



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 PM UTC

PDB ID : 9HIC / pdb_00009hic
Title : K166 acetylated human muscle pyruvate kinase, isoform M2 (PKM2), in complex with FBP
Authors : Pavlenko, D.; Nudelman, H.; Shahar, A.; Arbely, E.
Deposited on : 2024-11-25
Resolution : 2.90 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

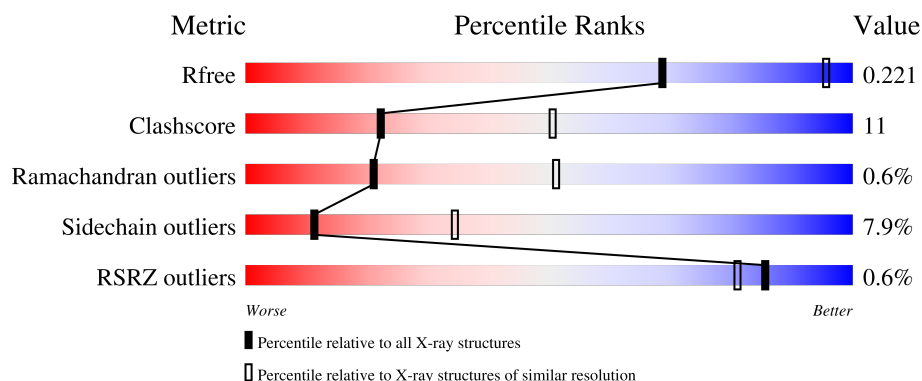
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	537	<div> <div></div> <div>71%22%...</div> </div>
1	B	537	<div> <div>%</div> <div>68%24%...</div> </div>
1	C	537	<div> <div>%</div> <div>67%24%...</div> </div>
1	D	537	<div> <div></div> <div>66%22%6%..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16087 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	1	0
			4006	2518	715	748	25			
1	B	518	Total	C	N	O	S	0	1	0
			3978	2500	708	745	25			
1	C	519	Total	C	N	O	S	0	2	0
			3993	2513	710	745	25			
1	D	518	Total	C	N	O	S	0	1	0
			3978	2500	708	745	25			

There are 24 discrepancies between the modelled and reference sequences:

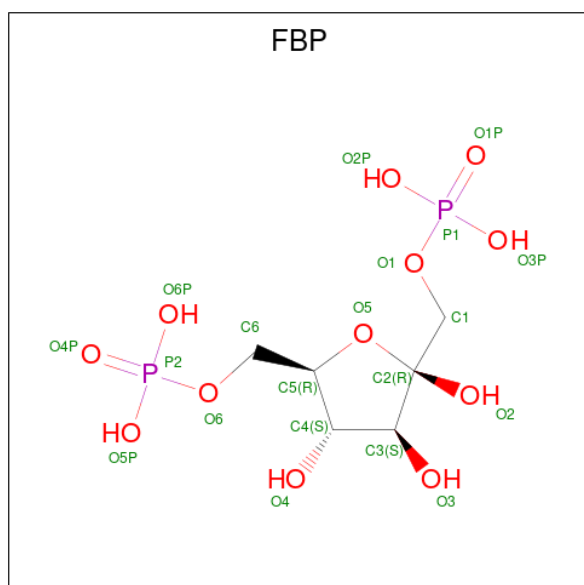
Chain	Residue	Modelled	Actual	Comment	Reference
A	532	HIS	-	expression tag	UNP P14618
A	533	HIS	-	expression tag	UNP P14618
A	534	HIS	-	expression tag	UNP P14618
A	535	HIS	-	expression tag	UNP P14618
A	536	HIS	-	expression tag	UNP P14618
A	537	HIS	-	expression tag	UNP P14618
B	532	HIS	-	expression tag	UNP P14618
B	533	HIS	-	expression tag	UNP P14618
B	534	HIS	-	expression tag	UNP P14618
B	535	HIS	-	expression tag	UNP P14618
B	536	HIS	-	expression tag	UNP P14618
B	537	HIS	-	expression tag	UNP P14618
C	532	HIS	-	expression tag	UNP P14618
C	533	HIS	-	expression tag	UNP P14618
C	534	HIS	-	expression tag	UNP P14618
C	535	HIS	-	expression tag	UNP P14618
C	536	HIS	-	expression tag	UNP P14618
C	537	HIS	-	expression tag	UNP P14618
D	532	HIS	-	expression tag	UNP P14618
D	533	HIS	-	expression tag	UNP P14618
D	534	HIS	-	expression tag	UNP P14618

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	535	HIS	-	expression tag	UNP P14618
D	536	HIS	-	expression tag	UNP P14618
D	537	HIS	-	expression tag	UNP P14618

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	Mg 2	0	0

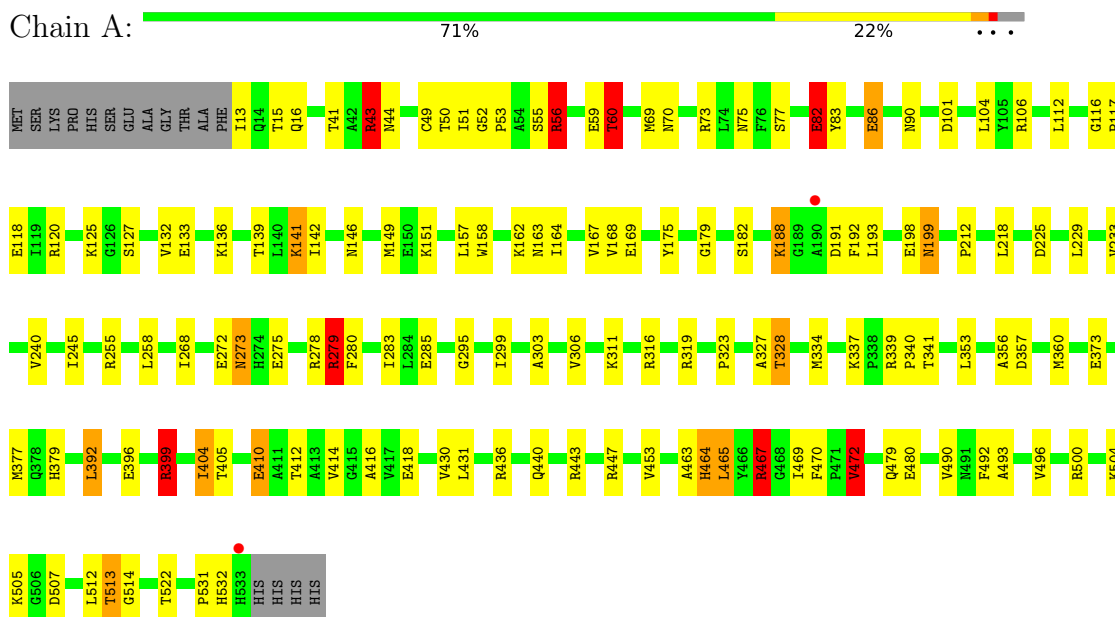
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	16	Total 16	O 16	0	0
4	C	6	Total 6	O 6	0	0
4	D	4	Total 4	O 4	0	0

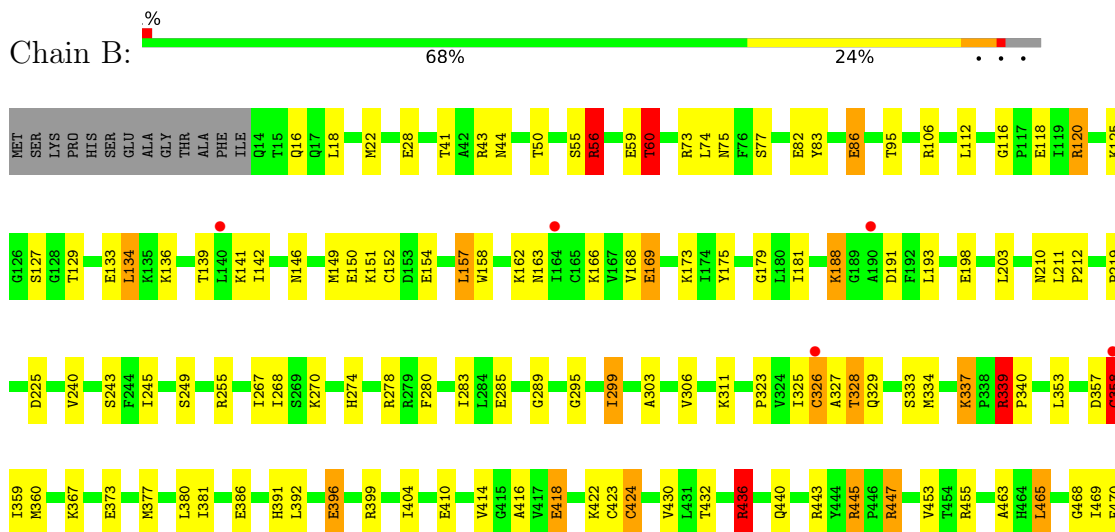
3 Residue-property plots

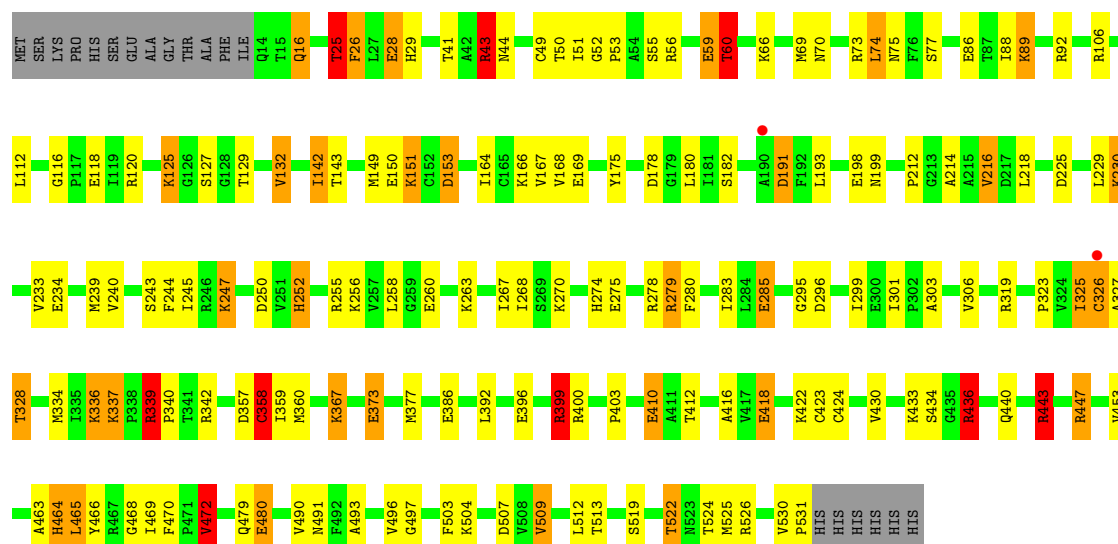
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.00Å 147.23Å 97.97Å 90.00° 103.72° 90.00°	Depositor
Resolution (Å)	49.38 – 2.90 49.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.38-2.90) 99.9 (49.38-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.197 , 0.252 (Not available) , 0.221	Depositor DCC
R_{free} test set	2326 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16087	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, MG, ALY

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	0.71	1/4059 (0.0%)	1.47	44/5482 (0.8%)
1	B	0.69	0/4029	1.45	42/5441 (0.8%)
1	C	0.68	0/4052	1.50	49/5472 (0.9%)
1	D	0.67	0/4029	1.49	56/5441 (1.0%)
All	All	0.69	1/16169 (0.0%)	1.48	191/21836 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	5
1	D	0	11
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	ARG	NE-CZ	5.20	1.38	1.33

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	CYS	CB-CA-C	-12.61	82.69	110.19
1	B	358	CYS	CB-CA-C	-12.50	82.94	110.19
1	D	358	CYS	CB-CA-C	-12.40	83.16	110.19
1	C	263	LYS	CB-CG-CD	10.84	136.23	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	10.37	128.54	119.20
1	A	43	ARG	NE-CZ-NH1	-10.37	111.13	121.50
1	C	487	ASP	CA-CB-CG	10.26	122.86	112.60
1	A	399	ARG	CA-CB-CG	9.81	133.73	114.10
1	A	470	PHE	CB-CA-C	-9.77	101.65	110.44
1	C	383	ARG	CG-CD-NE	9.15	132.14	112.00
1	D	198	GLU	CB-CG-CD	8.82	127.60	112.60
1	C	516	ARG	N-CA-CB	-8.81	101.84	111.10
1	C	263	LYS	CG-CD-CE	8.72	131.36	111.30
1	D	43	ARG	NE-CZ-NH2	-8.72	111.35	119.20
1	D	43	ARG	CD-NE-CZ	8.64	136.49	124.40
1	A	15	THR	CA-CB-OG1	-8.63	96.66	109.60
1	A	399	ARG	CB-CA-C	8.49	124.88	110.79
1	A	399	ARG	CB-CG-CD	8.43	130.69	111.30
1	B	516	ARG	N-CA-CB	-8.33	97.01	111.17
1	A	240	VAL	N-CA-CB	-8.32	99.93	111.41
1	D	132	VAL	N-CA-CB	-8.26	98.57	112.44
1	B	339	ARG	CG-CD-NE	-8.11	94.16	112.00
1	D	339	ARG	CD-NE-CZ	8.03	135.63	124.40
1	C	28	GLU	CB-CG-CD	7.93	126.08	112.60
1	D	326	CYS	N-CA-CB	-7.93	98.79	110.84
1	C	240	VAL	N-CA-CB	-7.86	100.57	111.41
1	B	240	VAL	N-CA-CB	-7.82	100.62	111.41
1	A	43	ARG	CD-NE-CZ	7.80	135.32	124.40
1	B	28	GLU	CB-CG-CD	7.73	125.74	112.60
1	D	339	ARG	CG-CD-NE	-7.72	95.03	112.00
1	D	240	VAL	N-CA-CB	-7.47	101.10	111.41
1	B	299	ILE	N-CA-C	-7.43	105.53	112.96
1	A	465	LEU	N-CA-CB	-7.41	97.37	110.42
1	A	500	ARG	CB-CG-CD	7.37	128.24	111.30
1	C	480	GLU	CB-CG-CD	7.36	125.11	112.60
1	B	465	LEU	N-CA-CB	-7.30	97.56	110.42
1	D	399[A]	ARG	CB-CA-C	7.25	124.58	110.67
1	D	399[B]	ARG	CB-CA-C	7.25	124.58	110.67
1	D	28	GLU	CB-CG-CD	7.21	124.86	112.60
1	A	532	HIS	CA-CB-CG	7.17	120.97	113.80
1	A	60	THR	CA-CB-OG1	-7.08	98.98	109.60
1	C	285	GLU	CB-CA-C	7.03	122.46	110.79
1	D	465	LEU	N-CA-CB	-7.02	98.07	110.42
1	A	82	GLU	CB-CG-CD	7.00	124.50	112.60
1	B	285	GLU	CB-CA-C	6.93	122.30	110.79
1	D	443	ARG	CG-CD-NE	6.89	127.16	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	THR	N-CA-CB	-6.80	99.97	110.85
1	D	299	ILE	N-CA-C	-6.80	106.16	112.96
1	C	299	ILE	N-CA-C	-6.78	106.18	112.96
1	B	139	THR	CA-CB-OG1	-6.78	99.43	109.60
1	D	252	HIS	CB-CA-C	6.77	122.36	110.85
1	C	445	ARG	NE-CZ-NH1	-6.76	114.74	121.50
1	C	150	GLU	CB-CG-CD	6.69	123.97	112.60
1	B	141	LYS	CG-CD-CE	6.66	126.63	111.30
1	A	285	GLU	CB-CA-C	6.62	121.79	110.79
1	C	465	LEU	N-CA-CB	-6.57	98.86	110.42
1	C	82	GLU	CB-CG-CD	6.57	123.76	112.60
1	C	60	THR	CA-CB-OG1	-6.56	99.76	109.60
1	A	255	ARG	NE-CZ-NH1	-6.55	114.95	121.50
1	D	336	LYS	N-CA-CB	6.50	119.70	110.67
1	A	106	ARG	CD-NE-CZ	6.46	133.44	124.40
1	B	326	CYS	N-CA-CB	-6.39	100.45	110.87
1	D	247	LYS	CA-CB-CG	6.38	126.87	114.10
1	A	405	THR	CA-CB-OG1	-6.38	100.04	109.60
1	C	516	ARG	CD-NE-CZ	6.35	133.29	124.40
1	B	60	THR	CA-CB-OG1	-6.32	100.11	109.60
1	C	373	GLU	CB-CA-C	6.26	122.69	110.67
1	B	447	ARG	CG-CD-NE	6.25	125.75	112.00
1	C	319	ARG	CD-NE-CZ	6.25	133.15	124.40
1	A	141	LYS	CG-CD-CE	6.24	125.65	111.30
1	A	414	VAL	N-CA-CB	6.18	118.94	110.54
1	A	299	ILE	N-CA-C	-6.18	106.78	112.96
1	D	60	THR	CA-CB-OG1	-6.17	100.35	109.60
1	A	272	GLU	CB-CG-CD	6.16	123.06	112.60
1	B	418	GLU	CB-CG-CD	6.16	123.06	112.60
1	A	278	ARG	CD-NE-CZ	6.10	132.94	124.40
1	B	396	GLU	CB-CG-CD	6.08	122.94	112.60
1	C	414	VAL	N-CA-CB	6.08	118.81	110.54
1	D	373	GLU	CB-CG-CD	6.04	122.88	112.60
1	A	464	HIS	CA-CB-CG	-6.01	107.79	113.80
1	C	143	THR	CA-CB-OG1	-5.99	100.62	109.60
1	D	373	GLU	CB-CA-C	5.97	120.69	110.79
1	D	296	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	325	ILE	CA-C-N	5.96	131.32	122.86
1	D	325	ILE	C-N-CA	5.96	131.32	122.86
1	D	43	ARG	NE-CZ-NH1	5.94	127.44	121.50
1	B	472	VAL	N-CA-CB	-5.94	103.20	111.99
1	C	236	ASP	CA-CB-CG	5.90	118.50	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	GLU	CB-CG-CD	5.90	122.63	112.60
1	C	86	GLU	CB-CG-CD	5.89	122.61	112.60
1	A	56	ARG	CA-CB-CG	5.88	125.85	114.10
1	B	526	ARG	CG-CD-NE	5.88	124.93	112.00
1	A	233	VAL	N-CA-CB	5.87	117.02	110.62
1	B	373	GLU	CB-CA-C	5.87	121.93	110.67
1	C	15	THR	CA-CB-OG1	-5.86	100.81	109.60
1	B	447	ARG	CA-CB-CG	5.85	125.81	114.10
1	D	422	LYS	CB-CG-CD	5.84	124.72	111.30
1	D	336	LYS	CA-CB-CG	5.79	125.68	114.10
1	A	162	LYS	CB-CG-CD	5.77	124.57	111.30
1	D	25	THR	CB-CA-C	5.77	119.92	109.37
1	B	169	GLU	CB-CG-CD	5.72	122.33	112.60
1	D	367	LYS	CB-CG-CD	5.72	124.46	111.30
1	D	447	ARG	CA-CB-CG	5.72	125.54	114.10
1	C	219	PRO	CB-CA-C	5.71	118.49	111.12
1	B	133	GLU	CB-CA-C	5.70	119.58	109.72
1	D	66	LYS	CG-CD-CE	5.66	124.33	111.30
1	D	491	ASN	CA-CB-CG	-5.66	106.94	112.60
1	D	89	LYS	CG-CD-CE	5.66	124.31	111.30
1	A	56	ARG	CB-CA-C	-5.65	98.50	110.31
1	C	410	GLU	CB-CG-CD	-5.64	103.00	112.60
1	B	414	VAL	N-CA-CB	5.63	118.19	110.54
1	B	445	ARG	CG-CD-NE	-5.62	99.63	112.00
1	A	132	VAL	N-CA-CB	5.62	121.88	112.44
1	C	154	GLU	CB-CG-CD	5.61	122.14	112.60
1	C	326	CYS	CB-CA-C	-5.61	103.26	111.23
1	B	498	LYS	CG-CD-CE	5.61	124.20	111.30
1	B	447	ARG	CD-NE-CZ	5.61	132.25	124.40
1	D	470	PHE	CA-CB-CG	-5.60	108.20	113.80
1	C	291	MET	CG-SD-CE	5.57	113.16	100.90
1	D	230	LYS	CB-CA-C	5.57	120.03	110.79
1	C	490	VAL	N-CA-CB	5.57	117.06	110.55
1	D	436	ARG	CD-NE-CZ	5.54	132.16	124.40
1	C	472	VAL	N-CA-CB	-5.52	103.82	111.99
1	D	59	GLU	CB-CA-C	5.52	120.06	110.68
1	D	422	LYS	CG-CD-CE	-5.51	98.62	111.30
1	B	56	ARG	CA-CB-CG	5.51	125.13	114.10
1	C	133	GLU	CB-CA-C	5.51	119.25	109.72
1	A	188	LYS	CA-CB-CG	5.50	125.11	114.10
1	B	154	GLU	N-CA-CB	5.50	118.85	110.44
1	A	470	PHE	CA-CB-CG	-5.49	108.31	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	VAL	N-CA-CB	5.47	116.95	110.55
1	C	337	LYS	CB-CG-CD	5.46	123.85	111.30
1	C	532	HIS	CA-CB-CG	5.45	119.25	113.80
1	C	132	VAL	N-CA-CB	-5.43	103.32	112.44
1	D	16	GLN	N-CA-CB	-5.43	104.00	112.41
1	D	25	THR	CA-CB-OG1	5.43	117.74	109.60
1	A	279	ARG	CG-CD-NE	5.42	123.93	112.00
1	B	149	MET	CB-CG-SD	-5.42	96.45	112.70
1	A	436	ARG	CB-CA-C	5.39	119.33	110.88
1	A	280	PHE	CA-CB-CG	-5.36	108.44	113.80
1	D	464	HIS	CA-CB-CG	-5.36	108.44	113.80
1	A	133	GLU	CB-CG-CD	5.36	121.71	112.60
1	B	436	ARG	N-CA-CB	5.34	117.89	109.94
1	D	522	THR	OG1-CB-CG2	5.33	119.96	109.30
1	A	472	VAL	N-CA-CB	-5.31	104.13	111.99
1	B	280	PHE	CA-CB-CG	-5.30	108.50	113.80
1	D	509	VAL	N-CA-CB	-5.30	102.55	112.36
1	B	470	PHE	CA-CB-CG	-5.29	108.51	113.80
1	C	152	CYS	CB-CA-C	-5.28	101.64	110.19
1	C	326	CYS	N-CA-CB	-5.27	101.83	110.95
1	D	472	VAL	N-CA-CB	-5.27	104.19	111.99
1	B	219	PRO	CB-CA-C	5.27	117.92	111.12
1	C	470	PHE	CA-CB-CG	-5.26	108.54	113.80
1	D	234	GLU	CB-CG-CD	5.25	121.53	112.60
1	C	509	VAL	N-CA-CB	-5.24	102.66	112.36
1	C	319	ARG	CB-CA-C	5.24	119.76	110.85
1	B	56	ARG	CG-CD-NE	-5.24	100.48	112.00
1	D	153	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	490	VAL	N-CA-CB	5.22	116.65	110.55
1	D	280	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	188	LYS	N-CA-CB	-5.20	102.93	110.84
1	C	339	ARG	CG-CD-NE	-5.20	100.56	112.00
1	C	139	THR	CA-CB-OG1	-5.18	101.83	109.60
1	B	516	ARG	CA-CB-CG	5.17	124.45	114.10
1	A	443	ARG	CG-CD-NE	5.17	123.37	112.00
1	C	418	GLU	CB-CG-CD	5.17	121.39	112.60
1	D	191	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	95	THR	CA-CB-OG1	-5.10	101.95	109.60
1	C	233	VAL	N-CA-CB	5.10	116.52	110.55
1	D	26	PHE	N-CA-CB	5.10	117.71	110.06
1	B	455	ARG	N-CA-C	-5.10	107.11	113.38
1	B	152	CYS	CB-CA-C	-5.09	101.95	110.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ARG	CD-NE-CZ	5.09	131.52	124.40
1	A	404	ILE	CA-CB-CG1	5.08	119.04	110.40
1	C	424	CYS	CB-CA-C	5.08	120.03	112.06
1	D	216	VAL	N-CA-CB	5.06	116.05	110.53
1	C	464	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	373	GLU	CB-CA-C	5.06	119.45	110.85
1	B	56	ARG	CB-CA-C	-5.05	99.44	109.99
1	B	491	ASN	CA-CB-CG	-5.04	107.56	112.60
1	A	139	THR	CA-CB-OG1	-5.03	102.05	109.60
1	A	319	ARG	CD-NE-CZ	5.03	131.45	124.40
1	B	521	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	418	GLU	CG-CD-OE1	-5.02	106.86	118.40
1	B	418	GLU	CB-CA-C	-5.02	102.78	110.81
1	D	151	LYS	CB-CG-CD	5.02	122.84	111.30
1	D	339	ARG	O-C-N	-5.02	117.49	121.80
1	D	490	VAL	N-CA-CB	5.01	116.07	110.51
1	B	43	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	C	504	LYS	CB-CG-CD	5.01	122.81	111.30
1	D	74	LEU	CB-CG-CD1	-5.01	95.68	110.70

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ARG	Sidechain
1	A	316	ARG	Sidechain
1	A	43	ARG	Sidechain
1	A	467	ARG	Sidechain
1	A	56	ARG	Sidechain
1	B	106	ARG	Sidechain
1	B	339	ARG	Sidechain
1	B	358	CYS	Peptide
1	B	56	ARG	Sidechain
1	C	214	ALA	Peptide
1	C	339	ARG	Sidechain
1	C	358	CYS	Peptide
1	C	516	ARG	Sidechain
1	C	56	ARG	Sidechain
1	D	106	ARG	Sidechain
1	D	278	ARG	Sidechain
1	D	279	ARG	Sidechain
1	D	319	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	339	ARG	Sidechain
1	D	342	ARG	Sidechain
1	D	358	CYS	Peptide
1	D	399[A]	ARG	Sidechain
1	D	400	ARG	Sidechain
1	D	43	ARG	Sidechain
1	D	443	ARG	Sidechain

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	4006	0	4087	72	0
1	B	3978	0	4059	104	0
1	C	3993	0	4077	92	0
1	D	3978	0	4058	105	0
2	A	20	0	10	1	0
2	B	20	0	10	2	0
2	C	20	0	10	1	0
2	D	20	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	21	0	0	0	0
4	B	16	0	0	0	0
4	C	6	0	0	0	0
4	D	4	0	0	0	0
All	All	16087	0	16321	342	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 11.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ILE:HA	1:C:358:CYS:SG	1.65	1.36
1:B:325:ILE:HA	1:B:358:CYS:SG	1.65	1.35
1:D:325:ILE:HA	1:D:358:CYS:SG	1.65	1.34
1:B:326:CYS:SG	1:B:359:ILE:HA	1.87	1.15
1:C:326:CYS:SG	1:C:359:ILE:HA	1.88	1.14
1:D:326:CYS:SG	1:D:359:ILE:HA	1.87	1.13
1:C:150:GLU:HG3	1:D:252:HIS:CB	1.84	1.08
1:C:150:GLU:HG3	1:D:252:HIS:HB3	1.14	1.07
1:B:418:GLU:OE2	1:D:399[B]:ARG:HD2	1.58	1.04
1:B:525:MET:HE3	1:D:525:MET:HE3	1.40	1.00
1:D:125:LYS:HE3	1:D:153:ASP:HB3	1.49	0.95
1:C:325:ILE:CA	1:C:358:CYS:SG	2.56	0.93
1:C:150:GLU:CG	1:D:252:HIS:HB3	1.99	0.91
1:B:325:ILE:CA	1:B:358:CYS:SG	2.57	0.91
1:B:358:CYS:SG	1:B:358:CYS:O	2.30	0.89
1:B:418:GLU:OE1	1:D:399[A]:ARG:HD3	1.72	0.89
1:C:358:CYS:SG	1:C:358:CYS:O	2.30	0.89
1:D:325:ILE:CA	1:D:358:CYS:SG	2.58	0.89
1:D:358:CYS:SG	1:D:358:CYS:O	2.31	0.88
1:A:101:ASP:OD2	1:A:104:LEU:HD13	1.73	0.87
1:B:173:LYS:HE2	1:B:175:TYR:OH	1.76	0.84
1:A:356:ALA:O	1:A:467:ARG:NH1	2.09	0.84
1:C:150:GLU:HG3	1:D:252:HIS:CG	2.12	0.84
1:C:26:PHE:HE2	1:C:30:MET:HE3	1.40	0.83
1:A:175:TYR:CE2	1:A:212:PRO:HG3	2.15	0.81
1:B:418:GLU:HG3	1:D:418:GLU:HG3	1.64	0.80
1:C:323:PRO:HA	1:C:357:ASP:OD1	1.81	0.79
1:B:323:PRO:HA	1:B:357:ASP:OD1	1.82	0.79
1:C:175:TYR:CE2	1:C:212:PRO:HG3	2.19	0.77
1:D:175:TYR:CE2	1:D:212:PRO:HG3	2.19	0.77
1:B:268:ILE:HD12	1:B:289:GLY:HA3	1.66	0.76
1:B:418:GLU:CG	1:D:418:GLU:HG3	2.17	0.74
1:C:405:THR:HG21	1:C:410:GLU:OE2	1.87	0.73
1:B:422:LYS:HE3	1:D:403:PRO:O	1.90	0.72
1:A:472:VAL:HG21	1:A:496:VAL:HG11	1.74	0.70
1:B:418:GLU:OE2	1:D:399[B]:ARG:CD	2.39	0.69
1:D:125:LYS:HE3	1:D:153:ASP:CB	2.22	0.69
1:D:164:ILE:O	1:D:168:VAL:HG22	1.93	0.69
1:B:396:GLU:HG2	1:D:399[A]:ARG:HH21	1.59	0.68
1:B:118:GLU:OE1	1:B:120:ARG:HD2	1.94	0.68
1:B:494:MET:HE3	1:B:531:PRO:HD3	1.76	0.67
1:B:418:GLU:HG3	1:D:418:GLU:CG	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:PRO:HB3	1:C:465:LEU:O	1.95	0.67
1:C:221:VAL:HG13	1:C:225:ASP:HB3	1.76	0.66
1:D:323:PRO:HB3	1:D:465:LEU:O	1.95	0.66
1:B:323:PRO:HB3	1:B:465:LEU:O	1.95	0.66
1:C:118:GLU:OE1	1:C:120:ARG:HD2	1.95	0.66
1:A:164:ILE:O	1:A:168:VAL:HG22	1.95	0.66
1:A:323:PRO:HB3	1:A:465:LEU:O	1.95	0.65
1:B:479:GLN:HG2	1:B:480:GLU:HB2	1.77	0.65
1:A:43:ARG:HD3	1:A:379:HIS:ND1	2.11	0.65
1:B:163:ASN:HD22	1:B:166:ALY:HD3	1.62	0.65
1:A:118:GLU:OE1	1:A:120:ARG:HD2	1.98	0.64
1:C:117:PRO:HB2	1:C:218:LEU:HD13	1.80	0.64
1:D:118:GLU:OE1	1:D:120:ARG:HD2	1.97	0.64
1:A:268:ILE:HD11	1:A:465:LEU:HD21	1.79	0.63
1:A:279:ARG:HG2	1:A:279:ARG:HH21	1.64	0.63
1:D:285:GLU:OE2	1:D:285:GLU:HA	1.98	0.63
1:D:275:GLU:HG2	1:D:279:ARG:HD2	1.81	0.62
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.80	0.62
1:B:326:CYS:N	1:B:358:CYS:SG	2.72	0.61
1:D:326:CYS:SG	1:D:359:ILE:CA	2.79	0.61
1:B:422:LYS:HD3	1:D:399[B]:ARG:HH11	1.65	0.61
1:B:422:LYS:HD2	1:D:399[B]:ARG:NH1	2.16	0.61
1:C:326:CYS:N	1:C:358:CYS:SG	2.74	0.61
1:A:472:VAL:HG13	1:A:492:PHE:CE2	2.36	0.60
1:D:326:CYS:N	1:D:358:CYS:SG	2.75	0.60
1:C:326:CYS:SG	1:C:358:CYS:O	2.60	0.60
1:D:396:GLU:HG2	1:D:399[A]:ARG:NH2	2.17	0.60
1:C:168:VAL:HG11	1:C:185:VAL:HG21	1.83	0.59
1:D:88:ILE:CG2	1:D:92:ARG:HH11	2.16	0.59
1:A:396:GLU:HG2	1:A:399:ARG:NH2	2.18	0.59
1:C:472:VAL:HG13	1:C:492:PHE:CE2	2.38	0.59
1:A:353:LEU:CD1	1:B:311:LYS:HE2	2.33	0.59
1:B:326:CYS:SG	1:B:358:CYS:O	2.61	0.59
1:D:268:ILE:HD11	1:D:465:LEU:HD21	1.84	0.59
1:A:16:GLN:HG2	1:A:447[B]:ARG:HH21	1.66	0.59
1:D:25:THR:HG23	1:D:28:GLU:HB2	1.85	0.59
1:B:418:GLU:CD	1:D:399[B]:ARG:HD2	2.26	0.59
1:C:148:TYR:OH	1:D:263:LYS:HD3	2.03	0.59
1:B:268:ILE:CD1	1:B:289:GLY:HA3	2.33	0.58
1:D:472:VAL:HG21	1:D:496:VAL:HG11	1.84	0.58
1:B:157:LEU:HG	1:B:203:LEU:HD21	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:VAL:HG21	1:C:496:VAL:HG11	1.85	0.58
1:B:327:ALA:HB1	1:B:360:MET:HE2	1.86	0.58
1:D:326:CYS:SG	1:D:358:CYS:O	2.62	0.58
1:B:472:VAL:HG13	1:B:492:PHE:CE2	2.38	0.57
1:B:422:LYS:CD	1:D:399[B]:ARG:NH1	2.67	0.57
1:C:123:LEU:HD23	1:C:205:SER:HB3	1.86	0.57
1:A:273:ASN:N	1:A:273:ASN:HD22	2.02	0.57
1:C:126:GLY:HA2	1:D:256:LYS:HE3	1.87	0.57
1:B:326:CYS:SG	1:B:359:ILE:CA	2.79	0.57
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.87	0.57
1:A:341:THR:HA	1:B:329:GLN:OE1	2.04	0.57
1:C:410:GLU:HG3	1:C:440:GLN:NE2	2.20	0.56
1:B:136:LYS:HG3	1:B:198:GLU:O	2.05	0.56
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.86	0.56
1:C:326:CYS:SG	1:C:359:ILE:CA	2.79	0.56
1:D:25:THR:HG23	1:D:28:GLU:CB	2.36	0.56
1:B:396:GLU:HG2	1:D:399[A]:ARG:NH2	2.20	0.56
1:D:410:GLU:HG3	1:D:440:GLN:NE2	2.21	0.56
1:A:182:SER:HB3	1:A:199:ASN:HB2	1.88	0.55
1:C:303:ALA:O	1:C:306:VAL:HG23	2.07	0.55
1:B:274:HIS:HD2	1:B:278:ARG:HE	1.55	0.55
1:C:26:PHE:CE2	1:C:30:MET:HE3	2.32	0.55
1:C:325:ILE:HG12	1:C:358:CYS:HB3	1.88	0.55
1:C:327:ALA:HB1	1:C:360:MET:HE2	1.89	0.55
1:B:422:LYS:CD	1:D:399[B]:ARG:HH11	2.19	0.55
1:D:325:ILE:HG12	1:D:358:CYS:HB3	1.88	0.55
1:A:191:ASP:OD2	1:A:192:PHE:HD1	1.90	0.55
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.88	0.55
1:C:433:LYS:HE3	2:C:601:FBP:O5P	2.06	0.55
1:A:340:PRO:HG3	1:A:377:MET:HG2	1.89	0.55
1:B:325:ILE:HG12	1:B:358:CYS:HB3	1.89	0.54
1:D:51:ILE:HD11	1:D:69:MET:HE1	1.89	0.54
1:A:275:GLU:HG2	1:A:279:ARG:HD3	1.89	0.54
1:B:73:ARG:C	1:B:74:LEU:HD12	2.33	0.54
1:C:453:VAL:CG2	1:C:493:ALA:HB2	2.38	0.54
1:A:175:TYR:CD2	1:A:212:PRO:HG3	2.42	0.54
1:D:436:ARG:NH2	1:D:519:SER:OG	2.41	0.54
1:A:136:LYS:HG2	1:A:198:GLU:O	2.06	0.53
1:C:136:LYS:HG3	1:C:198:GLU:O	2.07	0.53
1:B:479:GLN:HE21	1:B:480:GLU:HB2	1.74	0.53
1:C:463:ALA:HB1	1:C:469:ILE:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:HIS:HD2	1:B:278:ARG:NE	2.06	0.53
1:D:327:ALA:HB1	1:D:360:MET:HE2	1.90	0.53
1:A:51:ILE:HD11	1:A:69:MET:CE	2.39	0.53
1:C:268:ILE:HD11	1:C:465:LEU:HD21	1.89	0.53
1:A:51:ILE:HD11	1:A:69:MET:HE1	1.90	0.53
1:B:118:GLU:CD	1:B:120:ARG:HH11	2.16	0.53
1:B:268:ILE:HD12	1:B:289:GLY:CA	2.37	0.53
1:D:51:ILE:HD11	1:D:69:MET:CE	2.40	0.52
1:D:175:TYR:CD2	1:D:212:PRO:HG3	2.44	0.52
1:B:175:TYR:CD2	1:B:179:GLY:HA2	2.44	0.52
1:B:418:GLU:HG2	1:D:418:GLU:HG3	1.90	0.52
1:D:50:THR:HA	1:D:73:ARG:HB3	1.92	0.52
1:B:50:THR:HA	1:B:73:ARG:HB3	1.92	0.52
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.91	0.52
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.40	0.52
1:C:295:GLY:CA	1:C:328:THR:HG21	2.40	0.52
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.92	0.52
1:B:56:ARG:NH2	1:B:83:TYR:O	2.43	0.51
1:B:173:LYS:CE	1:B:175:TYR:OH	2.55	0.51
1:D:334:MET:HA	1:D:337:LYS:O	2.11	0.51
1:A:56:ARG:NH2	1:A:83:TYR:O	2.43	0.51
1:B:134:LEU:HD21	1:B:203:LEU:HB2	1.92	0.51
1:C:50:THR:HA	1:C:73:ARG:HB3	1.91	0.51
1:B:357:ASP:OD2	1:B:445:ARG:NH1	2.44	0.51
1:A:334:MET:HA	1:A:337:LYS:O	2.11	0.51
1:C:51:ILE:HD11	1:C:69:MET:CE	2.40	0.51
1:A:50:THR:HA	1:A:73:ARG:HB3	1.92	0.51
1:C:175:TYR:CD2	1:C:212:PRO:HG3	2.46	0.50
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.93	0.50
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.42	0.50
1:B:56:ARG:HH22	1:B:86:GLU:HB3	1.76	0.50
1:D:167:VAL:HG12	1:D:167:VAL:O	2.11	0.50
1:C:221:VAL:HG13	1:C:225:ASP:CB	2.40	0.50
1:A:56:ARG:HH22	1:A:86:GLU:HB3	1.76	0.50
1:C:56:ARG:NH2	1:C:83:TYR:O	2.45	0.50
1:D:239:MET:HE2	1:D:465:LEU:HD22	1.92	0.50
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.94	0.50
1:C:73:ARG:C	1:C:74:LEU:HD12	2.37	0.50
1:B:134:LEU:CD2	1:B:203:LEU:HB2	2.42	0.50
1:D:239:MET:CE	1:D:465:LEU:HD22	2.42	0.50
1:D:434:SER:OG	1:D:436:ARG:HD3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:HIS:CD2	1:B:278:ARG:HE	2.30	0.50
1:A:16:GLN:HG2	1:A:447[B]:ARG:NH2	2.26	0.50
1:B:334:MET:HA	1:B:337:LYS:O	2.11	0.50
1:D:430:VAL:HG22	1:D:512:LEU:HD12	1.94	0.49
1:B:295:GLY:CA	1:B:328:THR:HG21	2.42	0.49
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.95	0.49
1:C:334:MET:HA	1:C:337:LYS:O	2.11	0.49
1:C:405:THR:HG23	1:C:407:ASP:H	1.77	0.49
1:C:74:LEU:HD21	1:C:88:ILE:HG13	1.94	0.49
1:D:260:GLU:HG3	1:D:263:LYS:CE	2.43	0.49
1:D:453:VAL:HG21	1:D:493:ALA:HB2	1.95	0.49
1:A:167:VAL:O	1:A:167:VAL:HG22	2.13	0.49
1:C:270:LYS:HE3	1:C:291:MET:HE3	1.94	0.49
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.95	0.48
1:D:245:ILE:HG22	1:D:283:ILE:HD13	1.95	0.48
1:C:51:ILE:HD11	1:C:69:MET:HE1	1.95	0.48
1:D:260:GLU:HG3	1:D:263:LYS:HE3	1.95	0.48
1:A:49:CYS:HB2	1:A:69:MET:HE3	1.95	0.48
1:D:49:CYS:HB2	1:D:69:MET:HE3	1.94	0.48
1:D:326:CYS:SG	1:D:326:CYS:O	2.71	0.48
1:D:75:ASN:OD1	1:D:77:SER:HB2	2.14	0.48
1:A:295:GLY:CA	1:A:328:THR:HG21	2.42	0.48
1:A:323:PRO:HA	1:A:357:ASP:OD2	2.13	0.48
1:A:430:VAL:HG22	1:A:512:LEU:HD12	1.96	0.48
1:C:49:CYS:HB2	1:C:69:MET:HE3	1.96	0.48
1:C:116:GLY:HA2	1:C:225:ASP:OD2	2.14	0.48
1:B:399[A]:ARG:NE	1:D:418:GLU:OE2	2.35	0.48
1:D:295:GLY:CA	1:D:328:THR:HG21	2.43	0.48
1:B:377:MET:HE3	1:B:381:ILE:HD11	1.96	0.47
1:B:432:THR:HA	2:B:601:FBP:H12	1.96	0.47
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.43	0.47
1:A:16:GLN:HG2	1:A:16:GLN:O	2.15	0.47
1:B:399[A]:ARG:HE	1:D:418:GLU:CD	2.21	0.47
1:D:463:ALA:HB1	1:D:469:ILE:HG21	1.95	0.47
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.96	0.47
1:C:142:ILE:HB	1:C:193:LEU:HB2	1.96	0.47
1:C:86:GLU:O	1:C:86:GLU:HG3	2.08	0.47
1:A:16:GLN:O	1:A:447[B]:ARG:NH2	2.48	0.47
1:A:70:ASN:HB3	1:A:464:HIS:CD2	2.50	0.47
1:A:90:ASN:HD22	1:A:90:ASN:N	2.12	0.47
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ILE:HG22	1:C:283:ILE:HD13	1.97	0.47
1:A:142:ILE:HB	1:A:193:LEU:HB2	1.97	0.47
1:B:526:ARG:HG3	1:D:524:THR:HG23	1.96	0.47
1:A:396:GLU:HG2	1:A:399:ARG:HH21	1.78	0.46
1:B:127:SER:C	1:B:129:THR:H	2.23	0.46
1:B:430:VAL:HG22	1:B:512:LEU:HD12	1.97	0.46
1:D:16:GLN:HG2	1:D:16:GLN:O	2.15	0.46
1:A:75:ASN:OD1	1:A:77:SER:HB2	2.14	0.46
1:B:399[A]:ARG:HD3	1:D:418:GLU:OE1	2.16	0.46
1:C:123:LEU:HD12	1:C:150:GLU:OE1	2.16	0.46
1:D:182:SER:HB3	1:D:199:ASN:HD22	1.80	0.46
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.98	0.46
1:B:514:GLY:N	2:B:601:FBP:O4	2.48	0.46
1:C:326:CYS:SG	1:C:326:CYS:O	2.74	0.46
1:A:149:MET:HG2	1:A:158:TRP:CE2	2.50	0.46
1:A:410:GLU:OE2	1:A:440:GLN:NE2	2.48	0.46
1:D:142:ILE:HB	1:D:193:LEU:HB2	1.98	0.46
1:A:191:ASP:OD2	1:A:192:PHE:CD1	2.68	0.46
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.98	0.46
1:B:18:LEU:O	1:B:22:MET:HG2	2.15	0.46
1:C:430:VAL:HG22	1:C:512:LEU:HD12	1.98	0.46
1:D:229:LEU:HD22	1:D:258:LEU:HD21	1.97	0.46
1:D:323:PRO:HA	1:D:357:ASP:OD2	2.15	0.46
1:C:168:VAL:CG1	1:C:185:VAL:HG21	2.46	0.45
1:B:243:SER:HA	1:B:270:LYS:HD3	1.98	0.45
1:A:82:GLU:H	1:A:82:GLU:CD	2.24	0.45
1:C:243:SER:HA	1:C:270:LYS:HD3	1.98	0.45
1:C:453:VAL:HG21	1:C:493:ALA:HB2	1.97	0.45
1:C:127:SER:C	1:C:129:THR:H	2.24	0.45
1:D:247:LYS:HE2	1:D:250:ASP:OD1	2.17	0.45
1:B:116:GLY:HA2	1:B:225:ASP:OD2	2.17	0.45
1:B:326:CYS:SG	1:B:326:CYS:O	2.74	0.45
1:C:146:ASN:HD22	1:C:158:TRP:HE1	1.64	0.45
1:A:514:GLY:HA3	2:A:601:FBP:O4	2.16	0.45
1:D:112:LEU:C	1:D:112:LEU:HD23	2.42	0.45
1:D:530:VAL:HA	1:D:531:PRO:HD3	1.87	0.45
1:B:523:ASN:O	1:D:526:ARG:HA	2.17	0.45
1:A:311:LYS:HE3	1:B:353:LEU:CD1	2.47	0.44
1:C:112:LEU:C	1:C:112:LEU:HD23	2.42	0.44
1:C:505:LYS:HG2	1:C:531:PRO:O	2.17	0.44
1:A:392:LEU:HD13	1:A:392:LEU:HA	1.67	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:VAL:HG12	1:D:214:ALA:HB1	1.98	0.44
1:A:117:PRO:HB2	1:A:218:LEU:HD13	1.98	0.44
1:B:142:ILE:HB	1:B:193:LEU:HB2	2.00	0.44
1:C:125:LYS:HZ1	1:C:151:LYS:HB2	1.81	0.44
1:A:112:LEU:C	1:A:112:LEU:HD23	2.43	0.44
1:A:146:ASN:HD22	1:A:158:TRP:HE1	1.65	0.44
1:A:339:ARG:HE	1:A:339:ARG:HB2	1.58	0.44
1:D:243:SER:HA	1:D:270:LYS:HD3	2.00	0.44
1:A:245:ILE:HG22	1:A:283:ILE:HD13	2.00	0.43
1:C:82:GLU:CD	1:C:82:GLU:H	2.26	0.43
1:C:505:LYS:HE3	1:C:532:HIS:HA	2.00	0.43
1:A:149:MET:HG2	1:A:158:TRP:CZ2	2.54	0.43
1:B:16:GLN:O	1:B:16:GLN:HG2	2.19	0.43
1:B:463:ALA:HB1	1:B:469:ILE:HG21	2.00	0.43
1:C:423:CYS:O	1:C:424:CYS:C	2.59	0.43
1:A:268:ILE:CD1	1:A:465:LEU:HD11	2.48	0.43
1:B:75:ASN:OD1	1:B:77:SER:HB2	2.18	0.43
1:B:112:LEU:HD23	1:B:112:LEU:C	2.42	0.43
1:C:412:THR:HG22	1:C:512:LEU:HD22	2.00	0.43
1:D:43:ARG:HE	1:D:43:ARG:HB3	1.67	0.43
1:C:270:LYS:HG2	1:C:291:MET:HG2	2.00	0.43
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.99	0.43
1:A:44:ASN:CB	1:A:467:ARG:HD2	2.48	0.43
1:B:436:ARG:HA	1:B:436:ARG:HD2	1.66	0.43
1:A:303:ALA:O	1:A:306:VAL:HG23	2.19	0.43
1:C:367:LYS:HE2	1:C:367:LYS:HB3	1.87	0.43
1:B:188:LYS:HB3	1:B:188:LYS:HE3	1.50	0.43
1:D:116:GLY:HA2	1:D:225:ASP:OD2	2.18	0.43
1:A:273:ASN:HD22	1:A:273:ASN:H	1.65	0.43
1:B:423:CYS:O	1:B:424:CYS:C	2.60	0.43
1:C:157:LEU:HD13	1:C:203:LEU:HD21	2.01	0.43
1:D:127:SER:C	1:D:129:THR:H	2.26	0.43
1:C:168:VAL:HG13	1:C:172:SER:HB2	2.00	0.42
1:C:327:ALA:O	1:C:328:THR:HB	2.18	0.42
1:B:82:GLU:OE1	1:B:82:GLU:N	2.41	0.42
1:B:245:ILE:HG22	1:B:283:ILE:HD13	2.01	0.42
1:D:303:ALA:O	1:D:306:VAL:HG23	2.19	0.42
1:C:339:ARG:HE	1:C:339:ARG:HB2	1.43	0.42
1:D:423:CYS:O	1:D:424:CYS:C	2.63	0.42
1:B:146:ASN:HD22	1:B:158:TRP:HE1	1.66	0.42
1:D:412:THR:HG22	1:D:512:LEU:HD22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:THR:HG22	1:A:512:LEU:HD22	2.02	0.42
1:B:422:LYS:NZ	1:D:410:GLU:HB3	2.34	0.42
1:C:16:GLN:O	1:C:447[B]:ARG:NH2	2.52	0.42
1:B:55:SER:HA	1:B:60:THR:HG21	2.02	0.42
1:B:44:ASN:H	1:B:386:GLU:CD	2.28	0.42
1:C:186:LYS:C	1:C:187:GLN:HG2	2.44	0.42
1:B:339:ARG:HE	1:B:339:ARG:HB2	1.39	0.42
1:D:26:PHE:O	1:D:29:HIS:HB3	2.20	0.42
1:A:55:SER:HA	1:A:60:THR:HG21	2.00	0.42
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.01	0.42
1:B:268:ILE:CD1	1:B:289:GLY:CA	2.96	0.41
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.55	0.41
1:B:530:VAL:HA	1:B:531:PRO:HD3	1.93	0.41
1:C:455:ARG:HH11	1:C:455:ARG:HD2	1.74	0.41
1:A:327:ALA:O	1:A:328:THR:HB	2.19	0.41
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.83	0.41
1:B:410:GLU:HG2	1:B:440:GLN:OE1	2.20	0.41
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.56	0.41
1:A:116:GLY:HA2	1:A:225:ASP:OD2	2.21	0.41
1:C:255:ARG:CZ	1:C:267:ILE:HD12	2.51	0.41
1:D:44:ASN:HB3	1:D:468:GLY:HA2	2.02	0.41
1:B:479:GLN:NE2	1:B:480:GLU:HB2	2.35	0.41
1:D:216:VAL:HG21	1:D:244:PHE:HZ	1.84	0.41
1:C:146:ASN:HD22	1:C:146:ASN:HA	1.65	0.41
1:B:303:ALA:O	1:B:306:VAL:HG23	2.20	0.41
1:C:44:ASN:HB3	1:C:468:GLY:HA2	2.02	0.41
1:C:52:GLY:O	1:C:53:PRO:C	2.64	0.41
1:C:325:ILE:C	1:C:358:CYS:SG	3.04	0.41
1:D:74:LEU:HD11	1:D:88:ILE:CG1	2.50	0.41
1:C:166:ALY:HE2	1:C:166:ALY:HH31	1.80	0.41
1:C:229:LEU:HD22	1:C:258:LEU:HD21	2.01	0.41
1:C:387:ALA:O	1:C:447[B]:ARG:NH2	2.53	0.41
1:B:44:ASN:HB3	1:B:468:GLY:HA2	2.03	0.41
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.51	0.41
1:D:255:ARG:CZ	1:D:267:ILE:HD12	2.51	0.41
1:D:339:ARG:HE	1:D:339:ARG:HB2	1.18	0.41
1:B:337:LYS:HE2	1:B:337:LYS:HB3	1.87	0.41
1:D:52:GLY:O	1:D:53:PRO:C	2.63	0.41
1:B:146:ASN:HD22	1:B:146:ASN:HA	1.68	0.40
1:B:175:TYR:HD2	1:B:179:GLY:HA2	1.85	0.40
1:D:70:ASN:HB3	1:D:464:HIS:CD2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LYS:HE3	1:C:162:LYS:HB3	1.96	0.40
1:C:472:VAL:CG2	1:C:496:VAL:HG11	2.51	0.40
1:D:274:HIS:CE1	1:D:301:ILE:HG22	2.56	0.40
1:A:229:LEU:HD22	1:A:258:LEU:HD21	2.04	0.40
1:B:212:PRO:HB3	1:B:299:ILE:O	2.22	0.40
1:C:44:ASN:H	1:C:386:GLU:CD	2.28	0.40
1:A:52:GLY:O	1:A:53:PRO:C	2.64	0.40
1:B:391:HIS:O	1:B:392:LEU:C	2.63	0.40
1:D:44:ASN:H	1:D:386:GLU:CD	2.29	0.40
1:D:88:ILE:CG2	1:D:92:ARG:NH1	2.84	0.40
1:A:505:LYS:HG2	1:A:531:PRO:O	2.22	0.40
1:C:447[B]:ARG:HH11	1:C:447[B]:ARG:HD2	1.75	0.40
1:D:55:SER:HA	1:D:60:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

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	519/537 (97%)	494 (95%)	22 (4%)	3 (1%)	21	51
1	B	516/537 (96%)	490 (95%)	23 (4%)	3 (1%)	21	51
1	C	518/537 (96%)	491 (95%)	24 (5%)	3 (1%)	21	51
1	D	516/537 (96%)	491 (95%)	21 (4%)	4 (1%)	16	44
All	All	2069/2148 (96%)	1966 (95%)	90 (4%)	13 (1%)	21	51

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	LYS
1	D	125	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	125	LYS
1	C	507	ASP
1	A	125	LYS
1	A	328	THR
1	A	507	ASP
1	D	507	ASP
1	B	328	THR
1	B	507	ASP
1	C	328	THR
1	D	328	THR
1	D	480	GLU

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	429/441 (97%)	402 (94%)	27 (6%)	16	45
1	B	426/441 (97%)	390 (92%)	36 (8%)	10	31
1	C	428/441 (97%)	396 (92%)	32 (8%)	12	37
1	D	426/441 (97%)	385 (90%)	41 (10%)	8	26
All	All	1709/1764 (97%)	1573 (92%)	136 (8%)	11	34

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	41	THR
1	A	59	GLU
1	A	60	THR
1	A	82	GLU
1	A	86	GLU
1	A	127	SER
1	A	141	LYS
1	A	151	LYS
1	A	157	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	163	ASN
1	A	169	GLU
1	A	188	LYS
1	A	199	ASN
1	A	273	ASN
1	A	392	LEU
1	A	399	ARG
1	A	404	ILE
1	A	410	GLU
1	A	418	GLU
1	A	467	ARG
1	A	472	VAL
1	A	479	GLN
1	A	480	GLU
1	A	504	LYS
1	A	513	THR
1	A	522	THR
1	B	41	THR
1	B	59	GLU
1	B	60	THR
1	B	86	GLU
1	B	120	ARG
1	B	134	LEU
1	B	150	GLU
1	B	151	LYS
1	B	157	LEU
1	B	162	LYS
1	B	168	VAL
1	B	169	GLU
1	B	181	ILE
1	B	188	LYS
1	B	191	ASP
1	B	210	ASN
1	B	211	LEU
1	B	249	SER
1	B	333	SER
1	B	337	LYS
1	B	367	LYS
1	B	404	ILE
1	B	424	CYS
1	B	436	ARG
1	B	443	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	447	ARG
1	B	472	VAL
1	B	479	GLN
1	B	480	GLU
1	B	488	LEU
1	B	494	MET
1	B	504	LYS
1	B	509	VAL
1	B	513	THR
1	B	516	ARG
1	B	522	THR
1	C	14	GLN
1	C	41	THR
1	C	60	THR
1	C	86	GLU
1	C	125	LYS
1	C	132	VAL
1	C	133	GLU
1	C	141	LYS
1	C	151	LYS
1	C	162	LYS
1	C	167	VAL
1	C	173	LYS
1	C	178	ASP
1	C	181	ILE
1	C	247	LYS
1	C	261	LYS
1	C	263	LYS
1	C	291	MET
1	C	333	SER
1	C	367	LYS
1	C	422	LYS
1	C	443	ARG
1	C	472	VAL
1	C	475	LYS
1	C	480	GLU
1	C	484	GLU
1	C	488	LEU
1	C	504	LYS
1	C	509	VAL
1	C	513	THR
1	C	516	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	522	THR
1	D	25	THR
1	D	41	THR
1	D	43	ARG
1	D	56	ARG
1	D	59	GLU
1	D	60	THR
1	D	86	GLU
1	D	89	LYS
1	D	132	VAL
1	D	142	ILE
1	D	143	THR
1	D	149	MET
1	D	150	GLU
1	D	151	LYS
1	D	169	GLU
1	D	178	ASP
1	D	180	LEU
1	D	191	ASP
1	D	218	LEU
1	D	230	LYS
1	D	285	GLU
1	D	336	LYS
1	D	337	LYS
1	D	367	LYS
1	D	373	GLU
1	D	392	LEU
1	D	399[A]	ARG
1	D	399[B]	ARG
1	D	410	GLU
1	D	418	GLU
1	D	433	LYS
1	D	436	ARG
1	D	443	ARG
1	D	447	ARG
1	D	472	VAL
1	D	479	GLN
1	D	480	GLU
1	D	504	LYS
1	D	509	VAL
1	D	513	THR
1	D	522	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	90	ASN
1	A	146	ASN
1	A	163	ASN
1	A	252	HIS
1	A	264	ASN
1	A	273	ASN
1	A	318	ASN
1	A	391	HIS
1	A	439	HIS
1	A	458	GLN
1	A	464	HIS
1	A	479	GLN
1	A	495	ASN
1	A	532	HIS
1	B	16	GLN
1	B	146	ASN
1	B	163	ASN
1	B	184	GLN
1	B	199	ASN
1	B	227	GLN
1	B	252	HIS
1	B	274	HIS
1	B	318	ASN
1	B	391	HIS
1	B	479	GLN
1	B	495	ASN
1	C	16	GLN
1	C	146	ASN
1	C	199	ASN
1	C	227	GLN
1	C	264	ASN
1	C	318	ASN
1	C	458	GLN
1	D	14	GLN
1	D	16	GLN
1	D	199	ASN
1	D	227	GLN
1	D	318	ASN
1	D	439	HIS
1	D	458	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	462	GLN
1	D	464	HIS
1	D	495	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	ALY	B	166	1	10,11,12	0.52	0	7,12,14	0.85	0
1	ALY	A	166	1	10,11,12	0.43	0	7,12,14	0.68	0
1	ALY	C	166	1	10,11,12	0.59	0	7,12,14	1.22	1 (14%)
1	ALY	D	166	1	10,11,12	0.72	0	7,12,14	1.74	2 (28%)

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
1	ALY	B	166	1	-	3/9/10/12	-
1	ALY	A	166	1	-	1/9/10/12	-
1	ALY	C	166	1	-	5/9/10/12	-
1	ALY	D	166	1	-	7/9/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	ALY	CG-CD-CE	3.01	127.44	113.56
1	D	166	ALY	CE-NZ-CH	2.90	126.84	122.56
1	C	166	ALY	CE-NZ-CH	2.86	126.78	122.56

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	166	ALY	N-CA-CB-CG
1	B	166	ALY	C-CA-CB-CG
1	D	166	ALY	C-CA-CB-CG
1	C	166	ALY	OH-CH-NZ-CE
1	C	166	ALY	CH3-CH-NZ-CE
1	D	166	ALY	OH-CH-NZ-CE
1	D	166	ALY	CH3-CH-NZ-CE
1	D	166	ALY	CE-CD-CG-CB
1	D	166	ALY	CG-CD-CE-NZ
1	B	166	ALY	CE-CD-CG-CB
1	A	166	ALY	CG-CD-CE-NZ
1	D	166	ALY	CA-CB-CG-CD
1	C	166	ALY	C-CA-CB-CG
1	C	166	ALY	CG-CD-CE-NZ
1	C	166	ALY	N-CA-CB-CG
1	D	166	ALY	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	166	ALY	1	0
1	C	166	ALY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	A	601	-	18,20,20	1.13	1 (5%)	21,32,32	1.27	3 (14%)
2	FBP	C	601	-	18,20,20	1.06	1 (5%)	21,32,32	1.27	1 (4%)
2	FBP	D	601	-	18,20,20	0.60	0	21,32,32	0.93	0
2	FBP	B	601	-	18,20,20	0.80	0	21,32,32	0.84	1 (4%)

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	FBP	A	601	-	-	5/13/32/32	0/1/1/1
2	FBP	C	601	-	-	6/13/32/32	0/1/1/1
2	FBP	D	601	-	-	7/13/32/32	0/1/1/1
2	FBP	B	601	-	-	8/13/32/32	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FBP	P1-O1	2.74	1.68	1.60
2	A	601	FBP	P2-O6	2.28	1.67	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FBP	O4-C4-C5	-4.10	99.29	111.08
2	A	601	FBP	O4-C4-C5	-3.23	101.81	111.08
2	A	601	FBP	O6P-P2-O6	-2.52	100.09	106.67
2	A	601	FBP	O6-P2-O4P	2.18	112.33	106.44
2	B	601	FBP	O3P-P1-O2P	2.01	115.35	107.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	B	601	FBP	O1-C1-C2-O2
2	B	601	FBP	O5-C5-C6-O6
2	B	601	FBP	C6-O6-P2-O4P
2	B	601	FBP	C6-O6-P2-O5P
2	B	601	FBP	C6-O6-P2-O6P
2	C	601	FBP	C1-O1-P1-O2P
2	C	601	FBP	C1-O1-P1-O3P
2	C	601	FBP	O1-C1-C2-O2
2	C	601	FBP	O1-C1-C2-O5
2	D	601	FBP	C1-O1-P1-O2P
2	D	601	FBP	C1-O1-P1-O3P
2	D	601	FBP	O1-C1-C2-O2
2	D	601	FBP	O1-C1-C2-O5
2	D	601	FBP	C4-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C1-O1-P1-O1P
2	C	601	FBP	C5-C6-O6-P2
2	A	601	FBP	C6-O6-P2-O6P
2	B	601	FBP	O1-C1-C2-O5
2	A	601	FBP	C1-O1-P1-O1P
2	B	601	FBP	O1-C1-C2-C3

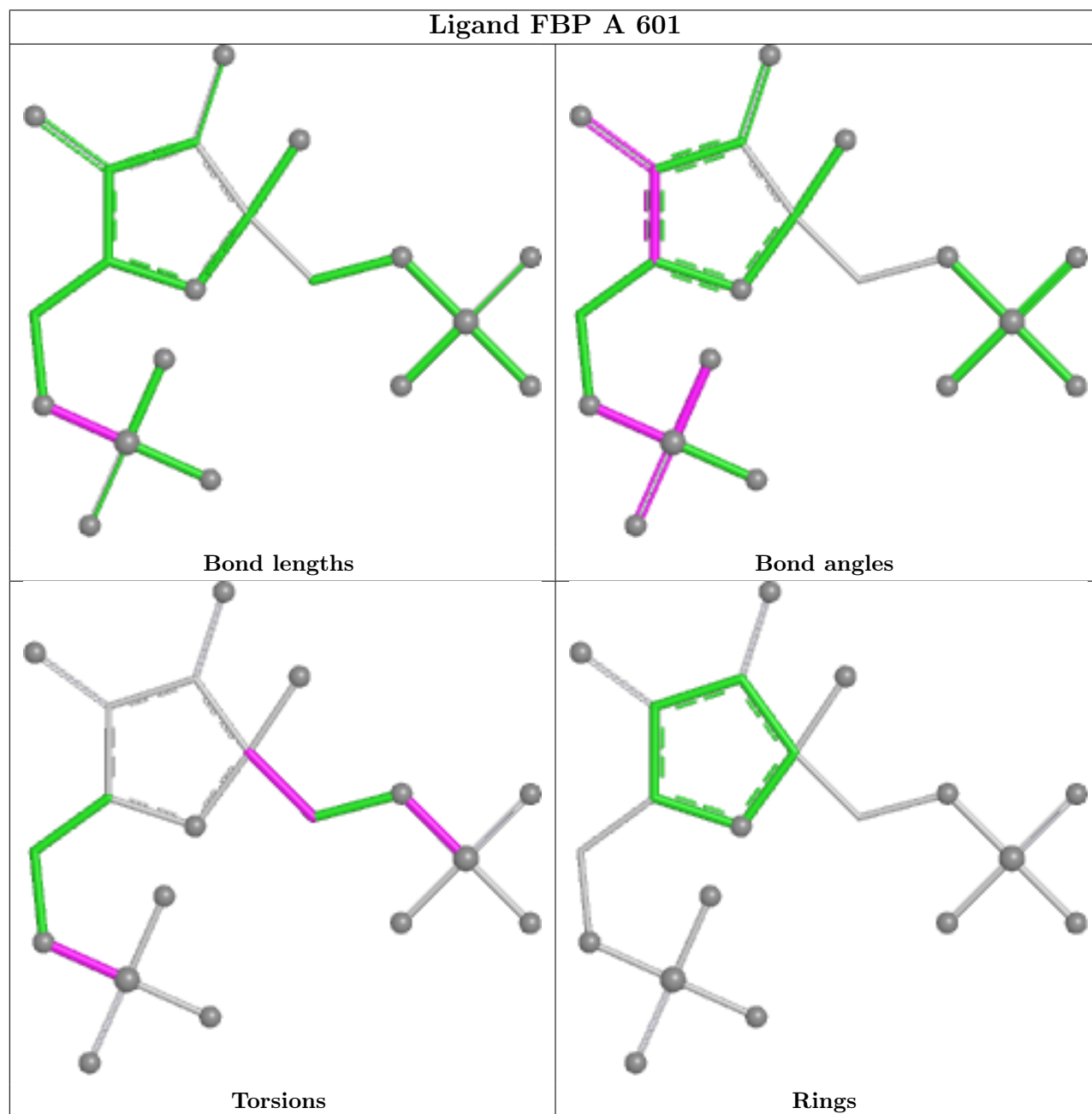
There are no ring outliers.

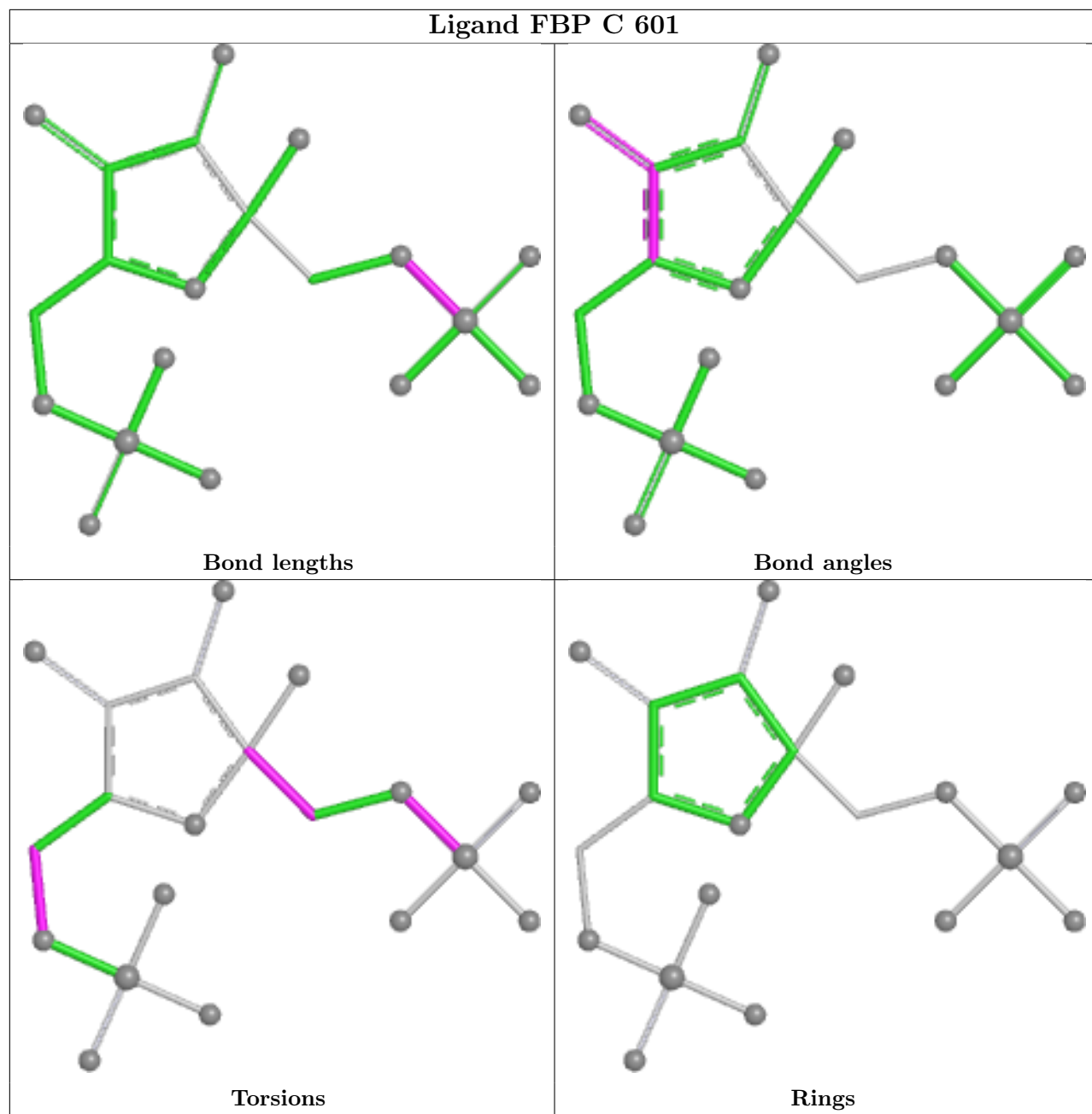
3 monomers are involved in 4 short contacts:

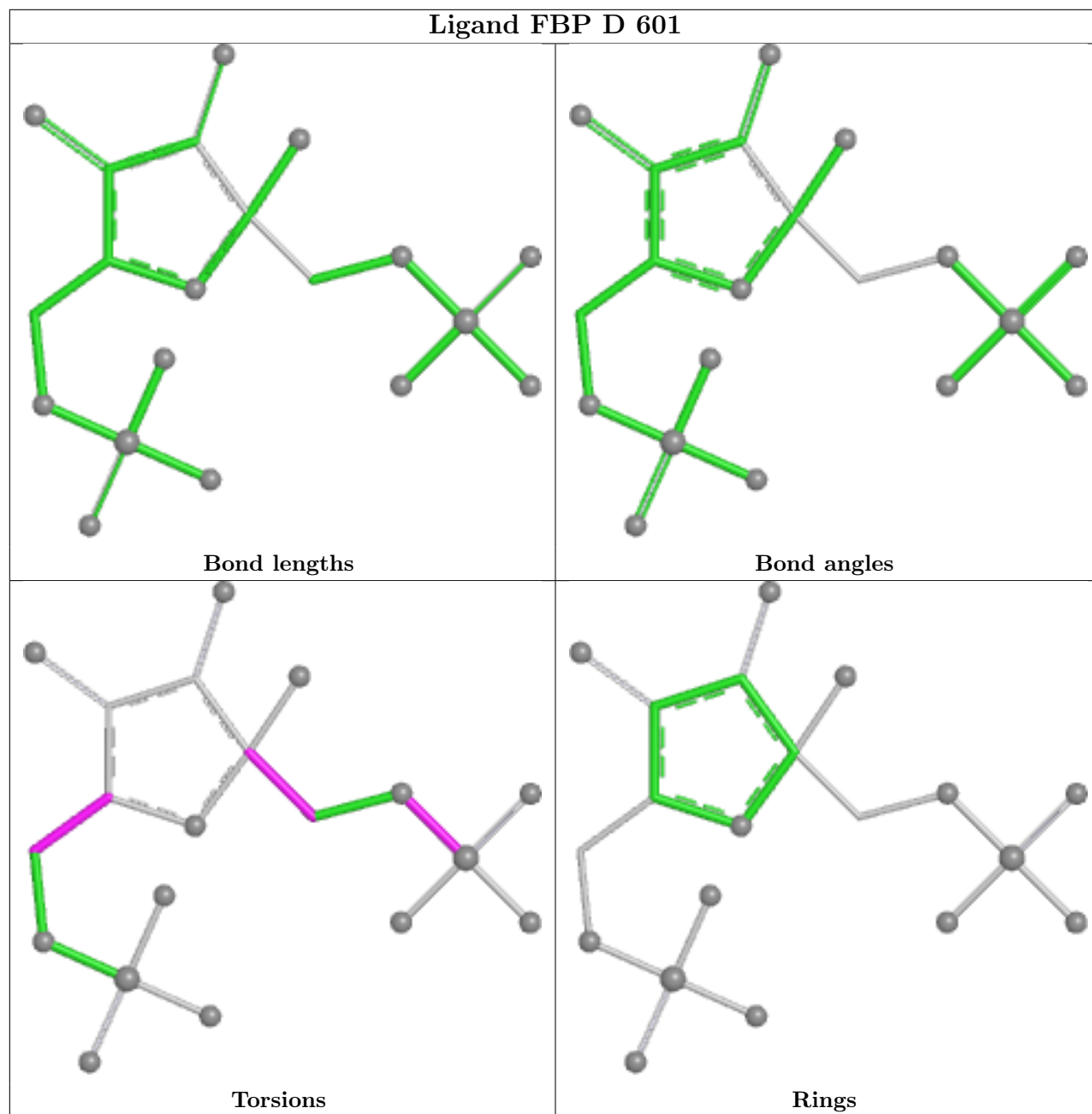
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FBP	1	0
2	C	601	FBP	1	0
2	B	601	FBP	2	0

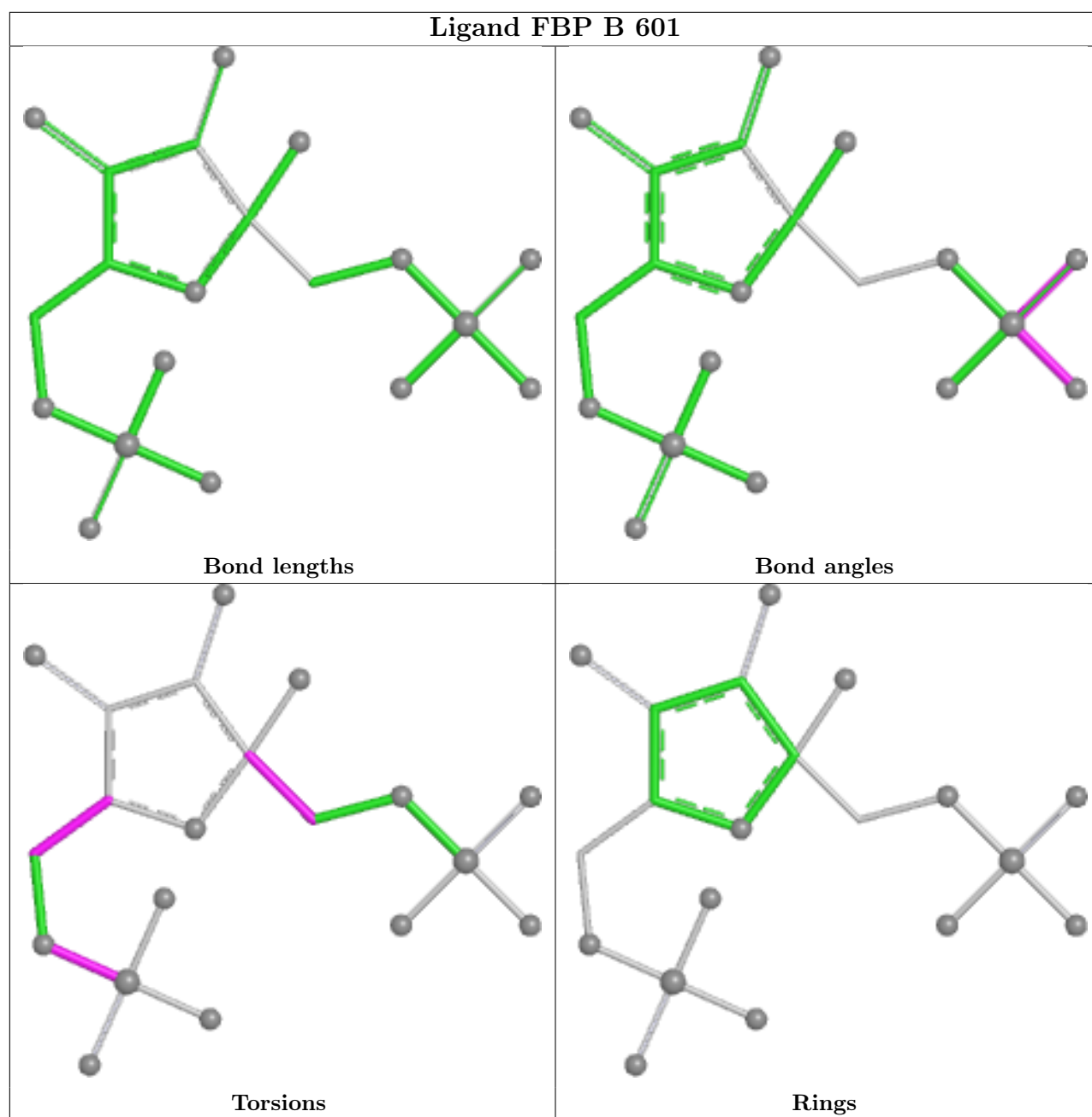
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	520/537 (96%)	-0.47	2 (0%) 88 85	21, 55, 115, 161	1 (0%)
1	B	517/537 (96%)	-0.35	5 (0%) 79 73	27, 59, 118, 153	1 (0%)
1	C	518/537 (96%)	-0.41	3 (0%) 85 81	24, 64, 99, 173	2 (0%)
1	D	517/537 (96%)	-0.28	2 (0%) 88 85	27, 70, 123, 229	1 (0%)
All	All	2072/2148 (96%)	-0.38	12 (0%) 85 81	21, 62, 117, 229	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	326	CYS	4.5
1	C	358	CYS	3.5
1	B	358	CYS	3.5
1	C	192[A]	PHE	3.2
1	B	164	ILE	3.0
1	D	190	ALA	2.9
1	D	326	CYS	2.5
1	B	326	CYS	2.5
1	B	140	LEU	2.3
1	A	533	HIS	2.2
1	A	190	ALA	2.2
1	B	190	ALA	2.1

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(\AA^2)	Q<0.9
1	ALY	B	166	12/13	0.63	0.14	107,111,126,126	0
1	ALY	D	166	12/13	0.69	0.17	118,124,127,128	0
1	ALY	C	166	12/13	0.78	0.13	83,96,128,128	0
1	ALY	A	166	12/13	0.81	0.14	89,109,137,140	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

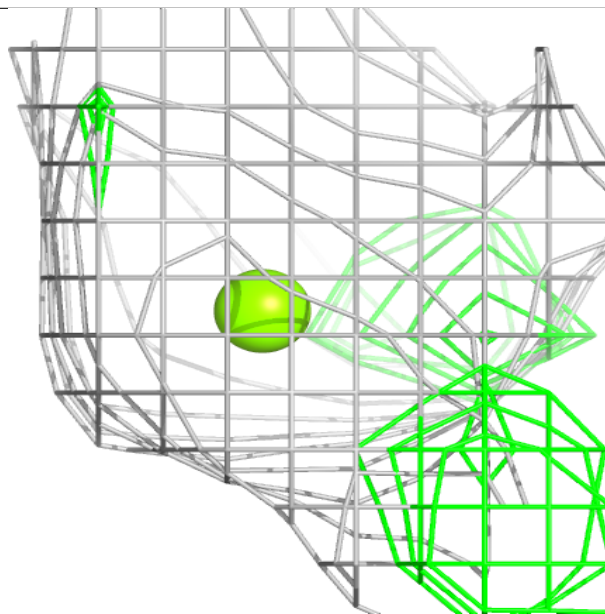
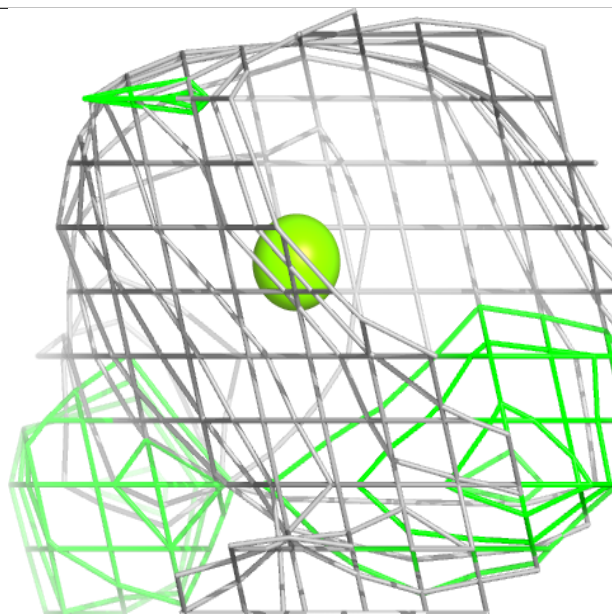
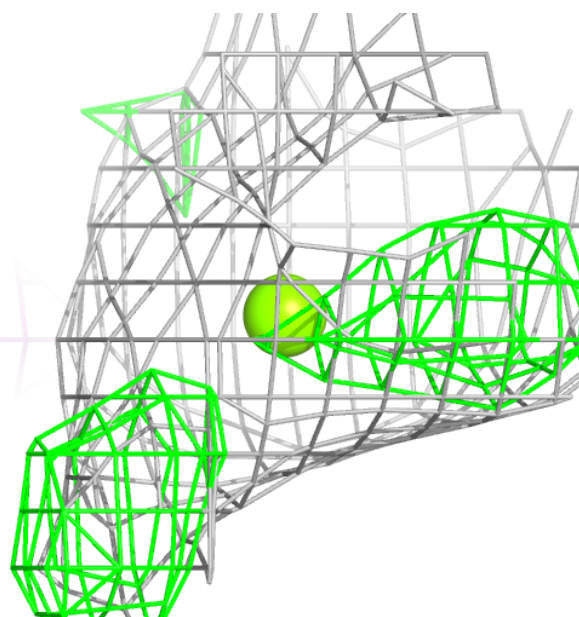
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	602	1/1	0.85	0.14	44,44,44,44	0
3	MG	D	603	1/1	0.85	0.18	61,61,61,61	0
3	MG	A	602	1/1	0.88	0.17	50,50,50,50	0
3	MG	D	602	1/1	0.92	0.13	51,51,51,51	0
2	FBP	C	601	20/20	0.93	0.08	54,72,79,83	0
2	FBP	B	601	20/20	0.94	0.07	68,85,91,102	0
2	FBP	A	601	20/20	0.96	0.06	40,47,49,50	0
2	FBP	D	601	20/20	0.96	0.06	67,77,84,85	0
3	MG	C	602	1/1	0.97	0.09	53,53,53,53	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.

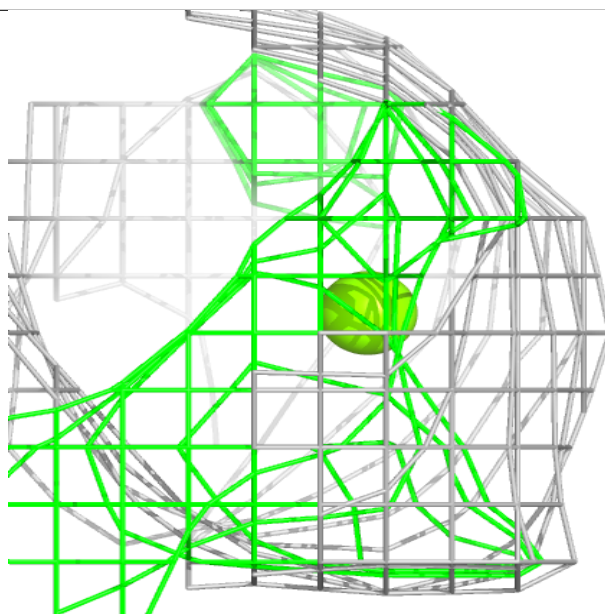
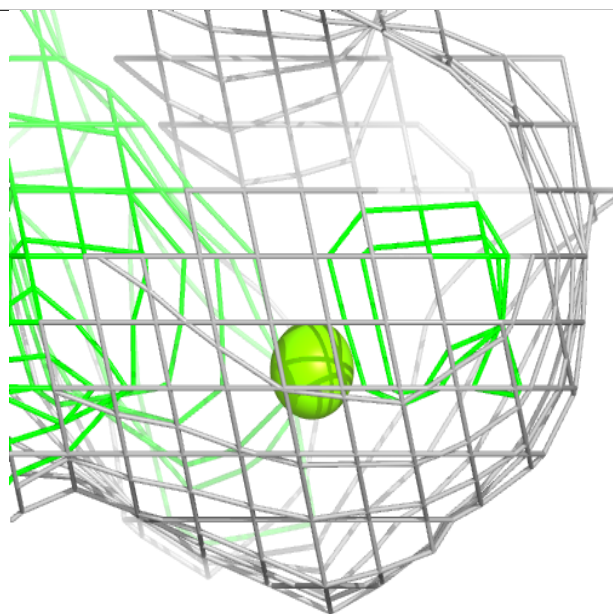
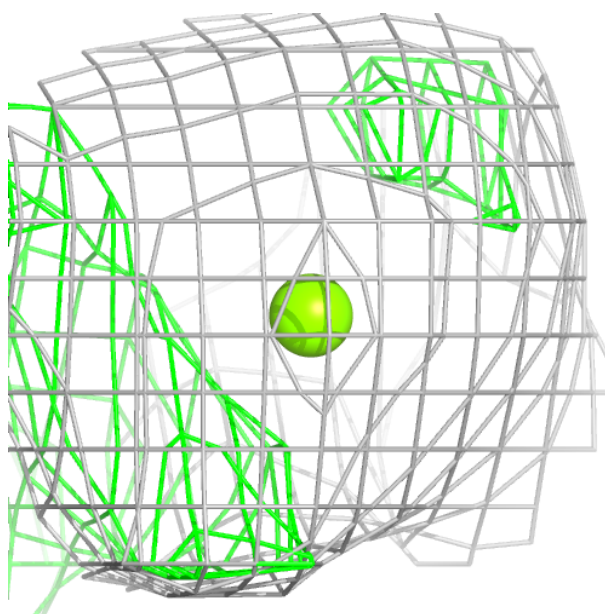
Electron density around MG B 602:

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



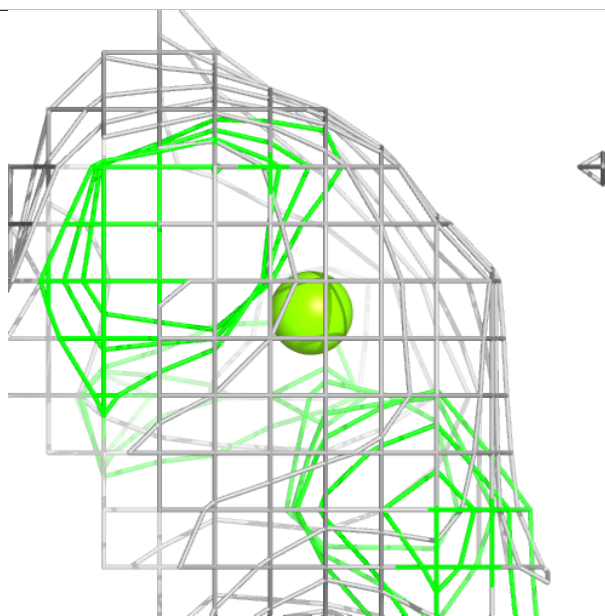
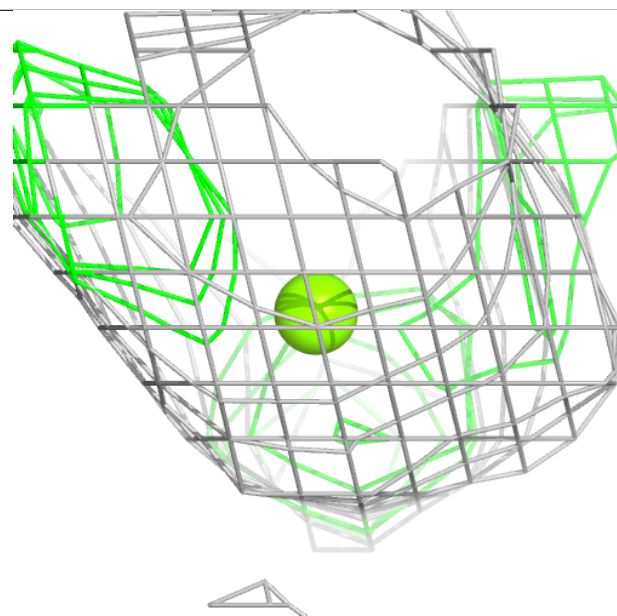
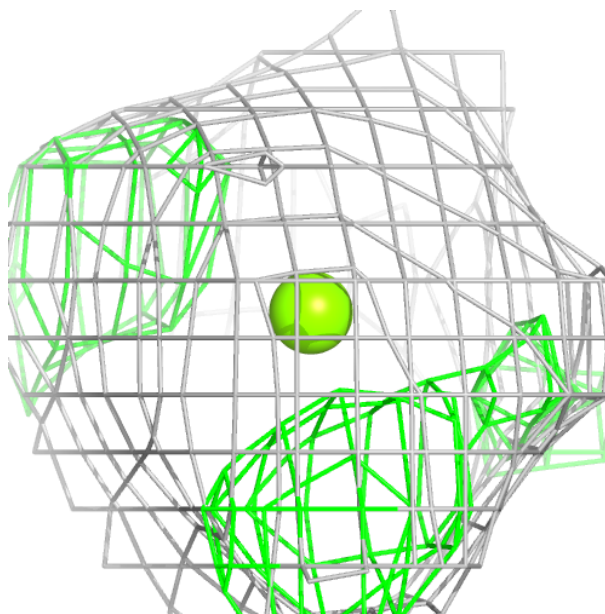
Electron density around MG D 603:

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



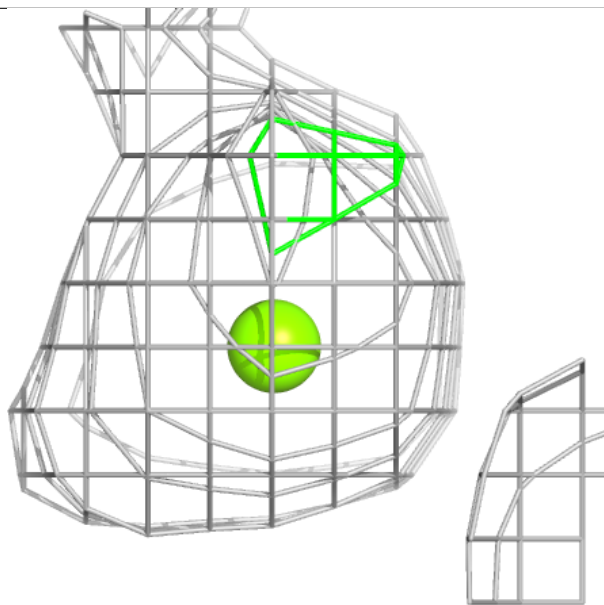
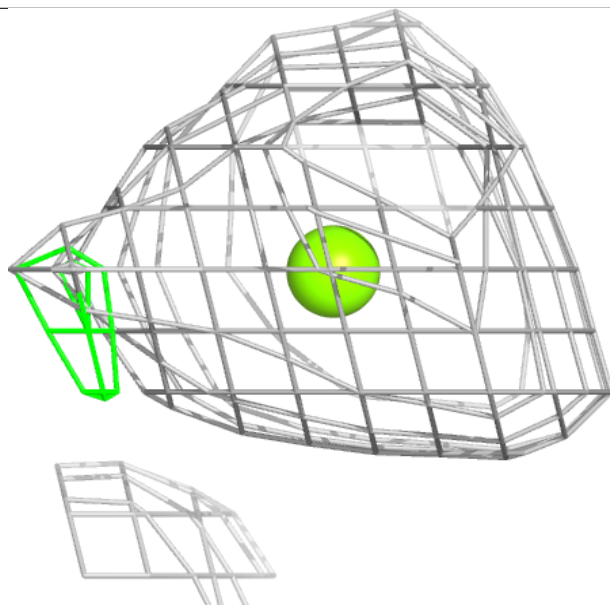
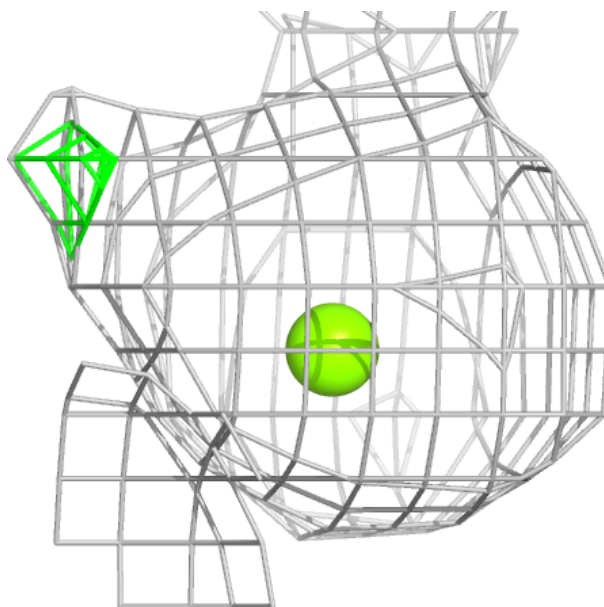
Electron density around MG A 602:

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



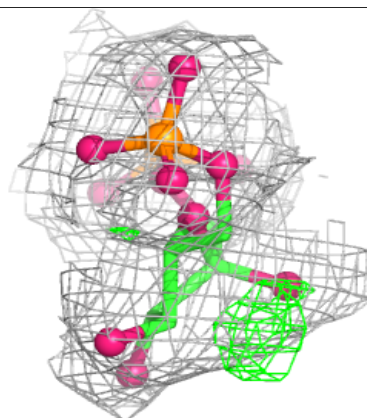
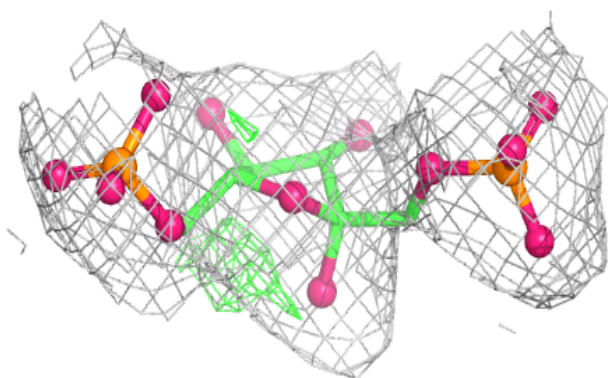
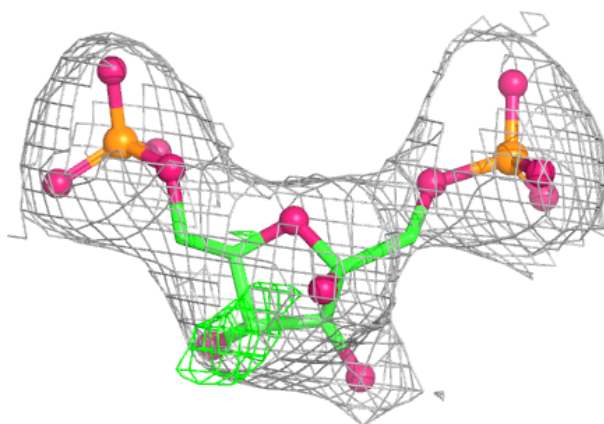
Electron density around MG D 602:

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



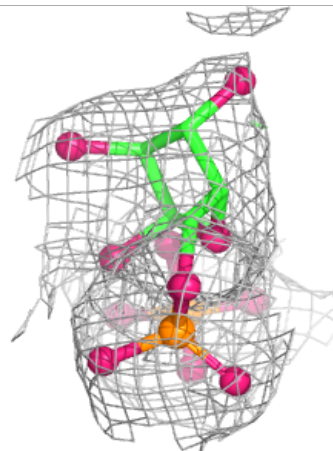
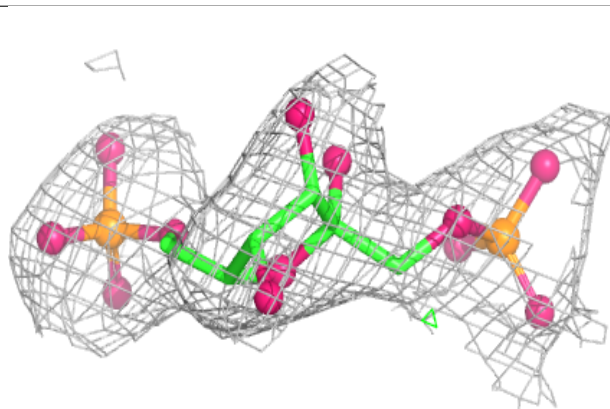
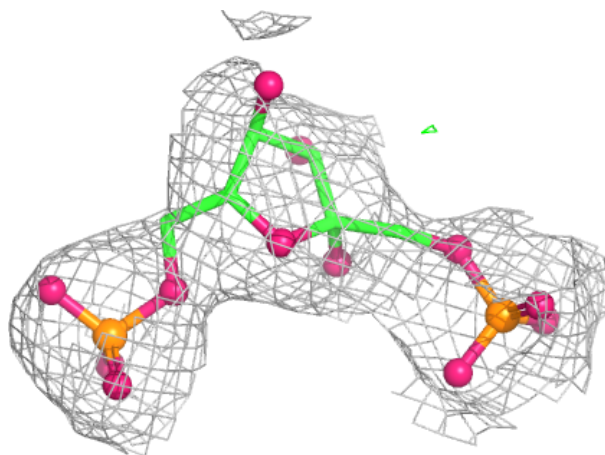
Electron density around FBP C 601:

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



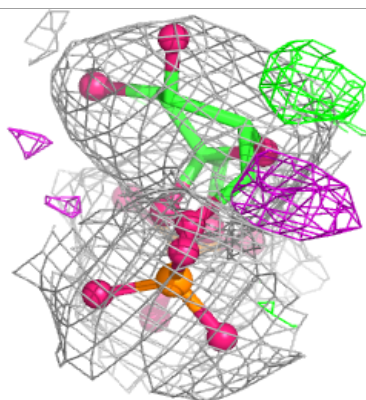
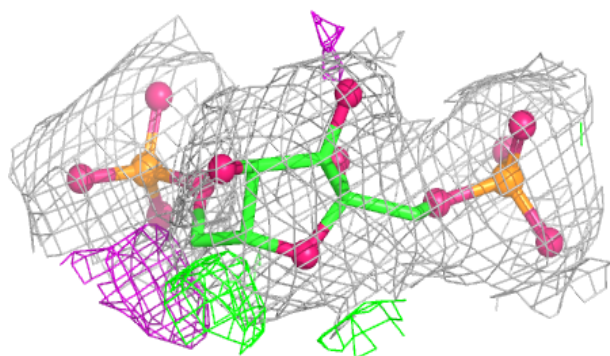
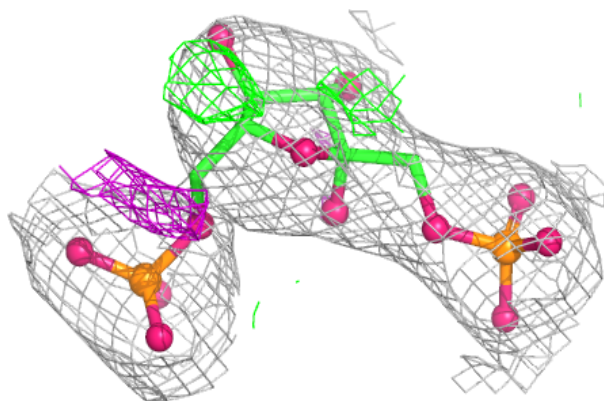
Electron density around FBP B 601:

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

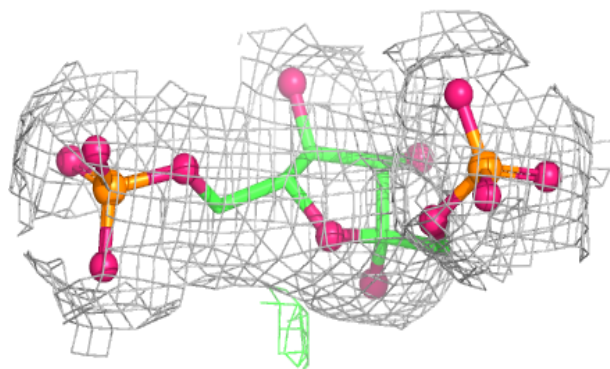
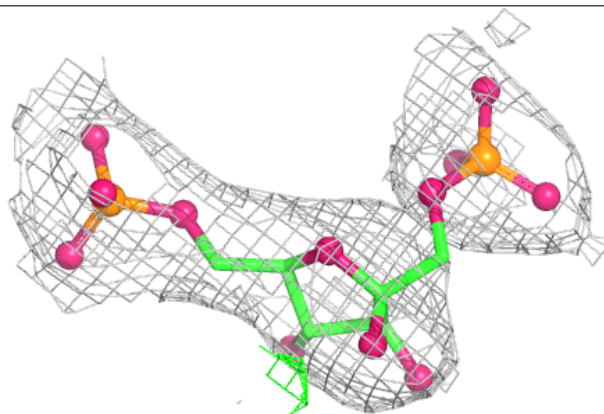


Electron density around FBP A 601:

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

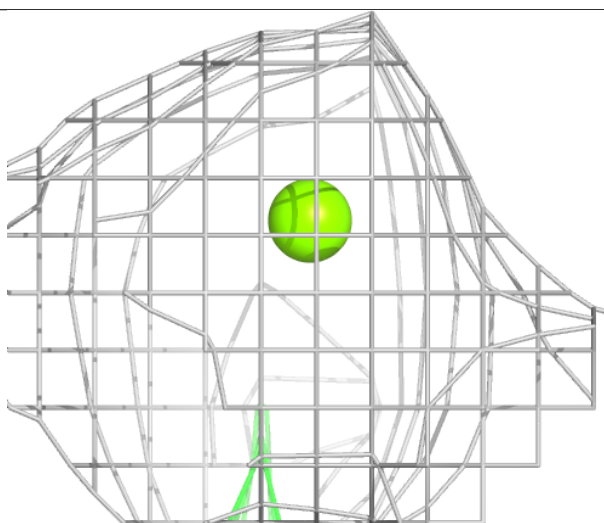
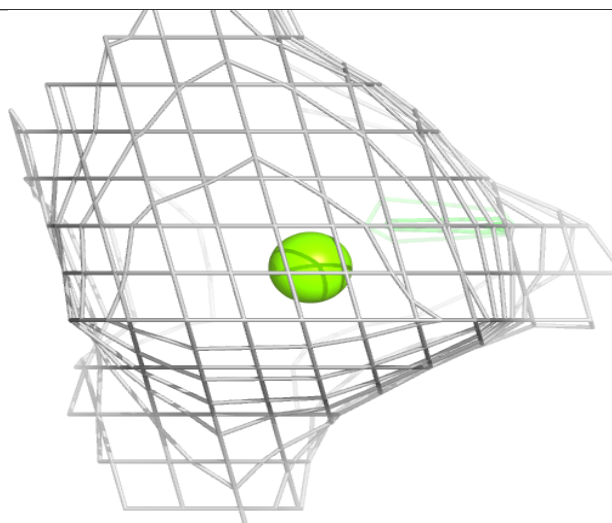
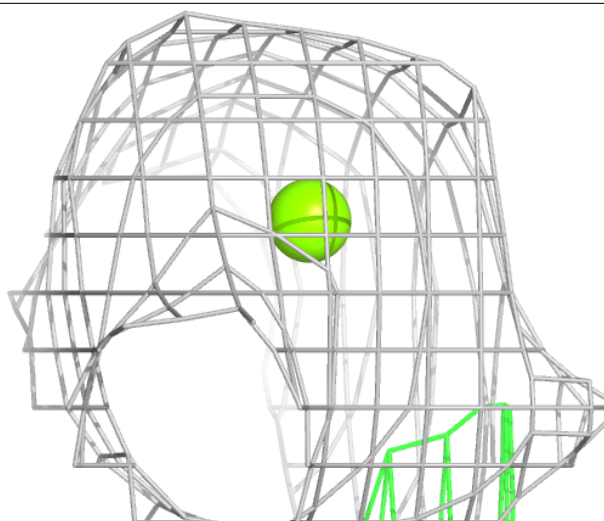
**Electron density around FBP D 601:**

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



Electron density around MG C 602:

$2mF_o-DF_c$ (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.