



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:49 PM UTC

PDB ID : 6SU1 / pdb_00006su1
Title : Trypanosoma congolense pyruvate kinase in complex with citrate and glycerol
Authors : Sterckx, Y.G.-J.; Pinto Torres, J.E.
Deposited on : 2019-09-12
Resolution : 3.00 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

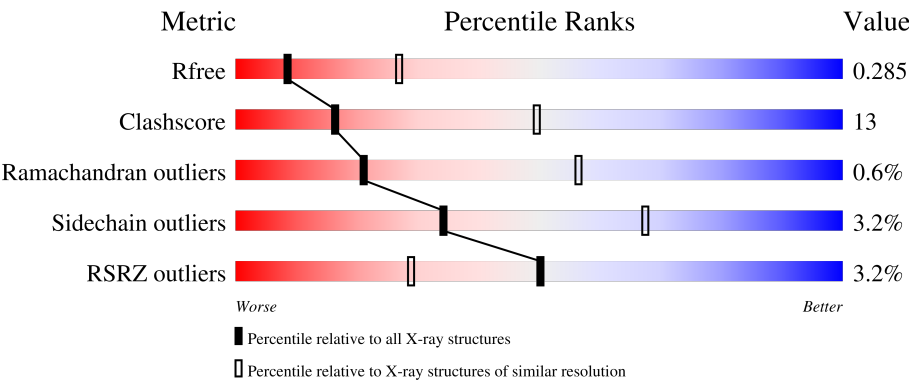
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	514	3% 65% 19% • 15%
1	B	514	4% 70% 20% • 7%
1	C	514	2% 75% 20% • •
1	D	514	4% 70% 25% • •
1	E	514	3% 70% 25% • •

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Mol	Chain	Length	Quality of chain
1	F	514	
1	G	514	
1	H	514	

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	CIT	H	601	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28228 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3226	2010	567	625	24			
1	B	476	Total	C	N	O	S	0	0	0
			3481	2164	623	667	27			
1	C	499	Total	C	N	O	S	0	1	0
			3726	2320	659	721	26			
1	D	498	Total	C	N	O	S	0	1	0
			3709	2306	660	717	26			
1	E	495	Total	C	N	O	S	0	0	0
			3710	2311	655	718	26			
1	F	498	Total	C	N	O	S	0	1	0
			3716	2316	658	716	26			
1	G	411	Total	C	N	O	S	0	1	0
			3054	1894	548	588	24			
1	H	449	Total	C	N	O	S	0	0	0
			3273	2029	586	635	23			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	GLU	-	expression tag	UNP G0UYF4
A	501	ASN	-	expression tag	UNP G0UYF4
A	502	LEU	-	expression tag	UNP G0UYF4
A	503	TYR	-	expression tag	UNP G0UYF4
A	504	PHE	-	expression tag	UNP G0UYF4
A	505	GLN	-	expression tag	UNP G0UYF4
A	506	SER	-	expression tag	UNP G0UYF4
A	507	GLY	-	expression tag	UNP G0UYF4
A	508	GLY	-	expression tag	UNP G0UYF4
A	509	HIS	-	expression tag	UNP G0UYF4
A	510	HIS	-	expression tag	UNP G0UYF4
A	511	HIS	-	expression tag	UNP G0UYF4
A	512	HIS	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	513	HIS	-	expression tag	UNP G0UYF4
A	514	HIS	-	expression tag	UNP G0UYF4
B	500	GLU	-	expression tag	UNP G0UYF4
B	501	ASN	-	expression tag	UNP G0UYF4
B	502	LEU	-	expression tag	UNP G0UYF4
B	503	TYR	-	expression tag	UNP G0UYF4
B	504	PHE	-	expression tag	UNP G0UYF4
B	505	GLN	-	expression tag	UNP G0UYF4
B	506	SER	-	expression tag	UNP G0UYF4
B	507	GLY	-	expression tag	UNP G0UYF4
B	508	GLY	-	expression tag	UNP G0UYF4
B	509	HIS	-	expression tag	UNP G0UYF4
B	510	HIS	-	expression tag	UNP G0UYF4
B	511	HIS	-	expression tag	UNP G0UYF4
B	512	HIS	-	expression tag	UNP G0UYF4
B	513	HIS	-	expression tag	UNP G0UYF4
B	514	HIS	-	expression tag	UNP G0UYF4
C	500	GLU	-	expression tag	UNP G0UYF4
C	501	ASN	-	expression tag	UNP G0UYF4
C	502	LEU	-	expression tag	UNP G0UYF4
C	503	TYR	-	expression tag	UNP G0UYF4
C	504	PHE	-	expression tag	UNP G0UYF4
C	505	GLN	-	expression tag	UNP G0UYF4
C	506	SER	-	expression tag	UNP G0UYF4
C	507	GLY	-	expression tag	UNP G0UYF4
C	508	GLY	-	expression tag	UNP G0UYF4
C	509	HIS	-	expression tag	UNP G0UYF4
C	510	HIS	-	expression tag	UNP G0UYF4
C	511	HIS	-	expression tag	UNP G0UYF4
C	512	HIS	-	expression tag	UNP G0UYF4
C	513	HIS	-	expression tag	UNP G0UYF4
C	514	HIS	-	expression tag	UNP G0UYF4
D	500	GLU	-	expression tag	UNP G0UYF4
D	501	ASN	-	expression tag	UNP G0UYF4
D	502	LEU	-	expression tag	UNP G0UYF4
D	503	TYR	-	expression tag	UNP G0UYF4
D	504	PHE	-	expression tag	UNP G0UYF4
D	505	GLN	-	expression tag	UNP G0UYF4
D	506	SER	-	expression tag	UNP G0UYF4
D	507	GLY	-	expression tag	UNP G0UYF4
D	508	GLY	-	expression tag	UNP G0UYF4
D	509	HIS	-	expression tag	UNP G0UYF4

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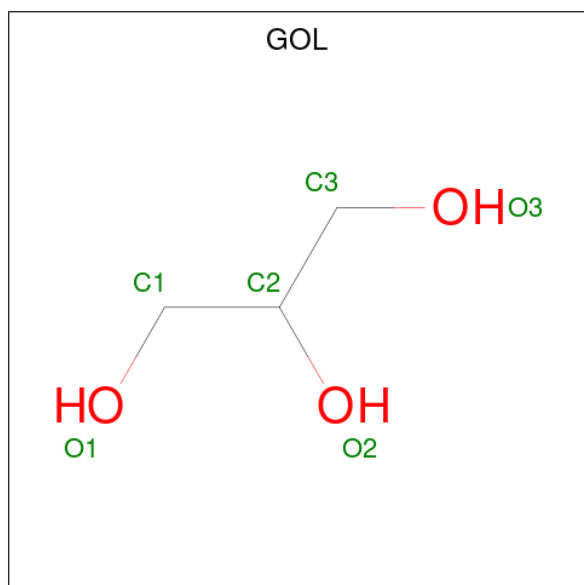
Chain	Residue	Modelled	Actual	Comment	Reference
D	510	HIS	-	expression tag	UNP G0UYF4
D	511	HIS	-	expression tag	UNP G0UYF4
D	512	HIS	-	expression tag	UNP G0UYF4
D	513	HIS	-	expression tag	UNP G0UYF4
D	514	HIS	-	expression tag	UNP G0UYF4
E	500	GLU	-	expression tag	UNP G0UYF4
E	501	ASN	-	expression tag	UNP G0UYF4
E	502	LEU	-	expression tag	UNP G0UYF4
E	503	TYR	-	expression tag	UNP G0UYF4
E	504	PHE	-	expression tag	UNP G0UYF4
E	505	GLN	-	expression tag	UNP G0UYF4
E	506	SER	-	expression tag	UNP G0UYF4
E	507	GLY	-	expression tag	UNP G0UYF4
E	508	GLY	-	expression tag	UNP G0UYF4
E	509	HIS	-	expression tag	UNP G0UYF4
E	510	HIS	-	expression tag	UNP G0UYF4
E	511	HIS	-	expression tag	UNP G0UYF4
E	512	HIS	-	expression tag	UNP G0UYF4
E	513	HIS	-	expression tag	UNP G0UYF4
E	514	HIS	-	expression tag	UNP G0UYF4
F	500	GLU	-	expression tag	UNP G0UYF4
F	501	ASN	-	expression tag	UNP G0UYF4
F	502	LEU	-	expression tag	UNP G0UYF4
F	503	TYR	-	expression tag	UNP G0UYF4
F	504	PHE	-	expression tag	UNP G0UYF4
F	505	GLN	-	expression tag	UNP G0UYF4
F	506	SER	-	expression tag	UNP G0UYF4
F	507	GLY	-	expression tag	UNP G0UYF4
F	508	GLY	-	expression tag	UNP G0UYF4
F	509	HIS	-	expression tag	UNP G0UYF4
F	510	HIS	-	expression tag	UNP G0UYF4
F	511	HIS	-	expression tag	UNP G0UYF4
F	512	HIS	-	expression tag	UNP G0UYF4
F	513	HIS	-	expression tag	UNP G0UYF4
F	514	HIS	-	expression tag	UNP G0UYF4
G	500	GLU	-	expression tag	UNP G0UYF4
G	501	ASN	-	expression tag	UNP G0UYF4
G	502	LEU	-	expression tag	UNP G0UYF4
G	503	TYR	-	expression tag	UNP G0UYF4
G	504	PHE	-	expression tag	UNP G0UYF4
G	505	GLN	-	expression tag	UNP G0UYF4
G	506	SER	-	expression tag	UNP G0UYF4

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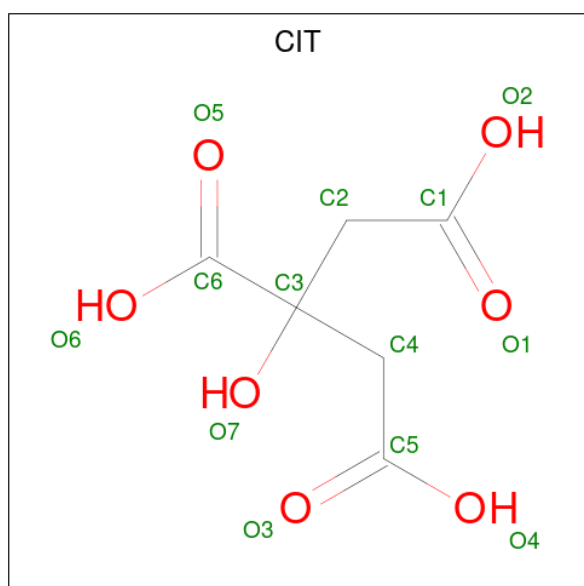
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G	507	GLY	-	expression tag	UNP G0UYF4
G	508	GLY	-	expression tag	UNP G0UYF4
G	509	HIS	-	expression tag	UNP G0UYF4
G	510	HIS	-	expression tag	UNP G0UYF4
G	511	HIS	-	expression tag	UNP G0UYF4
G	512	HIS	-	expression tag	UNP G0UYF4
G	513	HIS	-	expression tag	UNP G0UYF4
G	514	HIS	-	expression tag	UNP G0UYF4
H	500	GLU	-	expression tag	UNP G0UYF4
H	501	ASN	-	expression tag	UNP G0UYF4
H	502	LEU	-	expression tag	UNP G0UYF4
H	503	TYR	-	expression tag	UNP G0UYF4
H	504	PHE	-	expression tag	UNP G0UYF4
H	505	GLN	-	expression tag	UNP G0UYF4
H	506	SER	-	expression tag	UNP G0UYF4
H	507	GLY	-	expression tag	UNP G0UYF4
H	508	GLY	-	expression tag	UNP G0UYF4
H	509	HIS	-	expression tag	UNP G0UYF4
H	510	HIS	-	expression tag	UNP G0UYF4
H	511	HIS	-	expression tag	UNP G0UYF4
H	512	HIS	-	expression tag	UNP G0UYF4
H	513	HIS	-	expression tag	UNP G0UYF4
H	514	HIS	-	expression tag	UNP G0UYF4

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



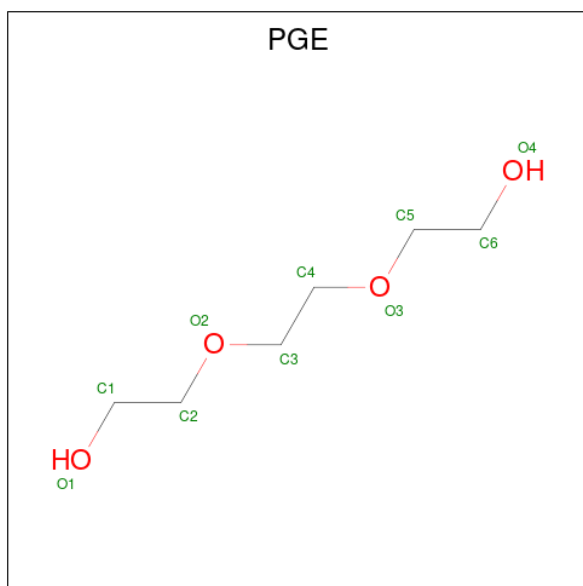
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		

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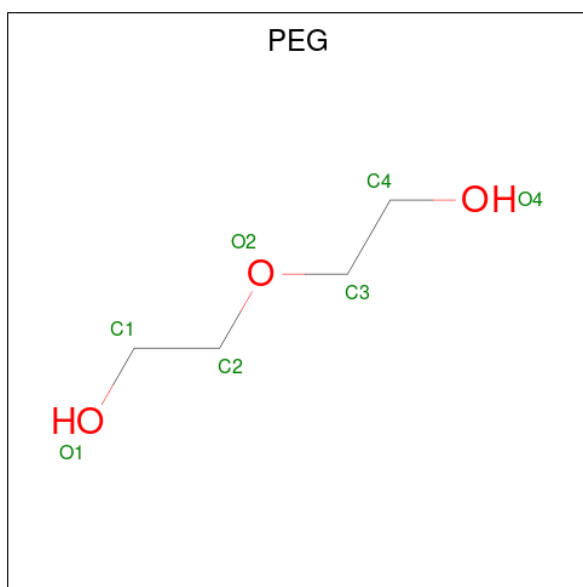
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		
3	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			10	6	4		

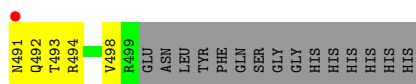
- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



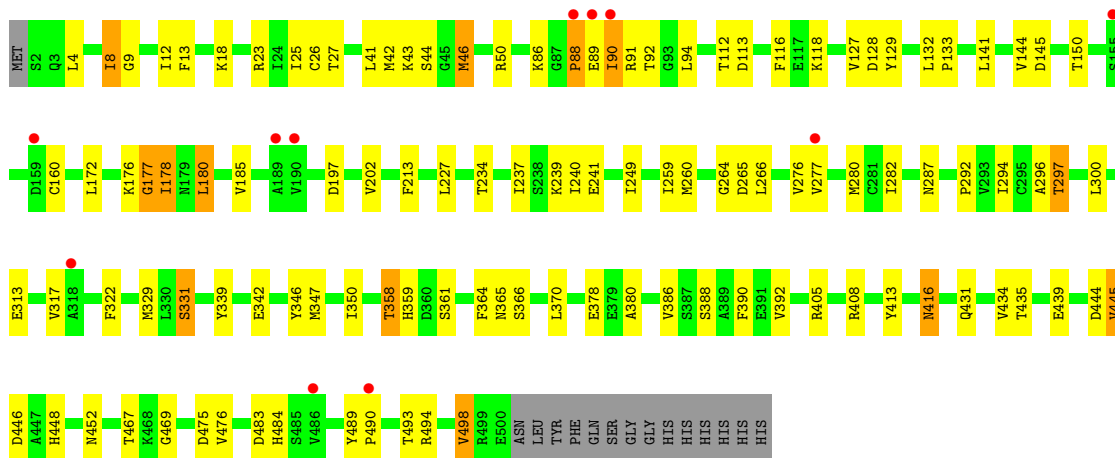
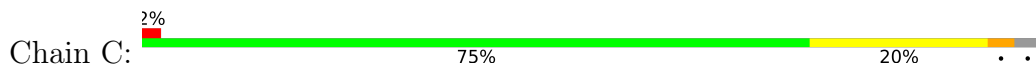
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

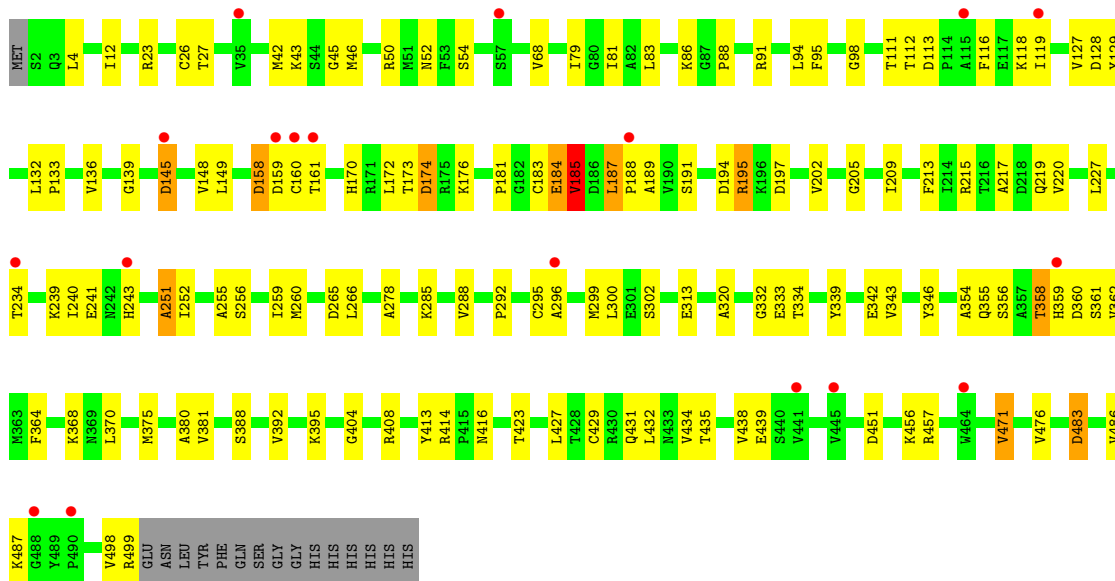
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	23	Total	O	0	0
			23	23		
6	C	32	Total	O	0	0
			32	32		
6	D	15	Total	O	0	0
			15	15		
6	E	22	Total	O	0	0
			22	22		
6	F	31	Total	O	0	0
			31	31		
6	G	20	Total	O	0	0
			20	20		
6	H	16	Total	O	0	0
			16	16		



• Molecule 1: Pyruvate kinase

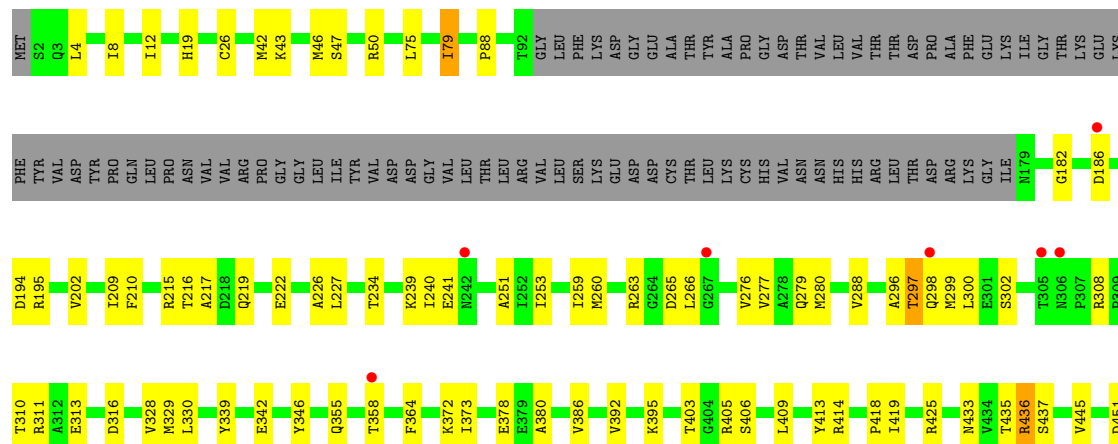


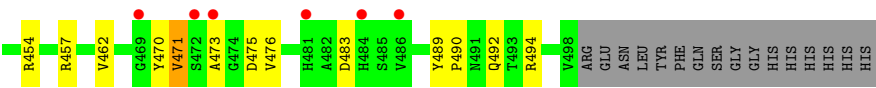
• Molecule 1: Pyruvate kinase



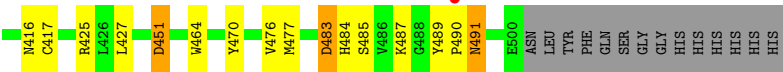
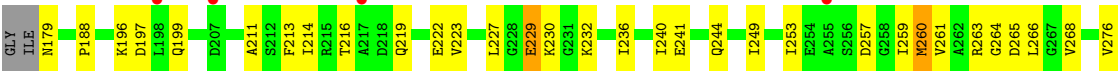
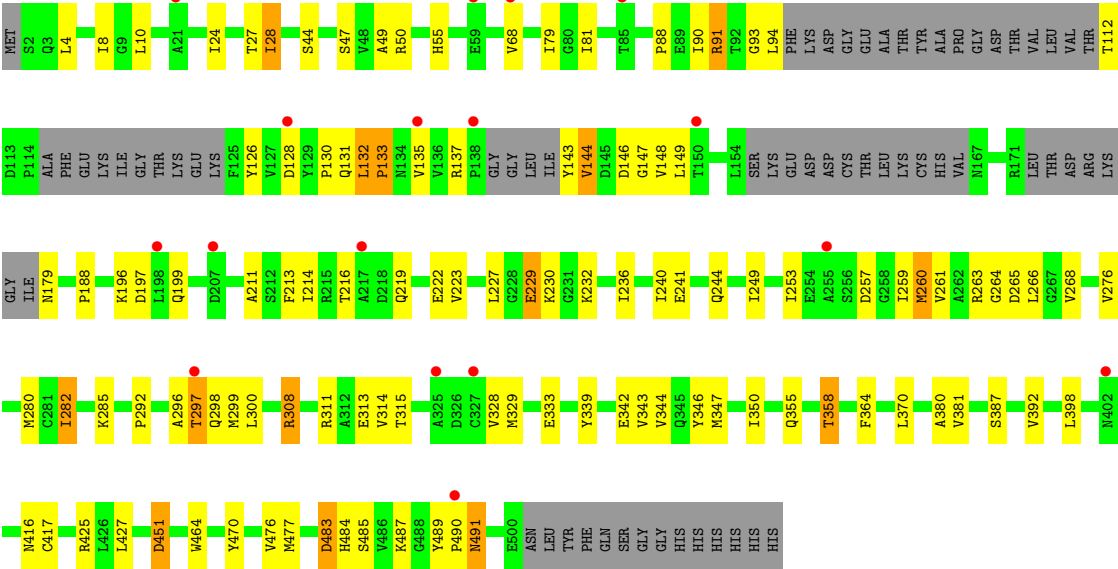
• Molecule 1: Pyruvate kinase







● Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.45Å 107.15Å 148.00Å 109.74° 90.51° 106.78°	Depositor
Resolution (Å)	49.33 – 3.00 49.33 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.33-3.00) 93.4 (49.33-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.208 , 0.257 (Not available) , 0.285	Depositor DCC
R_{free} test set	5317 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 102.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	28228	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, GOL, PEG, PGE

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	0.90	0/3268	1.49	23/4440 (0.5%)
1	B	0.97	3/3529 (0.1%)	1.52	33/4792 (0.7%)
1	C	0.94	2/3787 (0.1%)	1.49	23/5150 (0.4%)
1	D	0.87	2/3770 (0.1%)	1.47	37/5130 (0.7%)
1	E	0.90	2/3767 (0.1%)	1.45	26/5117 (0.5%)
1	F	0.91	0/3776	1.45	19/5133 (0.4%)
1	G	0.94	2/3098 (0.1%)	1.48	16/4201 (0.4%)
1	H	0.87	0/3317	1.46	17/4515 (0.4%)
All	All	0.91	11/28312 (0.0%)	1.48	194/38478 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	79	ILE	CG1-CD1	-8.15	1.20	1.51
1	E	51	MET	SD-CE	-7.34	1.61	1.79
1	B	358	THR	CA-C	6.26	1.61	1.52
1	B	414	ARG	CA-C	6.14	1.59	1.53
1	B	479	ILE	CA-C	5.86	1.60	1.52
1	C	180	LEU	CA-C	5.63	1.59	1.52
1	G	414	ARG	CA-C	5.38	1.58	1.53
1	C	358	THR	CA-C	5.26	1.60	1.52
1	E	299	MET	SD-CE	-5.19	1.66	1.79
1	D	358	THR	CA-C	5.15	1.59	1.53
1	D	414	ARG	CA-C	5.01	1.59	1.52

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ASP	N-CA-C	10.64	123.36	110.91
1	H	451	ASP	N-CA-C	9.32	123.86	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	SER	N-CA-C	9.31	123.26	111.24
1	D	145	ASP	N-CA-C	8.88	123.26	111.28
1	A	8	ILE	N-CA-C	-8.43	97.72	108.84
1	C	145	ASP	N-CA-C	8.35	122.55	111.28
1	B	296	ALA	N-CA-C	8.22	123.79	113.43
1	F	296	ALA	CA-C-N	-8.21	110.63	122.94
1	F	296	ALA	C-N-CA	-8.21	110.63	122.94
1	D	158	ASP	CA-C-N	7.80	130.58	120.44
1	D	158	ASP	C-N-CA	7.80	130.58	120.44
1	F	392	VAL	N-CA-C	-7.65	98.79	108.89
1	A	451	ASP	N-CA-C	7.64	121.59	111.28
1	B	366	SER	CA-C-N	7.59	130.28	120.56
1	B	366	SER	C-N-CA	7.59	130.28	120.56
1	E	354	ALA	N-CA-C	-7.49	103.06	111.07
1	D	296	ALA	CA-C-N	-7.32	110.87	122.73
1	D	296	ALA	C-N-CA	-7.32	110.87	122.73
1	A	391	GLU	CB-CG-CD	7.26	124.95	112.60
1	D	427	LEU	CA-C-N	7.23	130.55	120.29
1	D	427	LEU	C-N-CA	7.23	130.55	120.29
1	B	416	ASN	CA-CB-CG	7.10	119.70	112.60
1	E	296	ALA	N-CA-C	7.06	123.52	114.56
1	H	417	CYS	N-CA-C	6.97	121.16	109.87
1	G	329	MET	N-CA-C	6.89	120.40	108.76
1	E	296	ALA	CA-C-N	-6.76	111.77	122.73
1	E	296	ALA	C-N-CA	-6.76	111.77	122.73
1	C	498	VAL	CA-C-N	6.75	132.41	121.74
1	C	498	VAL	C-N-CA	6.75	132.41	121.74
1	E	226	ALA	CA-C-N	6.75	129.32	120.28
1	E	226	ALA	C-N-CA	6.75	129.32	120.28
1	D	361	SER	N-CA-C	-6.74	105.09	113.38
1	H	296	ALA	CA-C-N	-6.74	112.23	122.81
1	H	296	ALA	C-N-CA	-6.74	112.23	122.81
1	C	405	ARG	CA-C-N	6.65	129.20	120.28
1	C	405	ARG	C-N-CA	6.65	129.20	120.28
1	H	416	ASN	CA-CB-CG	6.59	119.19	112.60
1	B	358	THR	CB-CA-C	6.50	120.17	111.14
1	C	416	ASN	CA-CB-CG	6.49	119.09	112.60
1	B	197	ASP	CA-CB-CG	6.46	119.06	112.60
1	E	57	SER	N-CA-C	-6.46	99.64	109.85
1	F	453	ASP	N-CA-C	-6.41	105.09	114.39
1	D	183	CYS	N-CA-C	6.34	119.06	108.73
1	E	158	ASP	CA-CB-CG	6.32	118.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	ASN	CA-CB-CG	6.31	118.91	112.60
1	C	297	THR	CA-C-N	6.29	131.79	122.74
1	C	297	THR	C-N-CA	6.29	131.79	122.74
1	A	377	PRO	CA-C-N	6.20	128.59	120.28
1	A	377	PRO	C-N-CA	6.20	128.59	120.28
1	E	185	VAL	N-CA-C	-6.17	98.74	107.75
1	F	483	ASP	CA-C-N	6.17	128.83	120.38
1	F	483	ASP	C-N-CA	6.17	128.83	120.38
1	C	89	GLU	CA-C-N	6.13	133.01	121.97
1	C	89	GLU	C-N-CA	6.13	133.01	121.97
1	B	147	GLY	CA-C-N	6.13	128.80	120.77
1	B	147	GLY	C-N-CA	6.13	128.80	120.77
1	D	194	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	484	HIS	N-CA-C	6.08	121.40	111.37
1	E	159	ASP	CA-CB-CG	6.07	118.67	112.60
1	G	253	ILE	N-CA-CB	6.00	117.57	110.55
1	E	405	ARG	CA-C-N	5.98	128.29	120.28
1	E	405	ARG	C-N-CA	5.98	128.29	120.28
1	B	360	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	296	ALA	N-CA-C	5.95	121.40	114.62
1	B	341	ASN	CA-C-N	5.93	128.23	120.28
1	B	341	ASN	C-N-CA	5.93	128.23	120.28
1	G	406	SER	N-CA-C	-5.93	104.82	111.28
1	A	245	GLY	CA-C-N	5.90	129.17	120.74
1	A	245	GLY	C-N-CA	5.90	129.17	120.74
1	F	392	VAL	N-CA-CB	5.85	116.91	110.53
1	H	417	CYS	N-CA-CB	-5.81	102.31	110.04
1	D	205	GLY	N-CA-C	5.71	124.45	115.08
1	H	197	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	451	ASP	N-CA-C	5.69	118.97	111.28
1	A	457	ARG	CA-C-N	5.69	128.26	120.46
1	A	457	ARG	C-N-CA	5.69	128.26	120.46
1	D	145	ASP	CA-CB-CG	5.69	118.29	112.60
1	E	356	SER	N-CA-C	5.69	117.56	111.36
1	D	251	ALA	CA-C-N	5.67	128.23	120.46
1	D	251	ALA	C-N-CA	5.67	128.23	120.46
1	D	185	VAL	N-CA-C	5.66	115.79	110.30
1	C	365	ASN	CA-C-N	5.63	128.14	120.54
1	C	365	ASN	C-N-CA	5.63	128.14	120.54
1	C	197	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	483	ASP	CA-C-N	5.62	129.26	120.82
1	B	483	ASP	C-N-CA	5.62	129.26	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	373	ILE	N-CA-CB	5.62	118.35	111.21
1	A	297	THR	N-CA-C	5.55	118.53	109.59
1	G	296	ALA	CA-C-N	-5.55	113.93	122.87
1	G	296	ALA	C-N-CA	-5.55	113.93	122.87
1	D	361	SER	CA-C-N	5.55	127.56	120.56
1	D	361	SER	C-N-CA	5.55	127.56	120.56
1	E	360	ASP	N-CA-C	5.54	118.11	109.52
1	D	184	GLU	CA-C-N	5.52	127.60	120.70
1	D	184	GLU	C-N-CA	5.52	127.60	120.70
1	C	86	LYS	N-CA-C	-5.50	105.20	111.14
1	F	296	ALA	N-CA-C	5.49	122.50	110.80
1	F	362	VAL	N-CA-CB	5.46	116.94	110.55
1	A	359	HIS	CA-C-N	5.45	131.96	121.54
1	A	359	HIS	C-N-CA	5.45	131.96	121.54
1	C	287	ASN	CA-CB-CG	5.44	118.04	112.60
1	D	174	ASP	CA-CB-CG	5.44	118.04	112.60
1	H	297	THR	CA-C-N	5.44	130.29	122.40
1	H	297	THR	C-N-CA	5.44	130.29	122.40
1	G	297	THR	CB-CA-C	5.43	119.32	109.37
1	B	359	HIS	N-CA-C	5.42	117.27	111.36
1	D	332	GLY	CA-C-N	5.41	129.78	121.19
1	D	332	GLY	C-N-CA	5.41	129.78	121.19
1	D	197	ASP	CA-C-N	5.39	128.50	120.31
1	D	197	ASP	C-N-CA	5.39	128.50	120.31
1	B	405	ARG	CA-C-N	5.38	127.76	120.38
1	B	405	ARG	C-N-CA	5.38	127.76	120.38
1	F	118	LYS	N-CA-C	-5.38	101.46	109.96
1	B	2	SER	N-CA-C	5.37	118.01	110.23
1	F	112	THR	N-CA-C	-5.36	105.44	112.41
1	H	188	PRO	CA-C-N	5.36	127.72	120.38
1	H	188	PRO	C-N-CA	5.36	127.72	120.38
1	H	91	ARG	CB-CA-C	5.36	117.38	109.29
1	A	296	ALA	N-CA-C	5.32	122.14	110.80
1	F	147	GLY	N-CA-C	5.32	122.17	115.42
1	E	377	PRO	CA-C-N	5.32	127.67	120.65
1	E	377	PRO	C-N-CA	5.32	127.67	120.65
1	A	296	ALA	CA-C-N	-5.29	115.26	122.93
1	A	296	ALA	C-N-CA	-5.29	115.26	122.93
1	D	98	GLY	N-CA-C	5.29	122.57	115.59
1	B	91	ARG	CA-C-N	5.28	130.20	121.86
1	B	91	ARG	C-N-CA	5.28	130.20	121.86
1	B	93	GLY	N-CA-C	5.27	120.69	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	GLY	CA-C-N	5.26	124.97	119.92
1	D	139	GLY	C-N-CA	5.26	124.97	119.92
1	D	483	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	444	ASP	CA-C-N	5.26	128.79	120.47
1	E	444	ASP	C-N-CA	5.26	128.79	120.47
1	H	93	GLY	CA-C-O	-5.25	117.74	122.57
1	G	483	ASP	CA-C-N	5.23	127.29	120.28
1	G	483	ASP	C-N-CA	5.23	127.29	120.28
1	G	194	ASP	CA-CB-CG	5.22	117.82	112.60
1	F	287	ASN	CA-CB-CG	5.22	117.82	112.60
1	E	185	VAL	N-CA-CB	5.21	118.41	111.64
1	C	177	GLY	CA-C-N	5.20	129.81	123.10
1	C	177	GLY	C-N-CA	5.20	129.81	123.10
1	F	377	PRO	CA-C-N	5.20	127.20	120.44
1	F	377	PRO	C-N-CA	5.20	127.20	120.44
1	B	93	GLY	CA-C-N	5.19	128.47	121.05
1	B	93	GLY	C-N-CA	5.19	128.47	121.05
1	B	98	GLY	N-CA-C	5.18	120.89	114.37
1	D	457	ARG	CA-C-N	5.17	127.18	120.56
1	D	457	ARG	C-N-CA	5.17	127.18	120.56
1	C	476	VAL	N-CA-C	5.16	117.83	110.09
1	B	483	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	182	GLY	CA-C-N	5.15	128.03	120.71
1	B	182	GLY	C-N-CA	5.15	128.03	120.71
1	E	465	ALA	CA-C-N	5.15	127.14	120.44
1	E	465	ALA	C-N-CA	5.15	127.14	120.44
1	B	84	ASP	CA-C-N	5.14	128.38	120.82
1	B	84	ASP	C-N-CA	5.14	128.38	120.82
1	A	287	ASN	CA-C-N	5.14	127.72	120.42
1	A	287	ASN	C-N-CA	5.14	127.72	120.42
1	C	90	ILE	CA-C-N	5.14	130.66	122.59
1	C	90	ILE	C-N-CA	5.14	130.66	122.59
1	C	361	SER	CA-C-N	5.14	127.03	120.56
1	C	361	SER	C-N-CA	5.14	127.03	120.56
1	D	456	LYS	CA-C-N	5.12	127.14	120.28
1	D	456	LYS	C-N-CA	5.12	127.14	120.28
1	E	361	SER	CA-C-N	5.12	127.01	120.56
1	E	361	SER	C-N-CA	5.12	127.01	120.56
1	E	197	ASP	CA-CB-CG	5.12	117.72	112.60
1	G	297	THR	CA-C-N	5.12	129.38	122.07
1	G	297	THR	C-N-CA	5.12	129.38	122.07
1	F	483	ASP	CB-CA-C	5.11	119.94	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	GLY	CA-C-N	5.11	127.08	120.44
1	A	228	GLY	C-N-CA	5.11	127.08	120.44
1	A	84	ASP	CA-C-N	5.09	128.30	120.82
1	A	84	ASP	C-N-CA	5.09	128.30	120.82
1	E	474	GLY	CA-C-N	5.09	128.09	120.87
1	E	474	GLY	C-N-CA	5.09	128.09	120.87
1	A	19	HIS	CA-C-N	5.07	128.04	120.95
1	A	19	HIS	C-N-CA	5.07	128.04	120.95
1	H	229	GLU	N-CA-C	5.06	119.61	113.38
1	H	483	ASP	CA-CB-CG	5.06	117.66	112.60
1	G	19	HIS	CA-C-N	5.05	127.95	120.82
1	G	19	HIS	C-N-CA	5.05	127.95	120.82
1	H	244	GLN	CA-C-N	5.05	126.46	120.14
1	H	244	GLN	C-N-CA	5.05	126.46	120.14
1	G	186	ASP	CA-CB-CG	5.04	117.64	112.60
1	G	279	GLN	CA-C-N	5.04	127.00	120.44
1	G	279	GLN	C-N-CA	5.04	127.00	120.44
1	F	378	GLU	CB-CG-CD	5.04	121.16	112.60
1	F	145	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	186	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	173	THR	CA-C-N	5.03	129.40	121.56
1	D	173	THR	C-N-CA	5.03	129.40	121.56
1	B	485	SER	CA-C-N	5.01	127.40	120.49
1	B	485	SER	C-N-CA	5.01	127.40	120.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3226	0	3135	90	0
1	B	3481	0	3400	99	0
1	C	3726	0	3664	106	0
1	D	3709	0	3630	118	0
1	E	3710	0	3667	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3716	0	3671	94	0
1	G	3054	0	3026	82	0
1	H	3273	0	3139	84	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	2	0
2	G	6	0	8	1	0
2	H	6	0	8	0	0
3	B	13	0	5	4	0
3	C	13	0	5	1	0
3	D	13	0	5	1	0
3	E	13	0	5	0	0
3	F	13	0	5	0	0
3	H	13	0	5	3	0
4	F	10	0	14	0	0
5	F	7	0	10	0	0
6	A	19	0	0	0	0
6	B	23	0	0	0	0
6	C	32	0	0	2	0
6	D	15	0	0	0	0
6	E	22	0	0	0	0
6	F	31	0	0	0	0
6	G	20	0	0	0	0
6	H	16	0	0	0	0
All	All	28228	0	27466	723	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 13.

All (723) 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:G:299:MET:HE1	1:G:328:VAL:CG2	1.39	1.50
1:D:187:LEU:CD2	1:D:188:PRO:HD2	1.45	1.45
1:G:299:MET:CE	1:G:328:VAL:HG22	1.46	1.43
1:C:202:VAL:CG2	1:C:227:LEU:HD22	1.56	1.35
1:G:202:VAL:CG2	1:G:227:LEU:HD22	1.56	1.34
1:D:202:VAL:CG2	1:D:227:LEU:HD22	1.57	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:CG2	1:B:227:LEU:HD22	1.61	1.28
1:E:401:SER:O	1:E:423:THR:HG22	1.32	1.24
1:D:187:LEU:HD23	1:D:188:PRO:CD	1.70	1.19
1:E:12:ILE:HD11	1:F:278:ALA:HB2	1.24	1.14
1:A:202:VAL:CG2	1:A:227:LEU:HD22	1.77	1.14
1:B:292:PRO:HA	1:B:326:ASP:OD2	1.50	1.10
1:A:401:SER:O	1:A:423:THR:HG22	1.52	1.09
1:A:246:VAL:HG11	1:B:12:ILE:HD11	1.11	1.09
1:C:90:ILE:HD13	1:C:129:TYR:CB	1.82	1.08
1:A:292:PRO:HG3	1:A:435:THR:HG22	1.33	1.08
1:C:90:ILE:CD1	1:C:129:TYR:HB2	1.82	1.08
1:E:277:VAL:CG1	1:F:10:LEU:HD22	1.84	1.06
1:C:202:VAL:HG23	1:C:227:LEU:HD22	1.36	1.06
1:B:202:VAL:HG23	1:B:227:LEU:HD22	1.34	1.05
1:C:317:VAL:HG13	1:C:350:ILE:HG21	1.39	1.05
1:E:12:ILE:CD1	1:F:278:ALA:HB2	1.87	1.04
1:G:378:GLU:HB2	1:G:489:TYR:CD1	1.90	1.04
1:E:277:VAL:HG13	1:F:10:LEU:HD22	1.04	1.04
1:A:277:VAL:HG12	1:B:12:ILE:CG2	1.88	1.04
1:A:277:VAL:CG1	1:B:12:ILE:HG22	1.86	1.04
1:D:202:VAL:CG2	1:D:227:LEU:CD2	2.35	1.03
1:C:144:VAL:HG11	1:C:172:LEU:HD21	1.41	1.02
1:E:277:VAL:HG13	1:F:10:LEU:CD2	1.88	1.02
1:G:202:VAL:CG2	1:G:227:LEU:CD2	2.37	1.02
1:F:88:PRO:HA	1:F:187:LEU:HD22	1.39	1.01
1:A:421:CYS:SG	1:A:423:THR:HG23	2.00	1.01
1:C:202:VAL:CG2	1:C:227:LEU:CD2	2.40	0.99
1:D:187:LEU:HD22	1:D:188:PRO:HD2	1.42	0.98
1:A:472:SER:O	1:A:498:VAL:HG11	1.64	0.98
1:B:202:VAL:HG21	1:B:227:LEU:HD22	1.46	0.98
1:H:132:LEU:H	1:H:133:PRO:HD2	1.28	0.97
1:B:408:ARG:HG2	1:B:435:THR:HG21	1.47	0.96
1:A:399:VAL:HG21	1:A:410:ILE:HD12	1.45	0.96
1:A:277:VAL:HG12	1:B:12:ILE:HG22	0.98	0.96
1:G:202:VAL:HG23	1:G:227:LEU:HD22	1.43	0.96
1:C:144:VAL:CG1	1:C:172:LEU:HD21	1.97	0.95
1:G:378:GLU:HB2	1:G:489:TYR:CE1	2.00	0.95
1:H:50:ARG:HH22	3:H:601:CIT:H41	1.30	0.95
1:C:202:VAL:HG23	1:C:227:LEU:CD2	1.96	0.94
1:F:303:MET:HB3	1:F:343:VAL:HG12	1.50	0.94
1:C:144:VAL:HG12	1:C:172:LEU:CD2	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:VAL:HG23	1:G:227:LEU:CD2	1.98	0.94
1:E:12:ILE:HG23	1:E:13:PHE:CD2	2.03	0.93
1:D:187:LEU:HD23	1:D:188:PRO:HD2	0.95	0.93
1:D:202:VAL:HG23	1:D:227:LEU:HD22	1.49	0.93
1:E:410:ILE:HG22	1:E:419:ILE:CD1	1.99	0.93
1:C:144:VAL:HG22	1:C:178:ILE:CG2	1.98	0.92
1:F:489:TYR:HB2	1:F:490:PRO:HD2	1.49	0.92
1:C:144:VAL:CG1	1:C:172:LEU:CD2	2.47	0.92
1:C:292:PRO:HG3	1:C:435:THR:HG22	1.49	0.91
1:D:202:VAL:HG23	1:D:227:LEU:CD2	1.99	0.91
1:C:144:VAL:HG22	1:C:178:ILE:HG22	1.52	0.91
1:E:26:CYS:SG	1:E:46:MET:HG3	2.11	0.91
1:A:246:VAL:CG1	1:B:12:ILE:HD11	2.00	0.90
1:B:292:PRO:HG3	1:B:435:THR:HG22	1.53	0.90
1:E:12:ILE:HG23	1:E:13:PHE:CE2	2.06	0.90
1:A:202:VAL:HG23	1:A:227:LEU:HD22	1.54	0.89
1:A:292:PRO:HG3	1:A:435:THR:CG2	2.02	0.89
1:B:483:ASP:CG	1:B:491:ASN:HD21	1.80	0.89
1:G:202:VAL:HG21	1:G:227:LEU:HD22	1.53	0.88
1:A:242:ASN:OD1	1:A:245:GLY:HA3	1.73	0.88
1:G:395:LYS:HB2	1:G:471:VAL:HG23	1.55	0.88
1:C:202:VAL:HG21	1:C:227:LEU:HD22	1.57	0.86
1:F:7:ASN:HA	1:F:10:LEU:HD12	1.57	0.86
1:G:26:CYS:SG	1:G:46:MET:HG3	2.15	0.86
1:D:202:VAL:HG22	1:D:227:LEU:HD22	1.58	0.86
1:D:292:PRO:HG3	1:D:435:THR:HG22	1.55	0.85
1:A:246:VAL:HG11	1:B:12:ILE:CD1	2.03	0.85
1:A:472:SER:O	1:A:498:VAL:CG1	2.25	0.85
1:H:263:ARG:NH2	1:H:299:MET:SD	2.49	0.85
1:F:303:MET:HB3	1:F:343:VAL:CG1	2.07	0.85
1:C:317:VAL:HG13	1:C:350:ILE:CG2	2.06	0.85
1:D:359:HIS:O	1:D:359:HIS:ND1	2.10	0.85
1:E:410:ILE:HG22	1:E:419:ILE:HD13	1.58	0.83
1:A:150:THR:O	1:A:151:LEU:HG	1.77	0.83
1:A:391:GLU:OE1	1:D:375:MET:HE3	1.78	0.82
1:B:27:THR:HB	1:B:331:SER:O	1.80	0.82
1:F:187:LEU:HG	1:F:188:PRO:HD2	1.62	0.82
1:C:296:ALA:HB1	1:C:329:MET:HE2	1.60	0.82
1:D:202:VAL:HG21	1:D:227:LEU:HD22	1.56	0.82
1:H:143:TYR:HB2	1:H:179:ASN:O	1.79	0.81
1:D:158:ASP:HB2	1:D:161:THR:OG1	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:ILE:HG12	1:E:259:ILE:HG13	1.64	0.80
1:H:27:THR:HG22	1:H:50:ARG:HD3	1.63	0.80
1:A:399:VAL:CG2	1:A:410:ILE:HD12	2.11	0.80
1:A:421:CYS:SG	1:A:423:THR:CG2	2.69	0.80
1:F:88:PRO:CA	1:F:187:LEU:HD22	2.13	0.79
1:C:317:VAL:CG1	1:C:350:ILE:HG21	2.13	0.79
1:C:180:LEU:HD12	1:C:180:LEU:O	1.83	0.79
1:C:264:GLY:CA	1:C:297:THR:HG21	2.12	0.79
1:D:189:ALA:HB2	1:D:219:GLN:HE21	1.49	0.78
1:A:408:ARG:HG2	1:A:435:THR:HG21	1.63	0.78
1:E:425:ARG:HE	1:E:427:LEU:HD23	1.48	0.78
1:C:26:CYS:SG	1:C:46:MET:HG3	2.24	0.78
1:F:303:MET:CB	1:F:343:VAL:HG12	2.14	0.77
1:G:202:VAL:HG22	1:G:227:LEU:HD22	1.66	0.77
1:G:298:GLN:OE1	1:H:311:ARG:HG2	1.83	0.77
1:E:12:ILE:CD1	1:F:278:ALA:CB	2.61	0.77
1:F:489:TYR:HB2	1:F:490:PRO:CD	2.13	0.77
1:E:12:ILE:HD12	1:F:278:ALA:HA	1.65	0.76
1:F:483:ASP:OD2	1:G:494:ARG:HD3	1.85	0.76
1:H:299:MET:HE2	1:H:328:VAL:HG13	1.67	0.76
1:H:297:THR:HG21	3:H:601:CIT:O1	1.85	0.76
1:D:119:ILE:HG22	1:D:119:ILE:O	1.86	0.75
1:E:436:ARG:HG2	1:E:436:ARG:HH11	1.52	0.75
1:F:172:LEU:CD2	1:F:173:THR:O	2.35	0.75
1:A:202:VAL:CG2	1:A:227:LEU:CD2	2.61	0.75
1:C:4:LEU:O	1:C:8:ILE:HG13	1.85	0.75
1:C:90:ILE:HD13	1:C:129:TYR:HB2	0.89	0.75
1:A:370:LEU:HD22	1:B:4:LEU:HD23	1.69	0.75
1:D:187:LEU:CD2	1:D:188:PRO:CD	2.40	0.75
1:G:436:ARG:HG2	1:G:436:ARG:HH11	1.50	0.74
1:E:358:THR:O	1:E:358:THR:HG22	1.85	0.74
1:E:94:LEU:HB2	1:E:118:LYS:HA	1.68	0.73
1:G:299:MET:CE	1:G:328:VAL:CG2	2.27	0.73
1:B:254:GLU:OE1	1:B:254:GLU:C	2.32	0.73
1:F:92:THR:HG22	1:F:178:ILE:HD11	1.70	0.73
1:B:202:VAL:HG23	1:B:227:LEU:CD2	2.13	0.72
1:E:144:VAL:HG13	1:E:178:ILE:HD13	1.72	0.72
1:C:296:ALA:CB	1:C:329:MET:HE2	2.19	0.72
1:E:410:ILE:HG22	1:E:419:ILE:HD11	1.69	0.72
1:H:146:ASP:OD1	1:H:268:VAL:CG1	2.38	0.72
1:F:455:GLU:O	1:F:458:VAL:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG23	1:A:227:LEU:CD2	2.20	0.71
1:H:146:ASP:OD1	1:H:268:VAL:HG11	1.90	0.71
1:C:264:GLY:HA2	1:C:297:THR:HG21	1.70	0.71
1:E:410:ILE:CG2	1:E:419:ILE:HD13	2.21	0.71
1:E:12:ILE:HD12	1:F:278:ALA:CA	2.20	0.70
1:F:172:LEU:HD23	1:F:173:THR:O	1.92	0.70
1:D:202:VAL:HG21	1:D:227:LEU:CD2	2.16	0.70
1:G:202:VAL:HG21	1:G:227:LEU:CD2	2.17	0.70
1:B:359:HIS:O	1:B:416:ASN:ND2	2.25	0.70
1:C:4:LEU:HD23	1:D:370:LEU:HD22	1.72	0.69
1:E:307:PRO:HG3	1:F:170:HIS:CE1	2.27	0.69
1:B:326:ASP:OD1	1:B:414:ARG:NH2	2.25	0.69
1:B:354:ALA:O	1:B:358:THR:HG22	1.92	0.69
1:G:471:VAL:HG22	1:G:475:ASP:CB	2.22	0.69
1:E:145:ASP:O	1:E:148:VAL:HG23	1.92	0.69
1:D:354:ALA:O	1:D:358:THR:HG22	1.91	0.69
1:H:297:THR:CG2	3:H:601:CIT:O1	2.41	0.69
1:A:202:VAL:HG21	1:A:227:LEU:HD22	1.75	0.69
1:C:359:HIS:HA	1:C:416:ASN:OD1	1.93	0.68
1:C:8:ILE:HD11	1:D:288:VAL:HG21	1.76	0.68
1:F:132:LEU:CD1	1:F:180:LEU:HD11	2.23	0.68
1:G:88:PRO:HG2	1:G:215:ARG:HH22	1.58	0.68
1:D:483:ASP:OD1	1:D:486:VAL:HG12	1.93	0.68
1:C:364:PHE:HD1	1:C:413:TYR:HB3	1.59	0.68
1:E:253:ILE:CD1	1:E:286:CYS:SG	2.81	0.68
1:G:310:THR:OG1	1:H:298:GLN:HB3	1.94	0.68
1:C:202:VAL:HG22	1:C:227:LEU:HD22	1.68	0.67
1:C:133:PRO:HG2	1:C:160:CYS:HA	1.74	0.67
1:E:436:ARG:HH11	1:E:436:ARG:CG	2.08	0.66
1:G:298:GLN:HE22	1:H:308:ARG:HH12	1.42	0.66
1:B:333:GLU:OE1	1:B:333:GLU:N	2.25	0.66
1:A:42:MET:HG3	1:A:46:MET:HE2	1.78	0.66
1:H:88:PRO:HD2	1:H:213:PHE:HB2	1.75	0.66
1:C:144:VAL:CG2	1:C:178:ILE:HG22	2.25	0.66
1:F:453:ASP:OD1	1:F:453:ASP:N	2.27	0.66
1:B:239:LYS:NZ	3:B:601:CIT:H41	2.11	0.66
1:D:133:PRO:HG2	1:D:160:CYS:HA	1.76	0.66
1:A:242:ASN:OD1	1:A:245:GLY:CA	2.44	0.66
1:C:144:VAL:HG12	1:C:172:LEU:HD22	1.74	0.66
1:D:217:ALA:HB2	1:D:251:ALA:HB1	1.77	0.66
1:H:55:HIS:HE1	1:H:91:ARG:HH21	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ARG:HG2	1:D:435:THR:HG21	1.77	0.66
1:F:172:LEU:HD23	1:F:173:THR:N	2.11	0.66
1:A:46:MET:HE3	1:A:79:ILE:HG21	1.76	0.66
1:C:112:THR:OG1	1:C:160:CYS:HB2	1.95	0.66
1:E:253:ILE:HG12	1:E:259:ILE:CG1	2.26	0.66
1:D:356:SER:O	1:D:359:HIS:HD2	1.78	0.65
1:B:68:VAL:HG21	1:B:81:ILE:HG12	1.77	0.65
1:E:144:VAL:HG21	1:E:149:LEU:HD23	1.77	0.65
1:E:253:ILE:HD13	1:E:286:CYS:SG	2.37	0.65
1:H:260:MET:HE2	1:H:329:MET:HE1	1.78	0.65
1:E:21:ALA:N	1:E:355:GLN:HE22	1.94	0.65
1:E:42:MET:HE2	1:E:79:ILE:HG13	1.79	0.65
1:E:408:ARG:HG2	1:E:435:THR:HG21	1.79	0.64
1:C:8:ILE:CD1	1:D:288:VAL:HG21	2.27	0.64
1:D:355:GLN:HA	1:D:358:THR:CG2	2.28	0.64
1:D:23:ARG:NH2	1:D:438:VAL:O	2.29	0.64
1:G:288:VAL:HG22	1:H:4:LEU:HD21	1.79	0.64
1:D:68:VAL:HG21	1:D:81:ILE:HG12	1.79	0.64
1:F:401:SER:HA	2:F:602:GOL:H12	1.80	0.64
1:D:112:THR:OG1	1:D:160:CYS:HB2	1.98	0.64
1:D:42:MET:HE2	1:D:79:ILE:HG13	1.78	0.63
1:E:83:LEU:HB3	1:E:209:ILE:HD13	1.79	0.63
1:F:145:ASP:HB3	1:F:148:VAL:HG22	1.80	0.63
1:H:68:VAL:HG21	1:H:81:ILE:HG12	1.81	0.63
1:C:25:ILE:HB	1:C:329:MET:HG3	1.81	0.63
1:G:471:VAL:HG22	1:G:475:ASP:HB3	1.79	0.63
1:C:90:ILE:HG22	1:C:128:ASP:OD2	1.99	0.63
1:C:92:THR:HG22	1:C:176:LYS:H	1.63	0.63
1:A:180:LEU:N	1:A:180:LEU:HD12	2.13	0.63
1:C:112:THR:HG1	1:C:160:CYS:HB2	1.63	0.63
1:B:254:GLU:OE1	1:B:254:GLU:O	2.16	0.63
1:B:378:GLU:HG3	1:B:490:PRO:HD2	1.81	0.63
1:D:189:ALA:HB2	1:D:219:GLN:HG2	1.81	0.63
1:H:132:LEU:N	1:H:133:PRO:HD2	2.02	0.63
1:C:144:VAL:HG22	1:C:178:ILE:HG23	1.80	0.62
1:E:132:LEU:HD12	1:E:180:LEU:HD11	1.82	0.62
1:B:227:LEU:HD13	1:B:234:THR:OG1	1.98	0.62
1:E:21:ALA:CB	1:E:355:GLN:NE2	2.61	0.62
1:A:450:GLU:CD	1:A:452:ASN:ND2	2.57	0.62
1:G:308:ARG:HD3	1:H:147:GLY:CA	2.30	0.62
1:C:364:PHE:CD1	1:C:413:TYR:HB3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LEU:HB3	1:D:209:ILE:HD13	1.81	0.62
1:A:346:TYR:CE2	1:A:349:ARG:NH2	2.67	0.62
1:F:172:LEU:HD21	1:F:173:THR:O	1.99	0.62
1:G:195:ARG:NH2	1:G:226:ALA:HA	2.15	0.62
1:D:94:LEU:HB2	1:D:118:LYS:HA	1.82	0.62
1:A:399:VAL:CG2	1:A:410:ILE:CD1	2.78	0.62
1:B:247:GLN:O	1:B:247:GLN:HG2	1.98	0.61
1:D:220:VAL:HG11	1:D:255:ALA:HB3	1.81	0.61
1:E:133:PRO:HG2	1:E:160:CYS:HA	1.81	0.61
1:G:299:MET:HE1	1:G:328:VAL:HG23	1.69	0.61
1:G:355:GLN:HA	1:G:358:THR:HG22	1.82	0.61
1:A:227:LEU:HD13	1:A:234:THR:OG1	1.99	0.61
1:G:227:LEU:HD13	1:G:234:THR:OG1	2.00	0.61
1:C:41:LEU:O	1:C:44:SER:HB2	1.99	0.61
1:E:27:THR:CG2	1:E:50:ARG:HH11	2.14	0.61
1:D:111:THR:CB	1:D:161:THR:HG22	2.31	0.61
1:C:292:PRO:HG3	1:C:435:THR:CG2	2.26	0.60
1:C:127:VAL:HG21	1:C:132:LEU:HD22	1.82	0.60
1:D:127:VAL:HG21	1:D:132:LEU:HD22	1.82	0.60
1:D:355:GLN:HA	1:D:358:THR:HG22	1.83	0.60
1:E:127:VAL:HG21	1:E:132:LEU:HD22	1.82	0.60
1:F:127:VAL:HG21	1:F:132:LEU:HD22	1.82	0.60
1:A:465:ALA:C	1:A:471:VAL:HG22	2.26	0.60
1:C:227:LEU:HD13	1:C:234:THR:OG1	2.01	0.60
1:F:132:LEU:HD12	1:F:180:LEU:HD11	1.84	0.60
1:C:264:GLY:N	1:C:297:THR:HG21	2.16	0.60
1:F:494:ARG:HG2	1:G:492:GLN:HG3	1.82	0.60
1:D:112:THR:HG1	1:D:160:CYS:HB2	1.66	0.60
1:B:83:LEU:HB3	1:B:209:ILE:HD13	1.84	0.59
1:C:88:PRO:HD2	1:C:213:PHE:HB2	1.83	0.59
1:A:423:THR:HG21	1:A:428:THR:CG2	2.33	0.59
1:D:359:HIS:O	1:D:359:HIS:CG	2.53	0.59
1:F:94:LEU:HB2	1:F:118:LYS:HA	1.85	0.59
1:F:95:PHE:CE1	1:F:172:LEU:CD2	2.86	0.59
1:D:300:LEU:HD23	1:D:313:GLU:HB3	1.85	0.59
1:F:88:PRO:HA	1:F:187:LEU:CD2	2.23	0.59
1:G:298:GLN:OE1	1:H:311:ARG:N	2.32	0.59
1:H:24:ILE:HG23	1:H:347:MET:HE2	1.83	0.59
1:B:296:ALA:HA	1:B:329:MET:HE2	1.85	0.59
1:C:408:ARG:HG3	1:C:435:THR:HG21	1.84	0.59
1:E:144:VAL:HG13	1:E:178:ILE:CD1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:GLN:OE1	1:F:311:ARG:HD2	2.03	0.59
1:A:42:MET:CG	1:A:46:MET:HE2	2.33	0.58
1:E:88:PRO:CB	1:E:187:LEU:HB3	2.33	0.58
1:E:112:THR:OG1	1:E:160:CYS:HB2	2.03	0.58
1:H:489:TYR:HB3	1:H:490:PRO:HD2	1.84	0.58
1:B:202:VAL:CG2	1:B:227:LEU:CD2	2.57	0.58
1:D:220:VAL:HG13	1:D:255:ALA:HB1	1.83	0.58
1:E:12:ILE:CG2	1:E:13:PHE:CE2	2.84	0.58
1:H:28:ILE:HD11	1:H:49:ALA:HB1	1.84	0.58
1:A:36:GLU:O	1:A:36:GLU:HG3	2.02	0.58
1:B:145:ASP:H	1:B:178:ILE:HG13	1.68	0.58
1:D:240:ILE:HD11	1:D:252:ILE:HG21	1.85	0.58
1:F:132:LEU:HD11	1:F:180:LEU:HD11	1.86	0.58
1:C:90:ILE:CD1	1:C:178:ILE:HD11	2.34	0.58
1:F:95:PHE:CE1	1:F:172:LEU:HD22	2.38	0.58
1:C:26:CYS:SG	1:C:46:MET:CG	2.91	0.58
1:H:491:ASN:ND2	1:H:491:ASN:O	2.36	0.58
1:E:277:VAL:CG1	1:F:10:LEU:CD2	2.65	0.58
1:A:8:ILE:HG13	1:A:8:ILE:O	2.02	0.58
1:A:183:CYS:O	1:A:185:VAL:N	2.35	0.58
1:B:272:ALA:O	1:B:275:VAL:HG22	2.04	0.58
1:B:380:ALA:CB	1:C:392:VAL:HG13	2.33	0.58
1:E:253:ILE:CG1	1:E:259:ILE:HG13	2.33	0.58
1:G:471:VAL:HG22	1:G:475:ASP:HB2	1.86	0.58
1:C:90:ILE:HD12	1:C:178:ILE:HD11	1.86	0.57
1:D:227:LEU:HD13	1:D:234:THR:OG1	2.03	0.57
1:A:116:PHE:N	1:A:116:PHE:CD1	2.71	0.57
1:C:50:ARG:HH22	3:C:601:CIT:H42	1.70	0.57
1:D:27:THR:HG22	1:D:50:ARG:HD3	1.85	0.57
1:H:464:TRP:CZ3	1:H:470:TYR:HE2	2.21	0.57
1:C:202:VAL:HG21	1:C:227:LEU:CD2	2.22	0.57
1:B:492:GLN:HG3	1:C:494:ARG:HG2	1.87	0.57
1:B:27:THR:OG1	1:B:331:SER:HA	2.04	0.57
1:B:380:ALA:HB2	1:C:392:VAL:HG13	1.86	0.57
1:F:215:ARG:O	1:F:252:ILE:HD11	2.05	0.57
1:H:229:GLU:HA	1:H:232:LYS:HB3	1.86	0.57
1:A:466:LYS:HA	1:A:471:VAL:O	2.05	0.56
1:F:489:TYR:N	1:F:489:TYR:CD2	2.73	0.56
1:F:489:TYR:N	1:F:489:TYR:HD2	2.03	0.56
1:A:200:PHE:O	1:A:203:GLU:HG2	2.05	0.56
1:E:12:ILE:HD12	1:F:278:ALA:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:GLU:HG3	1:C:490:PRO:HD2	1.86	0.56
1:A:423:THR:HG21	1:A:428:THR:HG22	1.86	0.56
1:B:483:ASP:OD2	1:B:491:ASN:ND2	2.38	0.56
1:B:494:ARG:NE	1:C:483:ASP:OD2	2.38	0.55
1:D:241:GLU:HB2	1:D:265:ASP:HB2	1.88	0.55
1:F:378:GLU:HB2	1:F:489:TYR:HD1	1.70	0.55
1:G:489:TYR:HB2	1:G:490:PRO:HD2	1.87	0.55
1:A:183:CYS:O	1:A:185:VAL:HG12	2.07	0.55
1:E:88:PRO:HB2	1:E:187:LEU:HB3	1.88	0.55
1:C:322:PHE:HD1	1:C:358:THR:HG21	1.71	0.55
1:E:253:ILE:HD11	1:E:286:CYS:SG	2.47	0.55
1:H:27:THR:HG21	1:H:50:ARG:NH1	2.22	0.55
1:D:159:ASP:OD1	1:D:160:CYS:N	2.38	0.55
1:B:384:SER:HB3	6:C:704:HOH:O	2.06	0.55
1:C:241:GLU:HB2	1:C:265:ASP:HB2	1.89	0.55
1:G:403:THR:H	2:G:601:GOL:H12	1.72	0.55
1:H:483:ASP:OD1	1:H:484:HIS:N	2.38	0.54
1:C:144:VAL:CG1	1:C:172:LEU:HD22	2.34	0.54
1:G:419:ILE:HD12	1:G:437:SER:HB2	1.89	0.54
1:B:296:ALA:CA	1:B:329:MET:HE2	2.38	0.54
1:D:220:VAL:CG1	1:D:255:ALA:CB	2.86	0.54
1:F:187:LEU:CG	1:F:188:PRO:HD2	2.36	0.54
1:E:50:ARG:HH21	1:E:84:ASP:CG	2.16	0.54
1:H:211:ALA:HB1	1:H:214:ILE:HD11	1.89	0.54
1:F:144:VAL:HB	1:F:149:LEU:HB3	1.90	0.54
1:E:241:GLU:HB2	1:E:265:ASP:HB2	1.90	0.54
1:B:292:PRO:HG3	1:B:435:THR:CG2	2.31	0.54
1:D:23:ARG:NH2	1:D:439:GLU:OE2	2.39	0.54
1:D:145:ASP:CG	1:D:145:ASP:O	2.50	0.54
1:E:21:ALA:HB2	1:E:355:GLN:NE2	2.21	0.54
1:G:298:GLN:NE2	1:H:308:ARG:HH12	2.06	0.54
1:D:95:PHE:CZ	1:D:172:LEU:HD23	2.43	0.53
1:B:483:ASP:OD2	1:C:494:ARG:HD2	2.08	0.53
1:B:239:LYS:HE3	1:B:260:MET:HE2	1.90	0.53
1:D:94:LEU:HG	1:D:174:ASP:OD1	2.09	0.53
1:G:43:LYS:HE2	1:G:75:LEU:HD21	1.91	0.53
1:F:187:LEU:HG	1:F:188:PRO:CD	2.35	0.53
1:A:288:VAL:HG21	1:B:8:ILE:HD11	1.90	0.53
1:H:364:PHE:CZ	1:H:387:SER:HB3	2.44	0.53
1:E:112:THR:HG1	1:E:160:CYS:HB2	1.74	0.53
1:G:216:THR:HG22	1:G:219:GLN:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG13	1:D:380:ALA:HB2	1.91	0.53
1:B:249:ILE:O	1:B:252:ILE:HB	2.09	0.53
1:E:421:CYS:SG	1:E:423:THR:HG23	2.48	0.53
1:A:241:GLU:HB2	1:A:265:ASP:HB2	1.90	0.53
1:C:91:ARG:HA	1:C:177:GLY:HA2	1.90	0.53
1:E:410:ILE:CG2	1:E:419:ILE:CD1	2.79	0.53
1:B:239:LYS:HZ2	3:B:601:CIT:H41	1.73	0.53
1:A:391:GLU:OE1	1:D:375:MET:CE	2.54	0.52
1:F:241:GLU:HB2	1:F:265:ASP:HB2	1.91	0.52
1:C:8:ILE:HD11	1:D:288:VAL:CG2	2.38	0.52
1:D:86:LYS:HE2	1:D:91:ARG:HH22	1.73	0.52
1:E:292:PRO:HG3	1:E:435:THR:HG22	1.91	0.52
1:A:180:LEU:N	1:A:180:LEU:CD1	2.72	0.52
1:E:12:ILE:HD13	1:F:246:VAL:HG11	1.91	0.52
1:C:239:LYS:HE3	1:C:260:MET:HE2	1.89	0.52
1:G:8:ILE:HG23	1:H:285:LYS:HG2	1.91	0.52
1:C:475:ASP:O	1:C:498:VAL:HG22	2.09	0.52
1:G:47:SER:HB3	1:G:433:ASN:HB3	1.91	0.52
1:G:436:ARG:HH11	1:G:436:ARG:CG	2.17	0.52
1:A:260:MET:HE3	1:A:296:ALA:CB	2.40	0.52
1:A:378:GLU:HG3	1:A:489:TYR:HB3	1.90	0.52
1:B:137:ARG:HB3	1:B:138:PRO:HD2	1.91	0.52
1:B:144:VAL:HA	1:B:178:ILE:HB	1.91	0.52
1:C:90:ILE:HB	1:C:128:ASP:HB3	1.92	0.52
1:D:185:VAL:HG21	1:D:215:ARG:CZ	2.40	0.52
1:F:239:LYS:HE3	1:F:260:MET:HE2	1.90	0.52
1:H:241:GLU:HB2	1:H:265:ASP:HB2	1.91	0.52
1:G:241:GLU:HB2	1:G:265:ASP:HB2	1.91	0.52
1:H:55:HIS:CE1	1:H:91:ARG:HE	2.28	0.52
1:A:475:ASP:H	1:A:498:VAL:HG12	1.75	0.51
1:B:241:GLU:HB2	1:B:265:ASP:HB2	1.90	0.51
1:B:339:TYR:HB3	1:B:342:GLU:HB2	1.92	0.51
1:E:27:THR:HG23	1:E:50:ARG:HH11	1.75	0.51
1:F:240:ILE:HD13	1:F:259:ILE:HG23	1.92	0.51
1:A:450:GLU:OE1	1:A:452:ASN:ND2	2.43	0.51
1:C:180:LEU:O	1:C:180:LEU:CD1	2.57	0.51
1:G:263:ARG:NH2	1:G:297:THR:O	2.41	0.51
1:F:88:PRO:HD2	1:F:213:PHE:HB2	1.92	0.51
1:G:471:VAL:CG2	1:G:475:ASP:HB3	2.39	0.51
1:F:129:TYR:CZ	1:F:185:VAL:HG23	2.45	0.51
1:D:187:LEU:HD23	1:D:188:PRO:HD3	1.82	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:THR:HB	1:H:126:TYR:HE1	1.75	0.51
1:B:50:ARG:HH22	3:B:601:CIT:H42	1.74	0.51
1:B:91:ARG:HA	1:B:178:ILE:HD13	1.92	0.51
1:F:92:THR:CG2	1:F:178:ILE:HD11	2.41	0.51
1:G:239:LYS:HE3	1:G:260:MET:HE2	1.92	0.51
1:G:308:ARG:HD3	1:H:147:GLY:HA3	1.93	0.51
1:B:363:MET:O	1:B:366:SER:HB3	2.11	0.51
1:D:88:PRO:HD2	1:D:213:PHE:HB2	1.93	0.51
1:D:299:MET:HE1	1:D:320:ALA:HB2	1.92	0.51
1:H:24:ILE:HG21	1:H:344:VAL:HG13	1.93	0.51
1:C:23:ARG:NH2	1:C:439:GLU:OE2	2.44	0.50
1:C:94:LEU:HB2	1:C:118:LYS:HA	1.92	0.50
1:E:50:ARG:NH2	1:E:84:ASP:CG	2.70	0.50
1:F:145:ASP:HB2	1:F:172:LEU:HD12	1.93	0.50
1:B:248:ASN:O	1:B:252:ILE:HG12	2.11	0.50
1:D:302:SER:OG	1:D:313:GLU:OE1	2.24	0.50
1:E:401:SER:O	1:E:423:THR:CG2	2.28	0.50
1:A:424:THR:OG1	1:A:445:VAL:HG23	2.12	0.50
1:G:299:MET:HE1	1:G:328:VAL:HG22	0.58	0.50
1:A:427:LEU:H	2:A:601:GOL:H11	1.76	0.50
1:E:25:ILE:HG12	1:E:48:VAL:HB	1.93	0.50
1:E:239:LYS:HE3	1:E:260:MET:HE2	1.93	0.50
1:F:24:ILE:HG21	1:F:344:VAL:HG13	1.93	0.50
1:C:300:LEU:HD23	1:C:313:GLU:HB3	1.94	0.50
1:E:392:VAL:HG13	1:H:380:ALA:CB	2.42	0.49
1:G:277:VAL:HG13	1:H:10:LEU:HD13	1.93	0.49
1:E:263:ARG:NH2	1:E:299:MET:SD	2.85	0.49
1:A:424:THR:OG1	1:A:445:VAL:CG2	2.61	0.49
1:D:220:VAL:CG1	1:D:255:ALA:HB3	2.41	0.49
1:H:112:THR:HB	1:H:126:TYR:CE1	2.48	0.49
1:A:399:VAL:HG22	1:A:410:ILE:CD1	2.41	0.49
1:D:295:CYS:SG	1:D:299:MET:HE3	2.52	0.49
1:G:300:LEU:HD12	1:G:330:LEU:HD21	1.94	0.49
1:D:431:GLN:O	1:D:434:VAL:HG12	2.13	0.49
1:F:483:ASP:OD2	1:G:494:ARG:CD	2.58	0.49
1:D:240:ILE:HD13	1:D:259:ILE:HG23	1.94	0.49
1:E:90:ILE:HG22	1:E:178:ILE:HB	1.93	0.49
1:D:360:ASP:HB3	1:D:362:VAL:H	1.77	0.49
1:E:240:ILE:HD13	1:E:259:ILE:HG23	1.95	0.49
1:E:436:ARG:CG	1:E:436:ARG:NH1	2.73	0.49
1:B:493:THR:HB	1:C:493:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ARG:HD2	1:E:175:ARG:HB3	1.94	0.49
1:F:391:GLU:HA	1:G:373:ILE:HD12	1.95	0.49
1:G:240:ILE:HD13	1:G:259:ILE:HG23	1.95	0.49
1:A:240:ILE:HD13	1:A:259:ILE:HG23	1.95	0.48
1:E:380:ALA:CB	1:H:392:VAL:HG13	2.43	0.48
1:E:358:THR:O	1:E:358:THR:CG2	2.56	0.48
1:C:141:LEU:HD22	1:C:150:THR:HG22	1.95	0.48
1:D:119:ILE:O	1:D:119:ILE:CG2	2.58	0.48
1:D:423:THR:CG2	1:D:429:CYS:SG	3.02	0.48
1:B:88:PRO:HD2	1:B:213:PHE:HB2	1.95	0.48
1:B:392:VAL:HB	1:B:476:VAL:HG11	1.94	0.48
1:G:88:PRO:HG2	1:G:215:ARG:NH2	2.27	0.48
1:H:223:VAL:HG23	1:H:236:ILE:HD13	1.95	0.48
1:A:288:VAL:HG22	1:B:4:LEU:HD21	1.95	0.48
1:H:4:LEU:O	1:H:8:ILE:HG23	2.13	0.48
1:B:483:ASP:OD1	1:B:486:VAL:HB	2.13	0.48
1:C:90:ILE:CD1	1:C:129:TYR:CB	2.65	0.48
1:E:415:PRO:HG3	1:E:419:ILE:HD11	1.96	0.48
1:A:391:GLU:OE2	1:D:368:LYS:HE3	2.14	0.48
1:C:42:MET:C	1:C:44:SER:N	2.71	0.48
1:C:300:LEU:HA	1:C:313:GLU:HG2	1.95	0.48
1:E:88:PRO:HB3	1:E:187:LEU:HB3	1.96	0.48
1:E:454:ARG:HH22	1:E:484:HIS:HA	1.79	0.48
1:B:296:ALA:O	1:B:329:MET:CE	2.62	0.47
1:C:370:LEU:HD22	1:D:4:LEU:HD23	1.95	0.47
1:F:220:VAL:HG12	1:F:224:ARG:HH12	1.78	0.47
1:A:300:LEU:HD23	1:A:313:GLU:HB3	1.95	0.47
1:D:83:LEU:HB3	1:D:209:ILE:CD1	2.44	0.47
1:F:91:ARG:HG2	1:F:177:GLY:HA2	1.96	0.47
1:G:339:TYR:HB3	1:G:342:GLU:HB2	1.96	0.47
1:G:378:GLU:CB	1:G:489:TYR:CD1	2.80	0.47
1:C:27:THR:HB	1:C:331:SER:O	2.14	0.47
1:C:339:TYR:HB3	1:C:342:GLU:HB2	1.95	0.47
1:B:237:ILE:HG21	1:B:294:ILE:HD12	1.96	0.47
1:E:360:ASP:HB3	1:E:362:VAL:H	1.79	0.47
1:F:304:THR:HG22	1:F:333:GLU:HA	1.96	0.47
1:A:278:ALA:HA	1:B:12:ILE:HG21	1.97	0.47
1:A:302:SER:OG	1:A:313:GLU:OE1	2.25	0.47
1:C:240:ILE:HD13	1:C:259:ILE:HG23	1.96	0.47
1:G:405:ARG:O	1:G:409:LEU:N	2.41	0.47
1:A:421:CYS:HG	1:A:423:THR:HG23	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ILE:O	1:D:285:LYS:NZ	2.44	0.47
1:C:277:VAL:HG12	1:D:12:ILE:HG13	1.97	0.47
1:D:434:VAL:O	1:D:434:VAL:HG22	2.14	0.47
1:B:359:HIS:O	1:B:416:ASN:CG	2.57	0.47
1:D:54:SER:HA	1:D:86:LYS:HG3	1.95	0.47
1:D:145:ASP:O	1:D:145:ASP:OD1	2.32	0.47
1:D:220:VAL:CG1	1:D:255:ALA:HB1	2.45	0.47
1:E:294:ILE:HG21	1:E:329:MET:HE3	1.96	0.47
1:E:339:TYR:HB3	1:E:342:GLU:HB2	1.97	0.47
1:G:4:LEU:HD23	1:H:370:LEU:HD22	1.97	0.47
1:C:9:GLY:HA3	6:C:726:HOH:O	2.14	0.47
1:F:392:VAL:HG13	1:G:380:ALA:CB	2.45	0.47
1:H:314:VAL:HG13	1:H:350:ILE:HG12	1.97	0.47
1:B:296:ALA:HB1	1:B:329:MET:HE1	1.97	0.46
1:D:471:VAL:HG11	1:D:498:VAL:HG11	1.97	0.46
1:E:364:PHE:HD1	1:E:413:TYR:HB3	1.80	0.46
1:G:436:ARG:CG	1:G:436:ARG:NH1	2.78	0.46
1:G:454:ARG:HG2	1:G:457:ARG:NH2	2.30	0.46
1:B:292:PRO:CA	1:B:326:ASP:OD2	2.43	0.46
1:D:292:PRO:HB3	1:D:434:VAL:HG22	1.97	0.46
1:A:180:LEU:HB3	1:A:183:CYS:SG	2.55	0.46
1:C:13:PHE:CZ	1:D:243:HIS:ND1	2.81	0.46
1:D:423:THR:HG23	1:D:429:CYS:SG	2.55	0.46
1:E:144:VAL:HG23	1:E:149:LEU:O	2.16	0.46
1:G:12:ILE:HD12	1:G:12:ILE:H	1.80	0.46
1:H:146:ASP:OD1	1:H:268:VAL:HG13	2.12	0.46
1:A:339:TYR:HB3	1:A:342:GLU:HB2	1.97	0.46
1:D:95:PHE:HZ	1:D:172:LEU:HD23	1.81	0.46
1:F:402:ASN:H	2:F:602:GOL:H2	1.80	0.46
1:C:4:LEU:O	1:C:8:ILE:CG1	2.60	0.46
1:D:339:TYR:HB3	1:D:342:GLU:HB2	1.98	0.46
1:E:135:VAL:HG13	1:E:184:GLU:O	2.15	0.46
1:H:196:LYS:HA	1:H:199:GLN:HB2	1.97	0.46
1:B:244:GLN:O	1:B:248:ASN:HB2	2.16	0.46
1:C:42:MET:C	1:C:44:SER:H	2.24	0.46
1:G:209:ILE:HD13	1:G:227:LEU:HD11	1.96	0.46
1:H:355:GLN:HA	1:H:358:THR:HG22	1.96	0.46
1:G:276:VAL:HG22	1:H:315:THR:HG22	1.97	0.46
1:C:317:VAL:HG11	1:C:350:ILE:HD13	1.98	0.46
1:E:4:LEU:HD23	1:F:370:LEU:HD22	1.98	0.46
1:E:149:LEU:HA	1:E:168:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HB3	1:A:231:GLY:HA3	1.98	0.46
1:G:219:GLN:O	1:G:222:GLU:HB2	2.15	0.46
1:A:419:ILE:O	1:A:438:VAL:HA	2.16	0.45
1:B:129:TYR:CZ	1:B:131:GLN:HB2	2.51	0.45
1:E:50:ARG:HH12	1:E:52:ASN:HB2	1.81	0.45
1:H:216:THR:HG23	1:H:219:GLN:H	1.81	0.45
1:C:378:GLU:HB2	1:C:489:TYR:HB2	1.98	0.45
1:D:111:THR:HA	1:D:161:THR:HG22	1.97	0.45
1:D:129:TYR:HE1	1:D:187:LEU:HG	1.81	0.45
1:E:150:THR:HG23	1:E:167:ASN:HB2	1.98	0.45
1:F:142:ILE:HG12	1:F:180:LEU:HD21	1.97	0.45
1:H:47:SER:O	1:H:79:ILE:HG23	2.15	0.45
1:D:295:CYS:SG	1:D:299:MET:CE	3.05	0.45
1:E:27:THR:HA	1:E:50:ARG:HB3	1.98	0.45
1:F:88:PRO:CB	1:F:187:LEU:HD22	2.46	0.45
1:E:83:LEU:HB3	1:E:209:ILE:CD1	2.46	0.45
1:F:95:PHE:HE1	1:F:172:LEU:CD2	2.28	0.45
1:F:455:GLU:O	1:F:456:LYS:C	2.58	0.45
1:B:239:LYS:HZ1	3:B:601:CIT:H41	1.80	0.45
1:H:240:ILE:HD13	1:H:259:ILE:HG23	1.98	0.45
1:H:257:ASP:O	1:H:292:PRO:HD2	2.16	0.45
1:F:118:LYS:O	1:F:119:ILE:HG13	2.17	0.45
1:G:50:ARG:HD2	1:G:210:PHE:HD2	1.81	0.45
1:A:242:ASN:CG	1:A:245:GLY:H	2.25	0.45
1:B:240:ILE:HD13	1:B:259:ILE:HG23	1.99	0.45
1:C:446:ASP:C	1:C:448:HIS:H	2.25	0.45
1:D:364:PHE:HD1	1:D:413:TYR:HB3	1.82	0.45
1:E:27:THR:OG1	1:E:50:ARG:HD3	2.17	0.45
1:F:95:PHE:CZ	1:F:172:LEU:HD22	2.52	0.45
1:F:339:TYR:HB3	1:F:342:GLU:HB2	1.99	0.45
1:H:339:TYR:HB3	1:H:342:GLU:HB2	1.98	0.45
1:A:115:ALA:C	1:A:117:GLU:H	2.25	0.45
1:F:113:ASP:HB3	1:F:116:PHE:HD2	1.82	0.45
1:A:392:VAL:HG13	1:D:380:ALA:CB	2.46	0.45
1:C:113:ASP:HB3	1:C:116:PHE:HD2	1.82	0.45
1:E:21:ALA:N	1:E:355:GLN:NE2	2.65	0.45
1:G:298:GLN:HE22	1:H:308:ARG:NH1	2.10	0.45
1:G:418:PRO:HG2	1:G:470:TYR:CD1	2.52	0.45
1:C:249:ILE:HG12	1:C:282:ILE:HG12	2.00	0.44
1:C:276:VAL:O	1:C:280:MET:HG3	2.17	0.44
1:D:27:THR:HA	1:D:50:ARG:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:VAL:HB	1:F:476:VAL:HG11	1.98	0.44
1:H:398:LEU:HB2	1:H:477:MET:HE2	1.99	0.44
1:B:359:HIS:O	1:B:416:ASN:OD1	2.35	0.44
1:B:450:GLU:HG3	1:B:452:ASN:HD21	1.82	0.44
1:A:202:VAL:HG21	1:A:227:LEU:CD2	2.42	0.44
1:A:260:MET:HE3	1:A:296:ALA:HB1	1.99	0.44
1:B:157:GLU:H	1:B:162:LEU:HD12	1.82	0.44
1:D:215:ARG:HB2	1:D:219:GLN:OE1	2.16	0.44
1:D:300:LEU:HA	1:D:313:GLU:HG2	1.99	0.44
1:E:420:ILE:HA	1:E:439:GLU:O	2.17	0.44
1:E:474:GLY:H	1:E:498:VAL:C	2.24	0.44
1:B:116:PHE:CG	1:B:116:PHE:O	2.70	0.44
1:D:113:ASP:HB3	1:D:116:PHE:HD2	1.83	0.44
1:E:364:PHE:CD1	1:E:413:TYR:HB3	2.53	0.44
1:G:42:MET:HG2	1:G:79:ILE:HD13	2.00	0.44
1:H:264:GLY:N	1:H:297:THR:OG1	2.50	0.44
1:B:83:LEU:HB3	1:B:209:ILE:CD1	2.48	0.44
1:B:116:PHE:O	1:B:116:PHE:CD1	2.70	0.44
1:F:364:PHE:HD1	1:F:413:TYR:HB3	1.81	0.44
1:H:132:LEU:O	1:H:135:VAL:N	2.51	0.44
1:C:322:PHE:CE1	1:C:358:THR:HG23	2.52	0.44
1:C:467:THR:C	1:C:469:GLY:H	2.26	0.44
1:E:215:ARG:HG3	1:E:219:GLN:HE22	1.82	0.44
1:H:94:LEU:N	1:H:94:LEU:HD22	2.32	0.44
1:B:386:VAL:HG21	1:B:413:TYR:HB2	2.00	0.44
1:F:249:ILE:HG12	1:F:282:ILE:HG12	2.00	0.44
1:F:486:VAL:HG21	1:F:489:TYR:O	2.18	0.44
1:H:253:ILE:HG12	1:H:259:ILE:HG13	2.00	0.44
1:D:189:ALA:HB2	1:D:219:GLN:NE2	2.26	0.44
1:F:172:LEU:HD11	1:F:176:LYS:HB2	2.00	0.44
1:A:242:ASN:OD1	1:A:245:GLY:N	2.50	0.43
1:B:249:ILE:HG13	1:B:253:ILE:HD11	1.98	0.43
1:D:364:PHE:CD1	1:D:413:TYR:HB3	2.53	0.43
1:G:392:VAL:HB	1:G:476:VAL:HG11	1.99	0.43
1:A:314:VAL:HG13	1:A:350:ILE:HG12	2.00	0.43
1:C:317:VAL:CG1	1:C:350:ILE:HD13	2.48	0.43
1:F:364:PHE:CD1	1:F:413:TYR:HB3	2.53	0.43
1:H:144:VAL:HG12	1:H:148:VAL:HG21	2.01	0.43
1:C:388:SER:O	1:C:392:VAL:HG22	2.18	0.43
1:A:241:GLU:HA	1:A:266:LEU:HB2	2.00	0.43
1:B:35:VAL:HG21	1:G:372:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ILE:HG22	1:B:253:ILE:O	2.18	0.43
1:E:149:LEU:HD13	1:E:170:HIS:HB3	2.00	0.43
1:E:378:GLU:HB3	1:E:405:ARG:HH22	1.82	0.43
1:E:392:VAL:HB	1:E:476:VAL:HG11	1.99	0.43
1:E:405:ARG:HG3	1:E:406:SER:N	2.33	0.43
1:E:241:GLU:HA	1:E:266:LEU:HB2	2.00	0.43
1:G:302:SER:OG	1:G:313:GLU:OE1	2.20	0.43
1:H:261:VAL:HG13	1:H:282:ILE:HD11	2.01	0.43
1:B:25:ILE:HB	1:B:329:MET:HG3	2.00	0.43
1:E:113:ASP:HB3	1:E:116:PHE:HD2	1.83	0.43
1:H:249:ILE:HG12	1:H:282:ILE:HG22	1.99	0.43
1:B:189:ALA:HB2	1:B:219:GLN:HG2	2.00	0.43
1:D:129:TYR:HB3	1:D:132:LEU:HB2	2.01	0.43
1:E:378:GLU:CB	1:E:405:ARG:HH22	2.32	0.43
1:H:392:VAL:HB	1:H:476:VAL:HG11	2.01	0.43
1:A:278:ALA:O	1:A:282:ILE:HD12	2.19	0.43
1:E:21:ALA:H	1:E:355:GLN:NE2	2.17	0.43
1:E:144:VAL:CG2	1:E:149:LEU:HD23	2.45	0.43
1:G:46:MET:HE2	1:G:46:MET:HB3	1.82	0.43
1:H:425:ARG:HG3	1:H:427:LEU:H	1.84	0.43
1:E:392:VAL:HG13	1:H:380:ALA:HB2	1.99	0.43
1:E:397:ILE:HB	1:E:419:ILE:HG12	2.01	0.43
1:F:411:SER:OG	1:F:436:ARG:O	2.35	0.43
1:H:276:VAL:O	1:H:280:MET:HG3	2.19	0.43
1:A:12:ILE:HD12	1:A:12:ILE:H	1.84	0.42
1:B:51:MET:HE2	1:B:81:ILE:HG22	2.01	0.42
1:G:364:PHE:HD1	1:G:413:TYR:HB3	1.84	0.42
1:H:364:PHE:HZ	1:H:387:SER:HB3	1.83	0.42
1:D:42:MET:HG3	1:D:46:MET:CE	2.49	0.42
1:A:219:GLN:O	1:A:222:GLU:HB2	2.19	0.42
1:F:303:MET:CB	1:F:343:VAL:CG1	2.84	0.42
1:G:405:ARG:O	1:G:409:LEU:HB2	2.19	0.42
1:A:88:PRO:HD2	1:A:213:PHE:HB2	2.00	0.42
1:B:42:MET:HE2	1:B:79:ILE:HG13	2.01	0.42
1:D:241:GLU:HA	1:D:266:LEU:HB2	2.01	0.42
1:E:4:LEU:HD22	1:F:366:SER:HB3	2.01	0.42
1:E:292:PRO:HG3	1:E:435:THR:CG2	2.49	0.42
1:E:300:LEU:HD12	1:E:330:LEU:HD21	2.01	0.42
1:G:300:LEU:HD23	1:G:313:GLU:HB3	2.01	0.42
1:A:4:LEU:HD22	1:B:366:SER:OG	2.19	0.42
1:A:392:VAL:HB	1:A:476:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:TYR:OH	1:B:186:ASP:OD1	2.32	0.42
1:B:242:ASN:O	1:B:246:VAL:HG23	2.19	0.42
1:D:392:VAL:HB	1:D:476:VAL:HG11	2.00	0.42
1:D:486:VAL:HG22	1:D:487:LYS:H	1.85	0.42
1:E:21:ALA:HB3	1:E:355:GLN:NE2	2.35	0.42
1:H:241:GLU:HA	1:H:266:LEU:HB2	2.02	0.42
1:A:401:SER:O	1:A:423:THR:CG2	2.43	0.42
1:C:390:PHE:HE1	1:C:416:ASN:ND2	2.17	0.42
1:E:276:VAL:O	1:E:280:MET:HG3	2.18	0.42
1:F:294:ILE:HG21	1:F:329:MET:HE3	2.02	0.42
1:B:388:SER:O	1:B:392:VAL:HG22	2.19	0.42
1:D:191:SER:O	1:D:195:ARG:HG3	2.20	0.42
1:E:25:ILE:HG21	1:E:329:MET:HE2	2.02	0.42
1:E:451:ASP:HB2	1:E:456:LYS:HD2	2.01	0.42
1:G:217:ALA:HB2	1:G:251:ALA:HB1	2.01	0.42
1:B:450:GLU:HG3	1:B:452:ASN:ND2	2.35	0.42
1:E:330:LEU:HD13	1:E:343:VAL:HG13	2.02	0.42
1:F:451:ASP:OD2	1:F:456:LYS:CB	2.68	0.42
1:D:404:GLY:HA3	1:D:432:LEU:HD11	2.01	0.42
1:E:156:LYS:HA	1:E:162:LEU:HD23	2.01	0.42
1:E:388:SER:O	1:E:392:VAL:HG22	2.20	0.42
1:H:94:LEU:HD22	1:H:94:LEU:H	1.84	0.42
1:B:47:SER:HB3	1:B:433:ASN:HB3	2.01	0.41
1:B:202:VAL:HG21	1:B:227:LEU:CD2	2.32	0.41
1:B:241:GLU:HA	1:B:266:LEU:HB2	2.02	0.41
1:C:366:SER:HB3	1:D:4:LEU:HD22	2.02	0.41
1:D:388:SER:O	1:D:392:VAL:HG22	2.20	0.41
1:E:235:LEU:HD11	1:E:431:GLN:HG2	2.02	0.41
1:G:241:GLU:HA	1:G:266:LEU:HB2	2.02	0.41
1:H:132:LEU:N	1:H:133:PRO:CD	2.78	0.41
1:C:237:ILE:HG21	1:C:294:ILE:HD12	2.02	0.41
1:D:42:MET:HG3	1:D:46:MET:HE2	2.01	0.41
1:F:241:GLU:HA	1:F:266:LEU:HB2	2.01	0.41
1:F:406:SER:O	1:F:410:ILE:N	2.51	0.41
1:A:364:PHE:HD1	1:A:413:TYR:HB3	1.84	0.41
1:F:464:TRP:HZ3	1:F:470:TYR:HE2	1.69	0.41
1:H:94:LEU:H	1:H:94:LEU:CD2	2.33	0.41
1:A:386:VAL:HG21	1:A:413:TYR:HB2	2.02	0.41
1:G:299:MET:HA	1:G:316:ASP:OD2	2.20	0.41
1:H:451:ASP:CG	1:H:451:ASP:O	2.62	0.41
1:A:388:SER:O	1:A:392:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ILE:HD12	1:D:278:ALA:HA	2.03	0.41
1:C:317:VAL:HG21	1:C:347:MET:HG3	2.02	0.41
1:E:27:THR:HG21	1:E:50:ARG:NH1	2.36	0.41
1:E:315:THR:HG22	1:F:276:VAL:HG22	2.02	0.41
1:D:26:CYS:HB3	1:D:334:THR:HG21	2.02	0.41
1:G:364:PHE:CD1	1:G:413:TYR:HB3	2.55	0.41
1:C:431:GLN:O	1:C:434:VAL:HG22	2.21	0.41
1:D:111:THR:CA	1:D:161:THR:HG22	2.51	0.41
1:E:80:GLY:HA2	1:E:430:ARG:HB3	2.03	0.41
1:E:135:VAL:HG12	1:E:183:CYS:HB3	2.02	0.41
1:E:307:PRO:HG3	1:F:170:HIS:HE1	1.80	0.41
1:H:227:LEU:HD11	1:H:236:ILE:HD11	2.03	0.41
1:D:333:GLU:HB3	1:D:343:VAL:HG11	2.03	0.41
1:G:311:ARG:HG2	1:H:298:GLN:OE1	2.20	0.41
1:H:143:TYR:CB	1:H:179:ASN:O	2.61	0.41
1:B:360:ASP:CG	1:B:362:VAL:HG23	2.46	0.41
1:B:408:ARG:CG	1:B:435:THR:HG21	2.35	0.41
1:D:52:ASN:HD21	3:D:601:CIT:C1	2.34	0.41
1:H:263:ARG:HB2	1:H:297:THR:OG1	2.21	0.41
1:A:129:TYR:CZ	1:A:185:VAL:HG23	2.56	0.41
1:C:322:PHE:CD1	1:C:358:THR:HG21	2.54	0.41
1:D:113:ASP:HB3	1:D:116:PHE:CD2	2.56	0.41
1:D:158:ASP:HB2	1:D:161:THR:HG1	1.84	0.41
1:D:172:LEU:HD11	1:D:176:LYS:CB	2.51	0.41
1:D:220:VAL:HG21	1:D:256:SER:OG	2.21	0.41
1:B:392:VAL:HG13	1:C:380:ALA:CB	2.51	0.40
1:B:472:SER:O	1:B:498:VAL:HB	2.21	0.40
1:G:451:ASP:CG	1:G:454:ARG:HA	2.46	0.40
1:A:202:VAL:HG22	1:A:227:LEU:HD22	1.85	0.40
1:A:292:PRO:CG	1:A:435:THR:CG2	2.88	0.40
1:E:150:THR:HG22	1:E:168:ASN:HD21	1.86	0.40
1:F:118:LYS:HD3	1:F:119:ILE:H	1.86	0.40
1:F:219:GLN:O	1:F:222:GLU:HB2	2.20	0.40
1:G:386:VAL:HG21	1:G:413:TYR:HB2	2.03	0.40
1:H:90:ILE:HA	1:H:128:ASP:HB3	2.04	0.40
1:H:132:LEU:HD12	1:H:132:LEU:HA	1.82	0.40
1:H:219:GLN:O	1:H:222:GLU:HB2	2.21	0.40
1:H:333:GLU:HB3	1:H:343:VAL:HG11	2.03	0.40
1:A:276:VAL:O	1:A:280:MET:HG3	2.21	0.40
1:C:386:VAL:HG21	1:C:413:TYR:HB2	2.04	0.40
1:D:220:VAL:HG11	1:D:255:ALA:CB	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ASP:HB3	1:E:116:PHE:CD2	2.57	0.40
1:E:219:GLN:O	1:E:222:GLU:HB2	2.22	0.40
1:B:229:GLU:HA	1:B:232:LYS:HD3	2.02	0.40
1:B:276:VAL:O	1:B:280:MET:HG3	2.21	0.40
1:D:292:PRO:CB	1:D:434:VAL:HG22	2.51	0.40
1:E:25:ILE:HB	1:E:329:MET:HG3	2.03	0.40
1:E:227:LEU:HD22	1:E:236:ILE:HD11	2.03	0.40
1:E:294:ILE:HG12	1:E:327:CYS:HB2	2.04	0.40
1:F:377:PRO:HB2	1:F:489:TYR:HE1	1.87	0.40
1:F:378:GLU:HB2	1:F:489:TYR:CD1	2.52	0.40
1:B:329:MET:HE2	1:B:329:MET:HB3	1.63	0.40
1:B:355:GLN:HA	1:B:358:THR:HG22	2.04	0.40
1:C:241:GLU:HA	1:C:266:LEU:HB2	2.03	0.40
1:D:149:LEU:HD13	1:D:170:HIS:HB3	2.02	0.40
1:D:239:LYS:HE3	1:D:260:MET:HE2	2.03	0.40
1:F:118:LYS:C	1:F:119:ILE:HG13	2.47	0.40
1:F:237:ILE:HG21	1:F:294:ILE:HD12	2.04	0.40
1:G:276:VAL:O	1:G:280:MET:HG3	2.22	0.40
1:H:24:ILE:HG23	1:H:347:MET:CE	2.51	0.40
1:H:300:LEU:HD23	1:H:313:GLU:HB3	2.03	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	427/514 (83%)	387 (91%)	33 (8%)	7 (2%)	7 34
1	B	468/514 (91%)	429 (92%)	38 (8%)	1 (0%)	43 76
1	C	498/514 (97%)	454 (91%)	41 (8%)	3 (1%)	21 56
1	D	497/514 (97%)	457 (92%)	38 (8%)	2 (0%)	30 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	491/514 (96%)	466 (95%)	25 (5%)	0	100	100
1	F	497/514 (97%)	460 (93%)	36 (7%)	1 (0%)	43	76
1	G	408/514 (79%)	382 (94%)	24 (6%)	2 (0%)	24	60
1	H	437/514 (85%)	399 (91%)	33 (8%)	5 (1%)	11	43
All	All	3723/4112 (90%)	3434 (92%)	268 (7%)	21 (1%)	21	56

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	LYS
1	A	110	VAL
1	A	184	GLU
1	C	445	VAL
1	C	484	HIS
1	A	45	GLY
1	A	112	THR
1	A	181	PRO
1	H	131	GLN
1	A	113	ASP
1	A	116	PHE
1	C	88	PRO
1	G	473	ALA
1	H	132	LEU
1	H	487	LYS
1	H	130	PRO
1	H	133	PRO
1	D	181	PRO
1	F	119	ILE
1	D	45	GLY
1	G	182	GLY

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	338/435 (78%)	330 (98%)	8 (2%)	43	73
1	B	364/435 (84%)	352 (97%)	12 (3%)	33	67
1	C	401/435 (92%)	391 (98%)	10 (2%)	42	72
1	D	397/435 (91%)	384 (97%)	13 (3%)	33	67
1	E	402/435 (92%)	388 (96%)	14 (4%)	32	65
1	F	400/435 (92%)	383 (96%)	17 (4%)	26	60
1	G	327/435 (75%)	320 (98%)	7 (2%)	47	75
1	H	340/435 (78%)	326 (96%)	14 (4%)	27	61
All	All	2969/3480 (85%)	2874 (97%)	95 (3%)	34	67

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	116	PHE
1	A	178	ILE
1	A	180	LEU
1	A	190	VAL
1	A	199	GLN
1	A	346	TYR
1	A	460	LEU
1	B	44	SER
1	B	121	THR
1	B	135	VAL
1	B	162	LEU
1	B	199	GLN
1	B	248	ASN
1	B	254	GLU
1	B	329	MET
1	B	346	TYR
1	B	414	ARG
1	B	457	ARG
1	B	487	LYS
1	C	8	ILE
1	C	18	LYS
1	C	43	LYS
1	C	46	MET
1	C	178	ILE
1	C	185	VAL
1	C	346	TYR

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Mol	Chain	Res	Type
1	C	444	ASP
1	C	445	VAL
1	C	452	ASN
1	D	43	LYS
1	D	128	ASP
1	D	136	VAL
1	D	148	VAL
1	D	184	GLU
1	D	185	VAL
1	D	187	LEU
1	D	195	ARG
1	D	346	TYR
1	D	381	VAL
1	D	395	LYS
1	D	471	VAL
1	D	499	ARG
1	E	39	LYS
1	E	44	SER
1	E	46	MET
1	E	136	VAL
1	E	144	VAL
1	E	172	LEU
1	E	187	LEU
1	E	190	VAL
1	E	199	GLN
1	E	345	GLN
1	E	346	TYR
1	E	349	ARG
1	E	436	ARG
1	E	445	VAL
1	F	10	LEU
1	F	55	HIS
1	F	118	LYS
1	F	144	VAL
1	F	148	VAL
1	F	156	LYS
1	F	157	GLU
1	F	187	LEU
1	F	227	LEU
1	F	346	TYR
1	F	360	ASP
1	F	381	VAL

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Mol	Chain	Res	Type
1	F	453	ASP
1	F	485	SER
1	F	486	VAL
1	F	487	LYS
1	F	489	TYR
1	G	346	TYR
1	G	425	ARG
1	G	435	THR
1	G	436	ARG
1	G	445	VAL
1	G	462	VAL
1	G	471	VAL
1	H	28	ILE
1	H	44	SER
1	H	137	ARG
1	H	144	VAL
1	H	149	LEU
1	H	230	LYS
1	H	260	MET
1	H	282	ILE
1	H	308	ARG
1	H	346	TYR
1	H	358	THR
1	H	381	VAL
1	H	485	SER
1	H	491	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	243	HIS
1	A	244	GLN
1	A	319	ASN
1	A	323	ASN
1	A	345	GLN
1	A	369	ASN
1	A	452	ASN
1	B	3	GLN
1	B	7	ASN
1	B	67	ASN
1	B	78	HIS

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Mol	Chain	Res	Type
1	B	167	ASN
1	B	244	GLN
1	B	279	GLN
1	B	298	GLN
1	B	319	ASN
1	B	365	ASN
1	B	393	GLN
1	B	452	ASN
1	B	492	GLN
1	C	3	GLN
1	C	6	HIS
1	C	19	HIS
1	C	55	HIS
1	C	167	ASN
1	C	492	GLN
1	D	3	GLN
1	D	52	ASN
1	D	55	HIS
1	D	167	ASN
1	D	219	GLN
1	D	345	GLN
1	D	359	HIS
1	D	365	ASN
1	D	369	ASN
1	E	3	GLN
1	E	22	ASN
1	E	167	ASN
1	E	244	GLN
1	E	319	ASN
1	E	359	HIS
1	E	369	ASN
1	E	402	ASN
1	E	416	ASN
1	F	243	HIS
1	F	244	GLN
1	F	247	GLN
1	F	319	ASN
1	F	365	ASN
1	F	369	ASN
1	G	3	GLN
1	G	19	HIS
1	G	22	ASN

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Mol	Chain	Res	Type
1	G	199	GLN
1	G	243	HIS
1	G	319	ASN
1	G	369	ASN
1	G	393	GLN
1	G	402	ASN
1	G	416	ASN
1	G	459	GLN
1	G	492	GLN
1	H	3	GLN
1	H	6	HIS
1	H	55	HIS
1	H	369	ASN
1	H	402	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CIT	C	601	-	12,12,12	1.63	4 (33%)	17,17,17	1.53	4 (23%)
2	GOL	A	602	-	5,5,5	0.15	0	5,5,5	0.30	0
3	CIT	B	601	-	12,12,12	0.31	0	17,17,17	0.68	1 (5%)
2	GOL	C	602	-	5,5,5	0.11	0	5,5,5	0.31	0
3	CIT	E	601	-	12,12,12	1.85	6 (50%)	17,17,17	2.41	6 (35%)
3	CIT	H	601	-	12,12,12	1.95	6 (50%)	17,17,17	2.39	7 (41%)
2	GOL	C	603	-	5,5,5	0.07	0	5,5,5	0.20	0
2	GOL	H	602	-	5,5,5	0.06	0	5,5,5	0.35	0
2	GOL	G	601	-	5,5,5	0.08	0	5,5,5	0.28	0
2	GOL	F	602	-	5,5,5	0.09	0	5,5,5	0.70	0
4	PGE	F	603	-	9,9,9	0.16	0	8,8,8	0.12	0
2	GOL	A	601	-	5,5,5	0.14	0	5,5,5	0.46	0
2	GOL	E	602	-	5,5,5	0.10	0	5,5,5	0.18	0
2	GOL	B	602	-	5,5,5	0.11	0	5,5,5	0.23	0
3	CIT	F	601	-	12,12,12	0.30	0	17,17,17	0.89	1 (5%)
5	PEG	F	604	-	6,6,6	0.26	0	5,5,5	0.16	0
3	CIT	D	601	-	12,12,12	1.97	6 (50%)	17,17,17	2.39	8 (47%)
2	GOL	D	602	-	5,5,5	0.12	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	C	601	-	-	0/16/16/16	-
2	GOL	A	602	-	-	2/4/4/4	-
3	CIT	B	601	-	-	3/16/16/16	-
2	GOL	C	602	-	-	0/4/4/4	-
3	CIT	E	601	-	-	0/16/16/16	-
3	CIT	H	601	-	-	5/16/16/16	-
2	GOL	C	603	-	-	0/4/4/4	-
2	GOL	H	602	-	-	1/4/4/4	-
2	GOL	G	601	-	-	3/4/4/4	-
2	GOL	F	602	-	-	1/4/4/4	-
4	PGE	F	603	-	-	3/7/7/7	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	E	602	-	-	0/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
3	CIT	F	601	-	-	5/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	F	604	-	-	1/4/4/4	-
3	CIT	D	601	-	-	0/16/16/16	-
2	GOL	D	602	-	-	0/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	CIT	O4-C5	-3.29	1.19	1.30
3	C	601	CIT	O1-C1	3.16	1.32	1.22
3	D	601	CIT	O5-C6	3.03	1.31	1.22
3	H	601	CIT	O5-C6	2.98	1.31	1.22
3	D	601	CIT	O1-C1	2.96	1.31	1.22
3	H	601	CIT	O3-C5	2.95	1.31	1.22
3	H	601	CIT	O2-C1	-2.93	1.21	1.30
3	E	601	CIT	O1-C1	2.87	1.31	1.22
3	C	601	CIT	O3-C5	2.77	1.31	1.22
3	E	601	CIT	O4-C5	-2.74	1.21	1.30
3	H	601	CIT	O1-C1	2.70	1.30	1.22
3	E	601	CIT	O3-C5	2.68	1.30	1.22
3	H	601	CIT	O4-C5	-2.64	1.22	1.30
3	D	601	CIT	O3-C5	2.61	1.30	1.22
3	E	601	CIT	O2-C1	-2.58	1.22	1.30
3	C	601	CIT	O2-C1	-2.55	1.22	1.30
3	C	601	CIT	O4-C5	-2.50	1.22	1.30
3	E	601	CIT	O5-C6	2.48	1.29	1.22
3	D	601	CIT	O2-C1	-2.42	1.22	1.30
3	E	601	CIT	O6-C6	-2.27	1.22	1.30
3	H	601	CIT	O6-C6	-2.20	1.22	1.30
3	D	601	CIT	O6-C6	-2.07	1.23	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	CIT	O6-C6-C3	5.34	123.39	113.14
3	H	601	CIT	O6-C6-C3	5.31	123.33	113.14
3	E	601	CIT	O6-C6-C3	5.09	122.91	113.14
3	E	601	CIT	O5-C6-C3	-4.69	113.00	122.09
3	D	601	CIT	O5-C6-C3	-4.59	113.19	122.09
3	H	601	CIT	O5-C6-C3	-4.47	113.43	122.09
3	E	601	CIT	O1-C1-C2	-3.81	112.17	122.95
3	E	601	CIT	O3-C5-C4	-3.71	112.44	122.95
3	H	601	CIT	O3-C5-C4	-3.63	112.68	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	601	CIT	O1-C1-C2	-3.35	113.47	122.95
3	C	601	CIT	O3-C5-C4	-3.30	113.60	122.95
3	D	601	CIT	O1-C1-C2	-3.20	113.90	122.95
3	H	601	CIT	O4-C5-C4	3.11	124.19	114.35
3	E	601	CIT	O2-C1-C2	2.97	123.75	114.35
3	D	601	CIT	O3-C5-C4	-2.91	114.72	122.95
3	C	601	CIT	O4-C5-C4	2.91	123.55	114.35
3	E	601	CIT	O4-C5-C4	2.90	123.53	114.35
3	C	601	CIT	O1-C1-C2	-2.77	115.09	122.95
3	H	601	CIT	O2-C1-C2	2.77	123.13	114.35
3	D	601	CIT	O2-C1-C2	2.75	123.07	114.35
3	F	601	CIT	C3-C4-C5	2.68	121.24	113.92
3	D	601	CIT	O4-C5-C4	2.60	122.58	114.35
3	C	601	CIT	O2-C1-C2	2.47	122.17	114.35
3	B	601	CIT	C3-C2-C1	2.15	119.81	113.92
3	D	601	CIT	C3-C2-C1	2.09	119.65	113.92
3	H	601	CIT	C3-C4-C5	2.07	119.57	113.92
3	D	601	CIT	C4-C3-C2	-2.01	104.17	109.31

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3
3	F	601	CIT	C1-C2-C3-O7
3	F	601	CIT	C1-C2-C3-C6
3	B	601	CIT	C1-C2-C3-O7
3	B	601	CIT	C1-C2-C3-C6
3	F	601	CIT	C1-C2-C3-C4
3	H	601	CIT	C1-C2-C3-O7
3	H	601	CIT	C1-C2-C3-C6
2	F	602	GOL	C1-C2-C3-O3
2	G	601	GOL	O1-C1-C2-C3
2	H	602	GOL	O1-C1-C2-C3
3	B	601	CIT	C1-C2-C3-C4
3	H	601	CIT	C1-C2-C3-C4
4	F	603	PGE	C6-C5-O3-C4
4	F	603	PGE	C3-C4-O3-C5
4	F	603	PGE	C4-C3-O2-C2
3	F	601	CIT	C3-C4-C5-O4
2	G	601	GOL	O1-C1-C2-O2

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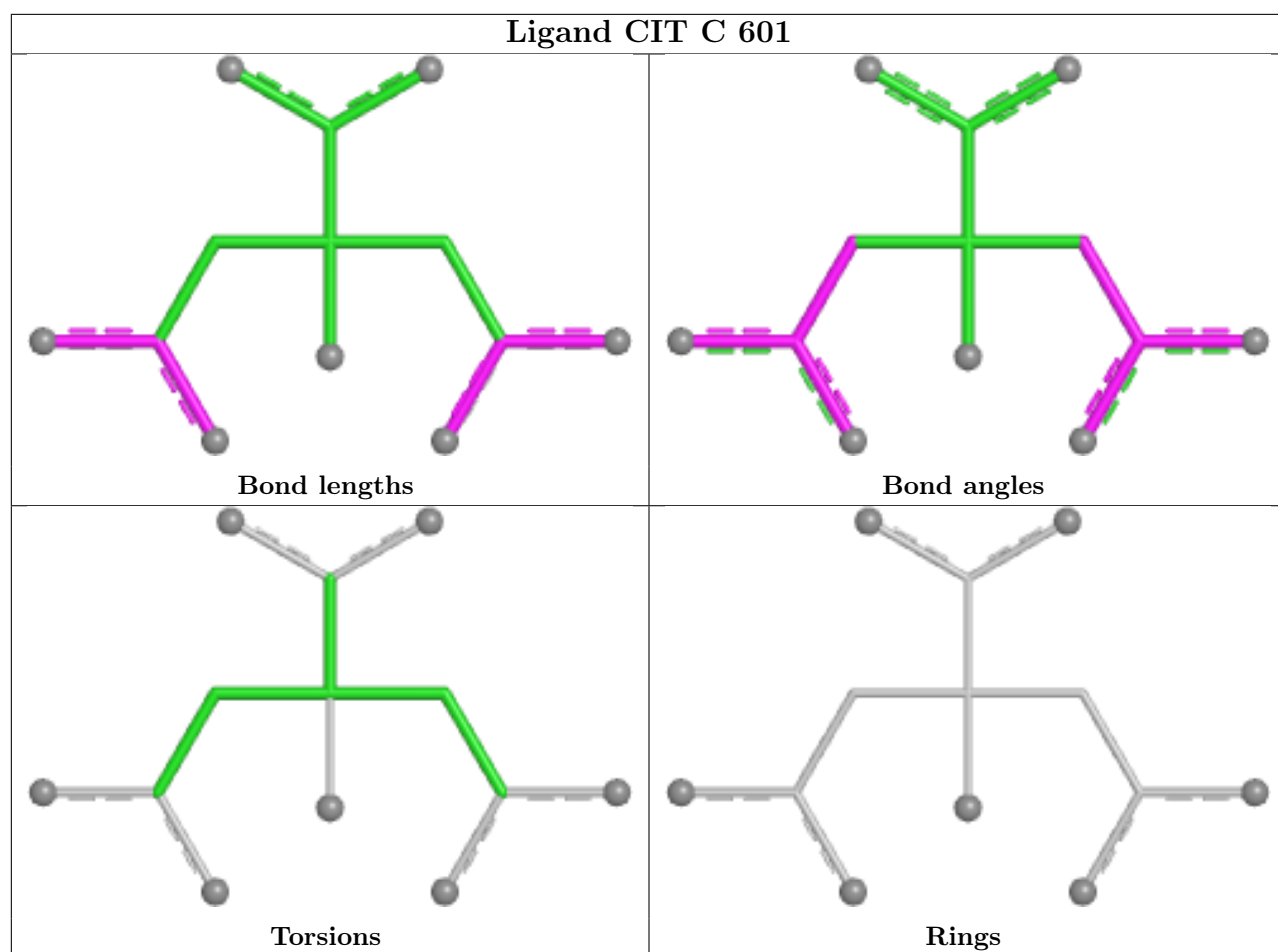
Mol	Chain	Res	Type	Atoms
3	F	601	CIT	C3-C4-C5-O3
3	H	601	CIT	C3-C4-C5-O4
3	H	601	CIT	C3-C4-C5-O3
2	G	601	GOL	O2-C2-C3-O3
5	F	604	PEG	O2-C3-C4-O4

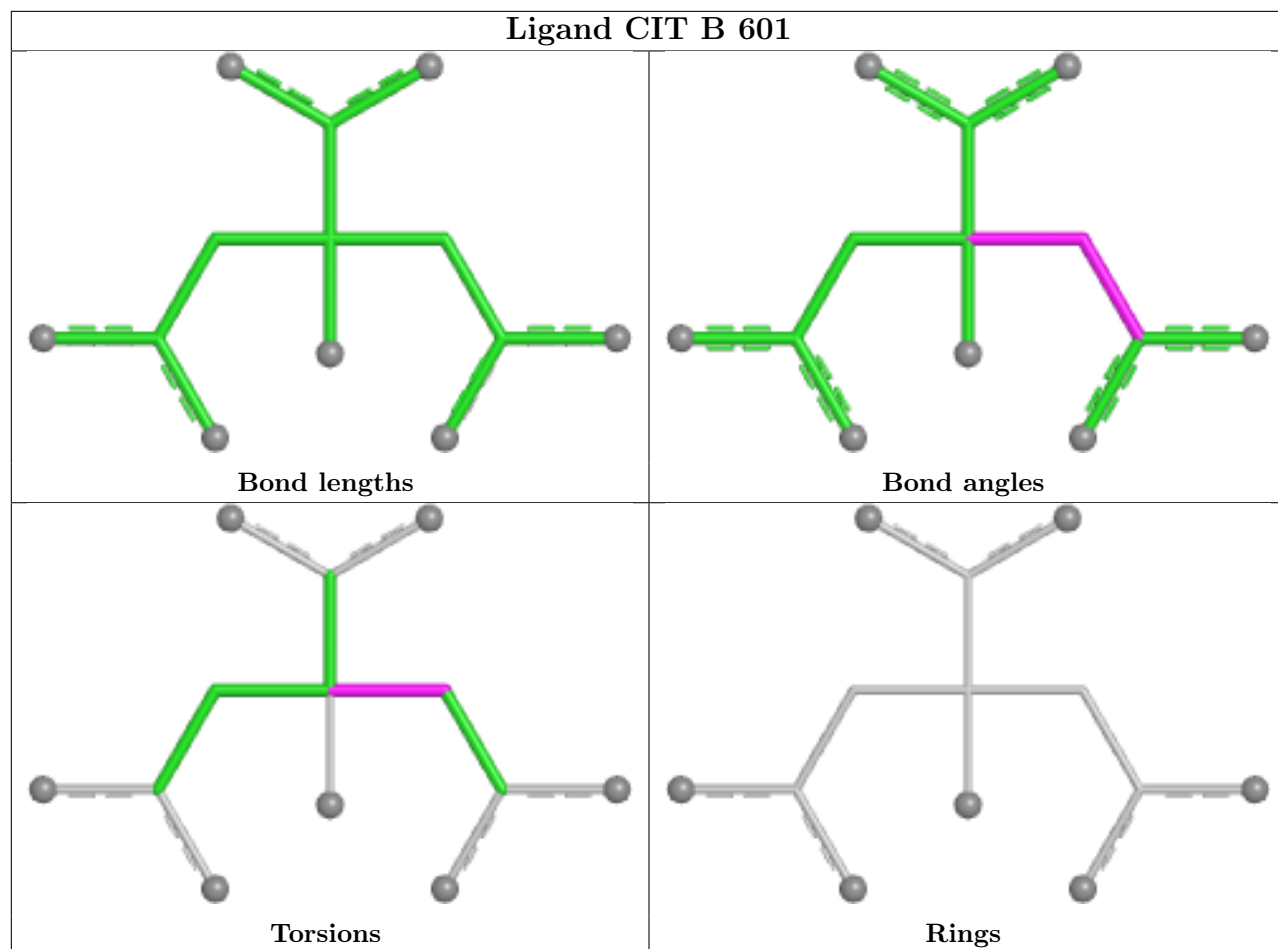
There are no ring outliers.

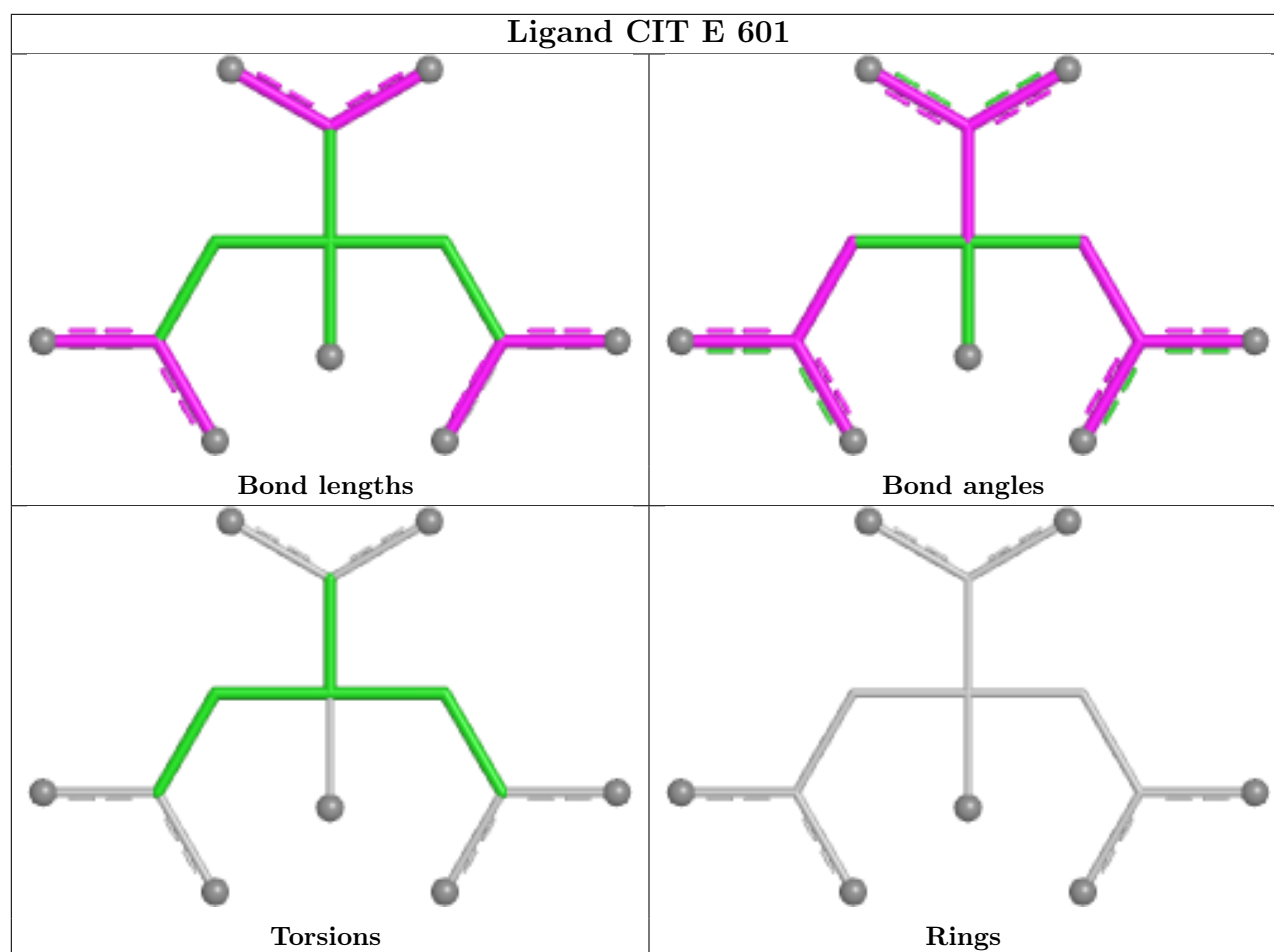
7 monomers are involved in 13 short contacts:

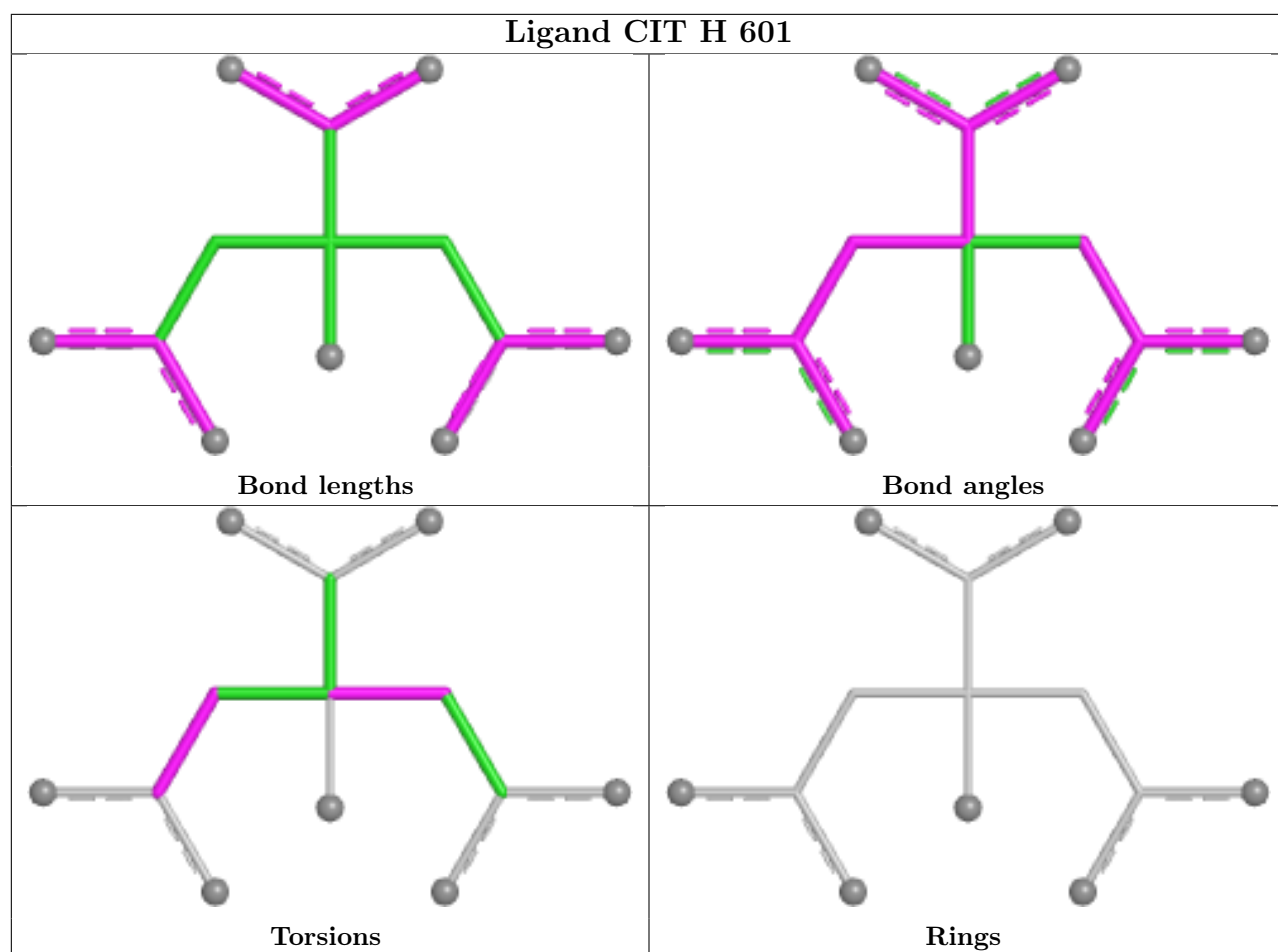
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	CIT	1	0
3	B	601	CIT	4	0
3	H	601	CIT	3	0
2	G	601	GOL	1	0
2	F	602	GOL	2	0
2	A	601	GOL	1	0
3	D	601	CIT	1	0

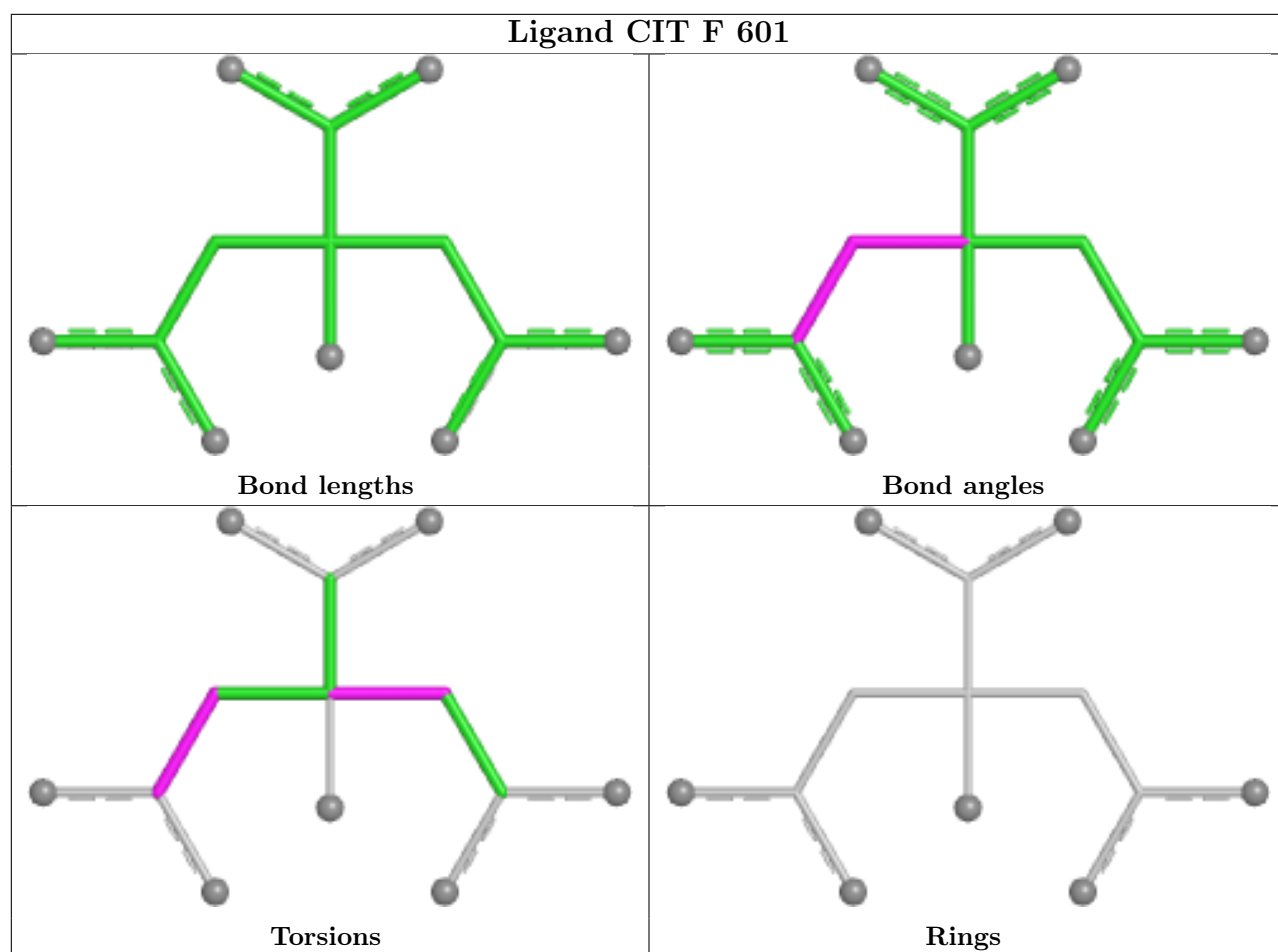
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

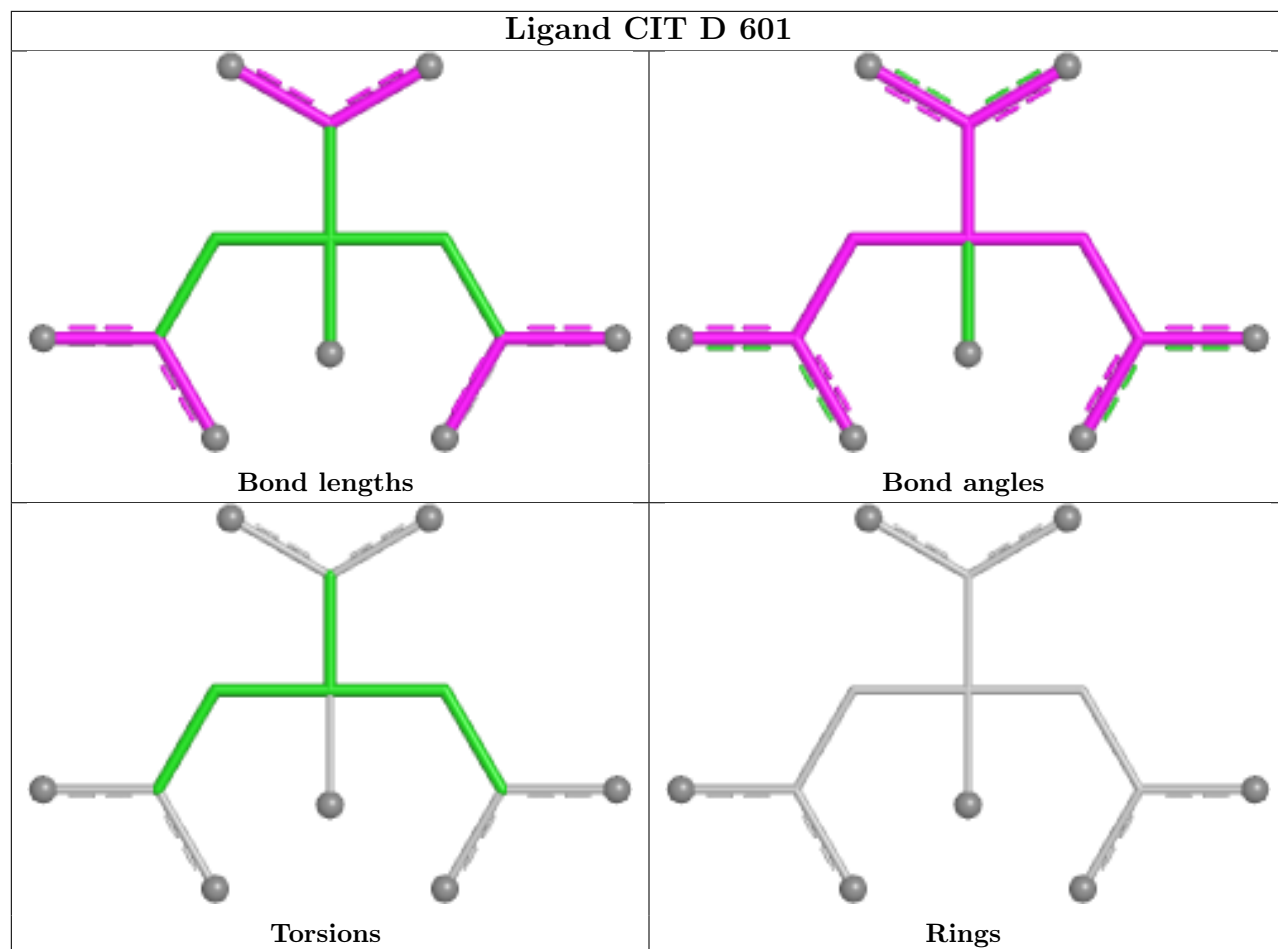












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	439/514 (85%)	0.54	15 (3%)	48	27	51, 85, 134, 165	0
1	B	476/514 (92%)	0.39	19 (3%)	42	23	41, 73, 174, 272	0
1	C	499/514 (97%)	0.40	11 (2%)	62	39	43, 80, 110, 137	1 (0%)
1	D	498/514 (96%)	0.53	18 (3%)	46	26	56, 88, 133, 179	1 (0%)
1	E	495/514 (96%)	0.39	16 (3%)	50	29	56, 79, 112, 171	0
1	F	498/514 (96%)	0.41	12 (2%)	59	36	39, 78, 107, 127	1 (0%)
1	G	411/514 (79%)	0.32	13 (3%)	50	29	42, 74, 115, 155	1 (0%)
1	H	449/514 (87%)	0.72	17 (3%)	44	24	56, 103, 144, 175	0
All	All	3765/4112 (91%)	0.46	121 (3%)	50	29	39, 82, 129, 272	4 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	155	SER	4.7
1	H	255	ALA	4.0
1	H	327	CYS	4.0
1	A	144	VAL	3.8
1	C	88	PRO	3.8
1	C	189	ALA	3.7
1	D	441	VAL	3.7
1	D	160	CYS	3.6
1	H	402	ASN	3.6
1	D	296	ALA	3.5
1	E	167	ASN	3.4
1	E	490	PRO	3.4
1	A	242	ASN	3.3
1	B	102	TYR	3.2
1	D	145	ASP	3.2
1	E	182	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	59	GLU	3.2
1	H	217	ALA	3.0
1	G	305	THR	3.0
1	C	89	GLU	3.0
1	C	486	VAL	2.9
1	B	160	CYS	2.9
1	F	335	ALA	2.9
1	D	115	ALA	2.9
1	H	150	THR	2.9
1	B	144	VAL	2.9
1	A	145	ASP	2.8
1	E	489	TYR	2.8
1	F	258	GLY	2.7
1	A	153	VAL	2.7
1	D	161	THR	2.7
1	D	359	HIS	2.7
1	B	166	VAL	2.7
1	H	207	ASP	2.7
1	F	76	GLY	2.7
1	E	361	SER	2.7
1	F	490	PRO	2.6
1	D	188	PRO	2.6
1	E	312	ALA	2.6
1	B	121	THR	2.6
1	H	85	THR	2.6
1	D	490	PRO	2.5
1	C	90	ILE	2.5
1	G	484	HIS	2.5
1	B	162	LEU	2.5
1	G	481	HIS	2.5
1	H	68	VAL	2.5
1	A	111	THR	2.5
1	C	277	VAL	2.4
1	C	318	ALA	2.4
1	B	167	ASN	2.4
1	H	138	PRO	2.4
1	B	164	CYS	2.4
1	B	491	ASN	2.4
1	G	186	ASP	2.4
1	D	488	GLY	2.4
1	B	385	ALA	2.4
1	E	357	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	156	LYS	2.4
1	C	190	VAL	2.4
1	C	159	ASP	2.4
1	G	469	GLY	2.4
1	D	57	SER	2.4
1	E	98	GLY	2.3
1	G	358	THR	2.3
1	F	166	VAL	2.3
1	G	486	VAL	2.3
1	H	490	PRO	2.3
1	E	479	ILE	2.3
1	A	299	MET	2.3
1	H	128	ASP	2.3
1	A	391	GLU	2.3
1	H	21	ALA	2.3
1	B	161	THR	2.3
1	F	369	ASN	2.3
1	B	159	ASP	2.3
1	E	157	GLU	2.2
1	A	142	ILE	2.2
1	G	242	ASN	2.2
1	B	13	PHE	2.2
1	B	92	THR	2.2
1	E	471	VAL	2.2
1	D	119	ILE	2.2
1	F	115	ALA	2.2
1	A	84	ASP	2.2
1	D	464	TRP	2.2
1	D	35	VAL	2.2
1	F	314	VAL	2.2
1	G	298	GLN	2.2
1	A	217	ALA	2.2
1	G	473	ALA	2.2
1	B	490	PRO	2.2
1	G	267	GLY	2.2
1	D	159	ASP	2.2
1	A	435	THR	2.1
1	D	445	VAL	2.1
1	H	135	VAL	2.1
1	H	297	THR	2.1
1	F	38	LEU	2.1
1	F	130	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	472	SER	2.1
1	F	168	ASN	2.1
1	F	100	ALA	2.1
1	E	14	GLU	2.1
1	H	198	LEU	2.1
1	D	243	HIS	2.1
1	A	326	ASP	2.1
1	H	325	ALA	2.1
1	E	267	GLY	2.1
1	C	155	SER	2.0
1	G	306	ASN	2.0
1	A	112	THR	2.0
1	B	97	ASP	2.0
1	D	234	THR	2.0
1	E	174	ASP	2.0
1	E	446	ASP	2.0
1	A	192	GLU	2.0
1	B	165	HIS	2.0
1	A	428	THR	2.0
1	C	490	PRO	2.0
1	B	149	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	602	6/6	0.49	0.27	91,93,93,94	0
5	PEG	F	604	7/7	0.65	0.20	83,84,87,87	0

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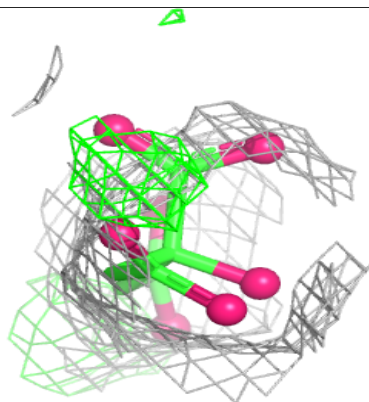
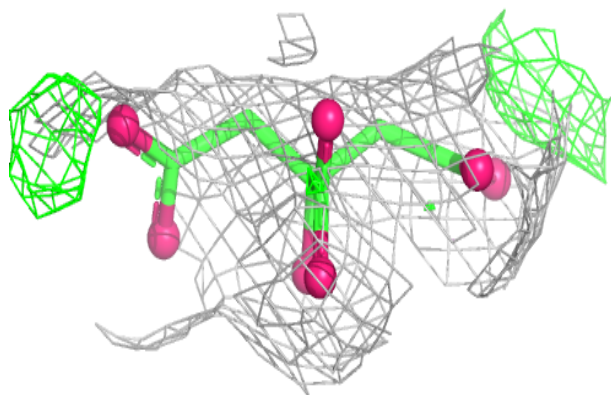
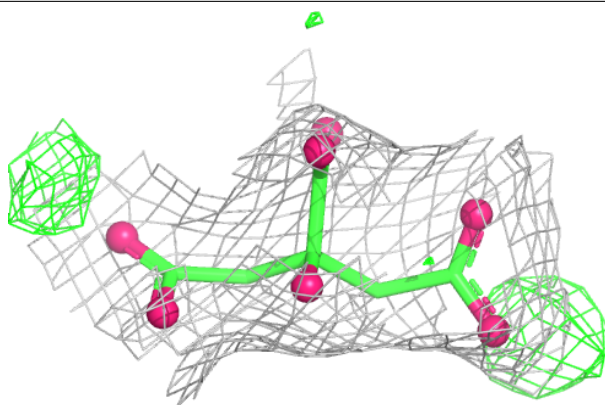
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CIT	D	601	13/13	0.67	0.17	112,123,127,128	0
2	GOL	F	602	6/6	0.69	0.15	85,88,89,91	0
2	GOL	E	602	6/6	0.73	0.15	71,79,82,82	0
2	GOL	C	603	6/6	0.75	0.21	85,89,89,89	0
4	PGE	F	603	10/10	0.75	0.14	90,98,101,101	0
2	GOL	H	602	6/6	0.75	0.12	80,83,86,88	0
3	CIT	B	601	13/13	0.77	0.14	107,121,124,127	0
2	GOL	A	602	6/6	0.78	0.14	76,80,81,81	0
2	GOL	G	601	6/6	0.80	0.17	88,89,89,90	0
2	GOL	D	602	6/6	0.80	0.22	76,80,83,84	0
2	GOL	B	602	6/6	0.82	0.21	80,82,84,85	0
3	CIT	E	601	13/13	0.82	0.14	103,108,111,115	0
3	CIT	C	601	13/13	0.85	0.12	96,105,108,110	0
3	CIT	F	601	13/13	0.87	0.11	101,109,117,117	0
3	CIT	H	601	13/13	0.87	0.13	141,145,149,150	0
2	GOL	A	601	6/6	0.88	0.08	59,67,68,69	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.

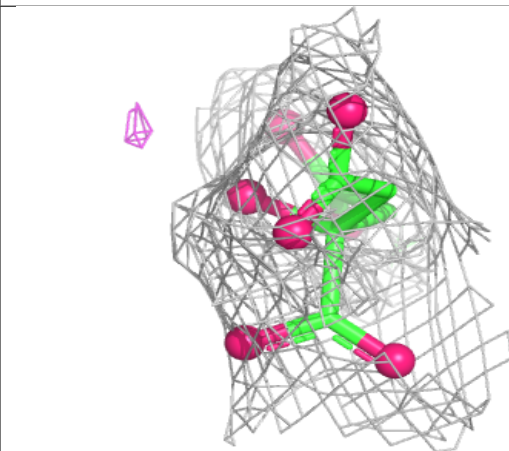
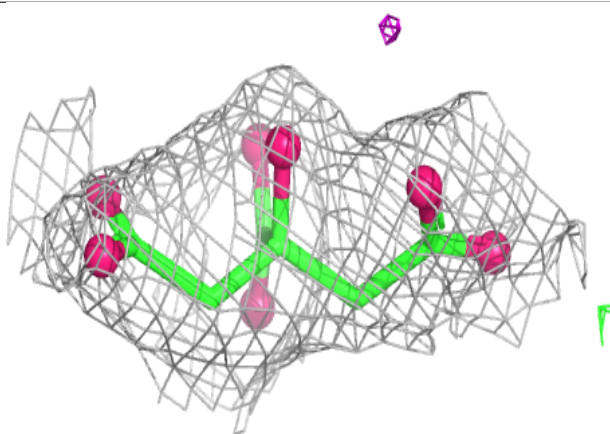
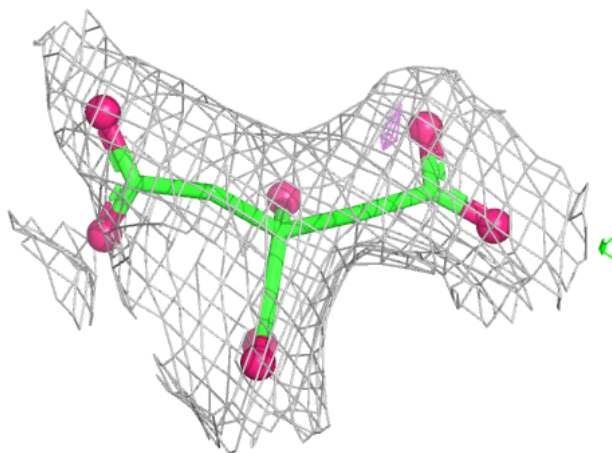
Electron density around CIT D 601:

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



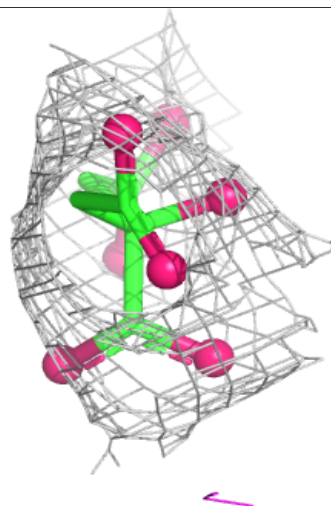
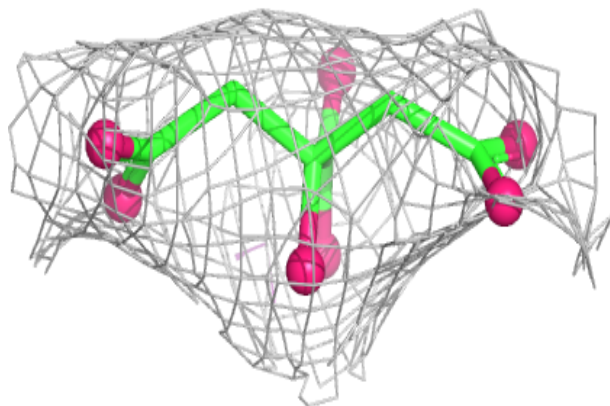
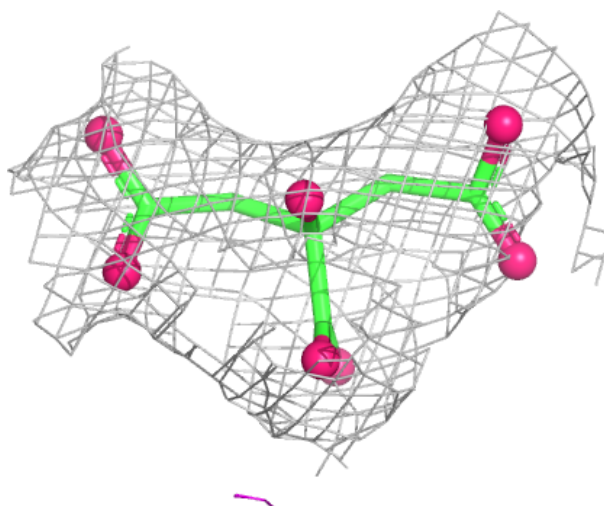
Electron density around CIT B 601:

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



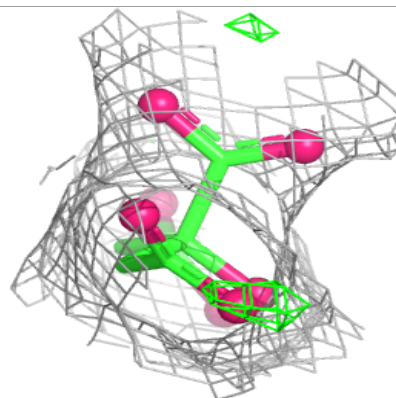
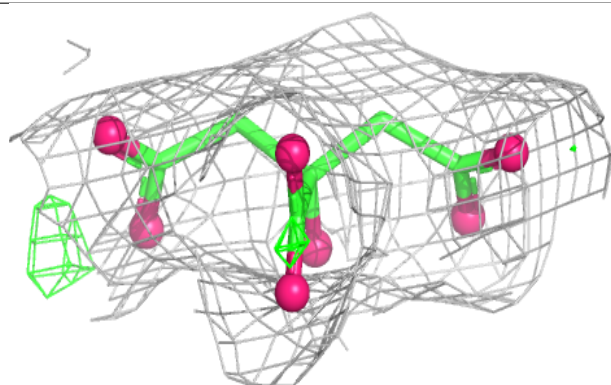
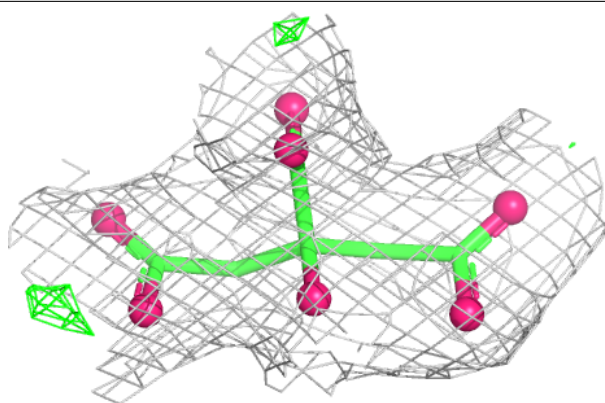
Electron density around CIT E 601:

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



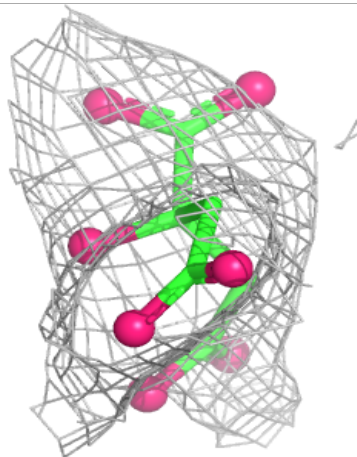
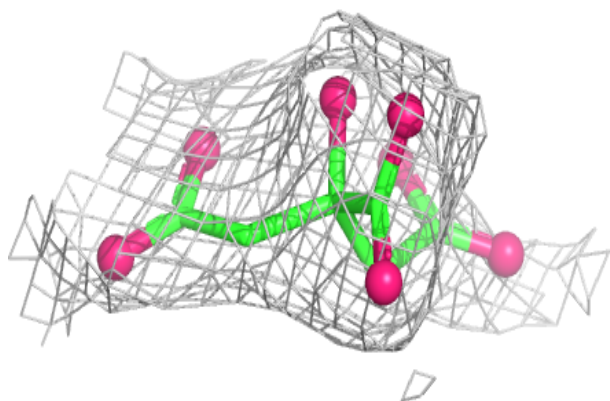
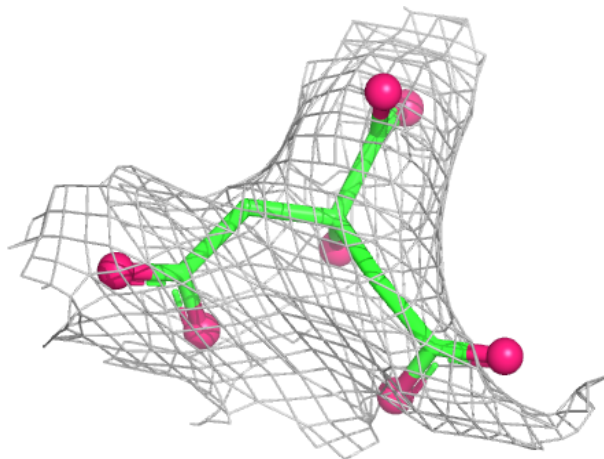
Electron density around CIT C 601:

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



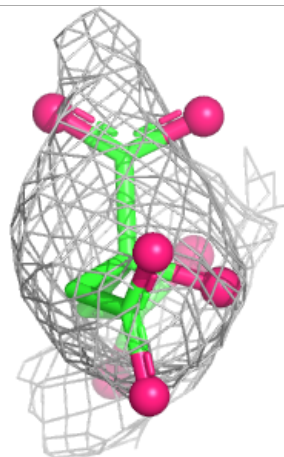
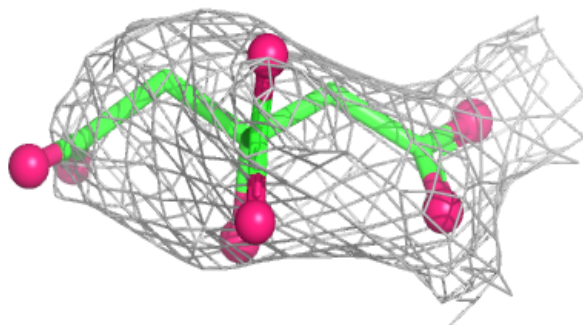
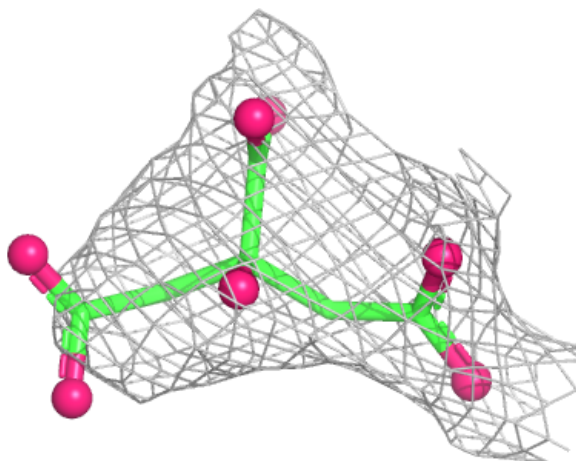
Electron density around CIT F 601:

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



Electron density around CIT H 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.