



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:39 AM UTC

PDB ID : 6R2E / pdb_00006r2e
Title : Crystal structure of the human thymidylate synthase (hTS) interface variant Q62R
Authors : Pozzi, C.; Mangani, M.
Deposited on : 2019-03-16
Resolution : 2.55 Å(reported)

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

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<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

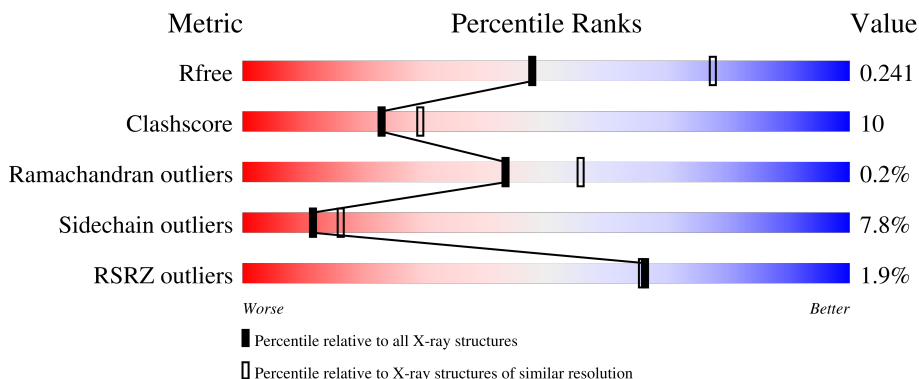
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	325	2% 64% 19% 5% 11%
1	B	325	2% 63% 20% 5% 11%
1	C	325	% 72% 14% • 11%
1	D	325	2% 65% 19% • 11%
1	F	325	2% 66% 19% • • 11%

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Mol	Chain	Length	Quality of chain
1	H	325	
2	E	325	
2	G	325	

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	A	401	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21357 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2312	1478	403	416	15			
1	C	288	Total	C	N	O	S	0	0	0
			2313	1478	401	419	15			
1	D	288	Total	C	N	O	S	0	1	0
			2329	1488	404	422	15			
1	B	289	Total	C	N	O	S	0	0	0
			2323	1486	406	416	15			
1	F	288	Total	C	N	O	S	0	0	0
			2323	1485	403	420	15			
1	H	288	Total	C	N	O	S	0	0	0
			2320	1484	403	418	15			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P04818
A	-10	ARG	-	expression tag	UNP P04818
A	-9	GLY	-	expression tag	UNP P04818
A	-8	SER	-	expression tag	UNP P04818
A	-7	HIS	-	expression tag	UNP P04818
A	-6	HIS	-	expression tag	UNP P04818
A	-5	HIS	-	expression tag	UNP P04818
A	-4	HIS	-	expression tag	UNP P04818
A	-3	HIS	-	expression tag	UNP P04818
A	-2	HIS	-	expression tag	UNP P04818
A	-1	GLY	-	expression tag	UNP P04818
A	0	SER	-	expression tag	UNP P04818
A	62	ARG	GLN	engineered mutation	UNP P04818
C	-11	MET	-	initiating methionine	UNP P04818
C	-10	ARG	-	expression tag	UNP P04818
C	-9	GLY	-	expression tag	UNP P04818
C	-8	SER	-	expression tag	UNP P04818

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	HIS	-	expression tag	UNP P04818
C	-6	HIS	-	expression tag	UNP P04818
C	-5	HIS	-	expression tag	UNP P04818
C	-4	HIS	-	expression tag	UNP P04818
C	-3	HIS	-	expression tag	UNP P04818
C	-2	HIS	-	expression tag	UNP P04818
C	-1	GLY	-	expression tag	UNP P04818
C	0	SER	-	expression tag	UNP P04818
C	62	ARG	GLN	engineered mutation	UNP P04818
D	-11	MET	-	initiating methionine	UNP P04818
D	-10	ARG	-	expression tag	UNP P04818
D	-9	GLY	-	expression tag	UNP P04818
D	-8	SER	-	expression tag	UNP P04818
D	-7	HIS	-	expression tag	UNP P04818
D	-6	HIS	-	expression tag	UNP P04818
D	-5	HIS	-	expression tag	UNP P04818
D	-4	HIS	-	expression tag	UNP P04818
D	-3	HIS	-	expression tag	UNP P04818
D	-2	HIS	-	expression tag	UNP P04818
D	-1	GLY	-	expression tag	UNP P04818
D	0	SER	-	expression tag	UNP P04818
D	62	ARG	GLN	engineered mutation	UNP P04818
B	-11	MET	-	initiating methionine	UNP P04818
B	-10	ARG	-	expression tag	UNP P04818
B	-9	GLY	-	expression tag	UNP P04818
B	-8	SER	-	expression tag	UNP P04818
B	-7	HIS	-	expression tag	UNP P04818
B	-6	HIS	-	expression tag	UNP P04818
B	-5	HIS	-	expression tag	UNP P04818
B	-4	HIS	-	expression tag	UNP P04818
B	-3	HIS	-	expression tag	UNP P04818
B	-2	HIS	-	expression tag	UNP P04818
B	-1	GLY	-	expression tag	UNP P04818
B	0	SER	-	expression tag	UNP P04818
B	62	ARG	GLN	engineered mutation	UNP P04818
F	-11	MET	-	initiating methionine	UNP P04818
F	-10	ARG	-	expression tag	UNP P04818
F	-9	GLY	-	expression tag	UNP P04818
F	-8	SER	-	expression tag	UNP P04818
F	-7	HIS	-	expression tag	UNP P04818
F	-6	HIS	-	expression tag	UNP P04818
F	-5	HIS	-	expression tag	UNP P04818

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	HIS	-	expression tag	UNP P04818
F	-3	HIS	-	expression tag	UNP P04818
F	-2	HIS	-	expression tag	UNP P04818
F	-1	GLY	-	expression tag	UNP P04818
F	0	SER	-	expression tag	UNP P04818
F	62	ARG	GLN	engineered mutation	UNP P04818
H	-11	MET	-	initiating methionine	UNP P04818
H	-10	ARG	-	expression tag	UNP P04818
H	-9	GLY	-	expression tag	UNP P04818
H	-8	SER	-	expression tag	UNP P04818
H	-7	HIS	-	expression tag	UNP P04818
H	-6	HIS	-	expression tag	UNP P04818
H	-5	HIS	-	expression tag	UNP P04818
H	-4	HIS	-	expression tag	UNP P04818
H	-3	HIS	-	expression tag	UNP P04818
H	-2	HIS	-	expression tag	UNP P04818
H	-1	GLY	-	expression tag	UNP P04818
H	0	SER	-	expression tag	UNP P04818
H	62	ARG	GLN	engineered mutation	UNP P04818

- Molecule 2 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	288	Total	C	N	O	S	0	0	0
			2321	1486	403	417	15			
2	G	288	Total	C	N	O	S	0	0	0
			2309	1478	399	417	15			

There are 26 discrepancies between the modelled and reference sequences:

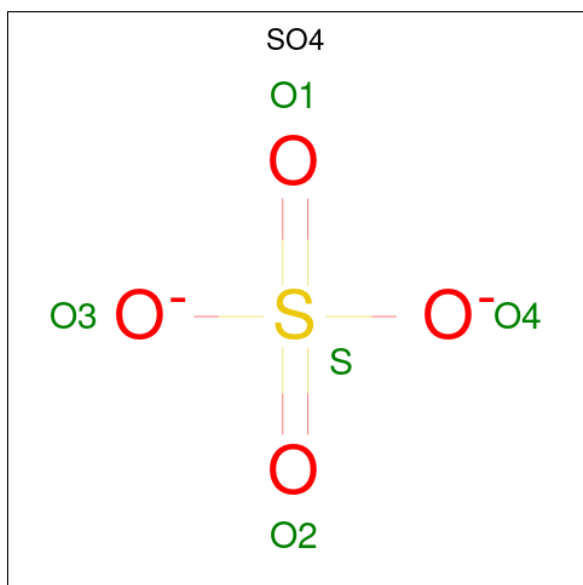
Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	MET	-	initiating methionine	UNP P04818
E	-10	ARG	-	expression tag	UNP P04818
E	-9	GLY	-	expression tag	UNP P04818
E	-8	SER	-	expression tag	UNP P04818
E	-7	HIS	-	expression tag	UNP P04818
E	-6	HIS	-	expression tag	UNP P04818
E	-5	HIS	-	expression tag	UNP P04818
E	-4	HIS	-	expression tag	UNP P04818
E	-3	HIS	-	expression tag	UNP P04818
E	-2	HIS	-	expression tag	UNP P04818
E	-1	GLY	-	expression tag	UNP P04818

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	UNP P04818
E	62	ARG	GLN	engineered mutation	UNP P04818
G	-11	MET	-	initiating methionine	UNP P04818
G	-10	ARG	-	expression tag	UNP P04818
G	-9	GLY	-	expression tag	UNP P04818
G	-8	SER	-	expression tag	UNP P04818
G	-7	HIS	-	expression tag	UNP P04818
G	-6	HIS	-	expression tag	UNP P04818
G	-5	HIS	-	expression tag	UNP P04818
G	-4	HIS	-	expression tag	UNP P04818
G	-3	HIS	-	expression tag	UNP P04818
G	-2	HIS	-	expression tag	UNP P04818
G	-1	GLY	-	expression tag	UNP P04818
G	0	SER	-	expression tag	UNP P04818
G	62	ARG	GLN	engineered mutation	UNP P04818

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



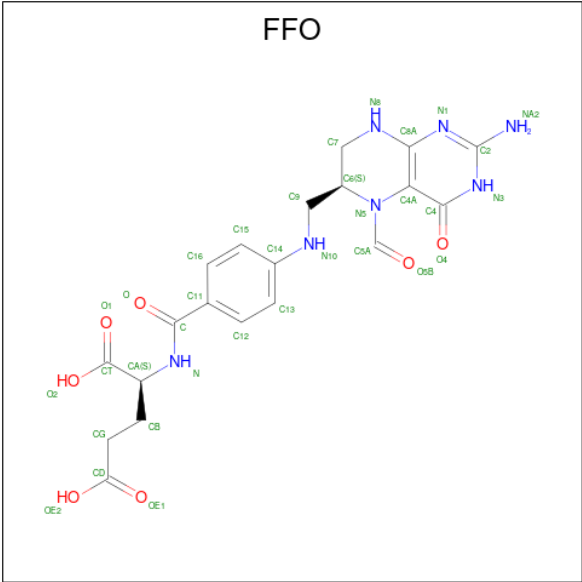
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (CCD ID: FFO) (formula: C₂₀H₂₃N₇O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			34	20	7	7		
4	C	1	Total	C	N	O	0	0
			34	20	7	7		
4	D	1	Total	C	N	O	0	0
			34	20	7	7		
4	B	1	Total	C	N	O	0	0
			34	20	7	7		
4	F	1	Total	C	N	O	0	0
			34	20	7	7		
4	H	1	Total	C	N	O	0	0
			34	20	7	7		
4	E	1	Total	C	N	O	0	0
			34	20	7	7		
4	G	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

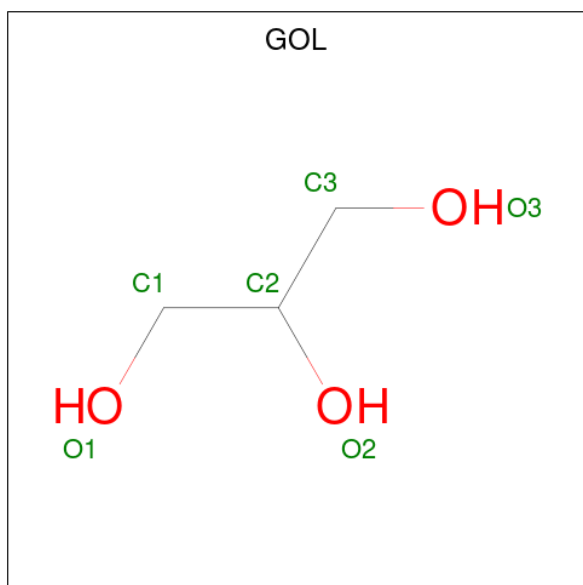
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	C	1	Total	Cl	0	0
			1	1		
5	D	2	Total	Cl	0	0
			2	2		
5	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 6 3 3	0	0
6	H	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	334	Total O 334 334	0	0
7	C	318	Total O 318 318	0	0
7	D	319	Total O 319 319	0	0
7	B	302	Total O 302 302	0	0
7	F	330	Total O 330 330	0	0

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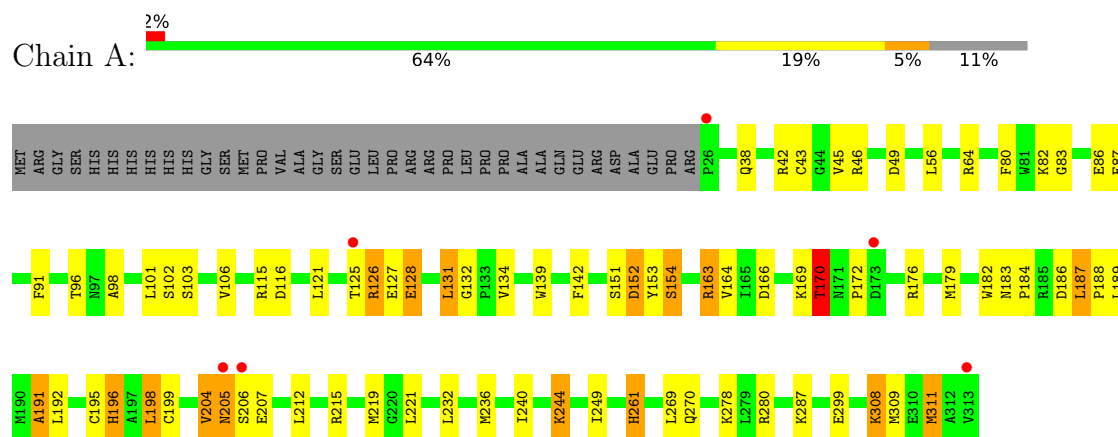
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	277	Total 277	O 277	0	0
7	E	311	Total 311	O 311	0	0
7	G	239	Total 239	O 239	0	0

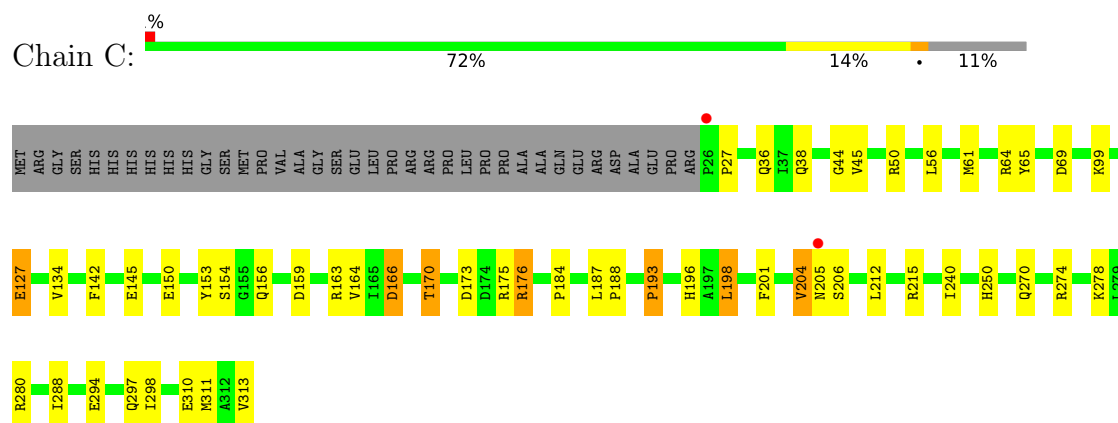
3 Residue-property plots [i](#)

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.

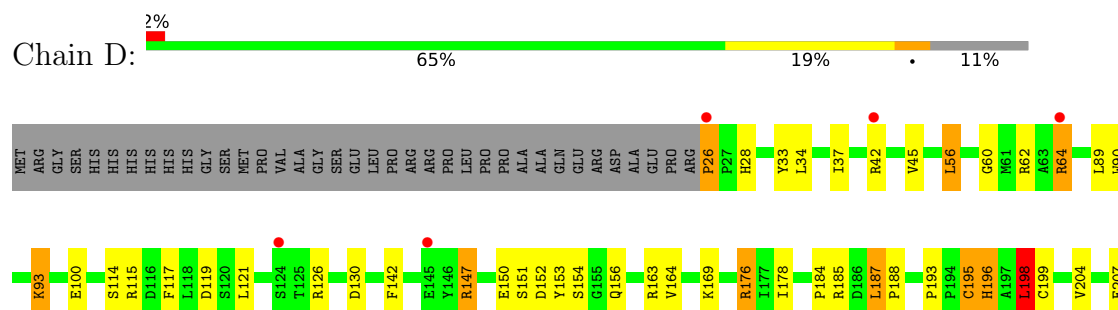
- Molecule 1: Thymidylate synthase

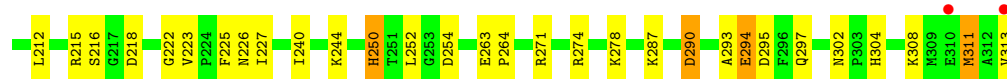


- Molecule 1: Thymidylate synthase

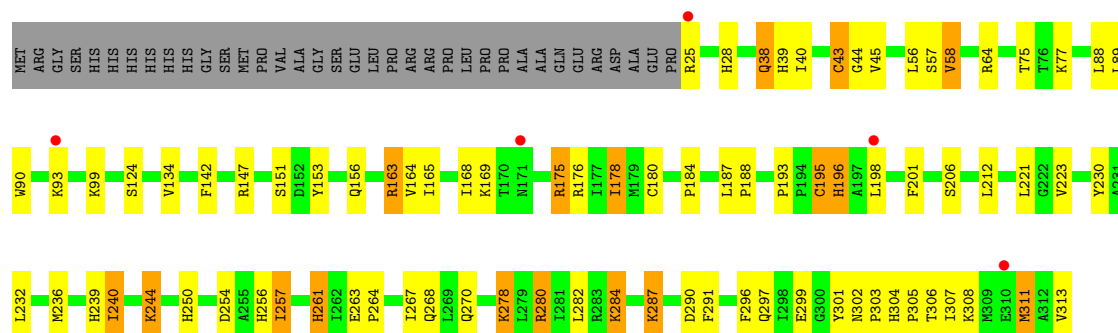


- Molecule 1: Thymidylate synthase

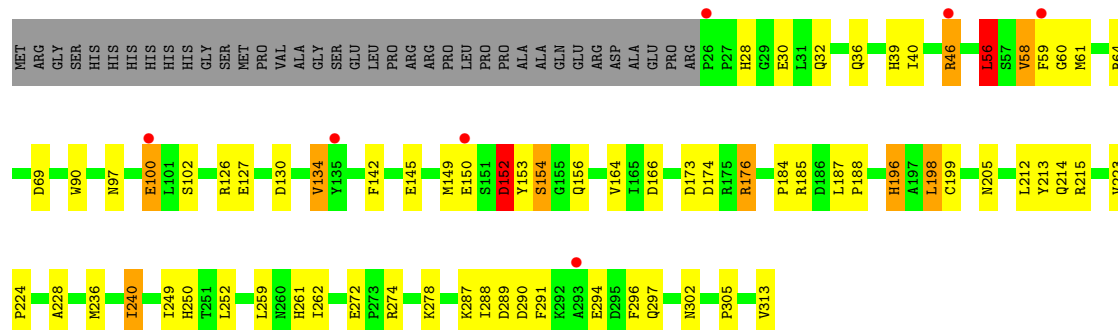




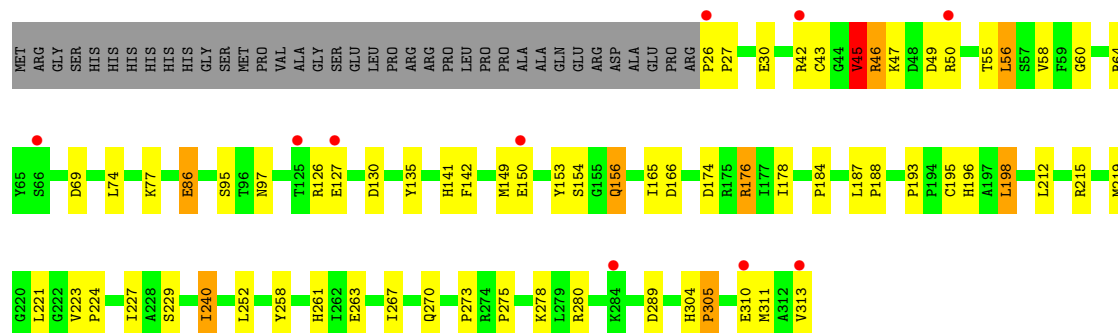
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase

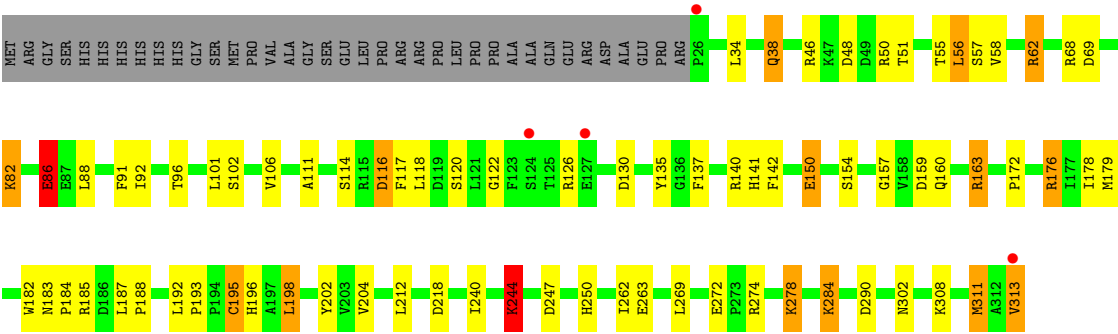


• Molecule 1: Thymidylate synthase

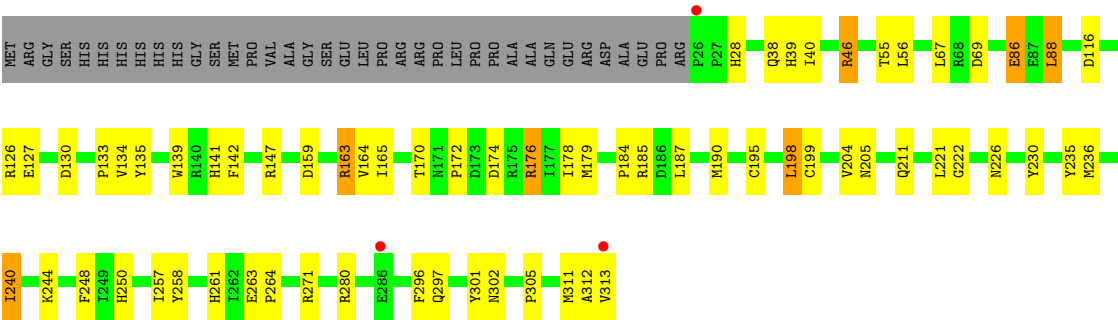


• Molecule 2: Thymidylate synthase





● Molecule 2: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.94Å 167.07Å 189.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.99 – 2.55 94.99 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (94.99-2.55) 99.8 (94.99-2.55)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.196 , 0.258 (Not available) , 0.241	Depositor DCC
R_{free} test set	7182 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21357	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6289e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, CME, SCH, SO4, FFO, GOL

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	0.84	1/2350 (0.0%)	1.43	24/3178 (0.8%)
1	B	0.90	2/2361 (0.1%)	1.47	16/3192 (0.5%)
1	C	0.86	1/2351 (0.0%)	1.41	14/3180 (0.4%)
1	D	0.86	3/2370 (0.1%)	1.40	10/3203 (0.3%)
1	F	0.91	2/2361 (0.1%)	1.43	17/3191 (0.5%)
1	H	0.84	0/2358	1.45	13/3187 (0.4%)
2	E	0.85	0/2361	1.45	22/3189 (0.7%)
2	G	0.83	3/2349 (0.1%)	1.40	8/3177 (0.3%)
All	All	0.86	12/18861 (0.1%)	1.43	124/25497 (0.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	HIS	CE1-NE2	7.24	1.39	1.32
1	F	250	HIS	CE1-NE2	6.01	1.38	1.32
1	C	250	HIS	CE1-NE2	5.97	1.38	1.32
1	F	261	HIS	CE1-NE2	5.85	1.38	1.32
1	D	28	HIS	CE1-NE2	5.82	1.38	1.32
2	G	250	HIS	CE1-NE2	5.64	1.38	1.32
1	A	261	HIS	CE1-NE2	5.60	1.38	1.32
1	D	250	HIS	CE1-NE2	5.57	1.38	1.32
2	G	28	HIS	CE1-NE2	5.44	1.38	1.32
2	G	39	HIS	CE1-NE2	5.28	1.37	1.32
1	B	250	HIS	CE1-NE2	5.20	1.37	1.32
1	D	187	LEU	C-O	-5.01	1.20	1.24

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	275	PRO	CB-CA-C	-8.75	100.52	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	116	ASP	CA-CB-CG	-8.61	103.99	112.60
1	C	193	PRO	N-CA-CB	7.94	107.35	103.22
2	E	86	GLU	CB-CG-CD	7.87	125.97	112.60
2	G	86	GLU	CB-CG-CD	7.69	125.67	112.60
1	F	196	HIS	CA-C-N	7.55	130.71	120.44
1	F	196	HIS	C-N-CA	7.55	130.71	120.44
1	C	127	GLU	CB-CG-CD	7.25	124.92	112.60
1	H	86	GLU	CB-CG-CD	6.95	124.42	112.60
1	A	91	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	219	MET	CA-C-N	6.86	127.42	119.94
1	A	219	MET	C-N-CA	6.86	127.42	119.94
1	C	170	THR	CA-C-N	-6.71	115.14	122.59
1	C	170	THR	C-N-CA	-6.71	115.14	122.59
2	E	290	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	188	PRO	CB-CA-C	-6.57	101.52	111.44
2	E	247	ASP	CA-CB-CG	-6.44	106.16	112.60
1	A	191	ALA	N-CA-C	-6.34	104.36	111.28
1	H	219	MET	CA-C-N	6.34	126.98	119.94
1	H	219	MET	C-N-CA	6.34	126.98	119.94
1	C	294	GLU	CB-CG-CD	6.27	123.27	112.60
2	E	172	PRO	CA-C-N	6.20	129.73	120.31
2	E	172	PRO	C-N-CA	6.20	129.73	120.31
1	B	306	THR	CB-CA-C	-6.12	99.85	109.70
1	A	308	LYS	CB-CA-C	6.11	118.95	110.16
1	F	294	GLU	CB-CG-CD	6.05	122.88	112.60
1	B	296	PHE	CA-CB-CG	-6.01	107.79	113.80
1	B	297	GLN	CB-CG-CD	-5.99	102.42	112.60
2	E	48	ASP	CA-C-N	-5.96	112.41	123.01
2	E	48	ASP	C-N-CA	-5.96	112.41	123.01
1	B	28	HIS	CA-CB-CG	-5.95	107.85	113.80
2	E	101	LEU	CA-C-N	5.93	128.50	120.38
2	E	101	LEU	C-N-CA	5.93	128.50	120.38
1	C	173	ASP	CA-C-N	5.93	129.25	120.90
1	C	173	ASP	C-N-CA	5.93	129.25	120.90
1	A	46	ARG	CB-CA-C	5.86	119.05	110.26
1	C	153	TYR	CB-CA-C	-5.81	102.10	111.28
1	B	230	TYR	CB-CA-C	5.79	120.40	110.79
1	F	56	LEU	CA-C-N	-5.78	112.39	121.87
1	F	56	LEU	C-N-CA	-5.78	112.39	121.87
2	E	274	ARG	CB-CA-C	5.78	117.81	109.09
1	H	45	VAL	CB-CA-C	-5.77	103.32	111.28
2	G	302	ASN	CB-CA-C	-5.76	102.80	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	HIS	CA-C-N	-5.73	113.27	121.52
1	B	239	HIS	C-N-CA	-5.73	113.27	121.52
1	C	201	PHE	CA-CB-CG	-5.70	108.10	113.80
1	C	27	PRO	CB-CA-C	5.70	118.44	110.98
1	A	170	THR	CB-CA-C	5.69	118.95	109.56
1	H	156	GLN	CB-CG-CD	-5.68	102.94	112.60
1	A	115	ARG	CB-CA-C	5.68	120.16	110.74
2	G	205	ASN	CA-CB-CG	5.66	118.26	112.60
1	H	227	ILE	N-CA-CB	5.65	117.17	110.55
1	A	170	THR	CA-C-N	-5.64	116.64	122.85
1	A	170	THR	C-N-CA	-5.64	116.64	122.85
1	D	34	LEU	CA-C-N	5.63	126.34	120.03
1	D	34	LEU	C-N-CA	5.63	126.34	120.03
1	A	244	LYS	CB-CA-C	5.62	116.50	108.68
1	F	228	ALA	CA-C-N	5.62	127.75	120.44
1	F	228	ALA	C-N-CA	5.62	127.75	120.44
1	A	127	GLU	CB-CG-CD	5.58	122.08	112.60
2	E	244	LYS	CB-CA-C	5.56	116.41	108.68
1	F	134	VAL	CA-C-N	5.55	130.02	121.19
1	F	134	VAL	C-N-CA	5.55	130.02	121.19
2	E	150	GLU	CB-CG-CD	5.55	122.03	112.60
1	D	115	ARG	CB-CA-C	5.52	119.64	110.81
1	B	201	PHE	CB-CA-C	5.46	119.55	109.71
2	E	91	PHE	CA-CB-CG	5.46	119.26	113.80
1	D	295	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	25	ARG	CA-C-N	5.45	123.59	119.66
1	B	25	ARG	C-N-CA	5.45	123.59	119.66
1	H	150	GLU	CB-CA-C	5.43	119.17	109.29
1	F	166	ASP	CB-CA-C	5.41	119.77	110.79
2	E	82	LYS	CA-C-N	5.40	126.09	119.99
2	E	82	LYS	C-N-CA	5.40	126.09	119.99
1	F	90	TRP	CA-C-O	-5.39	114.83	120.55
1	H	154	SER	N-CA-CB	5.39	117.97	109.83
1	B	305	PRO	N-CA-C	5.37	119.75	111.21
1	A	152	ASP	CB-CA-C	5.37	119.37	110.78
2	E	263	GLU	CB-CG-CD	5.37	121.72	112.60
1	A	205	ASN	CB-CA-C	-5.35	109.95	117.23
1	A	128	GLU	CB-CA-C	5.35	117.86	110.16
1	B	257	ILE	N-CA-CB	-5.34	104.96	111.21
1	B	57	SER	N-CA-C	5.34	117.30	109.24
1	F	152	ASP	CB-CA-C	5.33	119.01	110.16
1	B	223	VAL	N-CA-CB	5.32	113.85	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	119	ASP	CA-CB-CG	5.30	117.90	112.60
2	G	172	PRO	N-CA-C	5.30	120.81	113.98
1	A	169	LYS	CA-C-N	-5.29	112.37	122.53
1	A	169	LYS	C-N-CA	-5.29	112.37	122.53
2	E	150	GLU	CB-CA-C	5.28	118.91	110.09
2	G	226	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	308	LYS	CB-CA-C	5.26	118.51	109.51
1	C	127	GLU	CB-CA-C	5.24	118.99	109.62
1	H	49	ASP	CA-CB-CG	5.24	117.83	112.60
1	F	290	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	50	ARG	CB-CG-CD	5.22	123.31	111.30
1	F	205	ASN	CB-CA-C	5.20	119.27	111.89
1	A	163	ARG	CB-CA-C	5.19	119.68	110.85
2	E	192	LEU	O-C-N	-5.18	116.77	122.06
1	A	196	HIS	CB-CA-C	5.15	119.89	110.10
1	D	198	LEU	N-CA-CB	-5.15	101.87	110.99
1	F	32	GLN	CB-CG-CD	-5.15	103.85	112.60
1	A	126	ARG	CB-CA-C	-5.14	100.43	109.62
1	A	188	PRO	CB-CA-C	-5.14	104.56	111.85
1	B	299	GLU	CB-CA-C	5.13	118.99	109.70
1	D	26	PRO	CA-N-CD	-5.09	104.88	112.00
2	G	174	ASP	CA-CB-CG	5.08	117.68	112.60
2	E	183	ASN	CB-CA-C	5.07	115.92	110.65
1	A	101	LEU	CA-C-N	5.04	127.29	120.38
1	A	101	LEU	C-N-CA	5.04	127.29	120.38
1	D	290	ASP	CA-CB-CG	5.04	117.64	112.60
1	F	305	PRO	CA-C-N	5.04	128.81	121.31
1	F	305	PRO	C-N-CA	5.04	128.81	121.31
2	E	34	LEU	CA-C-N	5.04	125.57	119.98
2	E	34	LEU	C-N-CA	5.04	125.57	119.98
1	H	267	ILE	O-C-N	5.02	126.83	121.91
1	A	172	PRO	CB-CA-C	5.01	118.97	111.85
1	H	305	PRO	CA-C-N	5.01	128.22	121.05
1	H	305	PRO	C-N-CA	5.01	128.22	121.05
1	D	293	ALA	CA-C-N	5.00	128.69	120.63
1	D	293	ALA	C-N-CA	5.00	128.69	120.63
2	G	305	PRO	CA-C-N	5.00	127.87	120.82
2	G	305	PRO	C-N-CA	5.00	127.87	120.82

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	2312	0	2263	48	0
1	B	2323	0	2281	66	0
1	C	2313	0	2256	37	0
1	D	2329	0	2286	56	0
1	F	2323	0	2277	54	0
1	H	2320	0	2275	59	0
2	E	2321	0	2286	55	0
2	G	2309	0	2253	49	0
3	A	10	0	0	2	0
3	B	10	0	0	1	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	10	0	0	0	0
3	H	10	0	0	1	0
4	A	34	0	21	4	0
4	B	34	0	21	7	0
4	C	34	0	21	5	0
4	D	34	0	21	3	0
4	E	34	0	21	6	0
4	F	34	0	21	0	0
4	G	34	0	21	2	0
4	H	34	0	21	2	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	D	6	0	8	0	0
6	H	6	0	8	0	0
7	A	334	0	0	5	0
7	B	302	0	0	9	0
7	C	318	0	0	6	0
7	D	319	0	0	6	0
7	E	311	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	330	0	0	4	0
7	G	239	0	0	8	0
7	H	277	0	0	11	0
All	All	21357	0	18361	387	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (387) 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:26:PRO:HB2	1:H:27:PRO:CD	1.50	1.31
1:C:311:MET:HE3	4:C:404:FFO:H15	1.29	1.14
1:H:215:ARG:NH1	2:G:176:ARG:HG3	1.62	1.14
1:H:26:PRO:CB	1:H:27:PRO:CD	2.26	1.12
1:H:26:PRO:CB	1:H:27:PRO:HD3	1.82	1.10
1:A:215:ARG:NH1	1:B:176:ARG:HG3	1.69	1.08
1:H:26:PRO:HB2	1:H:27:PRO:HD2	1.30	1.07
2:E:195:CME:HZ3	2:E:218:ASP:HB2	1.36	1.05
1:A:221:LEU:HB3	7:A:584:HOH:O	1.59	1.01
1:B:280:ARG:HH11	1:B:280:ARG:HG2	1.24	1.00
2:G:185:ARG:HD2	7:G:503:HOH:O	1.64	0.98
2:E:311:MET:CE	4:E:403:FFO:H15	1.96	0.96
1:D:195:CME:HZ3	1:D:218:ASP:HB2	1.50	0.92
1:H:26:PRO:HB2	1:H:27:PRO:HD3	1.42	0.92
1:A:184:PRO:HD2	1:B:142:PHE:CE1	2.04	0.92
1:A:311:MET:HE3	4:A:403:FFO:H15	1.54	0.89
2:E:311:MET:HE3	4:E:403:FFO:H15	1.56	0.88
1:F:39:HIS:HD2	1:F:61:MET:HE1	1.38	0.87
1:F:46:ARG:HH21	1:F:46:ARG:HG3	1.40	0.87
1:B:38:GLN:HG3	7:B:645:HOH:O	1.76	0.85
1:F:39:HIS:CD2	1:F:61:MET:HE1	2.11	0.85
1:D:90:TRP:HA	1:D:93:LYS:HD2	1.59	0.84
1:H:153:TYR:O	1:H:156:GLN:HB2	1.77	0.83
1:C:310:GLU:HB3	7:C:732:HOH:O	1.78	0.82
1:B:280:ARG:HH11	1:B:280:ARG:CG	1.91	0.82
1:A:311:MET:HE2	4:A:403:FFO:N1	1.96	0.80
1:D:263:GLU:HB2	1:D:264:PRO:HD3	1.63	0.80
1:A:215:ARG:NH1	1:B:176:ARG:CG	2.43	0.80
1:F:39:HIS:CD2	1:F:61:MET:CE	2.65	0.78
1:H:26:PRO:HB3	1:H:27:PRO:HD3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLU:HG2	7:D:630:HOH:O	1.84	0.77
1:D:89:LEU:O	1:D:93:LYS:HG2	1.84	0.77
1:F:153:TYR:O	1:F:156:GLN:HB2	1.85	0.77
1:C:215:ARG:NH1	1:D:176:ARG:HG3	1.99	0.77
1:F:198:LEU:C	1:F:198:LEU:HD12	2.10	0.77
1:C:163:ARG:HB3	1:C:163:ARG:NH1	2.00	0.76
1:B:287:LYS:HD3	7:B:686:HOH:O	1.85	0.76
1:C:311:MET:HE2	4:C:404:FFO:N1	2.00	0.76
1:H:198:LEU:C	1:H:198:LEU:HD12	2.11	0.76
1:F:236:MET:HE2	1:F:296:PHE:CZ	2.20	0.75
2:G:198:LEU:C	2:G:198:LEU:HD12	2.12	0.74
1:B:39:HIS:O	1:B:43:CME:HB3	1.89	0.73
1:F:39:HIS:HD2	1:F:61:MET:CE	2.02	0.73
1:A:192:LEU:HD23	7:A:657:HOH:O	1.89	0.72
2:E:311:MET:HE3	4:E:403:FFO:C15	2.19	0.72
1:B:40:ILE:HG21	1:B:257:ILE:HG13	1.72	0.71
1:C:145:GLU:OE2	1:C:145:GLU:HA	1.90	0.71
2:G:163:ARG:HH11	2:G:163:ARG:HB3	1.56	0.71
1:C:44:GLY:O	2:G:46:ARG:NH1	2.24	0.71
1:H:30:GLU:HG3	1:H:74:LEU:HD22	1.73	0.70
2:E:195:CME:HZ3	2:E:218:ASP:CB	2.17	0.70
1:C:187:LEU:HD22	1:C:193:PRO:HB3	1.74	0.70
1:C:311:MET:HE3	4:C:404:FFO:C15	2.14	0.70
1:B:147:ARG:NH2	1:B:156:GLN:HE22	1.89	0.70
1:H:270:GLN:HG2	7:H:640:HOH:O	1.91	0.70
1:B:180:CYS:HB2	1:B:198:LEU:HD12	1.74	0.70
1:A:198:LEU:CD1	1:A:198:LEU:C	2.65	0.70
1:H:215:ARG:HH12	2:G:176:ARG:HG3	1.53	0.70
1:C:166:ASP:O	1:C:170:THR:HG23	1.92	0.70
1:H:126:ARG:HG2	1:H:130:ASP:HB3	1.74	0.70
1:H:97:ASN:ND2	1:H:149:MET:HE3	2.07	0.69
2:E:311:MET:HE2	4:E:403:FFO:H15	1.75	0.69
1:B:236:MET:HB3	1:B:291:PHE:CE2	2.27	0.68
1:A:184:PRO:HD2	1:B:142:PHE:CZ	2.28	0.68
1:B:164:VAL:O	1:B:168:ILE:HG13	1.93	0.68
1:B:257:ILE:HA	7:B:537:HOH:O	1.94	0.67
1:F:215:ARG:HB2	2:E:178:ILE:HD11	1.76	0.67
1:C:196:HIS:HB2	1:C:212:LEU:HD11	1.75	0.66
1:B:163:ARG:NH1	7:B:501:HOH:O	2.27	0.66
2:E:196:HIS:HB2	2:E:212:LEU:HD11	1.76	0.66
1:F:198:LEU:C	1:F:198:LEU:CD1	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HH12	1:B:176:ARG:HG3	1.55	0.66
1:B:64:ARG:HD2	7:B:661:HOH:O	1.95	0.66
1:B:280:ARG:HG2	1:B:280:ARG:NH1	1.99	0.65
1:F:215:ARG:NH1	2:E:176:ARG:HG3	2.12	0.65
2:G:236:MET:HE3	2:G:296:PHE:CZ	2.32	0.65
1:H:64:ARG:HG2	1:H:64:ARG:HH21	1.61	0.64
1:C:159:ASP:O	1:C:163:ARG:HG3	1.97	0.64
1:H:47:LYS:HG3	7:H:560:HOH:O	1.97	0.64
1:C:198:LEU:CD1	1:C:198:LEU:C	2.70	0.64
1:B:89:LEU:O	1:B:93:LYS:HG2	1.97	0.64
1:C:198:LEU:C	1:C:198:LEU:HD12	2.23	0.63
1:D:311:MET:CE	4:D:403:FFO:H15	2.28	0.62
1:A:126:ARG:NH2	1:A:189:LEU:O	2.32	0.62
1:F:145:GLU:OE1	1:F:185:ARG:NH2	2.29	0.62
1:D:147:ARG:NH2	1:D:152:ASP:O	2.32	0.62
1:B:221:LEU:HD22	4:B:403:FFO:C	2.29	0.62
7:C:599:HOH:O	1:D:185:ARG:HD2	1.98	0.62
1:A:215:ARG:NH1	1:B:175:ARG:O	2.32	0.62
1:C:36:GLN:HG2	1:C:61:MET:CE	2.30	0.62
1:D:90:TRP:O	1:D:93:LYS:HG3	2.00	0.61
1:D:90:TRP:HA	1:D:93:LYS:CD	2.30	0.61
1:F:174:ASP:OD2	1:F:176:ARG:HB2	2.00	0.61
1:H:165:ILE:CG2	1:H:240:ILE:HD11	2.32	0.60
1:C:45:VAL:HG21	1:D:204:VAL:HG21	1.81	0.60
1:A:261:HIS:CD2	1:A:309:MET:HB3	2.37	0.60
1:F:46:ARG:HG3	1:F:46:ARG:NH2	2.12	0.60
1:B:311:MET:HE3	4:B:403:FFO:H15	1.82	0.60
1:A:215:ARG:HH11	1:B:176:ARG:HG3	1.62	0.59
1:D:153:TYR:O	1:D:156:GLN:HB2	2.01	0.59
1:F:236:MET:HE2	1:F:296:PHE:HZ	1.63	0.59
1:B:90:TRP:HA	1:B:93:LYS:HD2	1.85	0.59
2:E:313:VAL:OXT	2:E:313:VAL:CG2	2.51	0.59
1:F:46:ARG:CZ	1:F:259:LEU:HD11	2.32	0.59
2:E:313:VAL:OXT	2:E:313:VAL:HG22	2.01	0.59
2:G:198:LEU:HD12	2:G:199:CYS:N	2.18	0.59
1:D:42:ARG:O	1:D:42:ARG:HG2	2.01	0.58
1:F:60:GLY:HA2	1:F:252:LEU:O	2.03	0.58
1:F:36:GLN:O	1:F:40:ILE:HG13	2.03	0.58
2:G:311:MET:HE2	4:G:403:FFO:H16	1.85	0.58
1:F:240:ILE:HD12	1:F:291:PHE:HE2	1.68	0.58
1:H:77:LYS:HE2	7:H:534:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:ASP:HB2	7:H:635:HOH:O	2.04	0.58
1:H:198:LEU:C	1:H:198:LEU:CD1	2.77	0.57
4:G:403:FFO:HG1	7:G:616:HOH:O	2.04	0.57
1:B:254:ASP:C	1:B:254:ASP:OD1	2.46	0.57
1:F:187:LEU:HB2	1:F:188:PRO:HD3	1.86	0.57
1:B:284:LYS:HD3	7:B:605:HOH:O	2.04	0.57
1:A:166:ASP:O	1:A:170:THR:HG23	2.05	0.56
2:E:68:ARG:O	2:E:69:ASP:CB	2.51	0.56
2:E:198:LEU:C	2:E:198:LEU:HD12	2.31	0.56
1:D:147:ARG:HA	7:D:619:HOH:O	2.06	0.56
1:B:221:LEU:HD22	4:B:403:FFO:N	2.21	0.56
1:H:126:ARG:HD3	1:H:130:ASP:O	2.06	0.55
1:A:207:GLU:HA	1:A:244:LYS:O	2.06	0.55
1:F:215:ARG:HD2	1:F:215:ARG:C	2.32	0.55
1:A:198:LEU:HD13	1:A:199:CYS:N	2.21	0.55
1:B:311:MET:CE	4:B:403:FFO:H15	2.36	0.55
1:H:215:ARG:HH11	2:G:176:ARG:HG3	1.64	0.55
2:E:111:ALA:HA	7:E:709:HOH:O	2.06	0.55
2:E:126:ARG:HD3	2:E:130:ASP:HB3	1.87	0.55
1:D:151:SER:HB2	1:D:153:TYR:CZ	2.42	0.55
1:B:64:ARG:NE	3:B:402:SO4:O2	2.31	0.55
1:B:90:TRP:O	1:B:93:LYS:HG3	2.07	0.55
1:B:163:ARG:HG2	7:B:697:HOH:O	2.05	0.55
1:B:196:HIS:HB2	1:B:212:LEU:HD11	1.89	0.55
2:E:50:ARG:NH1	2:E:51:THR:HG22	2.22	0.55
1:A:142:PHE:CE1	1:B:184:PRO:HD2	2.41	0.55
1:D:117:PHE:CE2	1:D:121:LEU:HD11	2.42	0.54
1:D:216:SER:HA	1:D:254:ASP:O	2.06	0.54
1:H:64:ARG:HG2	1:H:64:ARG:NH2	2.22	0.54
1:C:311:MET:HE2	4:C:404:FFO:C8A	2.37	0.54
1:D:263:GLU:CB	1:D:264:PRO:HD3	2.36	0.54
2:G:46:ARG:HG3	2:G:46:ARG:O	2.06	0.54
1:B:44:GLY:HA2	1:B:58:VAL:HG23	1.90	0.54
2:E:311:MET:HE1	7:E:509:HOH:O	2.08	0.54
1:B:175:ARG:O	1:B:176:ARG:HG3	2.08	0.54
2:E:46:ARG:HA	2:E:55:THR:O	2.08	0.54
1:A:287:LYS:HD3	7:A:706:HOH:O	2.07	0.54
1:H:165:ILE:HG21	1:H:240:ILE:HD11	1.90	0.53
1:A:198:LEU:C	1:A:198:LEU:HD12	2.33	0.53
1:C:99:LYS:HE3	7:C:686:HOH:O	2.09	0.53
2:G:86:GLU:HG3	7:G:576:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:ASP:HB2	7:F:521:HOH:O	2.08	0.53
1:F:142:PHE:CZ	2:E:184:PRO:HD2	2.44	0.53
2:G:46:ARG:HA	2:G:55:THR:O	2.09	0.53
1:C:204:VAL:HG23	1:D:45:VAL:HG11	1.91	0.52
1:B:187:LEU:HD22	1:B:193:PRO:HB3	1.89	0.52
1:F:154:SER:HA	7:F:729:HOH:O	2.08	0.52
1:H:196:HIS:HB2	1:H:212:LEU:HD11	1.90	0.52
2:E:163:ARG:HG2	2:E:163:ARG:HH11	1.74	0.52
1:H:215:ARG:NH1	2:G:176:ARG:CG	2.53	0.52
1:D:60:GLY:HA2	1:D:252:LEU:O	2.09	0.52
1:B:187:LEU:N	1:B:188:PRO:CD	2.72	0.52
1:H:184:PRO:HD2	2:G:142:PHE:CE1	2.45	0.52
1:B:90:TRP:HA	1:B:93:LYS:CG	2.39	0.52
1:C:142:PHE:CE1	1:D:184:PRO:HD2	2.45	0.51
2:E:135:TYR:CE1	2:E:196:HIS:CE1	2.98	0.51
1:C:176:ARG:HG3	1:D:215:ARG:NH1	2.24	0.51
2:E:157:GLY:HA2	7:E:652:HOH:O	2.09	0.51
1:F:240:ILE:HD12	1:F:291:PHE:CE2	2.44	0.51
1:H:187:LEU:HD22	1:H:193:PRO:HB3	1.92	0.51
1:H:64:ARG:HD3	7:H:562:HOH:O	2.10	0.51
1:H:42:ARG:O	1:H:42:ARG:HG2	2.11	0.50
1:H:45:VAL:HG11	2:G:204:VAL:HG23	1.92	0.50
2:G:67:LEU:HB3	2:G:235:TYR:HE1	1.75	0.50
2:G:301:TYR:HA	7:G:592:HOH:O	2.10	0.50
2:E:62:ARG:HA	2:E:250:HIS:O	2.11	0.50
1:H:273:PRO:HG2	7:H:655:HOH:O	2.11	0.50
4:B:403:FFO:HG2	7:B:564:HOH:O	2.10	0.50
1:H:215:ARG:HB2	2:G:178:ILE:HD11	1.94	0.50
2:E:56:LEU:HD22	2:E:262:ILE:HD11	1.94	0.50
2:E:163:ARG:HG2	2:E:163:ARG:NH1	2.27	0.50
1:D:311:MET:HE2	4:D:403:FFO:H15	1.92	0.49
1:F:126:ARG:HG2	1:F:130:ASP:HB3	1.94	0.49
1:B:268:GLN:HB2	1:B:307:ILE:HD13	1.94	0.49
2:G:67:LEU:HB3	2:G:235:TYR:CE1	2.48	0.49
1:D:274:ARG:HD2	1:D:302:ASN:O	2.13	0.49
1:B:75:THR:O	1:B:304:HIS:HD2	1.95	0.49
2:E:122:GLY:HA2	7:E:627:HOH:O	2.12	0.49
1:A:280:ARG:HD2	1:A:299:GLU:OE1	2.12	0.49
1:D:64:ARG:HH21	1:D:64:ARG:HB3	1.77	0.49
1:F:198:LEU:CD1	1:F:199:CYS:N	2.75	0.49
1:A:152:ASP:OD1	1:A:154:SER:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:VAL:HG21	1:D:204:VAL:CG2	2.43	0.48
1:F:212:LEU:HD12	1:F:213:TYR:N	2.28	0.48
1:C:163:ARG:HB3	1:C:163:ARG:HH11	1.76	0.48
1:B:195:CME:HZ3	1:B:256:HIS:CE1	2.48	0.48
2:E:82:LYS:O	2:E:86:GLU:HB2	2.12	0.48
1:D:147:ARG:HB2	1:D:151:SER:OG	2.14	0.48
1:H:280:ARG:HH11	1:H:280:ARG:HB2	1.79	0.48
1:F:184:PRO:HD2	2:E:142:PHE:CE1	2.48	0.48
2:E:311:MET:HE3	4:E:403:FFO:C16	2.44	0.48
1:C:311:MET:CE	4:C:404:FFO:H15	2.21	0.48
1:H:187:LEU:HB2	1:H:188:PRO:HD3	1.95	0.48
3:A:401:SO4:S	1:B:176:ARG:HD2	2.54	0.48
1:F:223:VAL:N	1:F:224:PRO:CD	2.76	0.48
1:H:60:GLY:HA2	1:H:252:LEU:O	2.14	0.48
1:A:204:VAL:CG2	1:B:45:VAL:HG21	2.43	0.48
1:D:89:LEU:O	1:D:93:LYS:CG	2.59	0.48
1:F:64:ARG:HG3	1:F:249:ILE:HG12	1.96	0.48
1:A:64:ARG:HG3	1:A:249:ILE:HG12	1.95	0.48
1:C:163:ARG:HH11	1:C:163:ARG:CB	2.26	0.48
1:D:163:ARG:NH1	7:D:507:HOH:O	2.45	0.48
2:G:159:ASP:O	2:G:163:ARG:HG3	2.13	0.48
1:A:311:MET:HE2	4:A:403:FFO:C8A	2.44	0.47
1:D:151:SER:HB2	1:D:153:TYR:CE2	2.49	0.47
2:E:185:ARG:HD2	7:E:583:HOH:O	2.14	0.47
1:H:46:ARG:HA	1:H:55:THR:O	2.14	0.47
1:A:198:LEU:C	1:A:198:LEU:HD13	2.37	0.47
3:A:401:SO4:O4	1:B:176:ARG:HD2	2.14	0.47
1:F:142:PHE:CE1	2:E:184:PRO:HD2	2.49	0.47
1:F:289:ASP:HB2	7:F:526:HOH:O	2.13	0.47
2:G:178:ILE:CG2	2:G:179:MET:N	2.77	0.47
2:G:198:LEU:C	2:G:198:LEU:CD1	2.86	0.47
1:C:175:ARG:HG2	1:D:254:ASP:OD2	2.14	0.47
1:A:87:GLU:HB3	7:A:503:HOH:O	2.14	0.47
1:C:297:GLN:HG2	1:F:297:GLN:OE1	2.15	0.47
1:D:196:HIS:HB2	1:D:212:LEU:HD11	1.97	0.47
1:H:135:TYR:OH	1:H:195:CME:N	2.46	0.47
1:C:205:ASN:O	1:C:206:SER:HB2	2.14	0.47
1:B:147:ARG:HH21	1:B:156:GLN:HE22	1.63	0.47
1:H:311:MET:HG3	4:H:403:FFO:H16	1.97	0.47
2:G:165:ILE:HD13	2:G:240:ILE:HD11	1.97	0.47
2:G:244:LYS:CB	7:G:699:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:TRP:HA	1:B:93:LYS:HG2	1.97	0.46
1:B:261:HIS:C	1:B:264:PRO:HD2	2.40	0.46
1:H:304:HIS:HB3	1:H:305:PRO:HD2	1.97	0.46
2:G:263:GLU:HB2	2:G:264:PRO:HD3	1.98	0.46
2:G:222:GLY:HA3	7:G:544:HOH:O	2.14	0.46
1:A:80:PHE:CE1	1:A:82:LYS:HB3	2.50	0.46
1:B:301:TYR:CE2	1:B:303:PRO:HG3	2.50	0.46
1:B:151:SER:HB2	1:B:153:TYR:CZ	2.50	0.46
1:F:274:ARG:HD2	1:F:302:ASN:O	2.15	0.46
1:H:165:ILE:HG23	1:H:240:ILE:HD11	1.96	0.46
1:H:46:ARG:CG	7:H:653:HOH:O	2.63	0.46
2:G:184:PRO:HA	2:G:187:LEU:HG	1.98	0.46
2:E:38:GLN:HG3	2:E:269:LEU:HD13	1.98	0.45
2:E:117:PHE:O	2:E:120:SER:OG	2.33	0.45
1:A:98:ALA:HB2	1:A:131:LEU:HD21	1.97	0.45
1:A:232:LEU:HG	1:A:236:MET:HE3	1.97	0.45
1:D:187:LEU:N	1:D:188:PRO:CD	2.78	0.45
1:H:95:SER:HA	7:H:673:HOH:O	2.16	0.45
1:A:182:TRP:CZ2	1:A:187:LEU:HD21	2.52	0.45
2:E:187:LEU:HD22	2:E:193:PRO:HB3	1.97	0.45
1:A:42:ARG:O	2:E:46:ARG:HD3	2.16	0.45
1:A:196:HIS:HB2	1:A:212:LEU:HD11	1.99	0.45
1:H:289:ASP:HB2	7:H:557:HOH:O	2.17	0.45
1:H:304:HIS:HB3	1:H:305:PRO:CD	2.47	0.45
2:G:126:ARG:HD3	2:G:130:ASP:HB3	1.98	0.45
1:C:184:PRO:HA	1:C:187:LEU:HG	1.99	0.45
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.81	0.45
2:E:141:HIS:O	2:E:142:PHE:C	2.58	0.45
1:D:114:SER:HA	7:D:593:HOH:O	2.17	0.45
1:A:183:ASN:HB3	1:A:186:ASP:HB2	1.99	0.45
1:A:139:TRP:CE2	1:A:179:MET:HE3	2.52	0.45
2:E:272:GLU:OE1	2:E:272:GLU:HA	2.16	0.45
1:D:195:CME:HB2	1:D:216:SER:O	2.17	0.45
1:D:294:GLU:CD	1:D:294:GLU:H	2.24	0.45
1:H:184:PRO:HD2	2:G:142:PHE:CZ	2.52	0.45
1:H:258:TYR:O	1:H:261:HIS:HB2	2.17	0.45
2:E:102:SER:HA	2:E:106:VAL:O	2.17	0.45
1:C:38:GLN:HG3	7:C:746:HOH:O	2.16	0.44
2:E:159:ASP:OD1	2:E:159:ASP:C	2.58	0.44
1:D:311:MET:HE3	4:D:403:FFO:H15	1.97	0.44
1:B:90:TRP:HA	1:B:93:LYS:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LYS:HD3	7:B:676:HOH:O	2.18	0.44
1:F:59:PHE:HB2	2:E:202:TYR:CD2	2.53	0.44
2:E:182:TRP:CZ2	2:E:187:LEU:HD11	2.52	0.44
2:E:284:LYS:HE3	2:E:284:LYS:HB2	1.86	0.44
2:G:221:LEU:HD23	2:G:221:LEU:HA	1.79	0.44
1:D:207:GLU:HA	1:D:244:LYS:O	2.17	0.44
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.68	0.44
1:F:46:ARG:NH2	1:F:46:ARG:CG	2.75	0.44
1:A:151:SER:HB2	1:A:153:TYR:CZ	2.53	0.44
2:G:133:PRO:O	2:G:190:MET:HE2	2.17	0.44
1:H:142:PHE:CD1	1:H:142:PHE:C	2.96	0.44
1:A:83:GLY:O	1:A:87:GLU:HB2	2.17	0.44
1:A:215:ARG:HH12	1:B:176:ARG:CG	2.23	0.44
1:H:97:ASN:HD21	1:H:149:MET:HE3	1.80	0.44
2:G:230:TYR:HB3	2:G:248:PHE:CE1	2.53	0.44
1:D:33:TYR:O	1:D:37:ILE:HG12	2.18	0.43
1:F:152:ASP:C	1:F:152:ASP:OD1	2.60	0.43
1:F:198:LEU:HD12	1:F:199:CYS:N	2.32	0.43
2:G:88:LEU:HD22	2:G:88:LEU:O	2.18	0.43
2:G:141:HIS:O	2:G:142:PHE:C	2.59	0.43
1:F:215:ARG:HD2	1:F:215:ARG:O	2.19	0.43
1:B:263:GLU:HB2	1:B:264:PRO:HD3	1.99	0.43
1:D:90:TRP:HA	1:D:93:LYS:CG	2.49	0.43
1:H:142:PHE:CZ	2:G:184:PRO:HD2	2.53	0.43
2:G:258:TYR:O	2:G:261:HIS:HB2	2.18	0.43
1:A:221:LEU:HD22	4:A:403:FFO:N	2.33	0.43
1:D:198:LEU:HD13	1:D:199:CYS:N	2.34	0.43
1:F:126:ARG:HD3	1:F:130:ASP:O	2.19	0.43
2:E:88:LEU:O	2:E:92:ILE:HG13	2.19	0.43
2:E:114:SER:O	2:E:118:LEU:HG	2.19	0.43
1:F:184:PRO:HD2	2:E:142:PHE:CZ	2.54	0.43
2:E:160:GLN:HB2	2:E:179:MET:HG3	2.01	0.43
2:G:163:ARG:NH2	7:G:513:HOH:O	2.52	0.43
2:G:311:MET:HG2	2:G:312:ALA:N	2.33	0.43
1:D:198:LEU:CD1	1:D:198:LEU:C	2.92	0.42
1:H:221:LEU:CD1	1:H:311:MET:HA	2.49	0.42
3:H:401:SO4:O1	2:G:176:ARG:HD2	2.19	0.42
1:A:195:CME:O	1:A:215:ARG:HG3	2.19	0.42
1:C:36:GLN:HG2	1:C:61:MET:HE2	1.99	0.42
2:E:244:LYS:HE2	2:E:244:LYS:HB2	1.38	0.42
1:D:62:ARG:HA	1:D:250:HIS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ASP:HB3	7:D:615:HOH:O	2.19	0.42
1:D:302:ASN:HD22	1:D:302:ASN:HA	1.60	0.42
1:B:267:ILE:O	1:B:270:GLN:HB2	2.18	0.42
1:F:196:HIS:HB3	1:F:212:LEU:HD21	2.00	0.42
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.93	0.42
4:E:403:FFO:H15	4:E:403:FFO:H92	1.73	0.42
4:H:403:FFO:H5A	4:H:403:FFO:O4	2.18	0.42
2:G:236:MET:CE	2:G:296:PHE:CZ	3.02	0.42
1:B:164:VAL:O	1:B:165:ILE:C	2.60	0.42
1:B:311:MET:HE3	4:B:403:FFO:C15	2.49	0.42
4:B:403:FFO:H15	4:B:403:FFO:H92	1.78	0.42
2:E:182:TRP:O	2:E:184:PRO:HD3	2.20	0.42
2:E:187:LEU:N	2:E:188:PRO:CD	2.83	0.42
1:B:196:HIS:CB	1:B:212:LEU:HD11	2.49	0.42
2:E:308:LYS:HA	7:E:620:HOH:O	2.18	0.42
1:D:126:ARG:HG2	1:D:130:ASP:HB3	2.02	0.42
1:F:28:HIS:CE1	1:F:30:GLU:HB2	2.55	0.42
1:F:142:PHE:CD1	1:F:142:PHE:C	2.97	0.42
2:G:40:ILE:HB	2:G:257:ILE:HD12	2.01	0.42
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.87	0.42
1:A:215:ARG:HB2	1:B:178:ILE:HD11	2.01	0.42
1:F:58:VAL:HG22	7:F:757:HOH:O	2.18	0.42
1:B:244:LYS:HA	1:B:244:LYS:HD3	1.87	0.41
1:F:130:ASP:OD2	1:F:149:MET:HG2	2.20	0.41
1:H:45:VAL:O	1:H:56:LEU:HA	2.19	0.41
1:F:187:LEU:N	1:F:188:PRO:CD	2.83	0.41
2:E:68:ARG:O	2:E:69:ASP:HB3	2.20	0.41
2:E:96:THR:CG2	2:E:137:PHE:HB2	2.50	0.41
1:C:156:GLN:NE2	7:C:506:HOH:O	2.51	0.41
1:C:184:PRO:HD2	1:D:142:PHE:CE1	2.56	0.41
1:B:77:LYS:HB3	1:B:307:ILE:HD12	2.01	0.41
2:G:139:TRP:CE2	2:G:179:MET:HE3	2.55	0.41
1:C:65:TYR:HA	7:C:530:HOH:O	2.20	0.41
1:C:215:ARG:HB2	1:D:178:ILE:HD11	2.03	0.41
1:D:271:ARG:HD3	1:D:304:HIS:CG	2.56	0.41
1:D:287:LYS:NZ	7:D:514:HOH:O	2.54	0.41
1:F:97:ASN:O	1:F:100:GLU:HB2	2.20	0.41
1:A:121:LEU:HD11	1:A:191:ALA:O	2.21	0.41
1:A:205:ASN:HB2	1:A:206:SER:H	1.62	0.41
1:F:145:GLU:CD	1:F:185:ARG:HH21	2.23	0.41
1:H:45:VAL:HG21	2:G:204:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:ARG:HG3	7:H:653:HOH:O	2.21	0.41
2:G:134:VAL:O	2:G:135:TYR:C	2.64	0.41
1:C:298:ILE:O	1:F:297:GLN:NE2	2.53	0.41
2:E:86:GLU:HB3	2:E:106:VAL:HG21	2.03	0.41
2:G:199:CYS:HA	2:G:211:GLN:O	2.19	0.41
1:D:187:LEU:HD22	1:D:193:PRO:HB3	2.02	0.41
1:F:56:LEU:HD22	1:F:262:ILE:HD11	2.02	0.41
1:F:127:GLU:HB3	1:F:149:MET:HE2	2.03	0.41
2:E:126:ARG:HB2	7:E:523:HOH:O	2.20	0.41
1:A:96:THR:HG21	1:A:132:GLY:O	2.21	0.41
1:F:214:GLN:HB3	1:F:252:LEU:HD23	2.02	0.41
2:E:278:LYS:NZ	7:E:518:HOH:O	2.53	0.41
1:A:221:LEU:CB	7:A:584:HOH:O	2.38	0.40
1:D:250:HIS:CE1	1:D:252:LEU:HD11	2.56	0.40
1:B:88:LEU:HD23	1:B:232:LEU:HD23	2.02	0.40
1:B:198:LEU:HD23	1:B:198:LEU:C	2.46	0.40
2:G:88:LEU:HD23	2:G:88:LEU:HA	1.94	0.40
1:A:86:GLU:HB2	1:A:106:VAL:HG21	2.02	0.40
1:C:163:ARG:NH1	1:C:163:ARG:CB	2.75	0.40
1:D:222:GLY:O	1:D:225:PHE:HB2	2.22	0.40
1:D:226:ASN:O	1:D:227:ILE:C	2.65	0.40
1:H:141:HIS:O	1:H:142:PHE:C	2.62	0.40
1:H:174:ASP:OD2	1:H:176:ARG:HB2	2.21	0.40
1:B:287:LYS:HB2	1:B:290:ASP:OD2	2.20	0.40
1:H:86:GLU:HG3	7:H:561:HOH:O	2.20	0.40
1:H:193:PRO:HG2	2:G:176:ARG:HG2	2.03	0.40
1:H:223:VAL:N	1:H:224:PRO:CD	2.84	0.40
2:G:297:GLN:HG3	7:G:690:HOH:O	2.20	0.40
1:B:240:ILE:HD12	1:B:240:ILE:HG21	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/325 (87%)	271 (95%)	12 (4%)	1 (0%)	30	39
1	B	285/325 (88%)	271 (95%)	13 (5%)	1 (0%)	30	39
1	C	284/325 (87%)	274 (96%)	9 (3%)	1 (0%)	30	39
1	D	285/325 (88%)	270 (95%)	15 (5%)	0	100	100
1	F	284/325 (87%)	276 (97%)	7 (2%)	1 (0%)	30	39
1	H	284/325 (87%)	268 (94%)	16 (6%)	0	100	100
2	E	284/325 (87%)	270 (95%)	14 (5%)	0	100	100
2	G	284/325 (87%)	270 (95%)	14 (5%)	0	100	100
All	All	2274/2600 (88%)	2170 (95%)	100 (4%)	4 (0%)	43	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	134	VAL
1	C	134	VAL
1	B	134	VAL
1	A	134	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/279 (87%)	219 (90%)	23 (10%)	8	9
1	B	243/279 (87%)	223 (92%)	20 (8%)	10	14
1	C	242/279 (87%)	225 (93%)	17 (7%)	14	19
1	D	246/279 (88%)	226 (92%)	20 (8%)	11	15
1	F	244/279 (88%)	226 (93%)	18 (7%)	13	17
1	H	243/279 (87%)	227 (93%)	16 (7%)	15	21
2	E	244/279 (88%)	223 (91%)	21 (9%)	10	13
2	G	241/279 (86%)	224 (93%)	17 (7%)	13	19
All	All	1945/2232 (87%)	1793 (92%)	152 (8%)	11	16

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	45	VAL
1	A	49	ASP
1	A	56	LEU
1	A	102	SER
1	A	103	SER
1	A	116	ASP
1	A	125	THR
1	A	128	GLU
1	A	131	LEU
1	A	154	SER
1	A	163	ARG
1	A	164	VAL
1	A	170	THR
1	A	176	ARG
1	A	187	LEU
1	A	198	LEU
1	A	204	VAL
1	A	240	ILE
1	A	270	GLN
1	A	278	LYS
1	A	308	LYS
1	A	311	MET
1	C	56	LEU
1	C	64	ARG
1	C	69	ASP
1	C	127	GLU
1	C	150	GLU
1	C	154	SER
1	C	164	VAL
1	C	176	ARG
1	C	198	LEU
1	C	204	VAL
1	C	240	ILE
1	C	270	GLN
1	C	274	ARG
1	C	278	LYS
1	C	280	ARG
1	C	288	ILE
1	C	313	VAL
1	D	26	PRO
1	D	56	LEU

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Mol	Chain	Res	Type
1	D	64	ARG
1	D	93	LYS
1	D	147	ARG
1	D	150	GLU
1	D	154	SER
1	D	164	VAL
1	D	169	LYS
1	D	176	ARG
1	D	196	HIS
1	D	198	LEU
1	D	223	VAL
1	D	240	ILE
1	D	278	LYS
1	D	294	GLU
1	D	297	GLN
1	D	308	LYS
1	D	311	MET
1	D	313	VAL
1	B	38	GLN
1	B	56	LEU
1	B	58	VAL
1	B	99	LYS
1	B	124	SER
1	B	163	ARG
1	B	169	LYS
1	B	175	ARG
1	B	178	ILE
1	B	196	HIS
1	B	206	SER
1	B	240	ILE
1	B	244	LYS
1	B	278	LYS
1	B	280	ARG
1	B	284	LYS
1	B	287	LYS
1	B	302	ASN
1	B	311	MET
1	B	313	VAL
1	F	46	ARG
1	F	56	LEU
1	F	58	VAL
1	F	69	ASP

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Mol	Chain	Res	Type
1	F	100	GLU
1	F	102	SER
1	F	150	GLU
1	F	152	ASP
1	F	154	SER
1	F	164	VAL
1	F	176	ARG
1	F	198	LEU
1	F	240	ILE
1	F	272	GLU
1	F	278	LYS
1	F	287	LYS
1	F	288	ILE
1	F	313	VAL
1	H	45	VAL
1	H	46	ARG
1	H	50	ARG
1	H	56	LEU
1	H	58	VAL
1	H	69	ASP
1	H	127	GLU
1	H	176	ARG
1	H	178	ILE
1	H	198	LEU
1	H	229	SER
1	H	240	ILE
1	H	263	GLU
1	H	278	LYS
1	H	310	GLU
1	H	313	VAL
2	E	38	GLN
2	E	56	LEU
2	E	57	SER
2	E	58	VAL
2	E	62	ARG
2	E	86	GLU
2	E	116	ASP
2	E	140	ARG
2	E	150	GLU
2	E	154	SER
2	E	163	ARG
2	E	176	ARG

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Mol	Chain	Res	Type
2	E	198	LEU
2	E	204	VAL
2	E	240	ILE
2	E	244	LYS
2	E	278	LYS
2	E	284	LYS
2	E	302	ASN
2	E	311	MET
2	E	313	VAL
2	G	38	GLN
2	G	46	ARG
2	G	56	LEU
2	G	69	ASP
2	G	88	LEU
2	G	116	ASP
2	G	127	GLU
2	G	147	ARG
2	G	163	ARG
2	G	164	VAL
2	G	170	THR
2	G	176	ARG
2	G	198	LEU
2	G	240	ILE
2	G	271	ARG
2	G	280	ARG
2	G	313	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	171	ASN
1	C	156	GLN
1	C	171	ASN
1	D	36	GLN
1	D	214	GLN
1	D	302	ASN
1	B	156	GLN
1	B	171	ASN
1	B	205	ASN
1	B	304	HIS
1	F	39	HIS

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Mol	Chain	Res	Type
1	F	171	ASN
1	H	36	GLN
1	H	156	GLN
1	H	171	ASN
2	E	156	GLN
2	E	171	ASN
2	E	214	GLN
2	E	226	ASN
2	G	171	ASN
2	G	297	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	CME	G	195	2	8,9,10	0.59	0	6,9,11	1.40	1 (16%)
1	CME	B	43	1	8,9,10	0.82	0	6,9,11	1.01	1 (16%)
1	CME	B	195	1	8,9,10	0.62	0	6,9,11	0.99	1 (16%)
1	CME	F	43	1	8,9,10	0.54	0	6,9,11	0.43	0
2	SCH	E	43	2	6,7,8	0.53	0	4,7,9	0.69	0
1	CME	F	195	1	8,9,10	0.47	0	6,9,11	0.90	0
1	CME	D	195	1	8,9,10	0.40	0	6,9,11	1.62	1 (16%)
1	CME	C	43	1	8,9,10	0.71	0	6,9,11	0.78	0
1	CME	A	43	1	8,9,10	0.50	0	6,9,11	1.40	1 (16%)
1	CME	A	195	1	8,9,10	0.60	0	6,9,11	1.35	0
1	CME	H	195	1	8,9,10	0.57	0	6,9,11	0.98	0
2	SCH	G	43	2	6,7,8	0.73	0	4,7,9	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	D	43	1	8,9,10	0.83	0	6,9,11	1.12	0
2	CME	E	195	2	8,9,10	0.75	0	6,9,11	1.88	2 (33%)
1	CME	C	195	1	8,9,10	0.52	0	6,9,11	0.88	0
1	CME	H	43	1	8,9,10	0.87	0	6,9,11	1.70	1 (16%)

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	CME	G	195	2	-	3/5/8/10	-
1	CME	B	43	1	-	1/5/8/10	-
1	CME	B	195	1	-	3/5/8/10	-
1	CME	F	43	1	-	1/5/8/10	-
2	SCH	E	43	2	-	0/2/6/8	-
1	CME	F	195	1	-	2/5/8/10	-
1	CME	D	195	1	-	1/5/8/10	-
1	CME	C	43	1	-	3/5/8/10	-
1	CME	A	43	1	-	2/5/8/10	-
1	CME	A	195	1	-	2/5/8/10	-
1	CME	H	195	1	-	1/5/8/10	-
2	SCH	G	43	2	-	0/2/6/8	-
1	CME	D	43	1	-	3/5/8/10	-
2	CME	E	195	2	-	2/5/8/10	-
1	CME	C	195	1	-	2/5/8/10	-
1	CME	H	43	1	-	1/5/8/10	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	CME	OH-CZ-CE	3.67	125.16	110.82
2	E	195	CME	OH-CZ-CE	3.47	124.37	110.82
1	H	43	CME	CZ-CE-SD	2.85	122.93	113.39
1	A	43	CME	CZ-CE-SD	-2.81	104.00	113.39
2	G	195	CME	CB-CA-C	2.61	117.89	110.80
1	B	43	CME	CZ-CE-SD	-2.26	105.84	113.39
2	E	195	CME	CB-CA-C	2.11	116.52	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	CME	OH-CZ-CE	2.07	118.88	110.82

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	43	CME	N-CA-CB-SG
1	A	43	CME	CE-SD-SG-CB
1	A	195	CME	CE-SD-SG-CB
1	C	43	CME	CE-SD-SG-CB
1	C	43	CME	CZ-CE-SD-SG
1	C	195	CME	SD-CE-CZ-OH
1	H	43	CME	SD-CE-CZ-OH
2	G	195	CME	SD-CE-CZ-OH
1	B	195	CME	CE-SD-SG-CB
1	F	195	CME	SD-CE-CZ-OH
1	D	43	CME	CE-SD-SG-CB
1	D	43	CME	SD-CE-CZ-OH
2	E	195	CME	SD-CE-CZ-OH
2	G	195	CME	CA-CB-SG-SD
1	C	195	CME	CZ-CE-SD-SG
1	F	43	CME	CZ-CE-SD-SG
1	F	195	CME	CZ-CE-SD-SG
1	A	195	CME	CA-CB-SG-SD
1	C	43	CME	SD-CE-CZ-OH
2	G	195	CME	CE-SD-SG-CB
1	D	43	CME	CZ-CE-SD-SG
1	D	195	CME	CZ-CE-SD-SG
1	B	43	CME	CZ-CE-SD-SG
1	B	195	CME	CZ-CE-SD-SG
1	H	195	CME	CZ-CE-SD-SG
2	E	195	CME	CZ-CE-SD-SG
1	B	195	CME	CA-CB-SG-SD

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	43	CME	1	0
1	B	195	CME	1	0
1	D	195	CME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	195	CME	1	0
1	H	195	CME	1	0
2	E	195	CME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 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	$\# Z > 2$
3	SO4	B	402	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	C	403	-	4,4,4	0.25	0	6,6,6	0.28	0
3	SO4	D	401	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.15	0
3	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.21	0
3	SO4	F	402	-	4,4,4	0.27	0	6,6,6	0.13	0
4	FFO	C	404	-	33,36,36	1.00	1 (3%)	35,50,50	1.68	7 (20%)
3	SO4	A	401	-	4,4,4	0.13	0	6,6,6	0.38	0
3	SO4	C	402	-	4,4,4	0.39	0	6,6,6	0.21	0
3	SO4	C	401	-	4,4,4	0.31	0	6,6,6	0.25	0
4	FFO	H	403	-	33,36,36	1.01	2 (6%)	35,50,50	1.57	4 (11%)
6	GOL	D	404	-	5,5,5	0.20	0	5,5,5	0.71	0
3	SO4	E	402	-	4,4,4	0.28	0	6,6,6	0.15	0
3	SO4	G	402	-	4,4,4	0.27	0	6,6,6	0.19	0
3	SO4	F	401	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	E	401	-	4,4,4	0.28	0	6,6,6	0.23	0
3	SO4	G	401	-	4,4,4	0.25	0	6,6,6	0.38	0
6	GOL	H	404	-	5,5,5	0.33	0	5,5,5	1.20	0
3	SO4	H	401	-	4,4,4	0.16	0	6,6,6	0.23	0
4	FFO	A	403	-	33,36,36	1.19	3 (9%)	35,50,50	1.90	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	402	-	4,4,4	0.26	0	6,6,6	0.15	0
4	FFO	D	403	-	33,36,36	1.16	3 (9%)	35,50,50	1.84	8 (22%)
3	SO4	H	402	-	4,4,4	0.28	0	6,6,6	0.07	0
4	FFO	B	403	-	33,36,36	1.03	1 (3%)	35,50,50	1.70	6 (17%)
4	FFO	F	403	-	33,36,36	1.09	2 (6%)	35,50,50	1.60	5 (14%)
4	FFO	G	403	-	33,36,36	1.02	1 (3%)	35,50,50	1.63	4 (11%)
4	FFO	E	403	-	33,36,36	0.98	1 (3%)	35,50,50	1.62	4 (11%)

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	FFO	A	403	-	-	7/24/37/37	0/3/3/3
4	FFO	C	404	-	-	4/24/37/37	0/3/3/3
4	FFO	D	403	-	-	7/24/37/37	0/3/3/3
4	FFO	B	403	-	-	5/24/37/37	0/3/3/3
4	FFO	F	403	-	-	7/24/37/37	0/3/3/3
4	FFO	G	403	-	-	11/24/37/37	0/3/3/3
4	FFO	H	403	-	-	5/24/37/37	0/3/3/3
6	GOL	H	404	-	-	4/4/4/4	-
6	GOL	D	404	-	-	3/4/4/4	-
4	FFO	E	403	-	-	3/24/37/37	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	403	FFO	C4A-N5	3.80	1.44	1.38
4	B	403	FFO	C4A-N5	3.55	1.43	1.38
4	A	403	FFO	C4A-N5	3.50	1.43	1.38
4	G	403	FFO	C4A-N5	3.50	1.43	1.38
4	E	403	FFO	C4A-N5	3.27	1.43	1.38
4	C	404	FFO	C4A-N5	3.26	1.43	1.38
4	D	403	FFO	C4A-N5	3.25	1.43	1.38
4	H	403	FFO	C4A-N5	3.08	1.43	1.38
4	D	403	FFO	C5A-N5	2.48	1.40	1.36
4	D	403	FFO	C8A-N1	2.34	1.39	1.36
4	A	403	FFO	C4A-C4	-2.31	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	FFO	O1-CT	2.25	1.28	1.22
4	H	403	FFO	C7-C6	2.11	1.54	1.52
4	F	403	FFO	O2-CT	-2.04	1.24	1.30

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	FFO	C4A-C4-N3	6.11	121.69	110.94
4	A	403	FFO	C4A-C4-N3	6.06	121.60	110.94
4	C	404	FFO	C4A-C4-N3	5.64	120.87	110.94
4	B	403	FFO	C4A-C4-N3	5.59	120.78	110.94
4	H	403	FFO	C4A-C4-N3	5.56	120.73	110.94
4	G	403	FFO	C4A-C4-N3	5.44	120.51	110.94
4	F	403	FFO	C4A-C4-N3	5.43	120.49	110.94
4	E	403	FFO	C4A-C4-N3	5.13	119.96	110.94
4	E	403	FFO	C2-N1-C8A	4.56	121.40	113.36
4	G	403	FFO	C2-N1-C8A	4.44	121.20	113.36
4	D	403	FFO	C2-N1-C8A	4.38	121.09	113.36
4	B	403	FFO	C2-N1-C8A	4.25	120.86	113.36
4	F	403	FFO	C2-N1-C8A	4.20	120.78	113.36
4	C	404	FFO	C2-N1-C8A	4.08	120.56	113.36
4	H	403	FFO	C2-N1-C8A	3.99	120.41	113.36
4	A	403	FFO	C2-N1-C8A	3.92	120.28	113.36
4	A	403	FFO	CB-CA-CT	3.80	119.37	110.35
4	D	403	FFO	C2-N3-C4	-3.16	119.39	125.11
4	H	403	FFO	C2-N3-C4	-3.08	119.53	125.11
4	E	403	FFO	C2-N3-C4	-3.06	119.56	125.11
4	B	403	FFO	C2-N3-C4	-3.02	119.63	125.11
4	G	403	FFO	C2-N3-C4	-3.02	119.64	125.11
4	F	403	FFO	C2-N3-C4	-3.00	119.67	125.11
4	D	403	FFO	CB-CA-CT	2.91	117.27	110.35
4	A	403	FFO	C2-N3-C4	-2.83	119.98	125.11
4	D	403	FFO	O4-C4-C4A	-2.80	120.75	127.62
4	A	403	FFO	OE1-CD-CG	-2.71	114.49	123.09
4	C	404	FFO	C2-N3-C4	-2.69	120.22	125.11
4	B	403	FFO	O4-C4-C4A	-2.63	121.16	127.62
4	D	403	FFO	OE1-CD-CG	-2.57	114.95	123.09
4	D	403	FFO	CT-CA-N	-2.55	104.65	110.57
4	A	403	FFO	O4-C4-C4A	-2.54	121.38	127.62
4	B	403	FFO	CT-CA-N	-2.54	104.68	110.57
4	E	403	FFO	O5B-C5A-N5	-2.39	120.64	124.67
4	A	403	FFO	C16-C11-C	-2.35	112.97	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	404	FFO	O4-C4-C4A	-2.31	121.95	127.62
4	C	404	FFO	OE2-CD-CG	2.26	121.13	114.00
4	A	403	FFO	OE2-CD-CG	2.23	121.05	114.00
4	G	403	FFO	O4-C4-C4A	-2.14	122.38	127.62
4	F	403	FFO	O4-C4-N3	-2.13	116.11	120.11
4	F	403	FFO	OE1-CD-CG	-2.12	116.37	123.09
4	B	403	FFO	NA2-C2-N3	2.11	121.22	116.76
4	C	404	FFO	OE1-CD-CG	-2.11	116.41	123.09
4	H	403	FFO	OE1-CD-CG	-2.10	116.44	123.09
4	C	404	FFO	CB-CA-CT	2.02	115.15	110.35
4	D	403	FFO	OE2-CD-CG	2.02	120.38	114.00

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	FFO	O5B-C5A-N5-C4A
4	A	403	FFO	O5B-C5A-N5-C6
4	C	404	FFO	O5B-C5A-N5-C4A
4	C	404	FFO	O5B-C5A-N5-C6
4	D	403	FFO	O5B-C5A-N5-C4A
4	D	403	FFO	O5B-C5A-N5-C6
4	D	403	FFO	N5-C6-C9-N10
4	D	403	FFO	CT-CA-CB-CG
4	B	403	FFO	O5B-C5A-N5-C4A
4	B	403	FFO	O5B-C5A-N5-C6
4	B	403	FFO	N5-C6-C9-N10
4	F	403	FFO	O5B-C5A-N5-C4A
4	F	403	FFO	O5B-C5A-N5-C6
4	F	403	FFO	N5-C6-C9-N10
4	F	403	FFO	C7-C6-C9-N10
4	H	403	FFO	N5-C6-C9-N10
4	G	403	FFO	O5B-C5A-N5-C4A
4	G	403	FFO	O5B-C5A-N5-C6
4	G	403	FFO	N5-C6-C9-N10
4	G	403	FFO	C7-C6-C9-N10
6	D	404	GOL	O1-C1-C2-C3
6	H	404	GOL	O1-C1-C2-C3
6	H	404	GOL	C1-C2-C3-O3
6	H	404	GOL	O2-C2-C3-O3
4	G	403	FFO	CT-CA-CB-CG
4	D	403	FFO	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
6	H	404	GOL	O1-C1-C2-O2
4	D	403	FFO	C11-C-N-CA
4	A	403	FFO	CT-CA-CB-CG
4	A	403	FFO	N-CA-CB-CG
4	D	403	FFO	C6-C9-N10-C14
4	B	403	FFO	C6-C9-N10-C14
4	E	403	FFO	C6-C9-N10-C14
4	G	403	FFO	C6-C9-N10-C14
4	G	403	FFO	C13-C14-N10-C9
6	D	404	GOL	O1-C1-C2-O2
4	H	403	FFO	C7-C6-C9-N10
4	G	403	FFO	N-CA-CB-CG
4	B	403	FFO	C11-C-N-CA
4	A	403	FFO	CB-CA-N-C
4	F	403	FFO	OE1-CD-CG-CB
4	F	403	FFO	OE2-CD-CG-CB
4	C	404	FFO	OE2-CD-CG-CB
4	E	403	FFO	OE2-CD-CG-CB
4	C	404	FFO	OE1-CD-CG-CB
4	G	403	FFO	OE2-CD-CG-CB
4	E	403	FFO	OE1-CD-CG-CB
4	G	403	FFO	C15-C14-N10-C9
4	F	403	FFO	C6-C9-N10-C14
4	H	403	FFO	C6-C9-N10-C14
4	H	403	FFO	OE2-CD-CG-CB
4	A	403	FFO	OE2-CD-CG-CB
4	G	403	FFO	OE1-CD-CG-CB
4	H	403	FFO	OE1-CD-CG-CB
4	A	403	FFO	OE1-CD-CG-CB
6	D	404	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 33 short contacts:

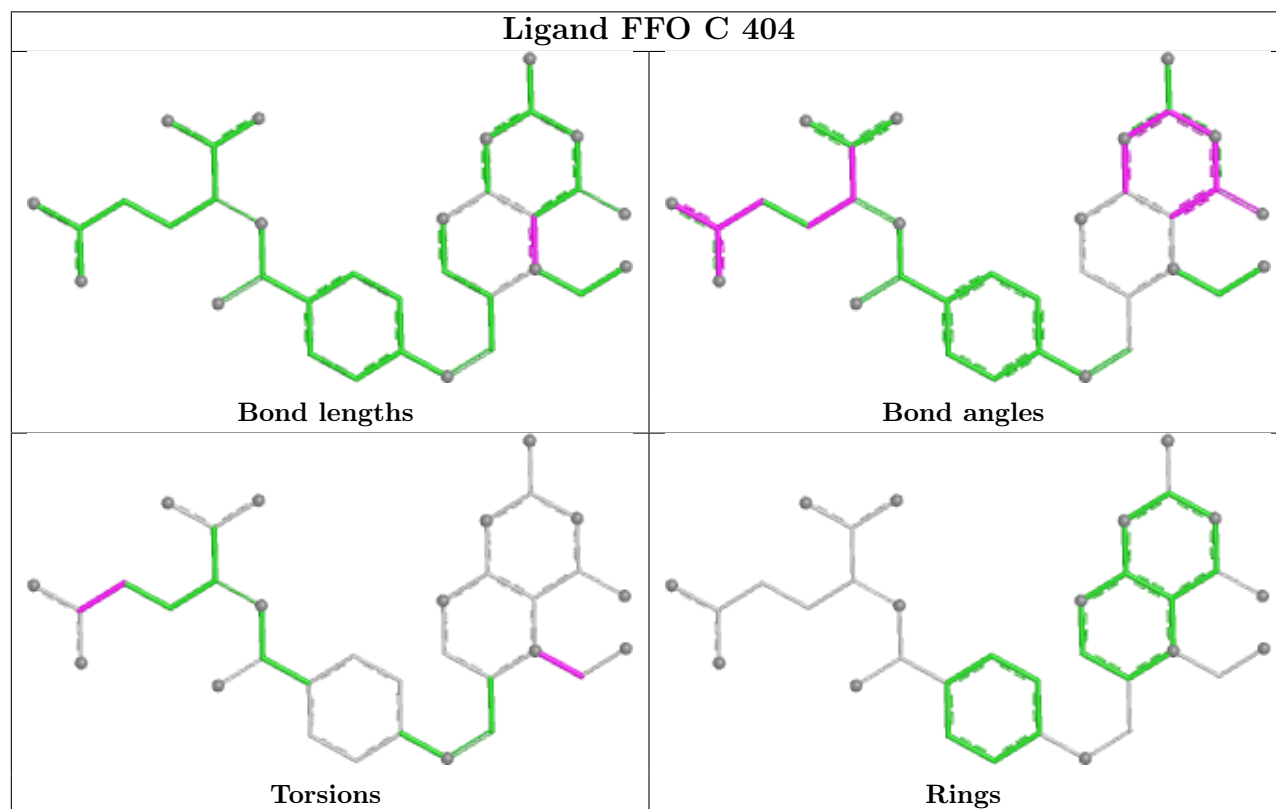
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	SO4	1	0
4	C	404	FFO	5	0
3	A	401	SO4	2	0
4	H	403	FFO	2	0
3	H	401	SO4	1	0
4	A	403	FFO	4	0
4	D	403	FFO	3	0

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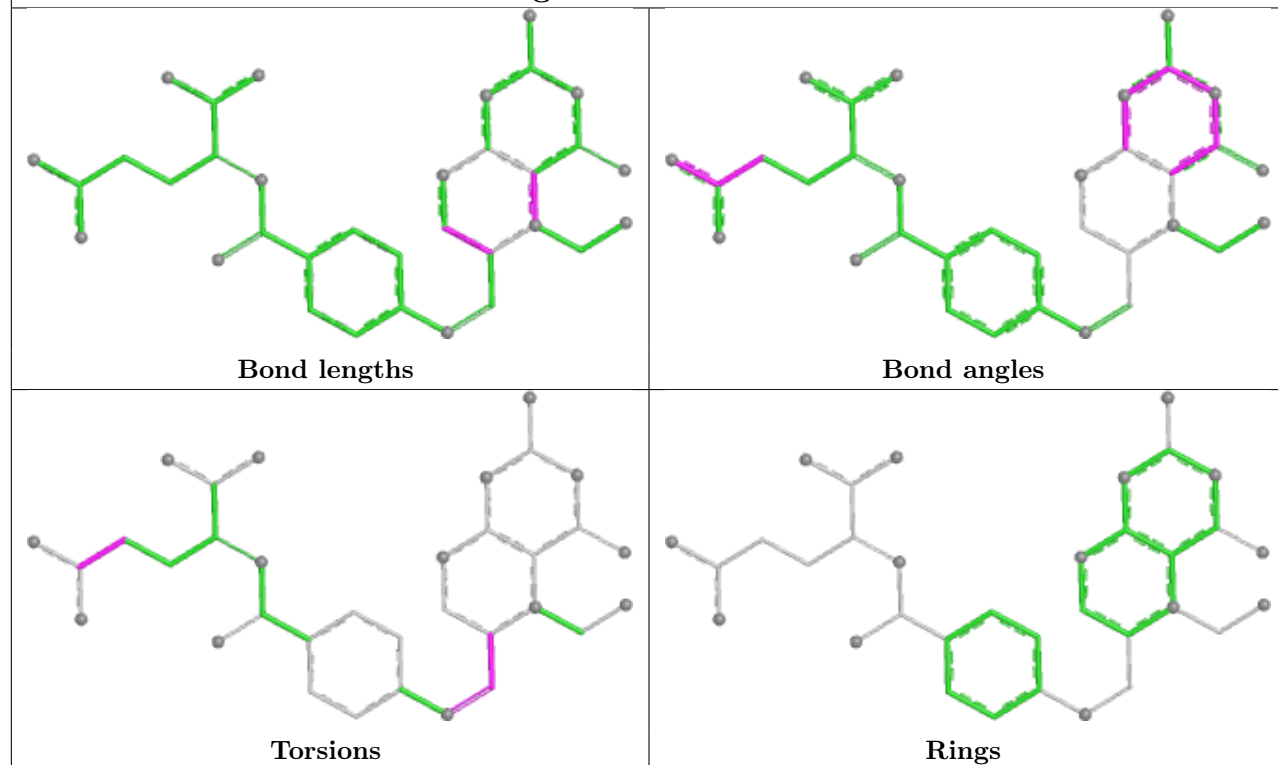
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	FFO	7	0
4	G	403	FFO	2	0
4	E	403	FFO	6	0

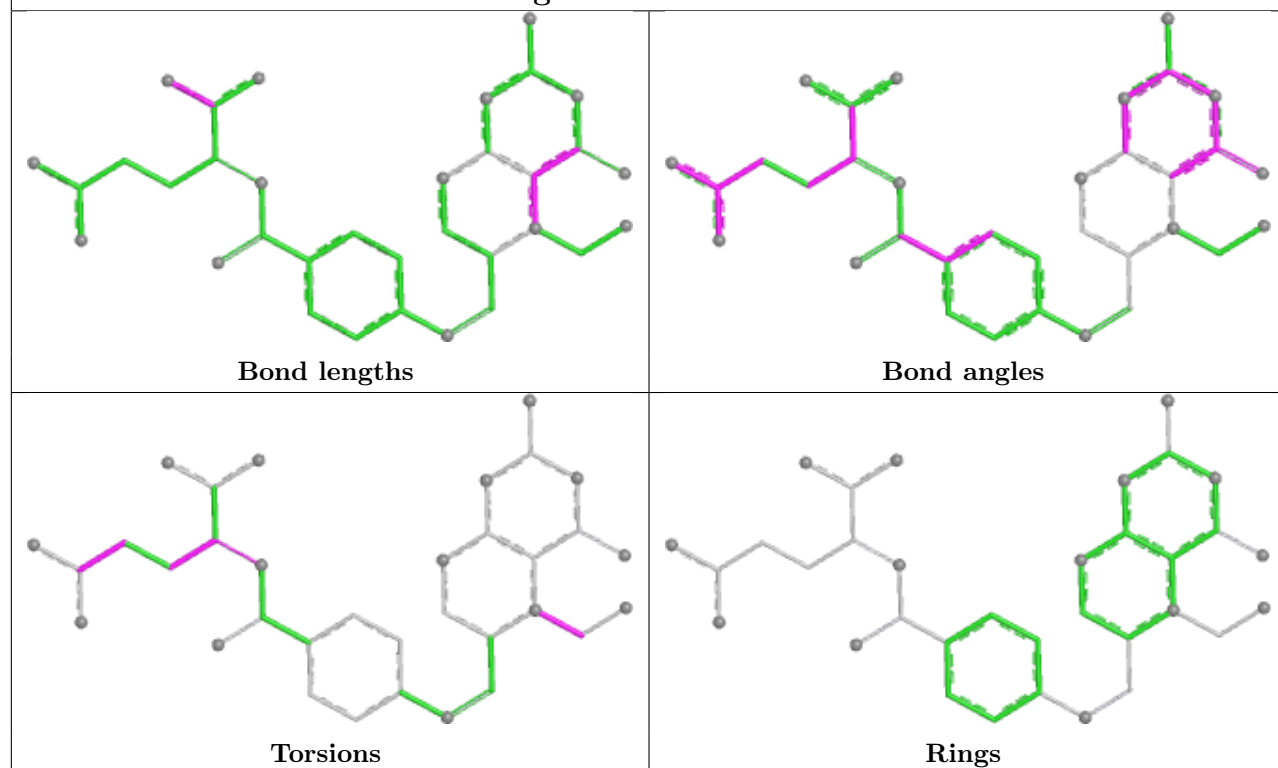
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

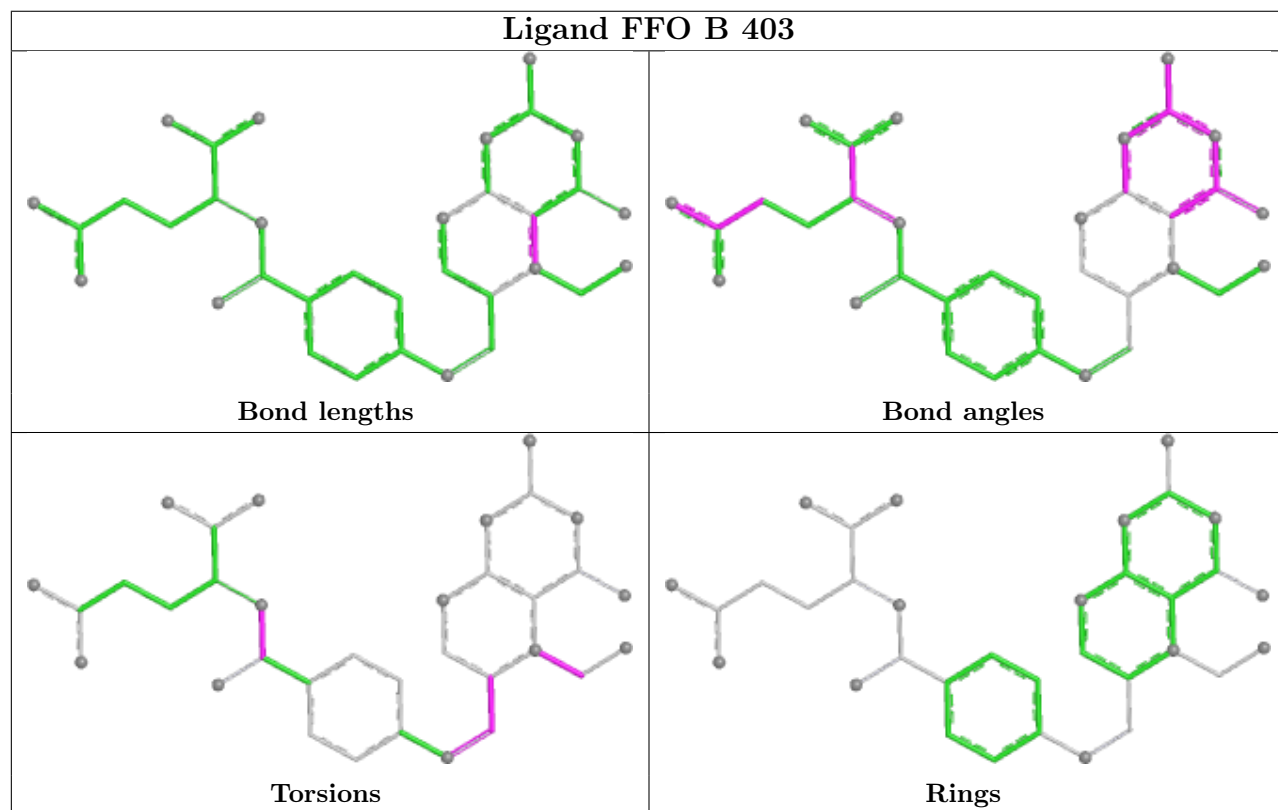
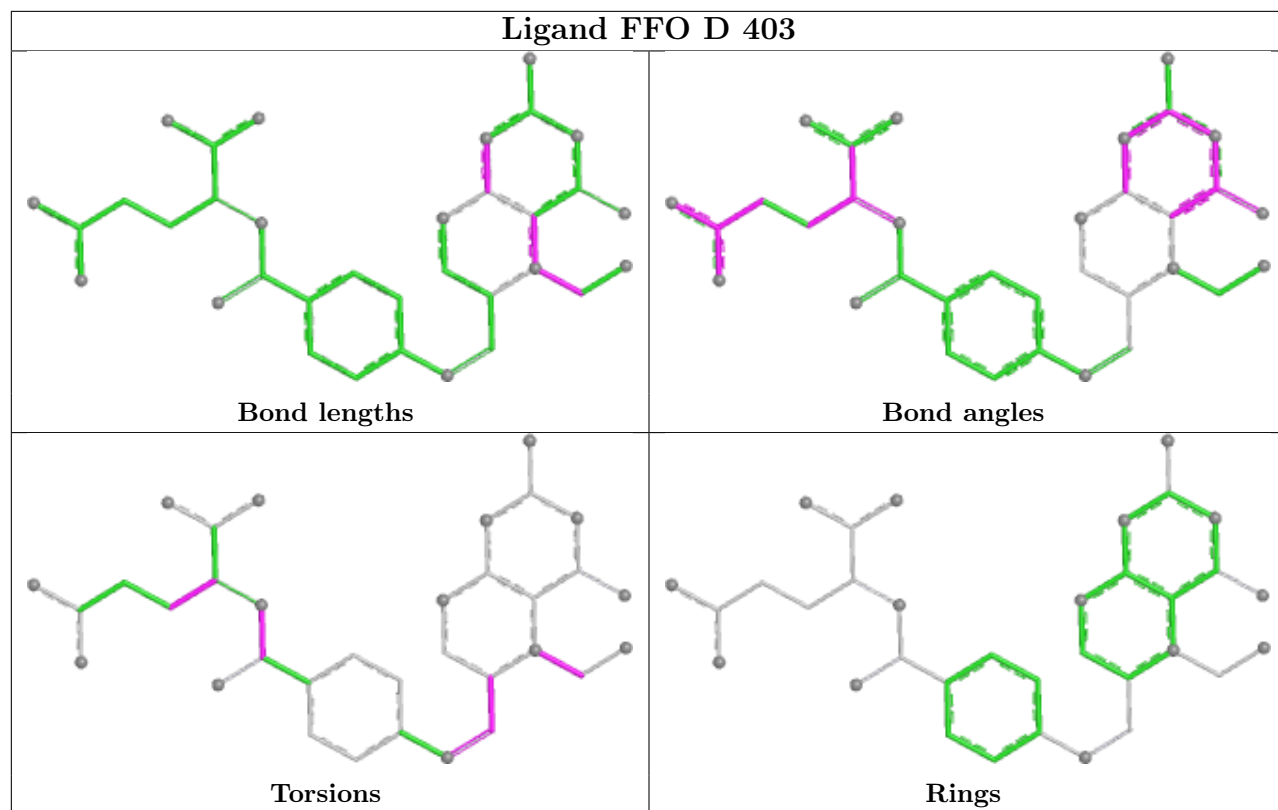


Ligand FFO H 403

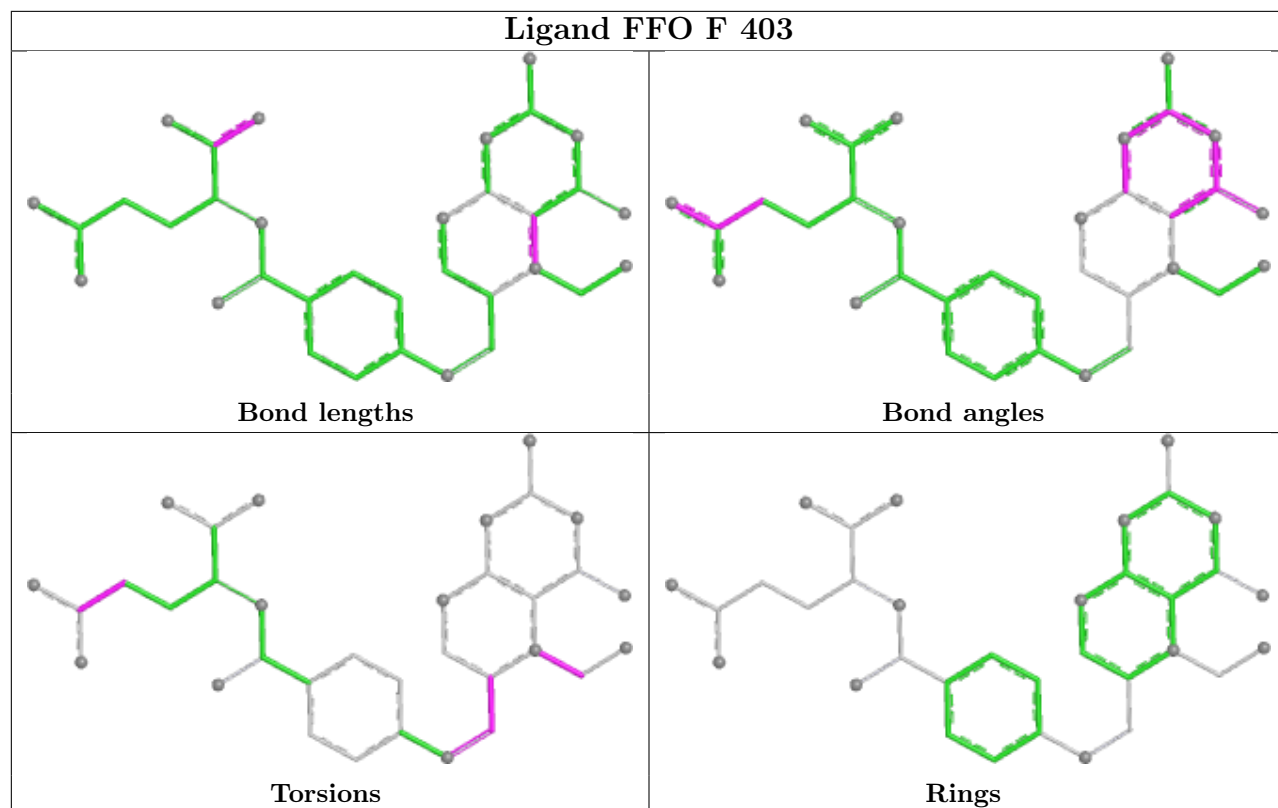


Ligand FFO A 403

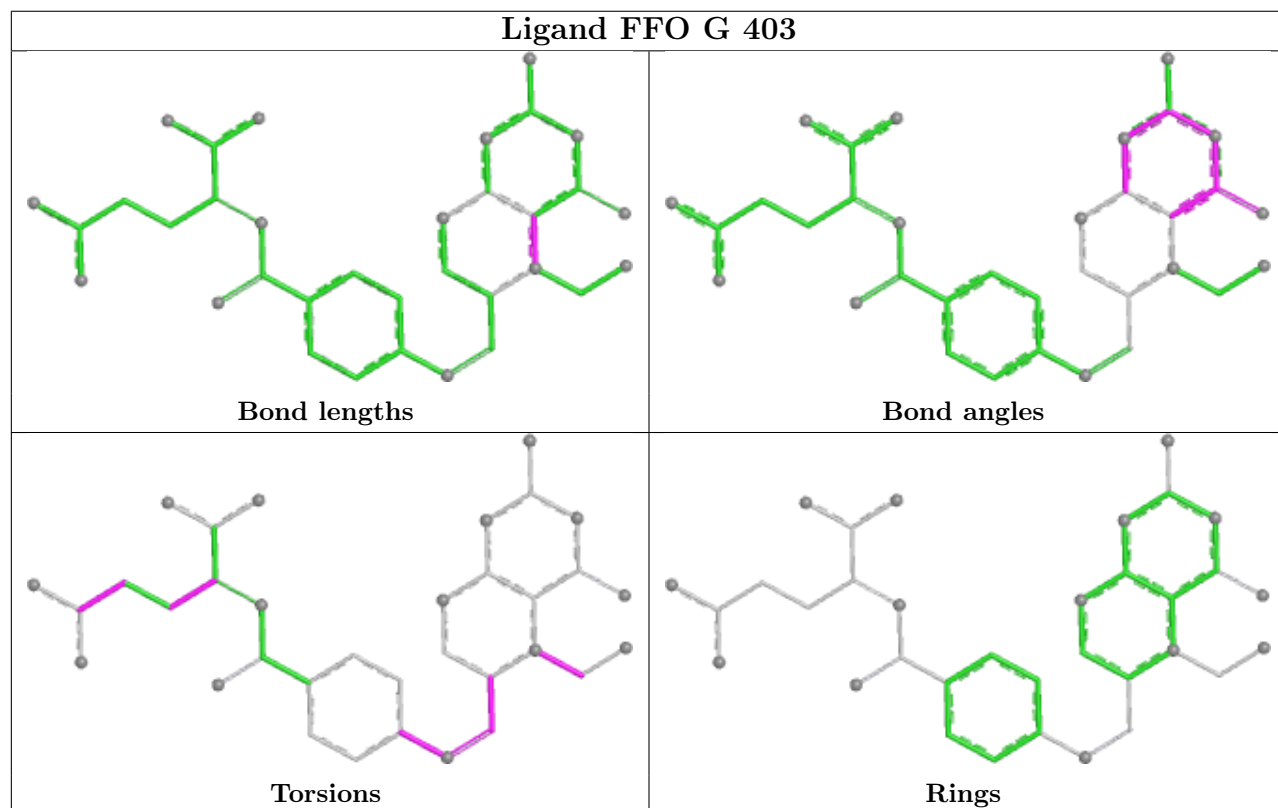


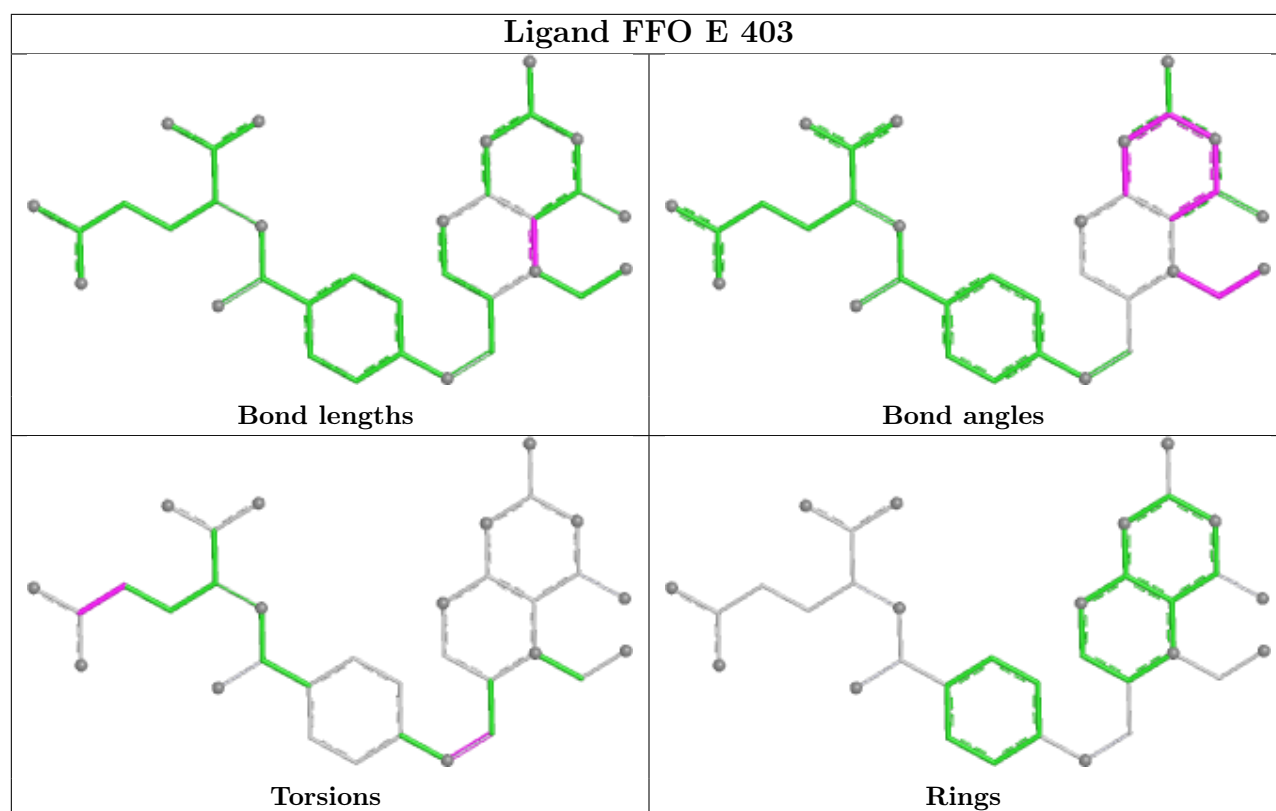


Ligand FFO F 403



Ligand FFO G 403





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	286/325 (88%)	-0.12	6 (2%) 63 64	26, 42, 67, 117	0
1	B	287/325 (88%)	-0.00	5 (1%) 69 69	26, 41, 67, 99	0
1	C	286/325 (88%)	-0.39	2 (0%) 84 86	24, 38, 62, 94	0
1	D	286/325 (88%)	-0.13	7 (2%) 59 61	25, 40, 66, 95	1 (0%)
1	F	286/325 (88%)	-0.17	7 (2%) 59 61	25, 40, 63, 108	0
1	H	286/325 (88%)	0.14	10 (3%) 47 48	27, 46, 73, 116	0
2	E	286/325 (88%)	-0.08	4 (1%) 73 74	25, 41, 69, 92	0
2	G	286/325 (88%)	-0.09	3 (1%) 79 80	26, 45, 71, 90	0
All	All	2289/2600 (88%)	-0.10	44 (1%) 66 66	24, 42, 68, 117	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	26	PRO	6.6
1	D	26	PRO	5.6
1	A	26	PRO	4.8
1	C	26	PRO	4.8
1	F	26	PRO	4.7
2	E	313	VAL	4.0
2	E	26	PRO	3.7
1	B	25	ARG	3.6
2	G	26	PRO	3.4
1	F	46	ARG	3.3
1	A	206	SER	3.3
1	D	145[A]	GLU	3.2
1	F	59	PHE	3.1
1	B	310	GLU	3.1
1	F	150	GLU	2.9
1	H	284	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	173	ASP	2.8
1	H	66	SER	2.7
1	F	135	TYR	2.7
1	C	205	ASN	2.7
1	A	125	THR	2.7
1	H	313	VAL	2.6
1	D	64	ARG	2.6
1	H	50	ARG	2.5
1	F	100	GLU	2.4
1	B	198	LEU	2.4
1	H	125	THR	2.4
1	D	124	SER	2.4
1	D	310	GLU	2.4
1	B	93	LYS	2.4
1	D	313	VAL	2.4
1	H	42	ARG	2.3
2	G	313	VAL	2.3
1	H	310	GLU	2.3
2	G	286	GLU	2.3
2	E	124	SER	2.3
1	A	205	ASN	2.2
1	B	171	ASN	2.1
1	D	42	ARG	2.1
1	H	127	GLU	2.1
1	A	313	VAL	2.1
1	H	150	GLU	2.1
1	F	293	ALA	2.0
2	E	127	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	F	43	10/11	0.87	0.16	30,35,53,53	0
2	SCH	E	43	8/9	0.91	0.14	37,40,81,90	0
1	CME	F	195	10/11	0.93	0.13	41,52,68,80	0
1	CME	D	43	10/11	0.94	0.12	33,41,76,76	0
1	CME	C	43	10/11	0.94	0.13	39,52,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CME	E	195	10/11	0.94	0.12	42,53,64,73	0
1	CME	H	195	10/11	0.95	0.12	45,50,71,76	0
1	CME	A	43	10/11	0.95	0.11	40,50,75,76	0
1	CME	H	43	10/11	0.95	0.11	34,36,48,51	0
2	SCH	G	43	8/9	0.95	0.13	35,38,63,65	0
2	CME	G	195	10/11	0.95	0.11	42,51,72,89	0
1	CME	C	195	10/11	0.96	0.09	35,48,59,74	0
1	CME	B	43	10/11	0.96	0.11	38,47,83,90	0
1	CME	B	195	10/11	0.97	0.10	36,47,80,82	0
1	CME	D	195	10/11	0.97	0.08	36,44,55,69	0
1	CME	A	195	10/11	0.97	0.09	34,44,63,69	0

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
6	GOL	H	404	6/6	0.70	0.21	64,71,86,87	0
6	GOL	D	404	6/6	0.82	0.15	52,63,66,67	0
3	SO4	H	402	5/5	0.84	0.20	96,101,106,119	0
3	SO4	F	402	5/5	0.87	0.11	87,93,103,108	0
3	SO4	A	402	5/5	0.87	0.11	91,92,98,108	0
3	SO4	C	403	5/5	0.88	0.17	78,85,89,96	0
3	SO4	G	402	5/5	0.91	0.13	63,63,69,73	0
3	SO4	D	402	5/5	0.92	0.15	70,72,75,80	0
5	CL	B	404	1/1	0.93	0.09	51,51,51,51	0
3	SO4	E	402	5/5	0.93	0.10	65,68,74,81	0
4	FFO	A	403	34/34	0.93	0.09	36,40,48,53	0
5	CL	E	404	1/1	0.94	0.10	47,47,47,47	0
5	CL	G	404	1/1	0.94	0.08	52,52,52,52	0
5	CL	A	404	1/1	0.94	0.10	55,55,55,55	0
4	FFO	D	403	34/34	0.94	0.09	26,39,44,47	0
4	FFO	G	403	34/34	0.95	0.09	35,48,54,64	0
3	SO4	B	402	5/5	0.95	0.10	66,70,74,79	0

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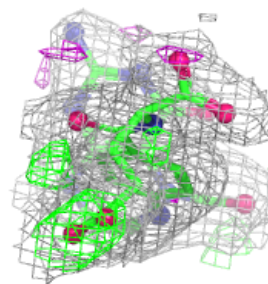
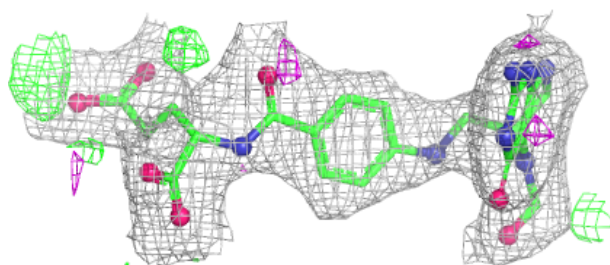
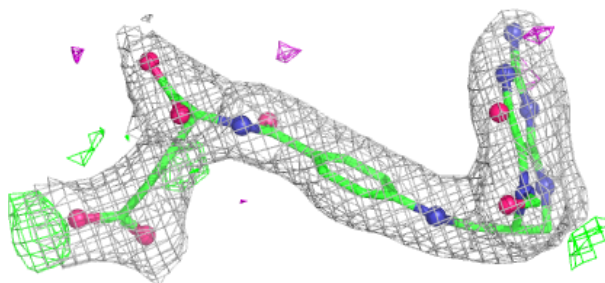
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	D	406	1/1	0.95	0.07	53,53,53,53	0
4	FFO	B	403	34/34	0.95	0.08	33,41,46,46	0
4	FFO	E	403	34/34	0.96	0.08	34,43,55,64	0
3	SO4	D	401	5/5	0.96	0.08	50,59,65,66	0
4	FFO	F	403	34/34	0.96	0.07	30,37,45,58	0
5	CL	C	405	1/1	0.96	0.07	48,48,48,48	0
4	FFO	H	403	34/34	0.96	0.07	34,45,54,69	0
5	CL	A	405	1/1	0.97	0.08	49,49,49,49	0
4	FFO	C	404	34/34	0.97	0.06	30,38,44,45	0
3	SO4	A	401	5/5	0.98	0.07	24,27,35,35	0
3	SO4	B	401	5/5	0.98	0.07	35,37,42,43	0
3	SO4	G	401	5/5	0.98	0.08	36,45,48,50	0
5	CL	D	405	1/1	0.98	0.10	54,54,54,54	0
3	SO4	H	401	5/5	0.98	0.07	34,38,39,41	0
3	SO4	C	401	5/5	0.99	0.06	27,32,35,36	0
3	SO4	F	401	5/5	0.99	0.05	31,32,33,34	0
3	SO4	E	401	5/5	0.99	0.07	42,44,52,53	0
3	SO4	C	402	5/5	0.99	0.07	33,34,39,40	0

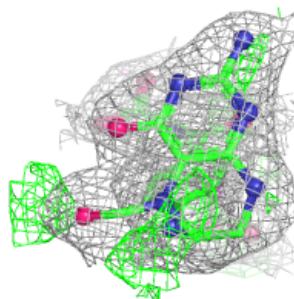
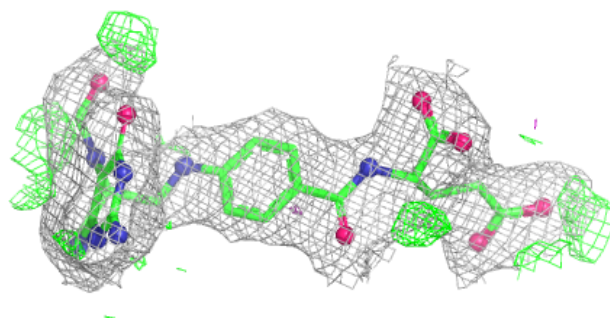
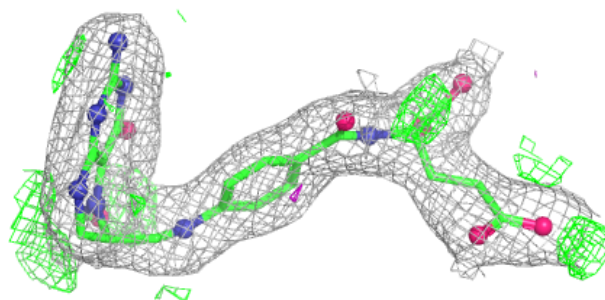
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FFO A 403:

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

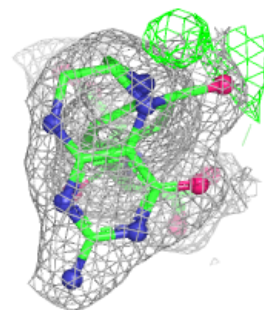
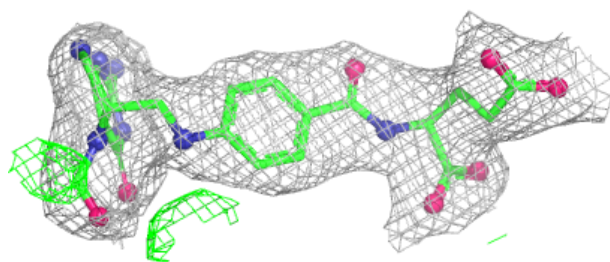
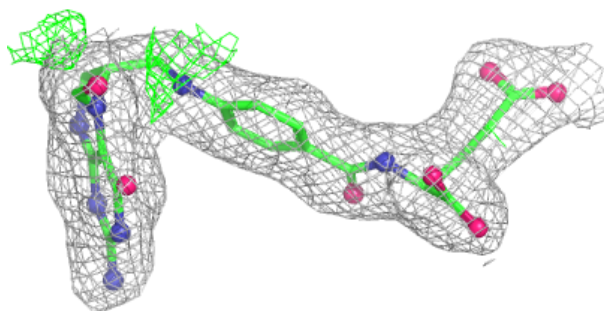
**Electron density around FFO D 403:**

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

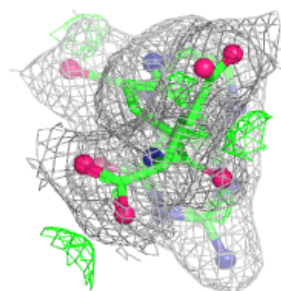
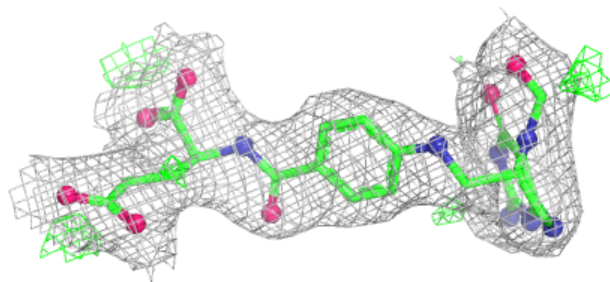
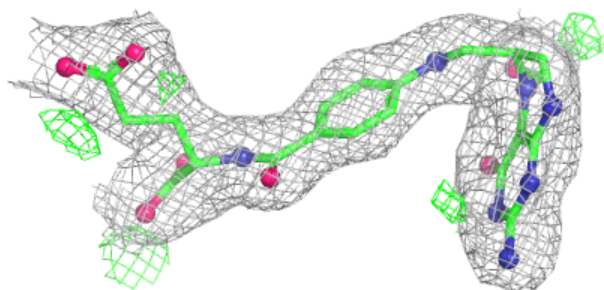


Electron density around FFO G 403:

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

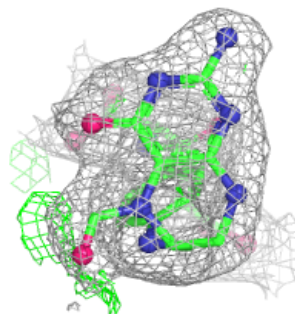
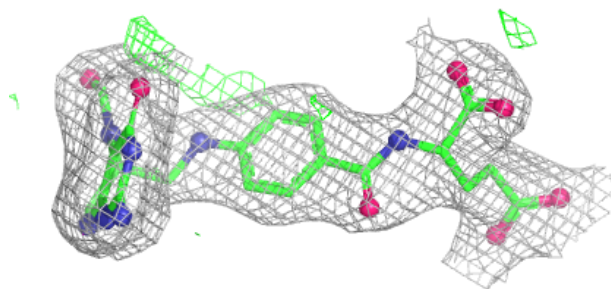
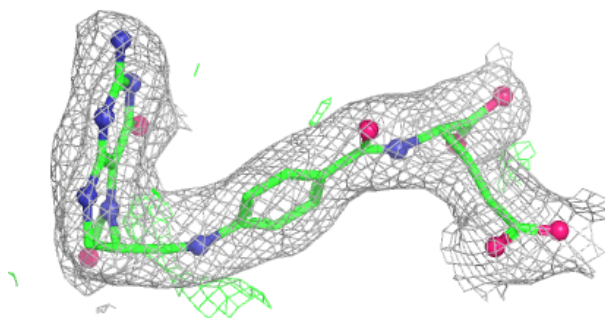
**Electron density around FFO B 403:**

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

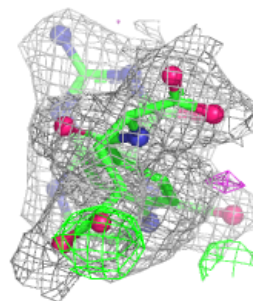
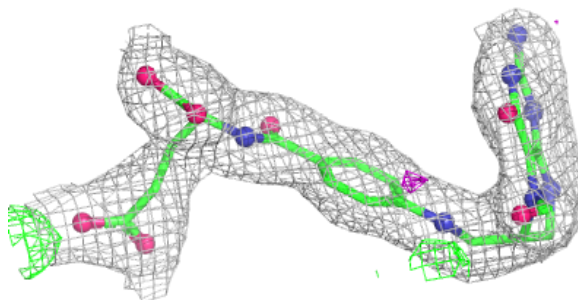


Electron density around FFO E 403:

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

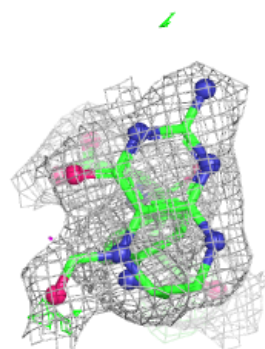
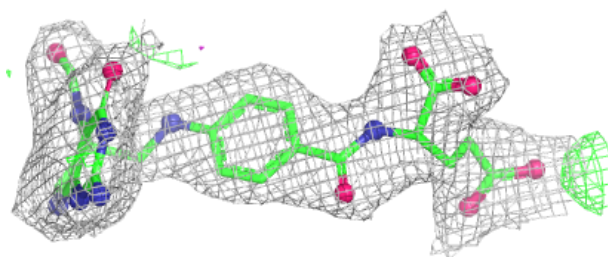
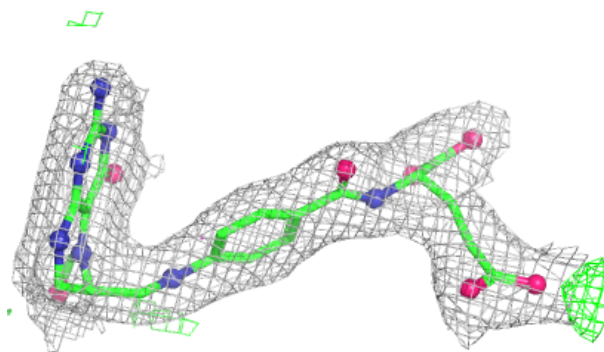
**Electron density around FFO F 403:**

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

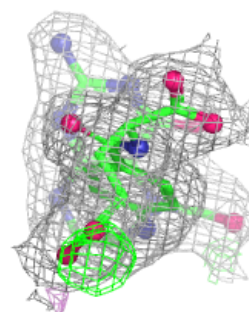
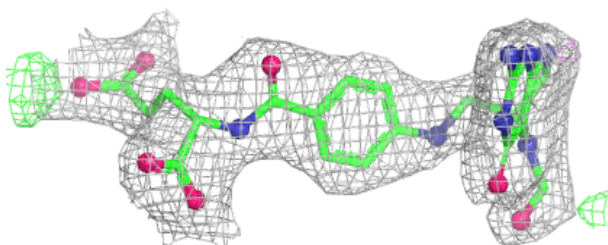
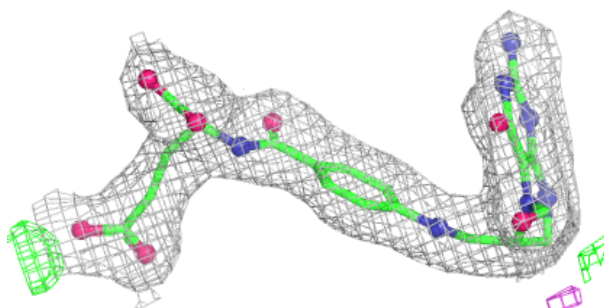


Electron density around FFO H 403:

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

**Electron density around FFO C 404:**

$2mF_o-DF_c$ (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.