



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:12 PM UTC

PDB ID : 8IH6 / pdb_00008ih6
Title : Crystal structure of decarboxylase-hydratase complex from Pseudomonas species AP-3
Authors : Shi, Q.L.; Su, D.
Deposited on : 2023-02-22
Resolution : 2.52 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

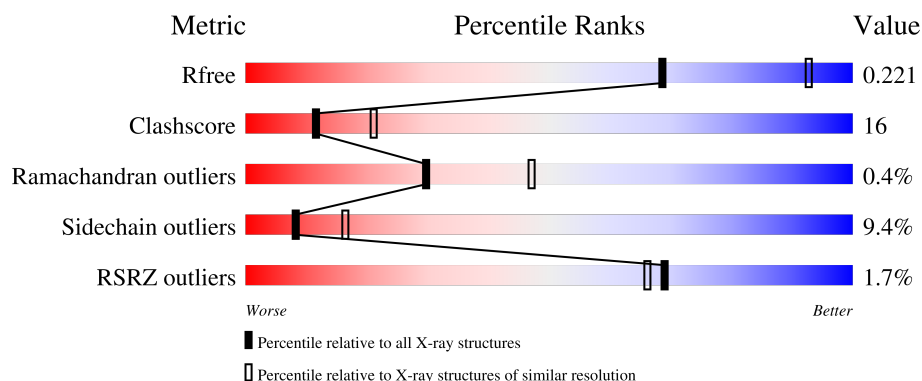
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	266	
1	B	266	
1	C	266	
1	D	266	
1	E	266	

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Mol	Chain	Length	Quality of chain
2	F	258	
2	G	258	
2	H	258	
2	I	258	
2	J	258	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19733 atoms, of which 32 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2-oxopent-4-enoate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			1945	1222	347	370	6			
1	B	264	Total	C	N	O	S	0	0	0
			1942	1220	343	372	7			
1	C	265	Total	C	N	O	S	0	0	0
			1947	1222	343	375	7			
1	D	263	Total	C	N	O	S	0	0	0
			1938	1219	343	369	7			
1	E	264	Total	C	N	O	S	0	0	0
			1948	1223	346	372	7			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	expression tag	UNP Q9KWS4
A	-3	ASP	-	expression tag	UNP Q9KWS4
A	-2	LEU	-	expression tag	UNP Q9KWS4
A	-1	ASN	-	expression tag	UNP Q9KWS4
A	0	TRP	-	expression tag	UNP Q9KWS4
B	-4	ALA	-	expression tag	UNP Q9KWS4
B	-3	ASP	-	expression tag	UNP Q9KWS4
B	-2	LEU	-	expression tag	UNP Q9KWS4
B	-1	ASN	-	expression tag	UNP Q9KWS4
B	0	TRP	-	expression tag	UNP Q9KWS4
C	-4	ALA	-	expression tag	UNP Q9KWS4
C	-3	ASP	-	expression tag	UNP Q9KWS4
C	-2	LEU	-	expression tag	UNP Q9KWS4
C	-1	ASN	-	expression tag	UNP Q9KWS4
C	0	TRP	-	expression tag	UNP Q9KWS4
D	-4	ALA	-	expression tag	UNP Q9KWS4
D	-3	ASP	-	expression tag	UNP Q9KWS4
D	-2	LEU	-	expression tag	UNP Q9KWS4
D	-1	ASN	-	expression tag	UNP Q9KWS4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	TRP	-	expression tag	UNP Q9KWS4
E	-4	ALA	-	expression tag	UNP Q9KWS4
E	-3	ASP	-	expression tag	UNP Q9KWS4
E	-2	LEU	-	expression tag	UNP Q9KWS4
E	-1	ASN	-	expression tag	UNP Q9KWS4
E	0	TRP	-	expression tag	UNP Q9KWS4

- Molecule 2 is a protein called 4-oxalocrotonate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	253	Total	C	N	O	S	0	0	0
			1815	1140	318	348	9			
2	G	256	Total	C	N	O	S	0	0	0
			1894	1184	337	363	10			
2	H	256	Total	C	N	O	S	0	0	0
			1874	1172	329	363	10			
2	I	257	Total	C	N	O	S	0	0	0
			1905	1190	341	364	10			
2	J	255	Total	C	N	O	S	0	0	0
			1876	1172	332	362	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	ALA	-	expression tag	UNP Q9KWS3
F	0	ALA	-	expression tag	UNP Q9KWS3
G	-1	ALA	-	expression tag	UNP Q9KWS3
G	0	ALA	-	expression tag	UNP Q9KWS3
H	-1	ALA	-	expression tag	UNP Q9KWS3
H	0	ALA	-	expression tag	UNP Q9KWS3
I	-1	ALA	-	expression tag	UNP Q9KWS3
I	0	ALA	-	expression tag	UNP Q9KWS3
J	-1	ALA	-	expression tag	UNP Q9KWS3
J	0	ALA	-	expression tag	UNP Q9KWS3

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		
3	J	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	63	Total	O	0	0
			63	63		
4	F	62	Total	O	0	0
			62	62		
4	C	62	Total	O	0	0
			62	62		
4	D	58	Total	O	0	0
			58	58		
4	E	66	Total	O	0	0
			66	66		
4	G	60	Total	O	0	0
			60	60		
4	H	66	Total	O	0	0
			66	66		

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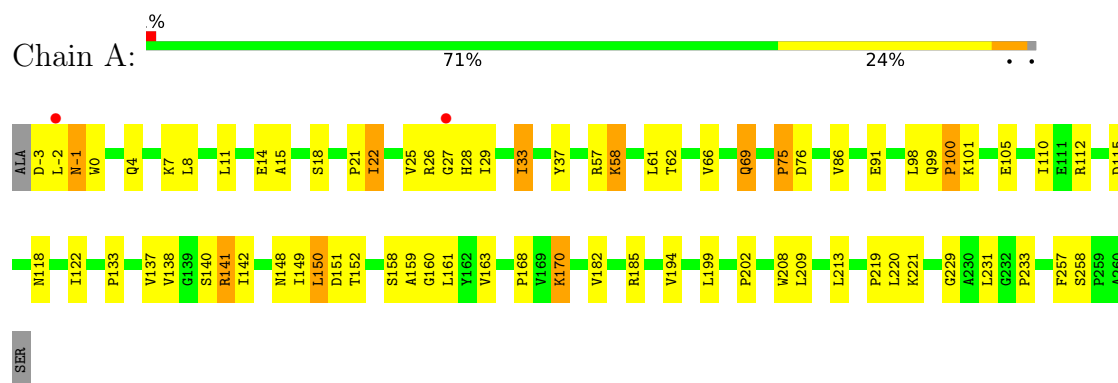
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	40	Total	O	0	0
			40	40		
4	J	76	Total	O	0	0
			76	76		

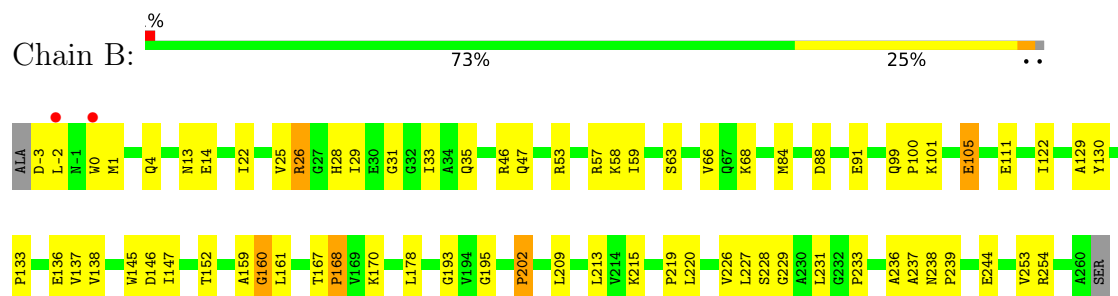
3 Residue-property plots [i](#)

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

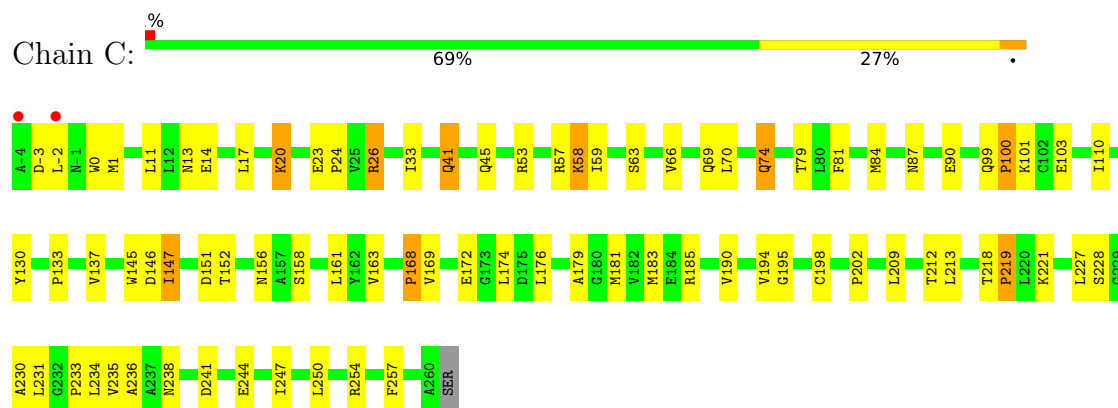
- Molecule 1: 2-oxopent-4-enoate hydratase



- Molecule 1: 2-oxopent-4-enoate hydratase

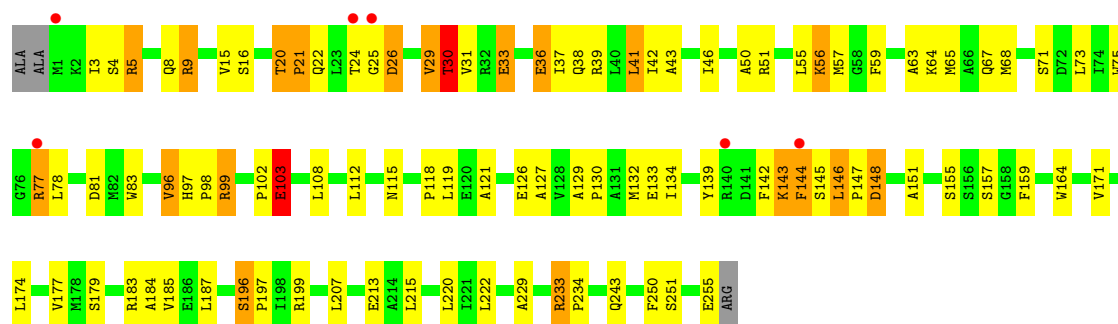


- Molecule 1: 2-oxopent-4-enoate hydratase



- Molecule 1: 2-oxopent-4-enoate hydratase

Chain H: 73% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.98Å 107.79Å 164.85Å 90.00° 124.46° 90.00°	Depositor
Resolution (Å)	30.35 – 2.52 30.35 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.35-2.52) 99.9 (30.35-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.174 , 0.222 0.185 , 0.221	Depositor DCC
R_{free} test set	4870 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19733	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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:
GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.43	8/1974 (0.4%)	1.38	4/2688 (0.1%)
1	B	1.47	8/1971 (0.4%)	1.33	2/2685 (0.1%)
1	C	1.46	8/1976 (0.4%)	1.38	5/2693 (0.2%)
1	D	1.44	8/1967 (0.4%)	1.34	3/2678 (0.1%)
1	E	1.49	12/1977 (0.6%)	1.36	2/2692 (0.1%)
2	F	1.31	4/1842 (0.2%)	1.45	5/2507 (0.2%)
2	G	1.38	11/1921 (0.6%)	1.39	3/2602 (0.1%)
2	H	1.43	10/1901 (0.5%)	1.33	2/2580 (0.1%)
2	I	1.42	10/1932 (0.5%)	1.40	4/2616 (0.2%)
2	J	1.42	10/1903 (0.5%)	1.42	5/2580 (0.2%)
All	All	1.43	89/19364 (0.5%)	1.38	35/26321 (0.1%)

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	102	PRO	C-O	-8.38	1.15	1.23
1	E	238	ASN	C-O	-7.90	1.16	1.24
1	E	133	PRO	C-O	-7.05	1.15	1.23
2	I	197	PRO	C-O	-6.90	1.15	1.24
1	C	133	PRO	C-O	-6.83	1.16	1.23
2	J	118	PRO	C-O	-6.76	1.15	1.24
2	H	197	PRO	C-O	-6.59	1.16	1.24
1	A	100	PRO	C-O	-6.57	1.16	1.23
1	E	219	PRO	C-O	-6.57	1.16	1.23
1	D	20	LYS	C-O	-6.55	1.19	1.25
2	F	102	PRO	C-O	-6.53	1.16	1.23
2	I	102	PRO	C-O	-6.47	1.17	1.23
1	B	133	PRO	C-O	-6.41	1.16	1.23
2	G	197	PRO	C-O	-6.35	1.15	1.24
2	H	118	PRO	C-O	-6.33	1.16	1.24
1	B	226	VAL	C-O	-6.24	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	ASN	C-O	-6.12	1.17	1.24
1	C	238	ASN	C-O	-6.10	1.16	1.24
2	J	234	PRO	C-O	-6.09	1.16	1.23
2	G	21	PRO	C-O	-6.08	1.16	1.23
1	A	168	PRO	C-O	-6.07	1.16	1.23
1	E	202	PRO	C-O	-6.07	1.16	1.24
2	I	225	ALA	C-O	-6.05	1.16	1.24
2	G	102	PRO	C-O	-6.04	1.17	1.23
1	D	233	PRO	C-O	-6.01	1.17	1.23
2	J	98	PRO	C-O	-6.00	1.17	1.23
2	G	98	PRO	C-O	-6.00	1.17	1.23
1	C	233	PRO	C-O	-5.86	1.16	1.23
1	D	103	GLU	C-O	-5.86	1.17	1.23
2	G	167	PRO	C-O	-5.86	1.16	1.24
1	A	202	PRO	C-O	-5.85	1.16	1.24
1	B	168	PRO	C-O	-5.83	1.17	1.23
1	C	100	PRO	C-O	-5.83	1.17	1.23
2	F	118	PRO	C-O	-5.79	1.16	1.24
2	I	167	PRO	C-O	-5.77	1.17	1.24
2	I	147	PRO	C-O	-5.74	1.17	1.24
2	H	147	PRO	C-O	-5.72	1.17	1.24
2	G	233	ARG	C-O	-5.69	1.19	1.24
1	C	163	VAL	C-O	-5.66	1.18	1.24
1	B	202	PRO	C-O	-5.65	1.16	1.24
1	E	20	LYS	C-O	-5.63	1.19	1.24
2	J	130	PRO	C-O	-5.63	1.17	1.23
1	E	168	PRO	C-O	-5.61	1.17	1.23
2	I	234	PRO	C-O	-5.57	1.17	1.23
1	A	233	PRO	C-O	-5.56	1.16	1.23
1	C	202	PRO	C-O	-5.55	1.17	1.24
2	I	128	VAL	C-O	-5.54	1.18	1.23
1	C	168	PRO	C-O	-5.52	1.17	1.23
2	G	118	PRO	C-O	-5.51	1.17	1.24
1	E	233	PRO	C-O	-5.50	1.17	1.23
1	B	233	PRO	C-O	-5.50	1.17	1.23
1	D	133	PRO	C-O	-5.48	1.17	1.23
2	J	21	PRO	C-O	-5.47	1.17	1.23
2	J	146	LEU	C-O	-5.46	1.19	1.24
2	I	118	PRO	C-O	-5.46	1.16	1.24
2	I	216	GLU	C-O	-5.46	1.16	1.23
2	H	130	PRO	C-O	-5.44	1.17	1.23
1	E	223	GLY	C-O	-5.36	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	167	PRO	C-O	-5.35	1.17	1.24
1	D	202	PRO	C-O	-5.34	1.17	1.24
2	J	196	SER	C-O	-5.32	1.17	1.24
2	H	102	PRO	C-O	-5.31	1.18	1.23
1	E	183	MET	C-O	-5.31	1.18	1.24
2	H	176	MET	C-O	-5.30	1.18	1.23
2	G	148	ASP	C-O	-5.28	1.18	1.24
1	B	219	PRO	C-O	-5.27	1.17	1.23
2	I	196	SER	C-O	-5.27	1.17	1.24
1	D	21	PRO	C-O	-5.25	1.17	1.23
2	F	137	SER	CA-CB	-5.24	1.46	1.53
1	C	198	CYS	C-O	-5.24	1.17	1.23
2	H	177	VAL	C-O	-5.22	1.18	1.24
1	B	239	PRO	C-O	-5.20	1.17	1.23
2	H	186	GLU	C-O	-5.19	1.17	1.23
1	A	133	PRO	C-O	-5.18	1.18	1.23
1	E	100	PRO	C-O	-5.18	1.17	1.23
1	A	182	VAL	C-O	-5.17	1.18	1.24
2	F	128	VAL	C-O	-5.17	1.18	1.24
2	H	233	ARG	C-O	-5.17	1.18	1.24
1	D	151	ASP	C-O	-5.15	1.18	1.24
2	G	247	SER	C-O	-5.11	1.17	1.24
1	A	112	ARG	C-O	-5.09	1.17	1.23
1	E	54	VAL	C-O	-5.08	1.19	1.24
2	G	234	PRO	C-O	-5.07	1.17	1.23
2	J	185	VAL	C-O	-5.06	1.19	1.24
1	E	247	ILE	C-O	-5.06	1.18	1.24
2	J	197	PRO	C-O	-5.05	1.17	1.24
2	G	128	VAL	C-O	-5.03	1.19	1.24
1	A	75	PRO	C-O	-5.02	1.17	1.24
1	D	219	PRO	C-O	-5.00	1.17	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ASP	CB-CA-C	-8.05	96.65	110.09
2	I	185	VAL	N-CA-C	-7.27	105.69	112.96
2	J	185	VAL	N-CA-C	-7.11	105.85	112.96
2	F	234	PRO	N-CA-C	6.46	121.65	111.38
2	G	185	VAL	N-CA-C	-6.34	106.00	113.42
1	C	74	GLN	CB-CA-C	-6.09	101.63	109.92
2	I	31	VAL	N-CA-C	-5.99	104.51	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	24	THR	CA-CB-OG1	-5.75	100.98	109.60
2	F	28	ALA	CA-C-N	5.72	132.27	121.97
2	F	28	ALA	C-N-CA	5.72	132.27	121.97
2	J	96	VAL	CB-CA-C	5.46	118.91	111.87
2	J	98	PRO	N-CA-C	5.44	120.77	111.68
1	C	24	PRO	CB-CA-C	-5.36	104.53	111.39
1	C	100	PRO	N-CA-C	5.36	119.50	111.14
1	A	75	PRO	CB-CA-C	-5.36	102.72	111.56
2	F	202	VAL	N-CA-C	-5.29	105.56	110.53
2	J	103	GLU	CB-CA-C	-5.25	100.75	113.19
2	H	98	PRO	N-CA-C	5.21	119.66	111.38
2	F	185	VAL	N-CA-C	-5.18	107.78	112.96
1	C	212	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	219	PRO	N-CA-C	5.16	119.41	111.57
1	E	24	PRO	CB-CA-C	-5.15	105.02	111.56
1	D	231	LEU	N-CA-C	-5.15	107.17	113.50
1	D	211	ARG	CB-CG-CD	-5.13	99.49	111.30
2	I	118	PRO	N-CA-C	-5.13	106.13	113.47
2	I	253	THR	CA-CB-OG1	-5.12	101.91	109.60
1	D	74	GLN	CB-CA-C	-5.12	103.02	110.03
1	C	219	PRO	N-CA-C	5.12	118.38	111.22
1	A	231	LEU	N-CA-C	-5.10	106.91	113.23
2	G	253	THR	CA-CB-OG1	-5.08	101.99	109.60
1	E	79	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	141	ARG	N-CA-C	-5.05	106.97	113.23
2	H	143	LYS	N-CA-C	-5.04	100.95	108.96
2	J	30	THR	CB-CA-C	5.04	118.11	109.80
1	B	233	PRO	CB-CA-C	-5.00	104.83	111.23

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	1945	0	1963	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1942	0	1952	43	0
1	C	1947	0	1950	49	0
1	D	1938	0	1959	41	0
1	E	1948	0	1963	41	0
2	F	1815	0	1790	88	0
2	G	1894	0	1915	88	0
2	H	1874	0	1871	50	0
2	I	1905	0	1931	109	0
2	J	1876	0	1879	82	0
3	B	6	8	8	0	0
3	G	6	8	8	0	0
3	H	6	8	8	0	0
3	J	6	8	8	0	0
4	A	40	0	0	0	0
4	B	63	0	0	1	0
4	C	62	0	0	0	0
4	D	58	0	0	1	0
4	E	66	0	0	0	0
4	F	62	0	0	2	0
4	G	60	0	0	3	0
4	H	66	0	0	2	0
4	I	40	0	0	1	0
4	J	76	0	0	2	0
All	All	19701	32	19205	611	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 16.

All (611) 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)
2:I:42:ILE:CD1	2:I:77:ARG:HD2	1.65	1.24
2:I:56:LYS:HD2	2:I:133:GLU:OE2	1.43	1.17
1:D:58:LYS:HE3	1:D:136:GLU:OE1	1.46	1.16
2:I:42:ILE:HD13	2:I:77:ARG:CD	1.78	1.10
2:J:9:ARG:HH11	2:J:20:THR:CG2	1.64	1.09
2:G:8:GLN:O	2:G:12:GLU:HG3	1.51	1.07
2:I:64:LYS:HE3	2:I:68:MET:HE2	1.18	1.07
2:J:57:MET:HE1	2:J:207:LEU:HD12	1.38	1.06
2:I:39:ARG:HG3	2:I:39:ARG:HH21	1.18	1.05
2:I:42:ILE:HD13	2:I:77:ARG:HD2	1.08	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:65:MET:HE2	2:I:73:LEU:HD23	1.38	1.03
2:G:8:GLN:HG3	2:G:12:GLU:OE2	1.61	0.98
2:F:11:ASP:OD2	2:F:44:HIS:HB3	1.64	0.97
2:F:59:PHE:CD2	2:F:74:ILE:HG23	1.98	0.96
2:I:23:LEU:HD12	2:I:28:ALA:HA	1.45	0.95
2:I:23:LEU:HD13	2:I:29:VAL:N	1.83	0.94
2:I:77:ARG:NH1	2:I:213:GLU:OE1	2.01	0.94
2:F:56:LYS:HD2	2:F:133:GLU:OE2	1.68	0.93
2:J:9:ARG:HH11	2:J:20:THR:HG23	1.35	0.91
2:G:51:ARG:HG3	2:G:51:ARG:HH11	1.33	0.91
2:F:59:PHE:CD2	2:F:74:ILE:CG2	2.53	0.90
2:I:29:VAL:HG22	2:I:33:GLU:HB2	1.54	0.89
2:I:23:LEU:CD1	2:I:28:ALA:HA	2.02	0.89
2:F:48:ARG:HG3	2:F:48:ARG:HH11	1.37	0.89
2:G:146:LEU:HB3	2:G:147:PRO:HD3	1.55	0.88
2:G:8:GLN:O	2:G:12:GLU:CG	2.21	0.88
2:F:82:MET:CE	2:F:156:SER:HB3	2.04	0.88
2:J:233:ARG:HH11	2:J:233:ARG:HG3	1.38	0.86
2:F:59:PHE:HD2	2:F:74:ILE:HG23	1.38	0.86
1:A:170:LYS:NZ	1:C:172:GLU:HG2	1.90	0.86
2:F:59:PHE:CE2	2:F:74:ILE:HG21	2.12	0.85
2:H:51:ARG:HG3	2:H:51:ARG:HH11	1.41	0.85
2:J:38:GLN:O	2:J:42:ILE:HD13	1.77	0.84
2:I:23:LEU:HB2	2:I:27:ASP:O	1.77	0.84
2:F:146:LEU:HB3	2:F:147:PRO:HD3	1.61	0.83
2:G:56:LYS:HD2	2:G:133:GLU:OE2	1.78	0.82
2:F:168:GLU:OE1	2:F:168:GLU:N	2.13	0.82
2:G:8:GLN:CG	2:G:12:GLU:OE2	2.28	0.82
2:I:23:LEU:HD13	2:I:29:VAL:H	1.44	0.82
2:J:38:GLN:O	2:J:42:ILE:CD1	2.28	0.81
2:G:111:ARG:HG2	2:G:111:ARG:HH11	1.46	0.81
2:I:58:GLY:O	2:I:73:LEU:HB3	1.81	0.81
1:D:190:VAL:HG23	1:D:235:VAL:HG21	1.64	0.80
2:F:11:ASP:OD2	2:F:44:HIS:CB	2.30	0.80
1:A:152:THR:HG1	1:A:158:SER:HG	1.23	0.80
1:A:8:LEU:HD13	1:A:29:ILE:HD11	1.61	0.79
2:I:39:ARG:HG3	2:I:39:ARG:NH2	1.92	0.79
2:G:89:GLU:OE2	2:G:253:THR:HG22	1.82	0.79
2:G:39:ARG:HH21	2:G:211:GLN:CD	1.91	0.78
1:E:211:ARG:O	1:E:215:LYS:HG2	1.83	0.77
2:F:201:LEU:O	2:F:204:ALA:HB3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:ARG:NH2	2:I:27:ASP:OD1	2.16	0.77
2:F:23:LEU:CD2	2:F:28:ALA:O	2.32	0.76
2:F:56:LYS:CD	2:F:133:GLU:OE2	2.33	0.76
1:E:-3:ASP:HB3	1:E:0:TRP:HB3	1.66	0.76
2:I:29:VAL:CG2	2:I:33:GLU:CB	2.63	0.76
2:I:29:VAL:CG2	2:I:33:GLU:HB2	2.16	0.76
1:D:84:MET:HE3	1:D:160:GLY:O	1.85	0.76
1:C:69:GLN:HG2	1:C:70:LEU:HD12	1.66	0.76
2:J:9:ARG:NH1	2:J:20:THR:CG2	2.47	0.76
2:F:23:LEU:HD22	2:F:28:ALA:O	1.85	0.75
1:D:130:TYR:CD2	1:D:168:PRO:HB3	2.21	0.75
2:I:23:LEU:CD1	2:I:29:VAL:H	1.98	0.75
2:I:97:HIS:HE1	2:I:137:SER:O	1.69	0.75
2:F:6:ILE:HD13	2:F:6:ILE:N	2.03	0.74
1:B:91:GLU:CD	2:G:183:ARG:HH21	1.96	0.73
2:F:63:ALA:O	2:F:67:GLN:HB2	1.87	0.73
2:F:48:ARG:HH11	2:F:48:ARG:CG	2.01	0.73
2:H:75:TRP:HZ2	2:H:211:GLN:HG3	1.53	0.73
2:F:99:ARG:HG2	2:F:231:ALA:HA	1.69	0.73
2:G:97:HIS:HE1	2:G:137:SER:O	1.72	0.73
2:H:5:ARG:NH1	2:H:27:ASP:OD1	2.21	0.73
2:J:57:MET:CE	2:J:207:LEU:HD12	2.17	0.73
1:D:117:GLU:OE1	1:D:215:LYS:CE	2.37	0.72
2:F:82:MET:CE	2:F:156:SER:CB	2.67	0.72
2:H:51:ARG:HG3	2:H:51:ARG:NH1	2.04	0.71
1:C:-3:ASP:HB3	1:C:0:TRP:HB3	1.72	0.71
2:J:139:TYR:CE2	2:J:148:ASP:HB3	2.26	0.71
1:B:91:GLU:OE1	2:G:183:ARG:NH2	2.22	0.71
1:E:57:ARG:HB2	1:E:209:LEU:HD21	1.73	0.71
2:H:23:LEU:HD23	2:H:23:LEU:N	2.05	0.71
1:C:101:LYS:HG2	1:C:236:ALA:HA	1.72	0.71
2:I:23:LEU:CD2	2:I:29:VAL:HG12	2.21	0.70
2:F:38:GLN:HA	2:F:41:LEU:HD12	1.74	0.70
1:D:58:LYS:CE	1:D:136:GLU:OE1	2.34	0.70
1:A:8:LEU:HD13	1:A:29:ILE:CD1	2.21	0.70
2:I:20:THR:OG1	2:I:21:PRO:HD2	1.90	0.70
2:I:29:VAL:HG23	2:I:33:GLU:HB3	1.73	0.70
2:J:36:GLU:HG2	2:J:39:ARG:NH1	2.07	0.70
2:I:23:LEU:HB2	2:I:27:ASP:C	2.16	0.69
2:J:55:LEU:HD11	2:J:77:ARG:NH2	2.08	0.69
1:A:170:LYS:HZ1	1:C:172:GLU:HG2	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLY:N	1:B:35:GLN:OE1	2.25	0.69
2:H:31:VAL:HG12	2:H:147:PRO:HG3	1.75	0.68
1:B:167:THR:HB	4:B:402:HOH:O	1.92	0.68
2:F:59:PHE:HD2	2:F:74:ILE:CG2	1.95	0.68
2:J:233:ARG:HG3	2:J:233:ARG:NH1	2.08	0.68
2:G:51:ARG:HG3	2:G:51:ARG:NH1	2.06	0.68
2:I:46:ILE:HD12	2:I:50:ALA:O	1.93	0.68
2:H:176:MET:HG2	2:H:242:VAL:HG22	1.74	0.68
2:G:22:GLN:OE1	2:G:143:LYS:N	2.20	0.68
2:I:146:LEU:HB3	2:I:147:PRO:HD3	1.74	0.68
1:E:81:PHE:HD2	1:E:84:MET:HE3	1.58	0.68
2:I:29:VAL:CG2	2:I:33:GLU:HB3	2.23	0.68
2:J:22:GLN:OE1	2:J:143:LYS:N	2.24	0.67
2:I:23:LEU:CD2	2:I:148:ASP:OD2	2.42	0.67
2:I:29:VAL:HG22	2:I:33:GLU:CB	2.25	0.67
2:J:20:THR:O	2:J:139:TYR:HA	1.95	0.67
2:J:5:ARG:O	2:J:9:ARG:HG2	1.95	0.67
1:A:66:VAL:HA	1:A:69:GLN:CG	2.25	0.66
2:G:145:SER:HB3	2:G:148:ASP:HB2	1.77	0.66
2:F:82:MET:HE2	2:F:156:SER:HB3	1.75	0.66
1:D:63:SER:O	1:D:67:GLN:HG3	1.95	0.66
2:F:176:MET:CG	2:F:242:VAL:HG22	2.26	0.66
2:F:196:SER:HB3	2:F:199:ARG:HD2	1.75	0.66
2:I:79:THR:N	2:I:82:MET:HE3	2.10	0.66
2:H:56:LYS:HE2	2:H:154:ALA:O	1.96	0.66
2:G:70:VAL:HG12	2:G:146:LEU:HD22	1.78	0.65
2:J:42:ILE:HD12	2:J:42:ILE:N	2.11	0.65
1:B:57:ARG:HG3	1:B:213:LEU:HD11	1.79	0.65
2:I:176:MET:HG3	2:I:242:VAL:HG22	1.78	0.65
1:E:211:ARG:O	1:E:215:LYS:HE2	1.96	0.65
2:I:29:VAL:HG23	2:I:33:GLU:CB	2.26	0.65
2:J:36:GLU:HG2	2:J:39:ARG:HH12	1.61	0.65
1:D:87:ASN:ND2	4:D:301:HOH:O	2.29	0.65
2:F:55:LEU:N	2:F:78:LEU:HD12	2.12	0.64
1:C:41:GLN:HE21	1:C:45:GLN:HG2	1.62	0.64
2:F:84:VAL:CG2	2:F:160:VAL:HB	2.26	0.64
1:D:137:VAL:HB	1:D:161:LEU:HB2	1.79	0.64
1:E:114:LEU:HB3	1:E:119:ILE:HD13	1.78	0.64
1:E:105:GLU:OE1	1:E:229:GLY:N	2.29	0.64
2:F:75:TRP:CD1	2:F:207:LEU:HD13	2.33	0.64
2:I:56:LYS:CD	2:I:133:GLU:OE2	2.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLU:OE1	1:D:215:LYS:HE2	1.98	0.63
2:J:81:ASP:OD1	2:J:81:ASP:N	2.24	0.63
2:F:34:ALA:HA	2:F:37:ILE:HG13	1.79	0.63
1:E:15:ALA:HB2	1:E:22:ILE:HG23	1.78	0.63
1:B:147:ILE:HD12	1:B:152:THR:HB	1.81	0.63
2:F:176:MET:HG2	2:F:242:VAL:HG22	1.81	0.63
1:C:190:VAL:HG23	1:C:235:VAL:HG21	1.81	0.63
1:B:244:GLU:HG3	1:B:254:ARG:HG3	1.81	0.62
1:D:72:VAL:HG11	1:D:149:ILE:HD13	1.81	0.62
1:E:176:LEU:O	1:E:195:GLY:HA3	1.99	0.62
1:C:137:VAL:HB	1:C:161:LEU:HB2	1.81	0.62
1:B:84:MET:HG2	1:B:160:GLY:O	2.00	0.62
1:C:20:LYS:O	1:C:20:LYS:HG2	1.98	0.62
2:F:48:ARG:HG3	2:F:48:ARG:NH1	2.10	0.62
1:D:257:PHE:O	2:J:183:ARG:NH2	2.29	0.62
2:F:59:PHE:HE2	2:F:74:ILE:HG21	1.60	0.61
1:B:58:LYS:HD2	1:B:136:GLU:OE2	2.01	0.61
1:B:111:GLU:HB3	1:B:129:ALA:HB2	1.82	0.61
2:G:57:MET:HE3	2:G:73:LEU:HD22	1.83	0.61
2:F:171:VAL:HA	2:F:174:LEU:HD11	1.83	0.60
1:E:147:ILE:HB	1:E:151:ASP:HB2	1.83	0.60
2:G:3:ILE:HG23	2:G:37:ILE:HG12	1.82	0.60
2:G:72:ASP:OD2	2:G:206:ARG:NH1	2.34	0.60
1:C:169:VAL:HG11	1:C:174:LEU:HD13	1.83	0.60
2:G:64:LYS:O	2:G:68:MET:HG2	2.01	0.60
2:H:75:TRP:CZ2	2:H:211:GLN:HG3	2.35	0.60
2:I:145:SER:HB3	2:I:148:ASP:OD1	2.02	0.60
1:D:190:VAL:CG2	1:D:235:VAL:HG21	2.31	0.60
2:H:83:TRP:CE3	2:J:115:ASN:HB3	2.37	0.60
2:I:77:ARG:HH22	2:I:213:GLU:CD	2.09	0.60
2:G:3:ILE:HD13	2:G:3:ILE:N	2.16	0.59
2:G:77:ARG:NH2	2:G:211:GLN:OE1	2.32	0.59
1:C:257:PHE:O	2:I:183:ARG:NH2	2.34	0.59
2:F:82:MET:HE1	2:F:156:SER:HB3	1.82	0.59
2:J:55:LEU:CD1	2:J:77:ARG:NH2	2.66	0.59
2:J:59:PHE:O	2:J:73:LEU:CD2	2.51	0.59
1:A:61:LEU:HD22	1:A:66:VAL:HG12	1.84	0.59
1:C:244:GLU:HG3	1:C:254:ARG:HG3	1.83	0.59
2:G:2:LYS:HD3	2:G:33:GLU:OE2	2.02	0.59
1:B:58:LYS:HD3	1:B:159:ALA:HB2	1.85	0.59
2:H:146:LEU:HB3	2:H:147:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASN:OD1	1:B:46:ARG:HD3	2.03	0.58
1:B:59:ILE:HD12	1:B:228:SER:HA	1.85	0.58
2:G:11:ASP:O	2:G:15:VAL:HG23	2.02	0.58
1:B:1:MET:O	1:B:1:MET:HG3	2.02	0.58
2:F:59:PHE:CE2	2:F:74:ILE:CG2	2.78	0.58
2:I:20:THR:O	2:I:139:TYR:HA	2.03	0.58
2:I:23:LEU:HD22	2:I:29:VAL:HG12	1.84	0.58
2:J:41:LEU:HD12	2:J:151:ALA:O	2.03	0.58
2:F:84:VAL:HG22	2:F:160:VAL:HB	1.85	0.58
1:E:244:GLU:HG3	1:E:254:ARG:HG3	1.85	0.58
2:G:210:GLN:NE2	4:G:401:HOH:O	2.36	0.58
2:J:30:THR:H	2:J:33:GLU:HB2	1.69	0.58
1:A:141:ARG:HD3	1:A:141:ARG:N	2.18	0.58
2:J:108:LEU:CD1	2:J:215:LEU:HB3	2.34	0.58
1:B:26:ARG:NH2	1:B:146:ASP:OD1	2.34	0.58
2:J:146:LEU:HB3	2:J:147:PRO:HD3	1.85	0.58
2:H:38:GLN:HG3	2:H:153:ASN:HA	1.85	0.57
2:J:171:VAL:HA	2:J:174:LEU:HD11	1.86	0.57
2:F:23:LEU:HD23	2:F:28:ALA:O	2.05	0.57
2:F:171:VAL:HA	2:F:174:LEU:CD1	2.34	0.57
2:H:211:GLN:NE2	4:H:401:HOH:O	2.37	0.57
2:I:42:ILE:HD13	2:I:77:ARG:HD3	1.83	0.57
2:F:57:MET:HE1	2:F:204:ALA:HA	1.86	0.57
2:F:44:HIS:O	2:F:48:ARG:NH1	2.37	0.57
2:F:142:PHE:CZ	2:F:144:PHE:HA	2.40	0.57
2:G:171:VAL:HA	2:G:174:LEU:CD1	2.33	0.57
1:D:117:GLU:OE1	1:D:215:LYS:HE3	2.05	0.57
2:J:139:TYR:CZ	2:J:148:ASP:HB3	2.39	0.57
1:C:147:ILE:HB	1:C:151:ASP:HB2	1.87	0.57
1:A:57:ARG:HG3	1:A:213:LEU:HD11	1.87	0.57
2:I:240:CYS:HB3	2:I:248:LEU:CD2	2.35	0.57
1:A:142:ILE:HD13	1:A:151:ASP:HB3	1.87	0.56
2:F:23:LEU:HD23	2:F:28:ALA:N	2.20	0.56
2:I:42:ILE:HD11	2:I:77:ARG:HD2	1.79	0.56
1:C:26:ARG:NH2	1:C:146:ASP:OD1	2.38	0.56
1:D:57:ARG:HG3	1:D:213:LEU:HD11	1.87	0.56
2:F:20:THR:HG23	2:F:20:THR:O	2.05	0.56
1:C:247:ILE:HB	1:C:250:LEU:HB3	1.87	0.56
2:G:107:LEU:HB2	2:H:119:LEU:HD21	1.87	0.56
2:I:23:LEU:CD1	2:I:29:VAL:N	2.60	0.56
2:I:65:MET:CE	2:I:73:LEU:HD23	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:LEU:C	2:F:78:LEU:CD1	2.79	0.56
2:G:103:GLU:OE1	2:G:222:LEU:HB3	2.05	0.56
2:J:145:SER:OG	2:J:148:ASP:OD1	2.24	0.56
1:A:137:VAL:HB	1:A:161:LEU:HB2	1.86	0.55
1:B:105:GLU:OE1	1:B:227:LEU:HB3	2.06	0.55
2:G:179:SER:HB2	2:G:183:ARG:C	2.31	0.55
2:H:107:LEU:HB2	2:J:119:LEU:HD21	1.86	0.55
1:B:14:GLU:OE2	1:B:14:GLU:HA	2.04	0.55
2:G:39:ARG:NH2	2:G:211:GLN:CD	2.63	0.55
2:F:55:LEU:HD21	2:F:75:TRP:CE3	2.42	0.55
2:F:142:PHE:CE2	2:F:144:PHE:HA	2.42	0.55
2:G:111:ARG:HG2	2:G:111:ARG:NH1	2.20	0.55
2:I:23:LEU:HD22	2:I:29:VAL:CG1	2.37	0.55
2:I:60:THR:HG21	2:I:224:GLY:HA3	1.89	0.55
1:E:130:TYR:CD2	1:E:168:PRO:HB3	2.42	0.54
1:B:195:GLY:HA2	1:B:231:LEU:HD22	1.89	0.54
2:J:67:GLN:HB3	2:J:68:MET:HE2	1.89	0.54
2:F:144:PHE:CD1	2:F:144:PHE:C	2.85	0.54
2:I:29:VAL:HG23	2:I:33:GLU:OE2	2.07	0.54
2:J:56:LYS:O	2:J:56:LYS:HG3	2.07	0.54
2:G:33:GLU:O	2:G:37:ILE:HG13	2.08	0.54
1:B:105:GLU:CG	1:B:229:GLY:O	2.56	0.54
1:D:97:THR:HB	1:D:100:PRO:HB3	1.90	0.54
1:D:114:LEU:HB3	1:D:119:ILE:HD13	1.89	0.54
2:I:97:HIS:CE1	2:I:137:SER:O	2.56	0.54
2:G:56:LYS:O	2:G:56:LYS:HG3	2.06	0.53
2:G:102:PRO:HB2	2:G:176:MET:HE2	1.89	0.53
1:B:-3:ASP:HB3	1:B:0:TRP:HB3	1.90	0.53
1:D:191:SER:OG	1:D:233:PRO:HD2	2.09	0.53
2:H:89:GLU:CD	2:H:253:THR:HG23	2.33	0.53
2:J:43:ALA:HA	2:J:46:ILE:HD12	1.90	0.53
1:A:61:LEU:CD2	1:A:66:VAL:HG12	2.38	0.53
1:A:62:THR:HG21	1:A:229:GLY:HA3	1.91	0.53
1:C:1:MET:O	1:C:1:MET:HG2	2.09	0.53
2:F:55:LEU:C	2:F:78:LEU:HD11	2.34	0.53
2:G:146:LEU:HB3	2:G:147:PRO:CD	2.35	0.53
2:G:164:TRP:HA	2:H:119:LEU:HD12	1.91	0.53
2:I:2:LYS:NZ	2:I:28:ALA:O	2.42	0.53
1:B:26:ARG:NH2	1:B:146:ASP:O	2.42	0.52
2:F:176:MET:HG3	2:F:242:VAL:HG22	1.90	0.52
2:G:30:THR:H	2:G:33:GLU:HB2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:215:LEU:N	2:J:215:LEU:HD23	2.24	0.52
1:C:57:ARG:HG3	1:C:213:LEU:HD11	1.90	0.52
2:G:59:PHE:CD2	2:G:74:ILE:HG12	2.44	0.52
2:I:20:THR:HG1	2:I:21:PRO:HD2	1.74	0.52
2:I:78:LEU:HA	2:I:82:MET:CE	2.40	0.52
2:J:196:SER:HB3	2:J:199:ARG:HD2	1.92	0.52
2:F:193:ILE:O	2:F:193:ILE:HG22	2.09	0.52
1:D:75:PRO:HD2	1:D:208:TRP:CE2	2.45	0.52
2:I:29:VAL:HA	2:I:33:GLU:OE2	2.10	0.52
2:I:41:LEU:HD12	2:I:151:ALA:O	2.10	0.52
2:G:72:ASP:CG	2:G:206:ARG:HH12	2.16	0.52
2:I:78:LEU:HA	2:I:82:MET:HE3	1.92	0.52
1:C:213:LEU:HB3	1:C:218:THR:O	2.10	0.52
2:G:20:THR:O	2:G:139:TYR:HA	2.10	0.52
1:C:244:GLU:OE1	2:I:239:ARG:NH1	2.36	0.51
1:D:213:LEU:HD12	1:D:220:LEU:HG	1.92	0.51
2:I:77:ARG:CZ	2:I:213:GLU:OE1	2.58	0.51
1:A:14:GLU:OE2	1:A:18:SER:HB3	2.09	0.51
1:B:88:ASP:HB2	1:B:253:VAL:HG23	1.92	0.51
2:I:60:THR:HA	2:I:73:LEU:HD22	1.91	0.51
2:I:79:THR:OG1	2:I:81:ASP:OD1	2.27	0.51
1:A:170:LYS:HZ2	1:C:172:GLU:HG2	1.72	0.51
2:G:176:MET:HE3	2:G:242:VAL:HG22	1.93	0.51
2:H:12:GLU:O	2:H:12:GLU:HG3	2.11	0.51
1:C:176:LEU:O	1:C:195:GLY:HA3	2.10	0.51
1:E:114:LEU:HB3	1:E:119:ILE:CD1	2.40	0.51
2:I:77:ARG:O	2:I:82:MET:HE1	2.10	0.51
2:F:29:VAL:O	2:F:29:VAL:HG13	2.10	0.51
2:F:145:SER:O	2:F:149:VAL:HG23	2.11	0.51
2:G:30:THR:HG23	2:G:33:GLU:H	1.76	0.51
2:I:23:LEU:HD13	2:I:28:ALA:C	2.33	0.51
2:F:100:VAL:HG13	2:F:178:MET:SD	2.51	0.51
2:H:23:LEU:HB3	2:H:27:ASP:O	2.10	0.51
2:I:127:ALA:HB2	2:I:164:TRP:NE1	2.26	0.51
2:F:8:GLN:NE2	2:F:44:HIS:CE1	2.79	0.51
1:C:53:ARG:NH1	1:D:118:ASN:O	2.43	0.51
2:H:20:THR:O	2:H:139:TYR:HA	2.10	0.51
2:I:51:ARG:O	2:I:79:THR:HA	2.11	0.51
2:F:44:HIS:C	2:F:48:ARG:HH12	2.19	0.51
2:G:2:LYS:HG3	2:G:3:ILE:HD13	1.92	0.51
1:C:99:GLN:N	1:C:100:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:MET:SD	1:C:181:MET:C	2.94	0.51
2:H:20:THR:OG1	2:H:21:PRO:HD2	2.11	0.51
2:J:38:GLN:O	2:J:42:ILE:HD12	2.09	0.51
2:J:103:GLU:OE1	2:J:222:LEU:HB3	2.11	0.51
1:E:63:SER:O	1:E:67:GLN:HG3	2.10	0.50
1:D:247:ILE:HB	1:D:250:LEU:HB3	1.92	0.50
2:J:9:ARG:NH1	2:J:20:THR:HG23	2.16	0.50
2:F:162:GLY:O	2:G:118:PRO:HB2	2.12	0.50
2:I:65:MET:HE2	2:I:73:LEU:CD2	2.26	0.50
1:C:59:ILE:HD12	1:C:228:SER:HA	1.94	0.50
1:E:99:GLN:N	1:E:100:PRO:CD	2.74	0.50
1:E:103:GLU:OE1	1:E:234:LEU:HD11	2.11	0.50
2:H:56:LYS:HZ3	2:H:133:GLU:CD	2.17	0.50
2:I:58:GLY:O	2:I:73:LEU:CB	2.56	0.50
1:A:76:ASP:OD1	1:A:76:ASP:N	2.43	0.50
1:B:105:GLU:HG2	1:B:229:GLY:O	2.11	0.50
1:B:213:LEU:HD12	1:B:220:LEU:HG	1.93	0.50
1:D:65:ALA:O	1:D:69:GLN:HG3	2.11	0.50
2:J:171:VAL:HA	2:J:174:LEU:CD1	2.41	0.50
1:E:81:PHE:HD2	1:E:84:MET:CE	2.23	0.50
2:I:23:LEU:CD1	2:I:28:ALA:CA	2.85	0.50
2:J:99:ARG:HB3	2:J:229:ALA:HB1	1.92	0.50
1:D:176:LEU:O	1:D:195:GLY:HA3	2.12	0.50
2:I:38:GLN:HB2	2:I:150:ILE:O	2.11	0.50
1:A:28:HIS:ND1	1:A:28:HIS:N	2.60	0.49
2:G:51:ARG:NH1	2:G:51:ARG:CG	2.74	0.49
2:H:99:ARG:HD3	4:H:448:HOH:O	2.11	0.49
2:I:23:LEU:HD13	2:I:28:ALA:HA	1.89	0.49
2:I:145:SER:CB	2:I:148:ASP:OD1	2.60	0.49
1:C:195:GLY:HA2	1:C:231:LEU:CD2	2.43	0.49
2:J:20:THR:HG23	2:J:21:PRO:HD2	1.94	0.49
1:C:219:PRO:HG2	1:C:221:LYS:NZ	2.27	0.49
1:D:142:ILE:HD13	1:D:151:ASP:HB3	1.94	0.49
2:H:77:ARG:NH2	2:H:213:GLU:OE2	2.44	0.49
2:H:171:VAL:HA	2:H:174:LEU:CD1	2.42	0.49
2:J:37:ILE:O	2:J:41:LEU:HB2	2.13	0.49
2:F:55:LEU:O	2:F:78:LEU:HD11	2.13	0.49
2:F:102:PRO:HG3	2:F:227:THR:OG1	2.12	0.49
1:D:1:MET:SD	1:D:1:MET:N	2.74	0.49
2:I:46:ILE:HD13	2:I:46:ILE:N	2.27	0.49
1:B:193:GLY:HA3	1:B:231:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:LEU:HD22	2:F:243:GLN:O	2.13	0.49
2:H:31:VAL:CG1	2:H:147:PRO:HG3	2.40	0.49
2:F:116:VAL:HG23	2:F:202:VAL:HG22	1.93	0.49
2:G:171:VAL:HA	2:G:174:LEU:HD11	1.94	0.49
2:J:56:LYS:HD2	2:J:133:GLU:OE2	2.13	0.49
2:J:127:ALA:HB2	2:J:164:TRP:NE1	2.27	0.49
2:J:148:ASP:OD1	2:J:148:ASP:N	2.46	0.49
1:C:41:GLN:NE2	1:C:45:GLN:HG2	2.26	0.49
1:A:-1:ASN:N	1:A:-1:ASN:OD1	2.46	0.49
1:E:1:MET:O	1:E:1:MET:HG2	2.13	0.49
1:E:213:LEU:HD12	1:E:220:LEU:HG	1.95	0.49
2:G:83:TRP:CE3	2:H:115:ASN:HB3	2.48	0.49
2:I:68:MET:HB2	2:I:70:VAL:HG23	1.95	0.49
2:I:75:TRP:CD1	2:I:207:LEU:HD13	2.48	0.49
2:F:82:MET:HG2	2:F:157:SER:O	2.13	0.48
1:E:181:MET:SD	1:E:181:MET:C	2.96	0.48
2:G:5:ARG:NH1	2:G:27:ASP:OD1	2.46	0.48
1:A:99:GLN:N	1:A:100:PRO:CD	2.76	0.48
2:J:159:PHE:CD1	2:J:159:PHE:C	2.90	0.48
2:G:111:ARG:HH11	2:G:111:ARG:CG	2.18	0.48
1:A:21:PRO:HA	1:A:141:ARG:O	2.14	0.48
1:D:77:PHE:CD1	1:D:77:PHE:C	2.91	0.48
2:J:24:THR:O	2:J:26:ASP:N	2.46	0.48
2:J:29:VAL:HG11	2:J:37:ILE:CD1	2.44	0.48
2:H:38:GLN:CG	2:H:153:ASN:HA	2.44	0.48
2:F:59:PHE:CE2	2:F:74:ILE:HD12	2.48	0.48
1:A:58:LYS:HB2	1:A:58:LYS:HE3	1.65	0.48
2:I:39:ARG:HH21	2:I:39:ARG:CG	2.06	0.48
2:H:54:GLY:HA3	2:H:220:LEU:O	2.14	0.48
2:H:56:LYS:CE	2:H:154:ALA:O	2.62	0.48
2:I:23:LEU:HD13	2:I:28:ALA:CA	2.43	0.48
2:I:23:LEU:HG	2:I:148:ASP:OD2	2.13	0.48
2:I:23:LEU:HD21	2:I:148:ASP:OD2	2.14	0.48
1:A:86:VAL:O	1:A:163:VAL:HA	2.14	0.47
1:C:152:THR:OG1	1:C:158:SER:OG	2.31	0.47
2:I:23:LEU:CB	2:I:27:ASP:O	2.56	0.47
2:I:30:THR:HB	2:I:33:GLU:HG3	1.96	0.47
2:J:142:PHE:CZ	2:J:144:PHE:HA	2.48	0.47
1:B:101:LYS:HG2	1:B:236:ALA:HA	1.97	0.47
1:D:105:GLU:OE1	1:D:229:GLY:N	2.47	0.47
2:H:83:TRP:CZ3	2:J:115:ASN:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:ASP:OD2	2:I:44:HIS:HB3	2.14	0.47
2:I:77:ARG:NH2	2:I:213:GLU:OE1	2.47	0.47
1:C:103:GLU:HB3	1:C:234:LEU:CD1	2.45	0.47
2:J:75:TRP:N	2:J:75:TRP:CD1	2.82	0.47
2:J:145:SER:CB	2:J:148:ASP:OD1	2.63	0.47
2:F:207:LEU:O	2:F:210:GLN:HB2	2.14	0.47
1:D:88:ASP:HB2	1:D:253:VAL:HG23	1.97	0.47
1:E:21:PRO:HA	1:E:141:ARG:O	2.14	0.47
2:G:241:GLU:HG2	2:G:247:SER:HB3	1.97	0.47
2:I:59:PHE:CD2	2:I:74:ILE:HG12	2.49	0.47
2:G:95:TYR:HB3	2:G:136:ASP:OD2	2.15	0.47
2:I:233:ARG:HB2	2:I:234:PRO:CD	2.44	0.47
2:J:5:ARG:O	2:J:9:ARG:CG	2.62	0.47
1:C:87:ASN:HB2	1:C:90:GLU:HG3	1.95	0.47
1:C:103:GLU:OE1	1:C:230:ALA:HB2	2.15	0.47
1:A:152:THR:OG1	1:A:158:SER:OG	2.04	0.47
2:I:23:LEU:CD2	2:I:29:VAL:CG1	2.92	0.47
2:I:42:ILE:CD1	2:I:77:ARG:CD	2.54	0.47
2:I:79:THR:H	2:I:82:MET:HE3	1.80	0.47
1:A:149:ILE:HG23	1:A:150:LEU:HD13	1.97	0.46
1:B:105:GLU:HG3	1:B:229:GLY:O	2.15	0.46
1:C:57:ARG:HB2	1:C:209:LEU:HD21	1.96	0.46
1:C:130:TYR:CG	1:C:168:PRO:HB3	2.50	0.46
1:E:193:GLY:HA3	1:E:231:LEU:O	2.15	0.46
2:J:64:LYS:O	2:J:68:MET:HG2	2.14	0.46
1:B:244:GLU:HG3	1:B:254:ARG:CG	2.45	0.46
2:G:97:HIS:CE1	2:G:137:SER:O	2.60	0.46
2:J:41:LEU:HD21	4:J:453:HOH:O	2.14	0.46
1:E:147:ILE:O	1:E:147:ILE:HG12	2.15	0.46
2:I:23:LEU:CD1	2:I:29:VAL:HG12	2.45	0.46
1:B:4:GLN:NE2	1:B:28:HIS:O	2.49	0.46
1:E:81:PHE:CD2	1:E:84:MET:HE3	2.44	0.46
2:G:193:ILE:O	2:G:193:ILE:HG22	2.15	0.46
1:A:219:PRO:HG2	1:A:221:LYS:NZ	2.31	0.46
1:B:13:ASN:OD1	1:B:46:ARG:CD	2.63	0.46
1:B:178:LEU:O	2:H:175:GLY:HA3	2.16	0.46
1:E:59:ILE:HD13	1:E:209:LEU:HB2	1.98	0.46
2:G:177:VAL:HG22	2:G:187:LEU:HD22	1.98	0.46
1:A:8:LEU:CD1	1:A:29:ILE:CD1	2.90	0.46
2:J:112:LEU:HD21	2:J:121:ALA:HA	1.98	0.46
2:J:133:GLU:HG3	2:J:222:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:139:TYR:CE2	2:I:152:ASP:HB2	2.51	0.46
2:F:166:LYS:NZ	4:F:304:HOH:O	2.48	0.45
1:C:13:ASN:O	1:C:17:LEU:HG	2.16	0.45
1:E:97:THR:HB	1:E:100:PRO:HB3	1.98	0.45
1:D:130:TYR:CG	1:D:168:PRO:HB3	2.49	0.45
2:G:179:SER:HB2	2:G:183:ARG:O	2.16	0.45
2:J:59:PHE:O	2:J:73:LEU:HD23	2.15	0.45
1:E:207:LEU:O	1:E:211:ARG:HG3	2.17	0.45
2:G:70:VAL:CG1	2:G:146:LEU:HD22	2.45	0.45
2:F:92:LEU:HD22	2:F:98:PRO:HG3	1.99	0.45
1:E:101:LYS:HG2	1:E:236:ALA:HA	1.98	0.45
1:C:69:GLN:HG2	1:C:70:LEU:CD1	2.43	0.45
1:E:57:ARG:HG3	1:E:213:LEU:HD11	1.98	0.45
1:E:211:ARG:O	1:E:215:LYS:CE	2.62	0.45
2:G:134:ILE:O	2:G:134:ILE:HG22	2.16	0.45
2:F:82:MET:CE	2:F:156:SER:HB2	2.47	0.45
1:C:11:LEU:HD23	1:C:11:LEU:HA	1.82	0.45
1:D:48:LEU:HD21	1:D:54:VAL:HG23	1.99	0.45
2:H:103:GLU:OE2	2:H:133:GLU:OE1	2.35	0.45
2:I:46:ILE:HA	2:I:50:ALA:O	2.16	0.45
2:J:3:ILE:HG23	2:J:37:ILE:HG13	1.97	0.45
2:J:67:GLN:HB3	2:J:68:MET:CE	2.46	0.45
2:F:55:LEU:O	2:F:78:LEU:CD1	2.65	0.45
1:E:15:ALA:CB	1:E:22:ILE:HG23	2.45	0.45
2:I:215:LEU:HD13	2:I:221:ILE:CD1	2.46	0.45
2:J:56:LYS:NZ	4:J:405:HOH:O	2.49	0.45
2:J:233:ARG:NH1	2:J:233:ARG:CG	2.73	0.45
1:D:99:GLN:N	1:D:100:PRO:CD	2.80	0.45
1:E:15:ALA:HB2	1:E:22:ILE:CG2	2.46	0.45
1:E:98:LEU:HD12	1:E:98:LEU:HA	1.82	0.45
2:G:61:SER:HB3	2:G:64:LYS:HB3	1.99	0.45
2:I:51:ARG:HG3	2:I:51:ARG:HH11	1.82	0.45
2:H:99:ARG:NH1	2:H:99:ARG:HG2	2.31	0.45
2:I:94:HIS:ND1	2:I:94:HIS:N	2.65	0.45
1:E:75:PRO:O	1:E:208:TRP:CZ2	2.70	0.45
1:A:57:ARG:HB2	1:A:209:LEU:HD21	1.99	0.44
1:A:86:VAL:HB	1:A:163:VAL:HG22	1.98	0.44
1:A:118:ASN:O	1:B:53:ARG:NH1	2.50	0.44
2:J:65:MET:HE2	2:J:73:LEU:CD2	2.47	0.44
1:A:26:ARG:HD3	1:A:148:ASN:CG	2.41	0.44
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:THR:O	2:F:139:TYR:HA	2.18	0.44
1:C:101:LYS:HE3	1:C:145:TRP:NE1	2.33	0.44
2:G:34:ALA:HB1	2:G:151:ALA:HB2	1.98	0.44
2:I:45:ARG:HG2	2:I:81:ASP:OD2	2.17	0.44
2:F:42:ILE:HD13	2:F:77:ARG:HD3	1.98	0.44
1:E:244:GLU:OE1	2:H:239:ARG:NH1	2.50	0.44
1:A:-3:ASP:HB3	1:A:0:TRP:HB3	2.00	0.44
1:B:63:SER:HB3	1:B:66:VAL:HG23	2.00	0.44
1:C:99:GLN:N	1:C:100:PRO:HD3	2.33	0.44
2:I:196:SER:HB3	2:I:199:ARG:HD2	2.00	0.44
2:J:177:VAL:HG22	2:J:187:LEU:CD2	2.48	0.44
1:D:58:LYS:NZ	1:D:157:ALA:O	2.41	0.44
2:G:41:LEU:HD12	2:G:151:ALA:O	2.17	0.44
2:H:41:LEU:HD23	2:H:41:LEU:HA	1.63	0.44
2:H:142:PHE:CE2	2:H:144:PHE:HA	2.53	0.44
1:A:101:LYS:HB2	1:A:138:VAL:CG2	2.47	0.44
2:F:103:GLU:OE2	2:F:133:GLU:OE1	2.35	0.44
1:C:79:THR:N	1:C:156:ASN:OD1	2.37	0.44
2:J:42:ILE:HD12	2:J:42:ILE:H	1.81	0.44
2:G:41:LEU:CD1	2:G:151:ALA:O	2.66	0.44
2:J:250:PHE:CD1	2:J:250:PHE:C	2.96	0.44
1:A:66:VAL:HA	1:A:69:GLN:HG3	1.98	0.43
1:C:58:LYS:HA	1:C:227:LEU:HB2	2.00	0.43
1:A:75:PRO:O	1:A:208:TRP:CZ2	2.71	0.43
1:B:57:ARG:HB2	1:B:209:LEU:HD21	1.99	0.43
2:F:102:PRO:CG	2:F:227:THR:OG1	2.66	0.43
1:C:179:ALA:O	1:C:194:VAL:HA	2.18	0.43
1:D:26:ARG:NH1	1:D:151:ASP:OD2	2.47	0.43
1:A:15:ALA:HB2	1:A:22:ILE:HG23	2.00	0.43
1:A:66:VAL:HA	1:A:69:GLN:HG2	1.99	0.43
1:A:194:VAL:HG23	2:G:175:GLY:HA3	2.00	0.43
2:G:183:ARG:HD2	4:G:443:HOH:O	2.19	0.43
1:D:141:ARG:HD3	1:D:141:ARG:N	2.34	0.43
1:E:52:ARG:HH11	1:E:52:ARG:HG2	1.83	0.43
2:G:162:GLY:O	2:H:118:PRO:HB2	2.18	0.43
2:J:174:LEU:HD22	2:J:243:GLN:O	2.19	0.43
2:F:68:MET:HG3	2:F:144:PHE:CE2	2.53	0.43
2:H:56:LYS:NZ	2:H:133:GLU:OE2	2.38	0.43
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.90	0.43
1:B:25:VAL:HG23	1:B:29:ILE:CD1	2.49	0.43
2:F:82:MET:HE1	2:F:156:SER:CB	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:ILE:HD13	2:F:104:ILE:HA	1.84	0.43
2:G:23:LEU:N	2:G:23:LEU:HD23	2.33	0.43
2:G:127:ALA:HB3	2:H:119:LEU:HD11	2.01	0.43
2:J:65:MET:HE2	2:J:73:LEU:HD23	2.00	0.43
2:J:145:SER:HB3	2:J:148:ASP:OD1	2.19	0.43
2:J:55:LEU:HD11	2:J:77:ARG:CZ	2.48	0.43
2:F:92:LEU:HD22	2:F:98:PRO:CG	2.49	0.43
1:D:57:ARG:HB2	1:D:209:LEU:HD21	2.00	0.43
2:G:22:GLN:OE1	2:G:142:PHE:HA	2.19	0.43
2:G:179:SER:CB	2:G:184:ALA:HA	2.49	0.43
2:G:183:ARG:HB2	4:G:443:HOH:O	2.19	0.43
2:H:73:LEU:HD21	2:H:194:LEU:HD11	2.01	0.43
2:J:179:SER:HB3	2:J:184:ALA:HA	2.01	0.43
1:B:137:VAL:HB	1:B:161:LEU:HB2	2.02	0.42
1:E:183:MET:HA	1:E:244:GLU:O	2.19	0.42
2:F:41:LEU:HD11	2:F:151:ALA:O	2.18	0.42
2:F:89:GLU:HA	2:F:251:SER:O	2.19	0.42
1:E:195:GLY:HA2	1:E:231:LEU:HD22	2.01	0.42
2:I:119:LEU:HD13	2:J:129:ALA:HB2	2.00	0.42
1:A:213:LEU:HD12	1:A:220:LEU:HG	2.00	0.42
2:I:115:ASN:HB3	2:J:83:TRP:CD2	2.53	0.42
1:C:58:LYS:HB2	1:C:58:LYS:HE3	1.62	0.42
2:G:112:LEU:HD12	2:G:112:LEU:HA	1.89	0.42
2:J:20:THR:HA	2:J:21:PRO:HD3	1.92	0.42
1:B:99:GLN:N	1:B:100:PRO:CD	2.82	0.42
1:B:130:TYR:CD1	1:B:168:PRO:HB3	2.54	0.42
2:G:207:LEU:HA	2:G:207:LEU:HD12	1.71	0.42
2:F:56:LYS:HD2	2:F:133:GLU:CD	2.39	0.42
1:D:141:ARG:NH2	1:D:155:ASP:O	2.52	0.42
1:E:52:ARG:HG2	1:E:52:ARG:NH1	2.34	0.42
2:H:176:MET:CG	2:H:242:VAL:HG22	2.46	0.42
2:I:142:PHE:CE2	2:I:144:PHE:HA	2.55	0.42
2:I:215:LEU:HD13	2:I:221:ILE:HD11	2.01	0.42
2:G:59:PHE:CE2	2:G:74:ILE:HG12	2.54	0.42
2:J:220:LEU:HD23	2:J:220:LEU:HA	1.91	0.42
1:C:81:PHE:HB2	1:C:84:MET:HE3	2.01	0.42
1:C:185:ARG:NH1	1:C:241:ASP:OD2	2.50	0.42
2:G:62:ARG:NH2	2:G:65:MET:HE3	2.35	0.42
2:G:67:GLN:HG2	2:G:68:MET:SD	2.59	0.42
2:H:101:GLU:CG	2:H:229:ALA:HB2	2.49	0.42
2:I:23:LEU:HD21	2:I:29:VAL:HG12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:GLU:HG3	2:H:229:ALA:HB2	2.01	0.42
2:J:9:ARG:NH1	2:J:20:THR:HG22	2.28	0.42
1:A:141:ARG:N	1:A:141:ARG:CD	2.83	0.41
1:D:239:PRO:HB3	1:D:259:PRO:HA	2.01	0.41
2:G:10:LEU:HB2	2:G:41:LEU:HD21	2.01	0.41
2:J:145:SER:HB3	2:J:148:ASP:CG	2.45	0.41
1:A:58:LYS:HD2	1:A:159:ALA:HB2	2.01	0.41
1:D:94:TRP:CH2	1:D:239:PRO:HD3	2.54	0.41
2:I:75:TRP:HD1	2:I:207:LEU:HD13	1.85	0.41
2:J:42:ILE:CD1	2:J:42:ILE:N	2.79	0.41
2:J:78:LEU:HD11	2:J:222:LEU:HD12	2.03	0.41
2:G:111:ARG:NH1	2:G:111:ARG:CG	2.79	0.41
2:I:23:LEU:CG	2:I:148:ASP:OD2	2.68	0.41
2:J:46:ILE:HA	2:J:50:ALA:O	2.20	0.41
1:B:101:LYS:HE3	1:B:145:TRP:NE1	2.35	0.41
1:B:244:GLU:OE1	2:G:239:ARG:NH1	2.50	0.41
1:C:-2:LEU:HD23	1:C:-2:LEU:HA	1.83	0.41
2:G:61:SER:HB3	2:G:64:LYS:CB	2.51	0.41
1:B:100:PRO:HB2	1:B:237:ALA:HB3	2.03	0.41
2:I:153:ASN:ND2	2:I:156:SER:HB2	2.36	0.41
2:F:204:ALA:HB1	2:F:215:LEU:HD11	2.02	0.41
2:G:127:ALA:HB2	2:G:164:TRP:NE1	2.35	0.41
1:D:211:ARG:HH11	1:D:211:ARG:HD3	1.71	0.41
2:G:129:ALA:HB2	2:H:119:LEU:HD13	2.03	0.41
2:G:139:TYR:HB2	2:G:142:PHE:HB2	2.03	0.41
2:I:240:CYS:O	2:I:247:SER:HA	2.21	0.41
1:E:-2:LEU:N	1:E:-2:LEU:CD2	2.84	0.41
2:G:56:LYS:HD2	2:G:133:GLU:CD	2.45	0.41
2:H:112:LEU:HB3	2:H:215:LEU:HB2	2.01	0.41
2:H:112:LEU:HD12	2:H:112:LEU:HA	1.89	0.41
1:A:33:ILE:HD13	1:A:37:TYR:HE2	1.85	0.41
2:F:60:THR:HG21	2:F:223:ALA:O	2.20	0.41
2:F:108:LEU:CD1	2:F:215:LEU:HB3	2.51	0.41
1:C:190:VAL:CG2	1:C:235:VAL:HG21	2.47	0.41
1:D:1:MET:O	1:D:1:MET:HG2	2.21	0.41
2:G:2:LYS:HE3	2:G:2:LYS:HB2	1.71	0.41
2:G:101:GLU:O	2:G:132:MET:HA	2.20	0.41
2:H:77:ARG:HH21	2:H:213:GLU:CD	2.28	0.41
2:I:30:THR:HG22	2:I:32:ARG:H	1.86	0.41
2:I:51:ARG:HG3	2:I:51:ARG:NH1	2.36	0.41
2:I:132:MET:HE2	2:I:248:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:68:MET:HB3	2:J:144:PHE:CZ	2.55	0.41
1:A:257:PHE:O	2:F:183:ARG:NH2	2.50	0.41
2:F:11:ASP:OD1	2:F:48:ARG:NH2	2.54	0.41
2:F:68:MET:C	2:F:70:VAL:H	2.28	0.41
1:C:183:MET:HA	1:C:244:GLU:O	2.21	0.41
2:I:97:HIS:ND1	2:I:97:HIS:N	2.67	0.41
2:G:198:ILE:HD12	2:G:198:ILE:HA	1.91	0.40
2:H:99:ARG:HG2	2:H:99:ARG:HH11	1.85	0.40
2:I:177:VAL:HG22	2:I:187:LEU:CD2	2.51	0.40
2:I:240:CYS:HB3	2:I:248:LEU:HD21	2.01	0.40
2:I:242:VAL:HB	2:I:245:LEU:HB2	2.02	0.40
1:B:105:GLU:HG2	1:B:229:GLY:H	1.86	0.40
1:C:169:VAL:CG1	1:C:174:LEU:HD13	2.50	0.40
1:E:58:LYS:HB2	1:E:58:LYS:HE3	1.89	0.40
2:G:62:ARG:HA	2:G:62:ARG:HD2	1.85	0.40
1:A:25:VAL:C	1:A:27:GLY:N	2.79	0.40
2:F:96:VAL:HG11	2:F:138:ARG:HG3	2.02	0.40
2:H:27:ASP:O	2:H:29:VAL:HG13	2.22	0.40
1:A:91:GLU:OE1	1:A:258:SER:OG	2.35	0.40
1:A:219:PRO:HG2	1:A:221:LYS:HZ1	1.85	0.40
1:B:101:LYS:HB2	1:B:138:VAL:CG2	2.51	0.40
2:F:55:LEU:C	2:F:78:LEU:HD12	2.46	0.40
2:F:59:PHE:CE2	2:F:74:ILE:CD1	3.05	0.40
2:G:60:THR:HG22	2:G:73:LEU:HD23	2.03	0.40
2:I:60:THR:OG1	4:I:301:HOH:O	2.22	0.40
2:F:56:LYS:NZ	4:F:307:HOH:O	2.54	0.40
2:J:63:ALA:O	2:J:67:GLN:HB2	2.21	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	262/266 (98%)	252 (96%)	9 (3%)	1 (0%)	30	47
1	B	262/266 (98%)	257 (98%)	4 (2%)	1 (0%)	30	47
1	C	263/266 (99%)	257 (98%)	6 (2%)	0	100	100
1	D	261/266 (98%)	256 (98%)	5 (2%)	0	100	100
1	E	262/266 (98%)	254 (97%)	8 (3%)	0	100	100
2	F	251/258 (97%)	240 (96%)	7 (3%)	4 (2%)	7	13
2	G	254/258 (98%)	247 (97%)	6 (2%)	1 (0%)	30	47
2	H	254/258 (98%)	247 (97%)	7 (3%)	0	100	100
2	I	255/258 (99%)	249 (98%)	6 (2%)	0	100	100
2	J	253/258 (98%)	245 (97%)	5 (2%)	3 (1%)	10	19
All	All	2577/2620 (98%)	2504 (97%)	63 (2%)	10 (0%)	30	47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	29	VAL
2	G	25	GLY
2	J	25	GLY
2	F	23	LEU
2	F	26	ASP
2	J	144	PHE
1	A	160	GLY
2	F	25	GLY
2	J	157	SER
1	B	160	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	198/203 (98%)	182 (92%)	16 (8%)	11	22
1	B	198/203 (98%)	187 (94%)	11 (6%)	19	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	198/203 (98%)	186 (94%)	12 (6%)	17	33
1	D	198/203 (98%)	186 (94%)	12 (6%)	17	33
1	E	199/203 (98%)	189 (95%)	10 (5%)	22	42
2	F	178/195 (91%)	149 (84%)	29 (16%)	2	4
2	G	193/195 (99%)	173 (90%)	20 (10%)	7	13
2	H	189/195 (97%)	173 (92%)	16 (8%)	10	20
2	I	194/195 (100%)	171 (88%)	23 (12%)	5	9
2	J	190/195 (97%)	158 (83%)	32 (17%)	2	4
All	All	1935/1990 (97%)	1754 (91%)	181 (9%)	8	16

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	LEU
1	A	-1	ASN
1	A	4	GLN
1	A	7	LYS
1	A	22	ILE
1	A	33	ILE
1	A	58	LYS
1	A	69	GLN
1	A	105	GLU
1	A	110	ILE
1	A	122	ILE
1	A	140	SER
1	A	150	LEU
1	A	170	LYS
1	A	185	ARG
1	A	199	LEU
1	B	-2	LEU
1	B	22	ILE
1	B	26	ARG
1	B	33	ILE
1	B	47	GLN
1	B	68	LYS
1	B	105	GLU
1	B	122	ILE
1	B	170	LYS
1	B	202	PRO

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Mol	Chain	Res	Type
1	B	215	LYS
2	F	6	ILE
2	F	22	GLN
2	F	30	THR
2	F	37	ILE
2	F	42	ILE
2	F	46	ILE
2	F	48	ARG
2	F	52	GLN
2	F	55	LEU
2	F	56	LYS
2	F	61	SER
2	F	68	MET
2	F	74	ILE
2	F	80	SER
2	F	82	MET
2	F	94	HIS
2	F	96	VAL
2	F	97	HIS
2	F	126	GLU
2	F	138	ARG
2	F	140	ARG
2	F	145	SER
2	F	150	ILE
2	F	155	SER
2	F	166	LYS
2	F	176	MET
2	F	189	THR
2	F	197	PRO
2	F	211	GLN
1	C	14	GLU
1	C	20	LYS
1	C	23	GLU
1	C	26	ARG
1	C	33	ILE
1	C	41	GLN
1	C	58	LYS
1	C	63	SER
1	C	66	VAL
1	C	74	GLN
1	C	110	ILE
1	C	147	ILE

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Mol	Chain	Res	Type
1	D	-2	LEU
1	D	14	GLU
1	D	23	GLU
1	D	25	VAL
1	D	58	LYS
1	D	68	LYS
1	D	70	LEU
1	D	74	GLN
1	D	117	GLU
1	D	191	SER
1	D	214	VAL
1	D	215	LYS
1	E	-2	LEU
1	E	20	LYS
1	E	33	ILE
1	E	59	ILE
1	E	63	SER
1	E	74	GLN
1	E	140	SER
1	E	147	ILE
1	E	185	ARG
1	E	199	LEU
2	G	1	MET
2	G	2	LYS
2	G	3	ILE
2	G	12	GLU
2	G	18	LYS
2	G	20	THR
2	G	22	GLN
2	G	32	ARG
2	G	51	ARG
2	G	55	LEU
2	G	56	LYS
2	G	80	SER
2	G	97	HIS
2	G	104	ILE
2	G	111	ARG
2	G	143	LYS
2	G	176	MET
2	G	189	THR
2	G	196	SER
2	G	207	LEU

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Mol	Chain	Res	Type
2	H	22	GLN
2	H	23	LEU
2	H	30	THR
2	H	42	ILE
2	H	46	ILE
2	H	51	ARG
2	H	56	LYS
2	H	64	LYS
2	H	67	GLN
2	H	71	SER
2	H	92	LEU
2	H	138	ARG
2	H	141	ASP
2	H	176	MET
2	H	222	LEU
2	H	253	THR
2	I	23	LEU
2	I	26	ASP
2	I	31	VAL
2	I	36	GLU
2	I	38	GLN
2	I	39	ARG
2	I	41	LEU
2	I	46	ILE
2	I	51	ARG
2	I	55	LEU
2	I	64	LYS
2	I	67	GLN
2	I	73	LEU
2	I	74	ILE
2	I	94	HIS
2	I	97	HIS
2	I	166	LYS
2	I	168	GLU
2	I	176	MET
2	I	189	THR
2	I	213	GLU
2	I	222	LEU
2	I	248	LEU
2	J	4	SER
2	J	5	ARG
2	J	8	GLN

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Mol	Chain	Res	Type
2	J	9	ARG
2	J	15	VAL
2	J	16	SER
2	J	20	THR
2	J	26	ASP
2	J	29	VAL
2	J	30	THR
2	J	31	VAL
2	J	33	GLU
2	J	36	GLU
2	J	41	LEU
2	J	51	ARG
2	J	56	LYS
2	J	71	SER
2	J	77	ARG
2	J	96	VAL
2	J	97	HIS
2	J	99	ARG
2	J	103	GLU
2	J	126	GLU
2	J	132	MET
2	J	134	ILE
2	J	143	LYS
2	J	148	ASP
2	J	155	SER
2	J	213	GLU
2	J	233	ARG
2	J	251	SER
2	J	255	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	248	GLN
1	B	248	GLN
2	F	8	GLN
2	F	52	GLN
1	C	13	ASN
1	C	41	GLN
1	C	47	GLN
1	C	148	ASN

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Mol	Chain	Res	Type
1	D	189	GLN
1	E	-1	ASN
1	E	45	GLN
1	E	118	ASN
2	G	97	HIS
2	H	38	GLN
2	H	210	GLN
2	I	97	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	GOL	J	301	-	5,5,5	0.12	0	5,5,5	0.32	0
3	GOL	H	301	-	5,5,5	0.24	0	5,5,5	0.26	0
3	GOL	B	301	-	5,5,5	0.22	0	5,5,5	0.16	0
3	GOL	G	301	-	5,5,5	0.17	0	5,5,5	0.27	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	GOL	J	301	-	-	0/4/4/4	-
3	GOL	H	301	-	-	2/4/4/4	-
3	GOL	B	301	-	-	4/4/4/4	-
3	GOL	G	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

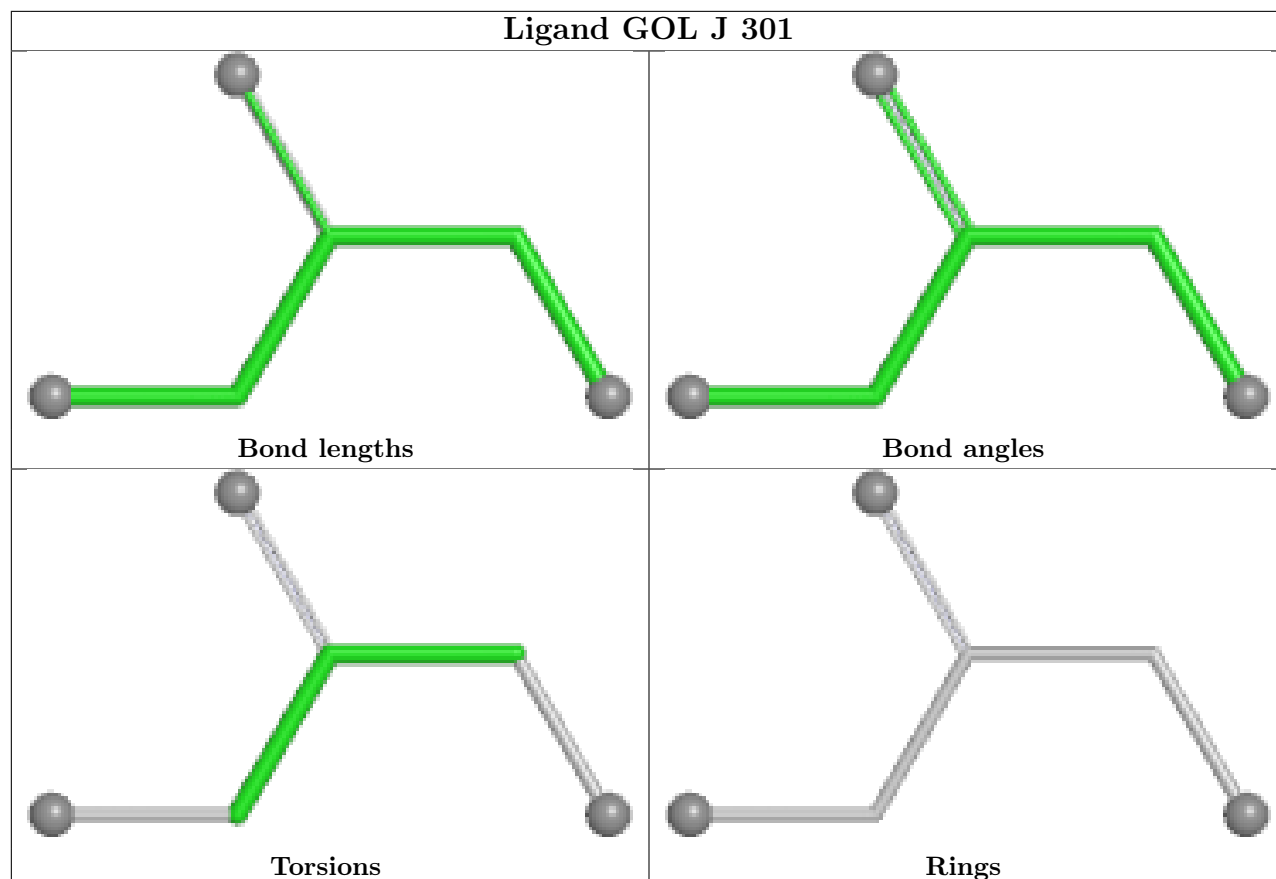
Mol	Chain	Res	Type	Atoms
3	B	301	GOL	C1-C2-C3-O3
3	H	301	GOL	C1-C2-C3-O3
3	H	301	GOL	O2-C2-C3-O3
3	G	301	GOL	O2-C2-C3-O3
3	B	301	GOL	O1-C1-C2-C3
3	G	301	GOL	O1-C1-C2-C3
3	G	301	GOL	C1-C2-C3-O3
3	B	301	GOL	O1-C1-C2-O2
3	B	301	GOL	O2-C2-C3-O3
3	G	301	GOL	O1-C1-C2-O2

There are no ring outliers.

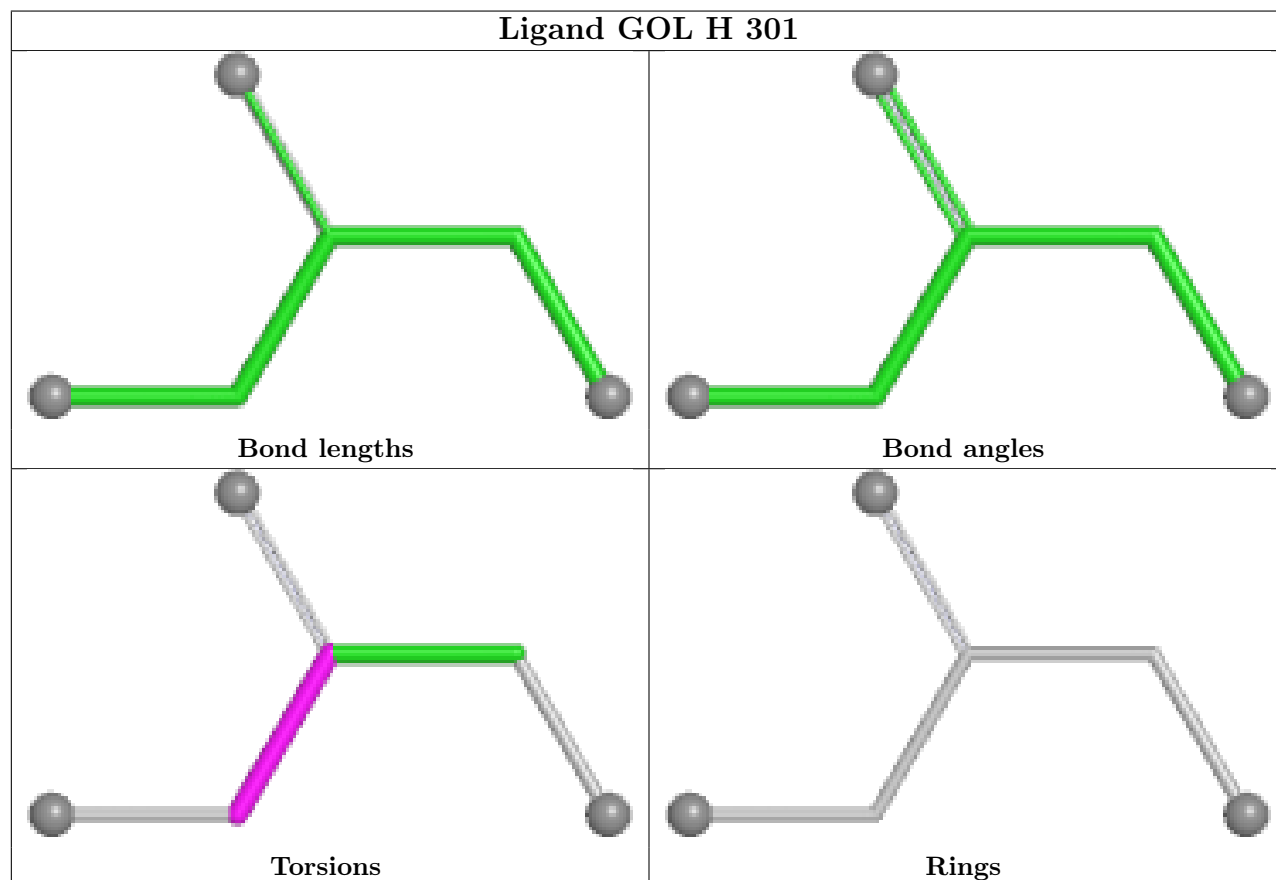
No monomer is involved in short contacts.

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

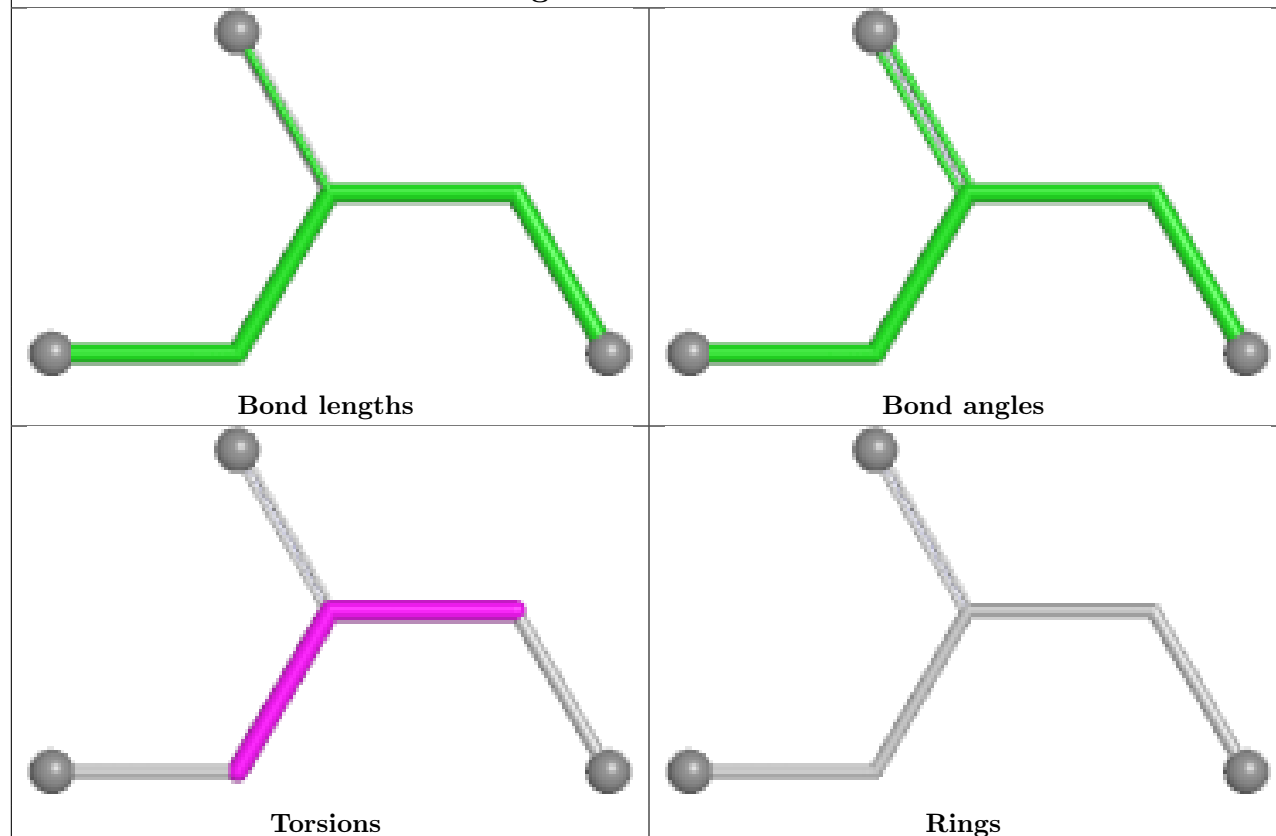
Ligand GOL J 301



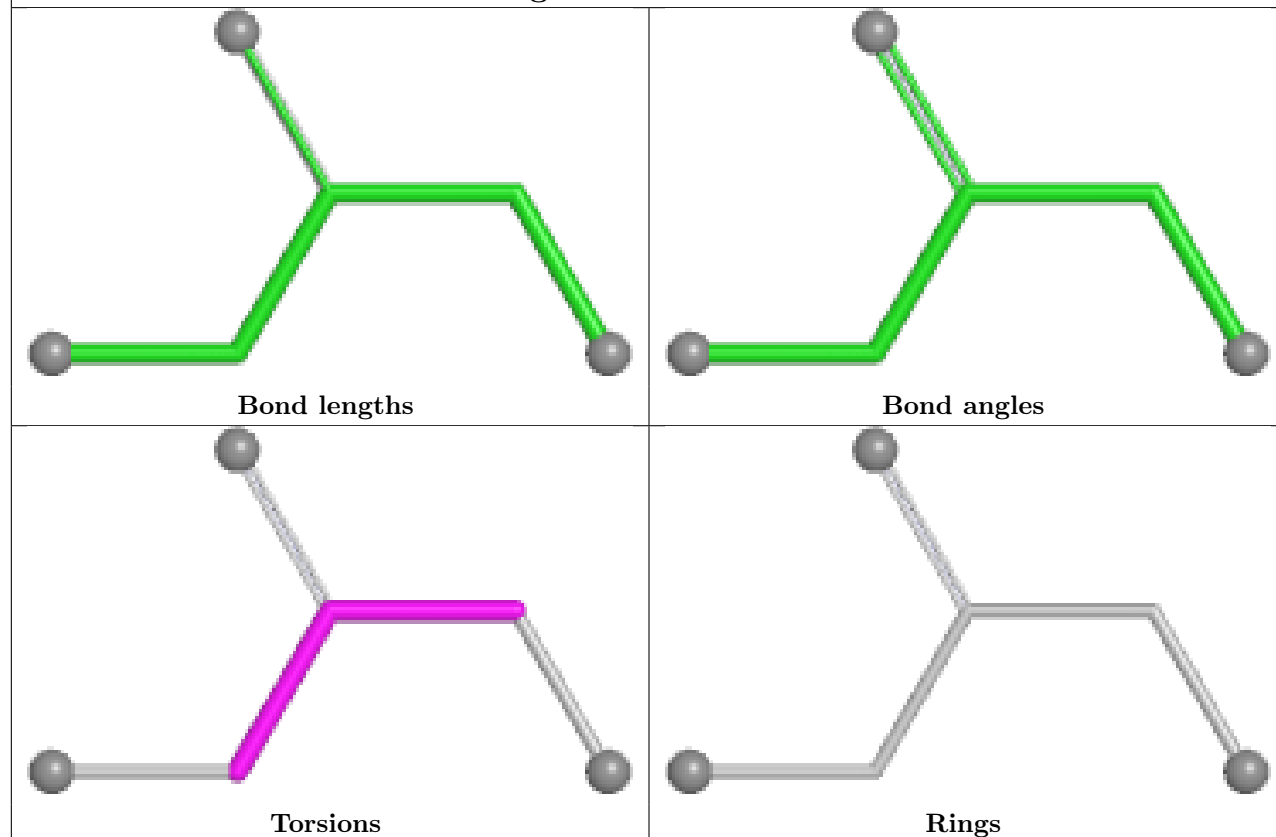
Ligand GOL H 301



Ligand GOL B 301



Ligand GOL G 301



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	264/266 (99%)	-0.12	2 (0%) 82 80	33, 49, 76, 108	0
1	B	264/266 (99%)	-0.20	2 (0%) 82 80	32, 46, 67, 104	0
1	C	265/266 (99%)	-0.16	2 (0%) 82 80	35, 47, 67, 115	0
1	D	263/266 (98%)	-0.14	1 (0%) 88 87	36, 47, 71, 87	0
1	E	264/266 (99%)	-0.16	2 (0%) 82 80	29, 46, 72, 103	0
2	F	253/258 (98%)	0.44	19 (7%) 20 18	37, 59, 116, 176	0
2	G	256/258 (99%)	0.12	2 (0%) 82 80	36, 54, 93, 120	0
2	H	256/258 (99%)	-0.08	2 (0%) 82 80	32, 51, 80, 109	0
2	I	257/258 (99%)	0.09	5 (1%) 66 63	37, 54, 86, 121	0
2	J	255/258 (98%)	0.10	6 (2%) 59 56	33, 52, 95, 115	0
All	All	2597/2620 (99%)	-0.01	43 (1%) 69 66	29, 50, 87, 176	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	-1	ALA	5.0
2	I	25	GLY	4.0
2	F	31	VAL	3.8
1	C	-4	ALA	3.8
2	F	27	ASP	3.6
2	F	144	PHE	3.5
2	F	26	ASP	3.4
2	F	3	ILE	3.3
2	G	23	LEU	3.2
1	B	0	TRP	3.2
2	F	147	PRO	3.1
2	F	28	ALA	3.1
2	F	97	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	260	ALA	3.0
2	I	23	LEU	2.9
2	F	7	ALA	2.9
2	I	27	ASP	2.9
1	B	-2	LEU	2.8
1	C	-2	LEU	2.8
2	F	6	ILE	2.7
1	E	260	ALA	2.7
2	J	1	MET	2.7
2	J	144	PHE	2.7
2	F	24	THR	2.6
2	J	140	ARG	2.5
2	F	36	GLU	2.4
2	F	143	LYS	2.4
2	F	25	GLY	2.3
2	H	254	GLY	2.3
1	A	27	GLY	2.3
1	E	-2	LEU	2.3
2	F	21	PRO	2.2
2	F	8	GLN	2.2
2	J	25	GLY	2.2
2	F	141	ASP	2.2
2	F	41	LEU	2.1
2	J	24	THR	2.1
2	J	77	ARG	2.1
1	A	-2	LEU	2.1
2	F	23	LEU	2.1
2	I	29	VAL	2.1
2	G	0	ALA	2.1
2	H	255	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

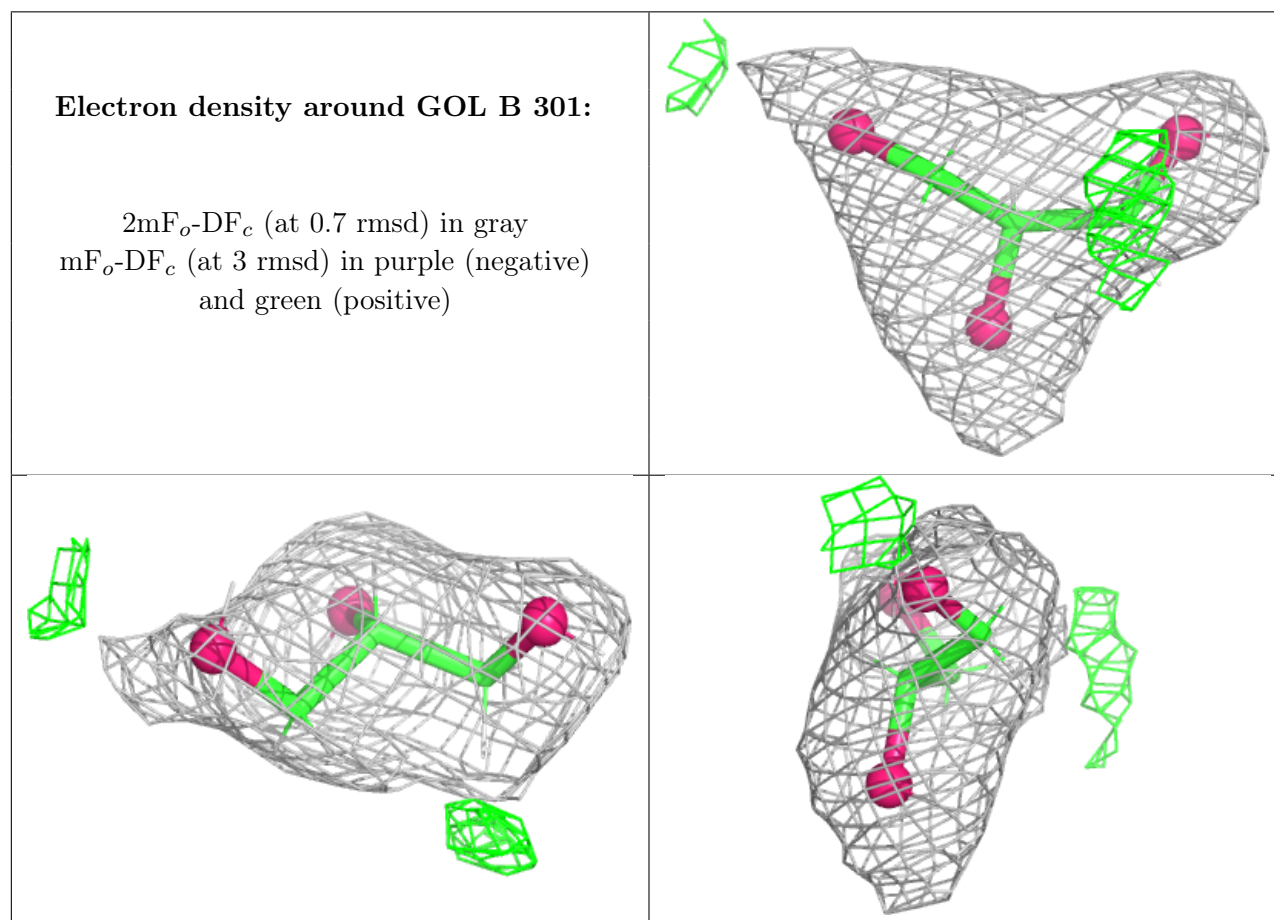
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

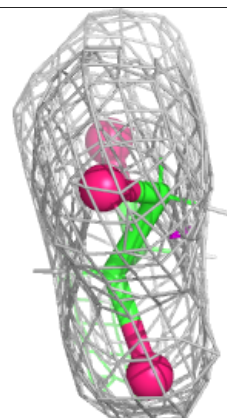
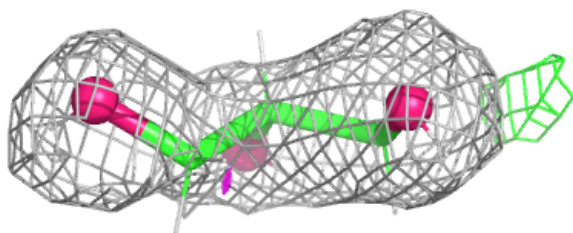
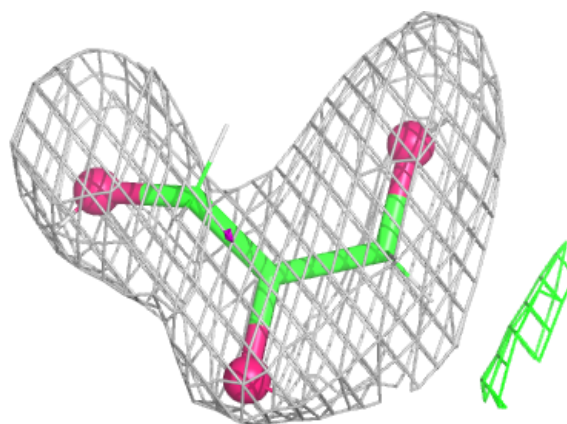
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	301	6/6	0.86	0.12	67,80,86,86	0
3	GOL	J	301	6/6	0.88	0.13	51,70,88,91	0
3	GOL	H	301	6/6	0.89	0.12	52,67,78,81	0
3	GOL	G	301	6/6	0.90	0.14	53,77,96,102	0

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.



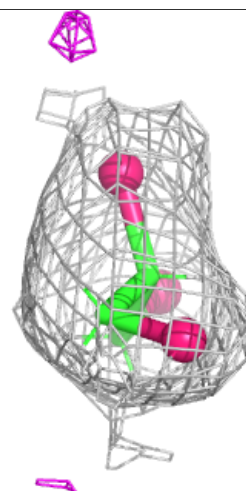
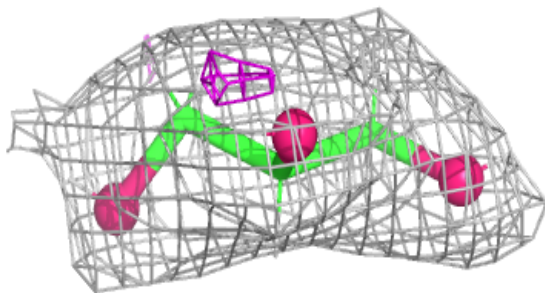
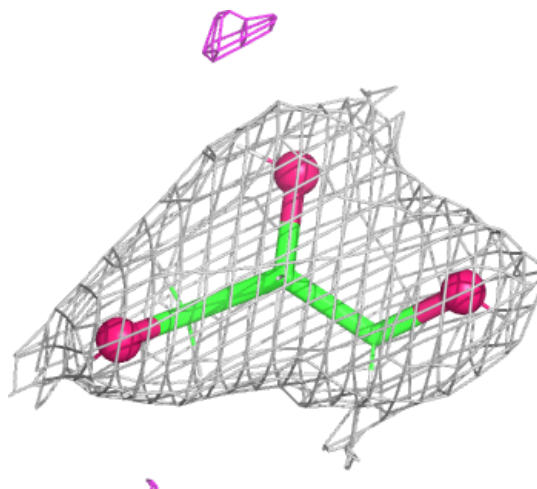
Electron density around GOL J 301:

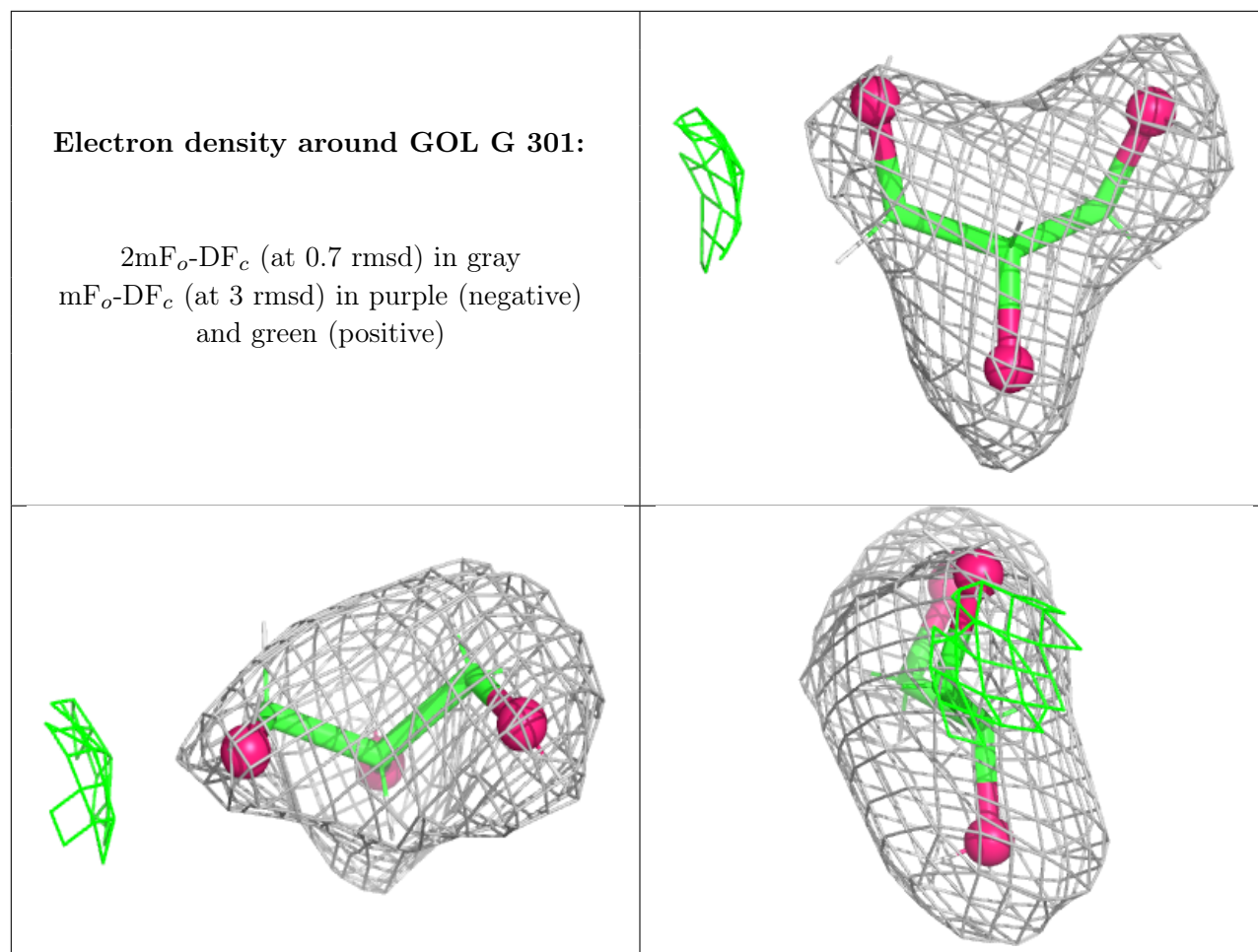
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL H 301:

$2mF_o-DF_c$ (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.