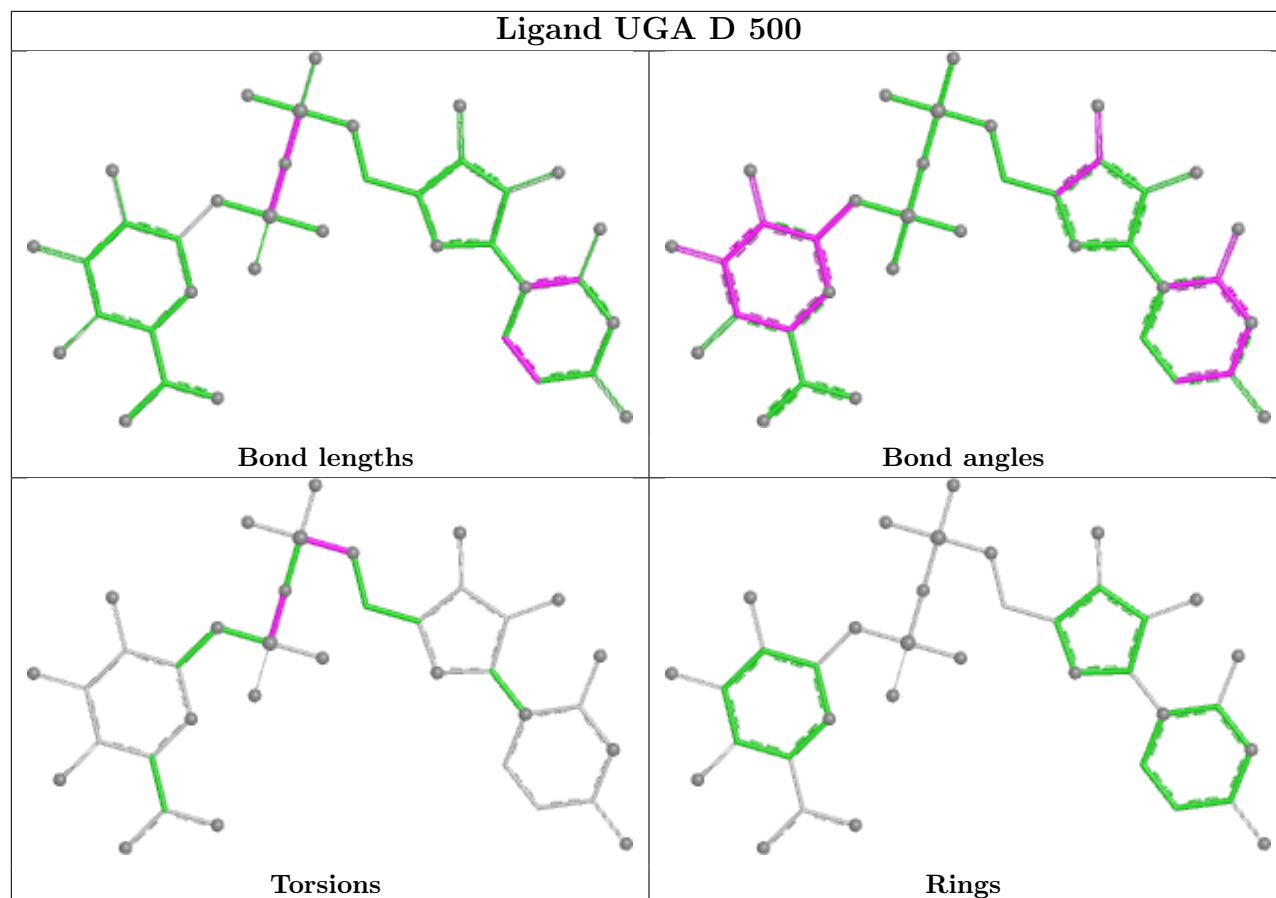
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1456	SO4	2	0
3	C	1455	SO4	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	455/478 (95%)	0.17	30 (6%) 24 18	8, 25, 68, 100	0
1	B	448/478 (93%)	0.23	28 (6%) 26 19	7, 26, 63, 98	0
1	C	451/478 (94%)	0.26	41 (9%) 15 11	7, 25, 64, 118	0
1	D	452/478 (94%)	0.30	34 (7%) 20 15	7, 26, 65, 118	0
All	All	1806/1912 (94%)	0.24	133 (7%) 20 15	7, 26, 67, 118	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	SER	7.5
1	B	198	ASN	6.3
1	A	93	SER	5.7
1	B	93	SER	5.5
1	D	92	GLY	5.1
1	C	437	GLU	4.9
1	C	93	SER	4.9
1	B	143	GLY	4.8
1	D	87	PRO	4.8
1	D	198	ASN	4.6
1	A	199	HIS	4.5
1	D	94	ALA	4.4
1	B	111	THR	4.4
1	B	199	HIS	4.1
1	A	0	SER	4.1
1	A	8	SER	4.1
1	B	87	PRO	4.0
1	C	111	THR	4.0
1	C	198	ASN	3.9
1	A	111	THR	3.9
1	C	199	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	196	ASN	3.8
1	C	139	ALA	3.8
1	B	437	GLU	3.8
1	C	441	GLU	3.8
1	B	94	ALA	3.8
1	B	145	GLN	3.7
1	D	199	HIS	3.7
1	A	87	PRO	3.7
1	C	145	GLN	3.7
1	A	416	VAL	3.6
1	D	25	ASP	3.5
1	C	87	PRO	3.5
1	A	456	GLN	3.5
1	B	453	GLY	3.4
1	A	454	SER	3.4
1	A	198	ASN	3.3
1	A	94	ALA	3.3
1	A	31	VAL	3.3
1	D	112	GLY	3.3
1	C	377	ASP	3.3
1	C	98	TYR	3.2
1	D	142	GLY	3.2
1	D	454	SER	3.2
1	A	144	ASP	3.1
1	C	112	GLY	3.1
1	C	453	GLY	3.0
1	C	197	ARG	3.0
1	C	135	ALA	3.0
1	C	0	SER	3.0
1	B	108	ARG	2.9
1	B	197	ARG	2.9
1	A	90	GLU	2.9
1	A	437	GLU	2.9
1	A	376	ALA	2.9
1	C	134	VAL	2.9
1	A	197	ARG	2.9
1	C	140	LYS	2.9
1	C	143	GLY	2.8
1	D	145	GLN	2.8
1	D	139	ALA	2.8
1	B	200	GLU	2.8
1	B	0	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	140	LYS	2.8
1	C	136	GLU	2.8
1	D	86	THR	2.7
1	D	88	PRO	2.7
1	B	416	VAL	2.7
1	D	35	LYS	2.7
1	A	112	GLY	2.7
1	C	131	ARG	2.7
1	D	108	ARG	2.7
1	A	32	ASP	2.7
1	D	0	SER	2.7
1	B	135	ALA	2.6
1	C	376	ALA	2.6
1	B	142	GLY	2.6
1	B	196	ASN	2.6
1	C	365	GLU	2.6
1	A	133	ALA	2.6
1	C	88	PRO	2.6
1	C	108	ARG	2.6
1	C	141	ARG	2.6
1	B	136	GLU	2.6
1	D	197	ARG	2.5
1	D	77	GLY	2.5
1	A	455	ARG	2.5
1	C	144	ASP	2.5
1	B	134	VAL	2.5
1	D	280	ARG	2.5
1	D	420	ARG	2.5
1	B	77	GLY	2.5
1	A	420	ARG	2.5
1	D	65	ARG	2.4
1	C	137	GLU	2.4
1	C	390	ASP	2.4
1	D	144	ASP	2.4
1	A	247	ARG	2.4
1	A	128	GLU	2.4
1	C	94	ALA	2.4
1	B	138	LEU	2.4
1	A	89	ASP	2.3
1	D	32	ASP	2.3
1	B	71	GLU	2.3
1	D	73	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	390	ASP	2.3
1	A	145	GLN	2.3
1	C	96	LEU	2.3
1	D	131	ARG	2.3
1	B	78	ASP	2.3
1	A	136	GLU	2.2
1	D	97	GLN	2.2
1	D	95	ASP	2.2
1	A	86	THR	2.2
1	D	316	GLU	2.2
1	C	142	GLY	2.1
1	C	284	GLU	2.1
1	C	316	GLU	2.1
1	D	98	TYR	2.1
1	B	441	GLU	2.1
1	C	97	GLN	2.1
1	C	113	PHE	2.1
1	D	71	GLU	2.1
1	C	47	HIS	2.1
1	A	179	VAL	2.1
1	C	86	THR	2.1
1	D	177	ASP	2.1
1	B	139	ALA	2.1
1	C	71	GLU	2.1
1	C	89	ASP	2.0
1	D	196	ASN	2.0
1	B	112	GLY	2.0
1	D	31	VAL	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.

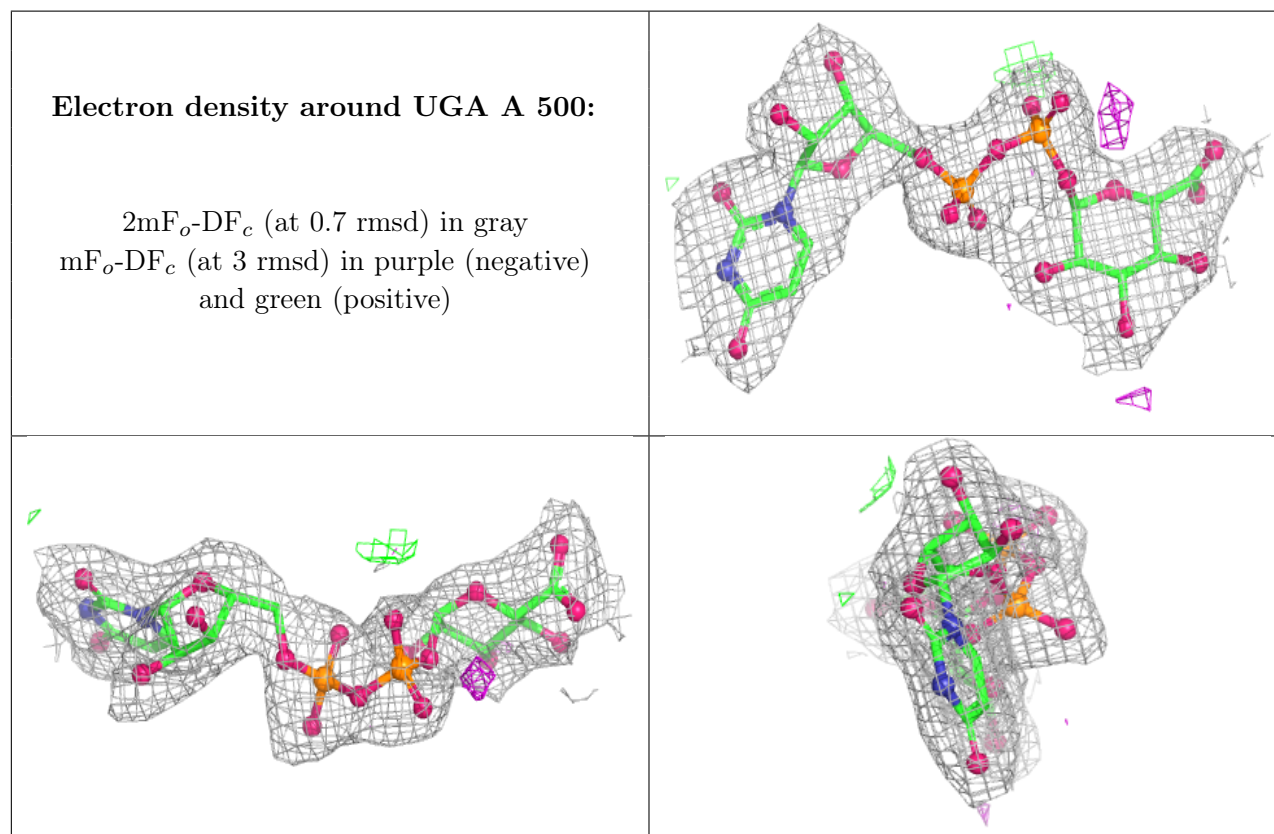
6.4 Ligands [i](#)

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.

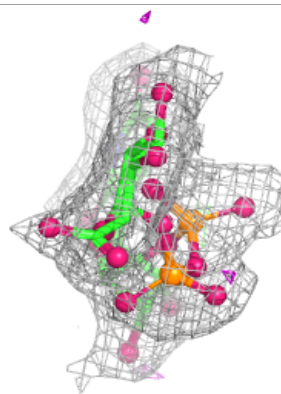
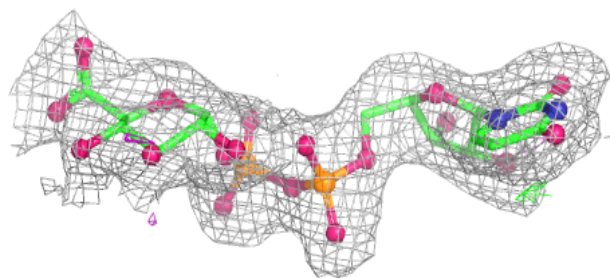
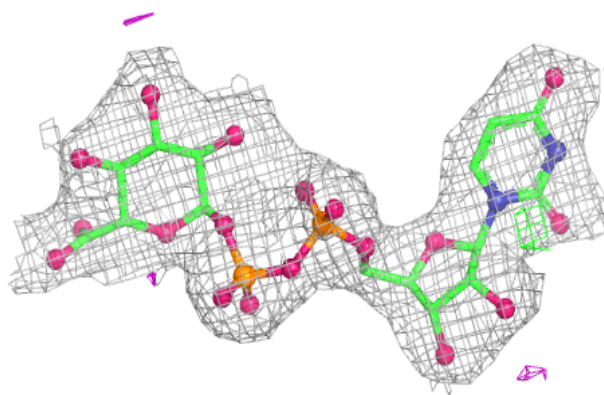
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	1456	5/5	0.84	0.15	69,87,90,97	0
3	SO4	A	1458	5/5	0.87	0.12	68,80,84,94	0
3	SO4	A	1459	5/5	0.88	0.14	37,45,56,71	0
3	SO4	C	1455	5/5	0.91	0.12	27,69,73,95	0
3	SO4	C	1454	5/5	0.95	0.11	30,32,51,63	0
3	SO4	A	1457	5/5	0.95	0.10	35,39,50,53	0
3	SO4	B	1454	5/5	0.95	0.08	30,39,47,49	0
3	SO4	D	1456	5/5	0.96	0.10	29,29,41,48	0
2	UGA	A	500	37/37	0.98	0.06	0,11,25,29	0
2	UGA	B	500	37/37	0.98	0.06	0,12,29,34	0
2	UGA	C	500	37/37	0.98	0.06	0,11,20,23	0
2	UGA	D	500	37/37	0.98	0.06	0,13,24,38	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.

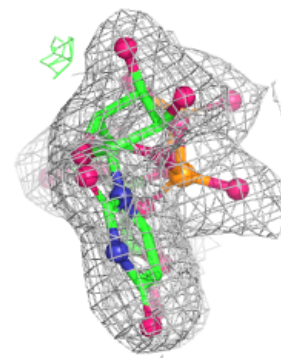
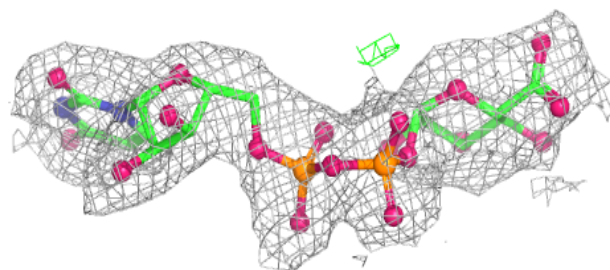
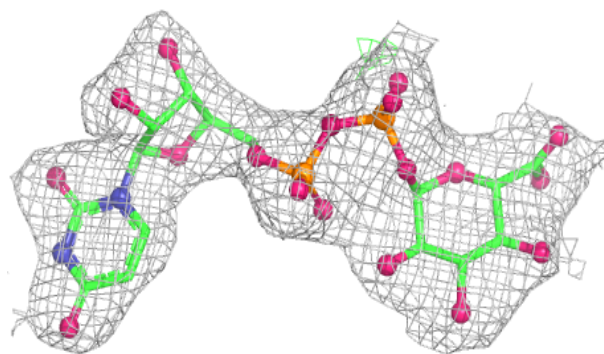


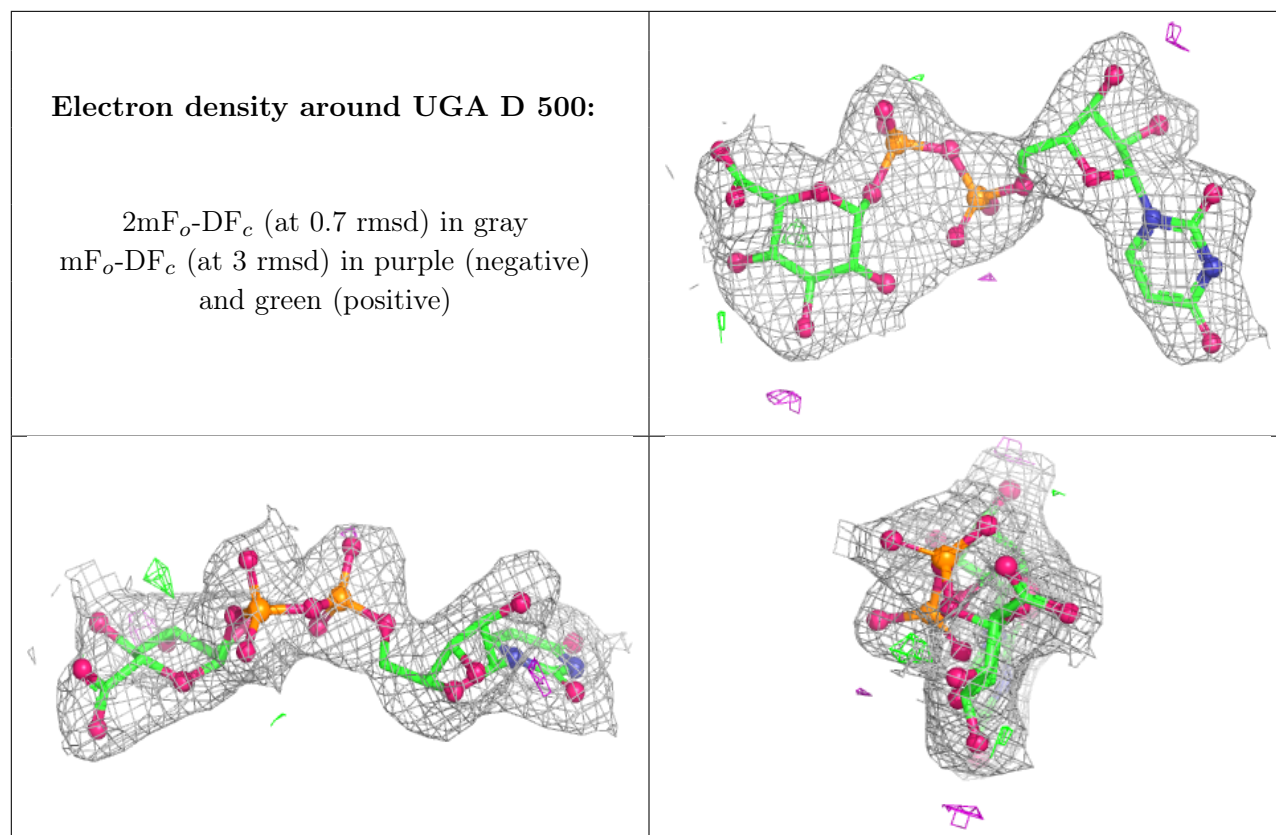
Electron density around UGA B 500:

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

**Electron density around UGA C 500:**

$2mF_o-DF_c$ (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.