Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:20 AM EDT

PDB ID	:	2QMI
Title	:	Structure of the octameric penicillin-binding protein homologue from Pyrococcus abyssi
Authors	:	Delfosse, V.; Girard, E.; Moulinier, L.; Schultz, P.; Mayer, C.
Deposited on	:	2007-07-16
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

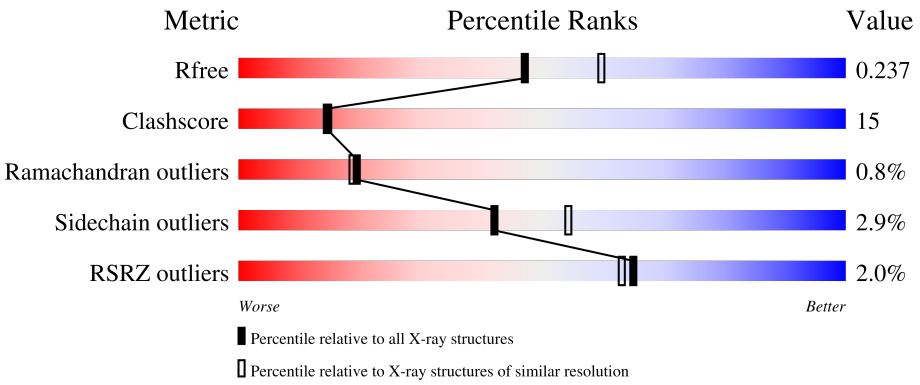
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	447	2% 70% 28% •
1	B	447	2% 74% 25% •
1	C	447	2% 76% 22% •
1	D	447	% 73% 25% •
1	E	447	2% 77% 22% •

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Mol	Chain	Length	Quality of chain
1	F	447	2% 74% 23%
1	G	447	2% 73% 24%
1	H	447	3% 75% 23%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30882 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 Pbp related beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3551	2325	558	654	14	0	0	0
1	B	447	3549	2325	555	655	14	0	0	0
1	C	446	3534	2317	553	650	14	0	0	0
1	D	446	3545	2323	555	653	14	0	0	0
1	E	446	3544	2322	556	652	14	0	0	0
1	F	447	3549	2325	555	655	14	0	0	0
1	G	447	3559	2331	559	655	14	0	0	0
1	H	447	3554	2326	558	656	14	0	0	0

- Molecule 2 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Lu		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	3	3	3	0	0

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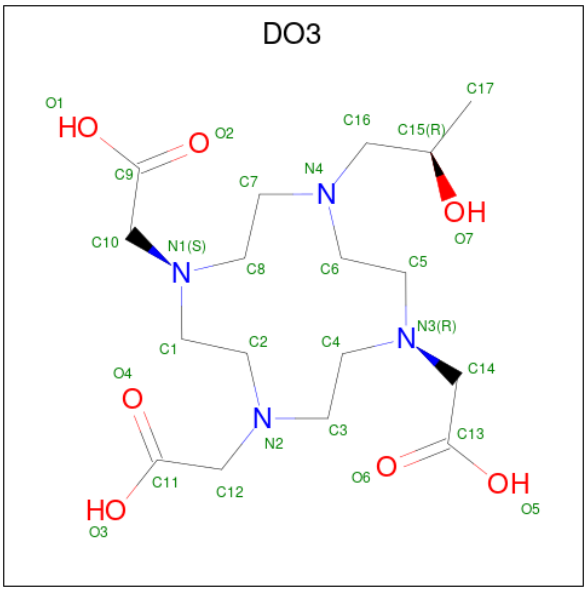
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Lu 3 3	0	0
2	H	1	Total Lu 1 1	0	0

- Molecule 3 is 10-((2R)-2-HYDROXYPROPYL)-1,4,7,10-TETRAAZACYCLODODECANE 1,4,7-TRIACETIC ACID (three-letter code: DO3) (formula: $C_{17}H_{32}N_4O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C N O 28 17 4 7	0	0
3	F	1	Total C N O 28 17 4 7	0	0
3	G	1	Total C N O 28 17 4 7	0	0
3	H	1	Total C N O 28 17 4 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	285	Total O 285 285	0	0
4	B	279	Total O 279 279	0	0
4	C	237	Total O 237 237	0	0

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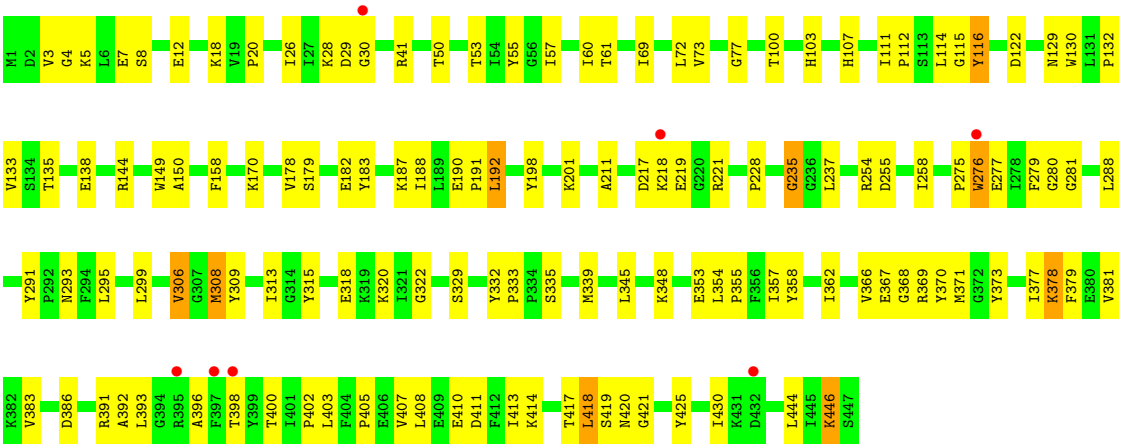
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	259	259	259	0	0
			Total	O		
4	E	337	337	337	0	0
			Total	O		
4	F	311	311	311	0	0
			Total	O		
4	G	351	351	351	0	0
			Total	O		
4	H	309	309	309	0	0

3 Residue-property plots (i)

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

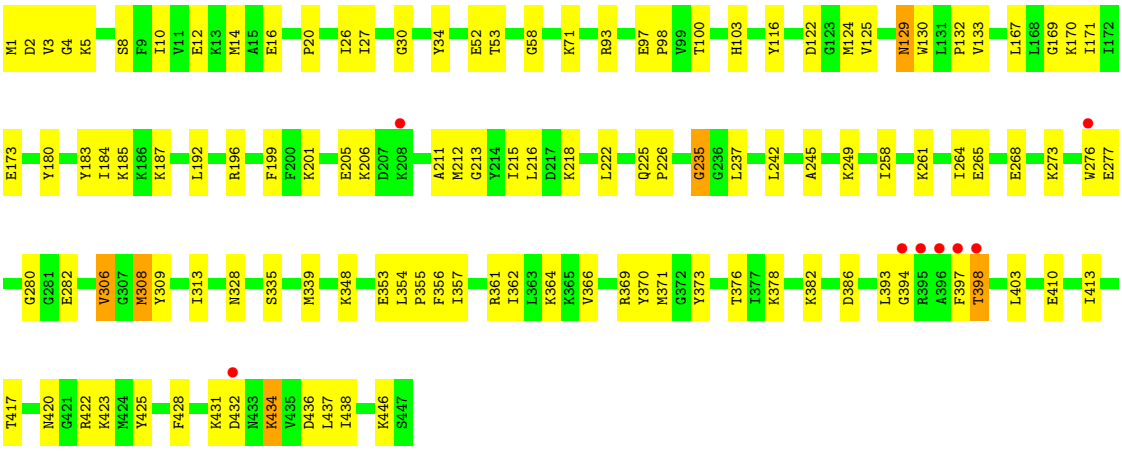
• Molecule 1: Pbp related beta-lactamase

Chain A:



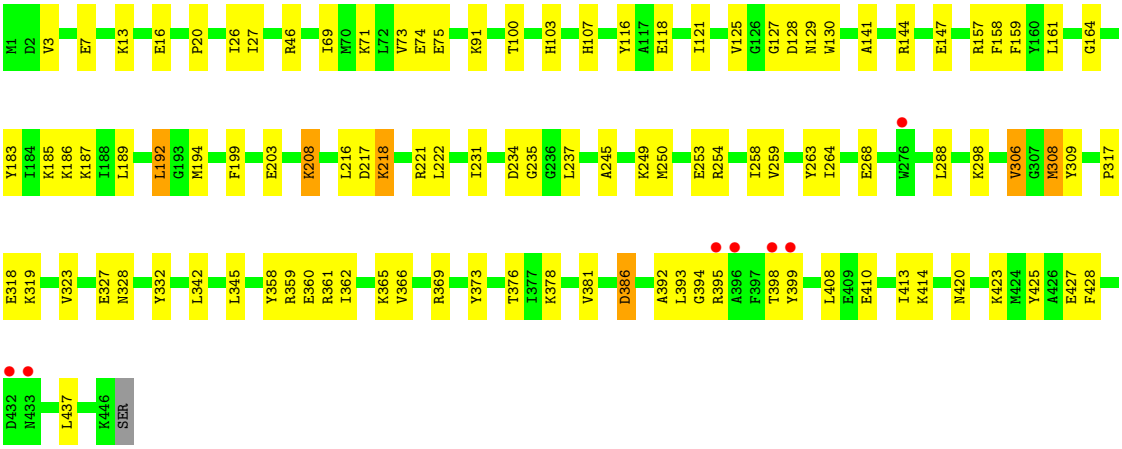
• Molecule 1: Pbp related beta-lactamase

Chain B:



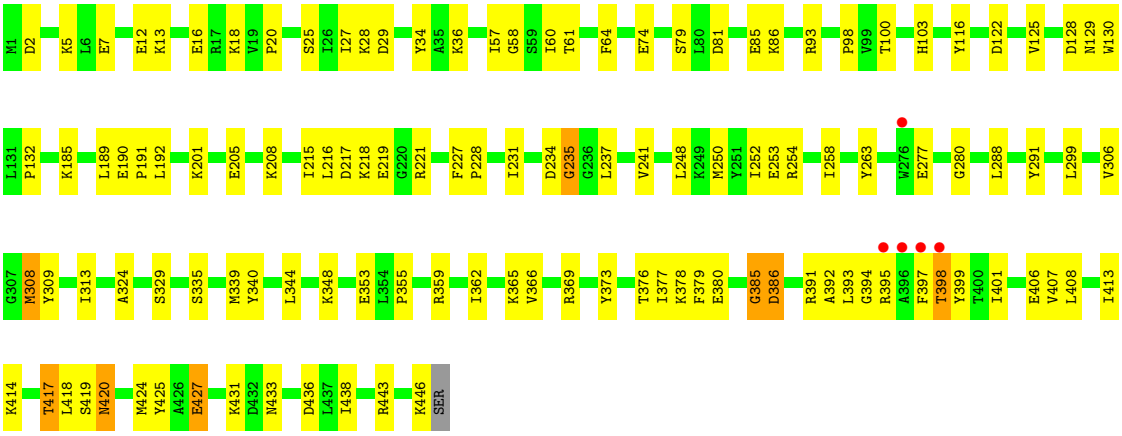
• Molecule 1: Pbp related beta-lactamase

Chain C:



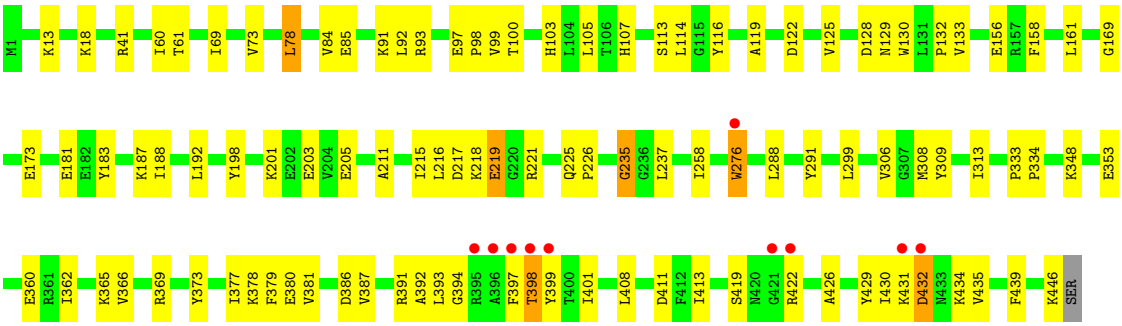
• Molecule 1: Pbp related beta-lactamase

Chain D:



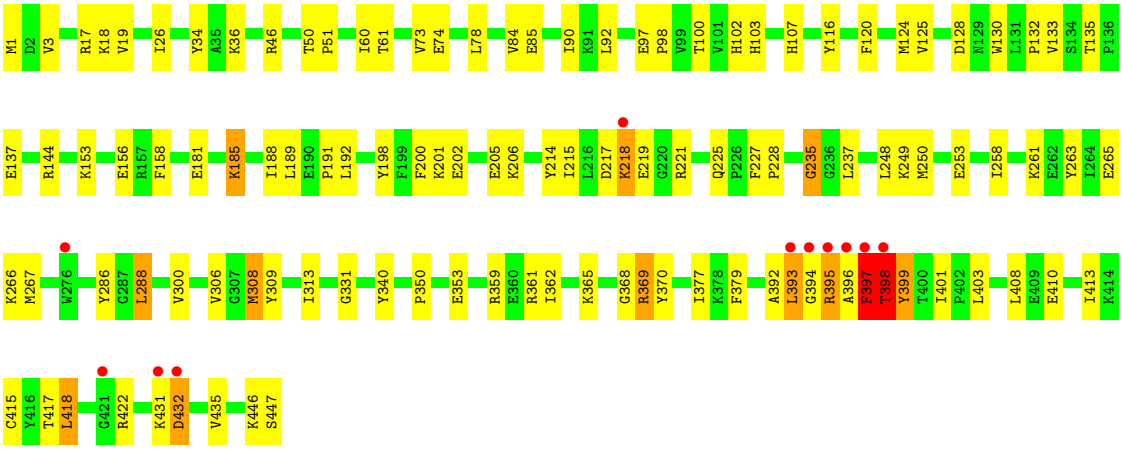
• Molecule 1: Pbp related beta-lactamase

Chain E:



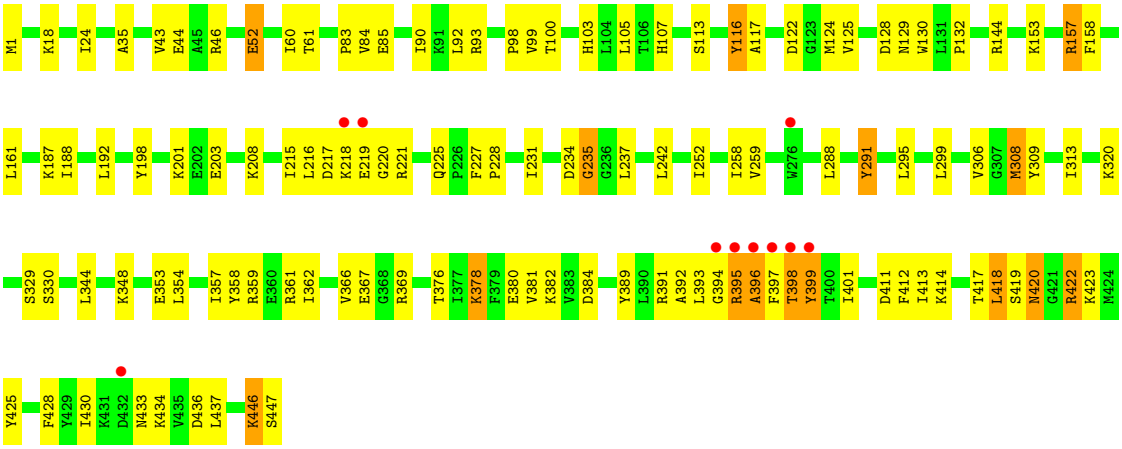
• Molecule 1: Pbp related beta-lactamase

Chain F:



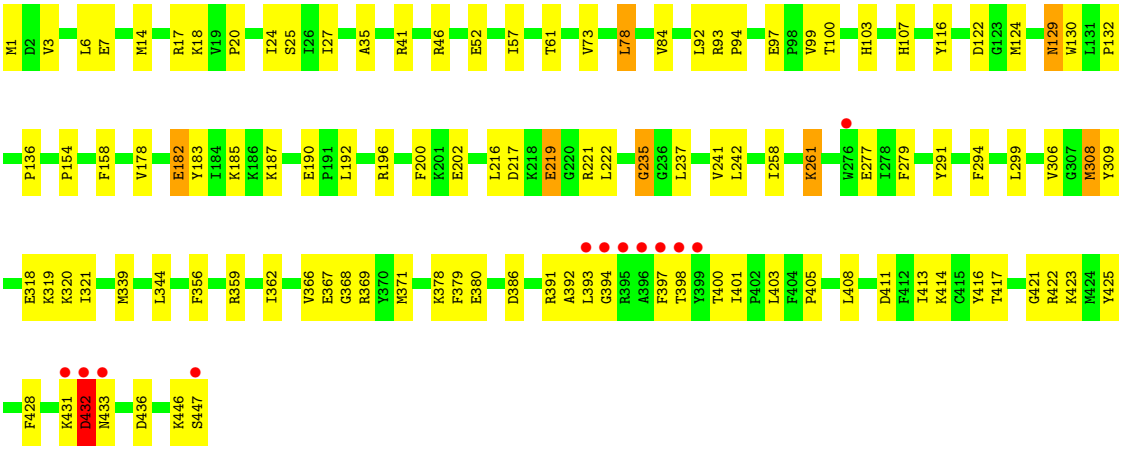
• Molecule 1: Pbp related beta-lactamase

Chain G:



• Molecule 1: Pbp related beta-lactamase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	100.94Å 105.63Å 112.92Å 72.17° 66.51° 81.39°	Depositor
Resolution (Å)	30.00 – 2.20 29.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (30.00-2.20) 96.1 (29.75-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.77 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.241 0.191 , 0.237	Depositor DCC
R_{free} test set	9931 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30882	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: LU, DO3

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	0.38	0/3637	0.61	1/4909 (0.0%)
1	B	0.37	0/3635	0.60	0/4906
1	C	0.37	0/3620	0.60	0/4889
1	D	0.38	0/3631	0.60	0/4902
1	E	0.38	0/3630	0.61	0/4901
1	F	0.38	0/3635	0.62	0/4906
1	G	0.38	0/3645	0.61	0/4917
1	H	0.39	0/3640	0.62	0/4913
All	All	0.38	0/29073	0.61	1/39243 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	LEU	N-CA-C	-5.32	96.63	111.00

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	3551	0	3588	123	0
1	B	3549	0	3586	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3534	0	3566	98	0
1	D	3545	0	3585	119	0
1	E	3544	0	3581	101	0
1	F	3549	0	3586	120	0
1	G	3559	0	3608	133	0
1	H	3554	0	3590	115	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	1	0	0	0	0
3	E	28	0	28	0	0
3	F	28	0	28	1	0
3	G	28	0	28	0	0
3	H	28	0	28	0	0
4	A	285	0	0	11	0
4	B	279	0	0	9	0
4	C	237	0	0	14	0
4	D	259	0	0	12	0
4	E	337	0	0	14	0
4	F	311	0	0	15	0
4	G	351	0	0	21	0
4	H	309	0	0	14	0
All	All	30882	0	28802	884	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 15.

All (884) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ASN:HD22	1:G:434:LYS:HD2	1.03	1.17
1:F:392:ALA:HB3	1:F:398:THR:HG21	1.14	1.12
1:D:369:ARG:HG3	1:D:378:LYS:HE3	1.36	1.08
1:H:431:LYS:HG3	1:H:432:ASP:H	1.22	1.00
1:H:84:VAL:HG21	1:H:92:LEU:HD12	1.44	0.98
1:E:156:GLU:HG2	4:E:599:HOH:O	1.64	0.98
1:D:433:ASN:ND2	1:G:434:LYS:HD2	1.80	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:422:ARG:HG3	1:H:422:ARG:HH11	1.29	0.96
1:D:221:ARG:CZ	1:G:395:ARG:HH21	1.77	0.96
1:F:125:VAL:HG23	1:F:225:GLN:HG3	1.47	0.96
1:C:361:ARG:HH11	1:C:361:ARG:HB3	1.31	0.96
1:H:392:ALA:HB3	1:H:398:THR:HB	1.48	0.95
1:E:125:VAL:HG11	1:E:215:ILE:HD12	1.45	0.95
1:C:100:THR:H	1:C:103:HIS:HD2	1.11	0.95
1:G:18:LYS:HD3	1:G:216:LEU:HD11	1.50	0.93
1:C:20:PRO:HG2	1:C:328:ASN:HB3	1.50	0.92
1:A:50:THR:O	1:A:53:THR:HG22	1.73	0.89
1:F:92:LEU:HG	4:F:688:HOH:O	1.72	0.89
1:F:308:MET:HE2	1:F:309:TYR:HD2	1.38	0.87
1:B:382:LYS:NZ	1:B:382:LYS:HB3	1.88	0.87
1:C:100:THR:H	1:C:103:HIS:CD2	1.93	0.87
1:G:422:ARG:HA	4:G:547:HOH:O	1.75	0.85
1:F:392:ALA:HB3	1:F:398:THR:CG2	2.04	0.85
1:A:291:TYR:HB2	1:A:299:LEU:HB3	1.58	0.85
1:G:418:LEU:HD12	1:G:418:LEU:O	1.76	0.84
1:E:215:ILE:HG23	4:E:547:HOH:O	1.78	0.84
1:H:405:PRO:HB3	1:H:408:LEU:HD21	1.60	0.84
1:H:306:VAL:HG23	1:H:308:MET:CE	2.08	0.84
1:C:369:ARG:HE	1:C:393:LEU:HD21	1.41	0.84
4:A:512:HOH:O	1:E:373:TYR:HB3	1.77	0.83
1:F:100:THR:H	1:F:103:HIS:HD2	1.24	0.83
1:H:306:VAL:HG23	1:H:308:MET:HE1	1.61	0.83
1:A:254:ARG:HH11	1:A:254:ARG:HG2	1.44	0.82
1:B:125:VAL:HG11	1:B:215:ILE:HD12	1.60	0.82
1:E:392:ALA:O	1:E:398:THR:HA	1.78	0.82
1:B:212:MET:HE2	1:B:213:GLY:H	1.42	0.82
1:C:192:LEU:HD23	1:C:194:MET:HE1	1.61	0.82
1:G:308:MET:HE2	1:G:309:TYR:HD2	1.42	0.82
1:B:382:LYS:HB3	1:B:382:LYS:HZ3	1.45	0.81
1:F:377:ILE:HD12	1:F:379:PHE:HE2	1.46	0.80
1:F:392:ALA:CB	1:F:398:THR:HG21	2.05	0.80
1:E:100:THR:H	1:E:103:HIS:HD2	1.29	0.80
1:H:100:THR:H	1:H:103:HIS:HD2	1.27	0.80
1:B:93:ARG:NH1	1:B:98:PRO:HG3	1.97	0.80
1:D:18:LYS:HD3	1:D:216:LEU:HD11	1.64	0.80
1:B:434:LYS:HB3	1:B:434:LYS:NZ	1.96	0.79
1:F:362:ILE:HG22	1:F:413:ILE:HD11	1.62	0.79
1:B:212:MET:HE1	1:B:226:PRO:HA	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:PRO:HD3	1:F:308:MET:HE1	1.62	0.79
1:G:391:ARG:HG3	4:G:723:HOH:O	1.82	0.78
1:F:250:MET:HE3	1:F:258:ILE:HD12	1.64	0.78
1:H:411:ASP:HB3	4:H:747:HOH:O	1.83	0.77
1:G:358:TYR:O	1:G:362:ILE:HG12	1.84	0.77
1:E:84:VAL:HG21	1:E:92:LEU:HD12	1.67	0.77
1:C:185:LYS:HE3	4:C:521:HOH:O	1.83	0.76
1:B:212:MET:CE	1:B:213:GLY:H	1.98	0.76
1:A:100:THR:H	1:A:103:HIS:CD2	2.04	0.76
1:F:100:THR:H	1:F:103:HIS:CD2	2.04	0.76
1:C:361:ARG:HB3	1:C:361:ARG:NH1	2.00	0.76
1:A:130:TRP:CD1	1:A:132:PRO:HD3	2.21	0.76
1:B:434:LYS:HB3	1:B:434:LYS:HZ3	1.49	0.75
1:F:228:PRO:HD3	1:F:308:MET:CE	2.16	0.74
1:A:100:THR:H	1:A:103:HIS:HD2	1.33	0.74
1:F:261:LYS:O	1:F:265:GLU:HG3	1.88	0.74
1:F:266:LYS:HE3	4:F:511:HOH:O	1.86	0.73
1:A:362:ILE:HG22	1:A:413:ILE:HD11	1.71	0.73
1:D:348:LYS:HD2	1:D:353:GLU:OE2	1.88	0.73
1:H:380:GLU:CB	1:H:393:LEU:HD11	2.19	0.73
1:H:196:ARG:HG3	1:H:196:ARG:HH11	1.54	0.73
1:D:377:ILE:HD12	1:D:379:PHE:HE2	1.52	0.72
1:E:100:THR:H	1:E:103:HIS:CD2	2.08	0.72
1:E:125:VAL:HG11	1:E:215:ILE:CD1	2.20	0.72
1:D:378:LYS:HE2	1:D:393:LEU:HD22	1.71	0.72
1:H:394:GLY:HA3	4:H:630:HOH:O	1.88	0.72
1:G:125:VAL:HG21	1:G:215:ILE:HG13	1.70	0.72
1:H:100:THR:H	1:H:103:HIS:CD2	2.07	0.72
1:H:93:ARG:HD3	4:H:570:HOH:O	1.89	0.72
1:B:100:THR:H	1:B:103:HIS:HD2	1.38	0.71
1:D:378:LYS:HG3	1:D:393:LEU:HB2	1.73	0.71
4:C:562:HOH:O	1:G:396:ALA:HB3	1.89	0.71
1:C:369:ARG:HE	1:C:393:LEU:CD2	2.02	0.71
1:E:188:ILE:O	1:E:192:LEU:HD13	1.90	0.71
1:H:306:VAL:CG2	1:H:308:MET:HE1	2.21	0.71
1:E:125:VAL:HG12	1:E:125:VAL:O	1.90	0.71
1:E:380:GLU:HB2	1:E:393:LEU:HD21	1.72	0.71
1:F:125:VAL:HG21	1:F:215:ILE:HG12	1.71	0.71
1:F:308:MET:HE2	1:F:309:TYR:CD2	2.24	0.70
1:G:228:PRO:CD	1:G:308:MET:HE1	2.21	0.70
1:G:369:ARG:O	1:G:447:SER:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:MET:HE2	1:G:309:TYR:CD2	2.25	0.70
1:A:281:GLY:N	4:A:711:HOH:O	2.21	0.70
1:B:306:VAL:HG23	1:B:308:MET:CE	2.22	0.70
1:B:125:VAL:O	1:B:125:VAL:HG12	1.92	0.70
1:B:369:ARG:HG3	1:B:369:ARG:HH11	1.56	0.70
1:D:369:ARG:CG	1:D:378:LYS:HE3	2.19	0.70
4:C:529:HOH:O	1:G:129:ASN:HB2	1.90	0.69
1:A:69:ILE:O	1:A:73:VAL:HG23	1.93	0.69
1:A:306:VAL:HG23	1:A:308:MET:CE	2.22	0.69
1:C:203:GLU:HG2	4:C:510:HOH:O	1.91	0.69
1:D:398:THR:HG22	1:D:398:THR:O	1.92	0.69
1:D:308:MET:HE2	1:D:309:TYR:HD2	1.57	0.69
1:G:100:THR:H	1:G:103:HIS:CD2	2.10	0.69
1:A:367:GLU:O	1:A:446:LYS:HE2	1.93	0.69
1:E:306:VAL:HG13	1:E:308:MET:SD	2.32	0.69
1:F:84:VAL:HG21	1:F:92:LEU:HD12	1.75	0.69
1:G:125:VAL:CG2	1:G:215:ILE:HG13	2.22	0.69
1:H:308:MET:HE2	1:H:308:MET:H	1.58	0.69
1:E:41:ARG:HG2	1:E:211:ALA:HA	1.75	0.69
1:E:362:ILE:HG22	1:E:413:ILE:HD11	1.74	0.68
1:E:397:PHE:O	1:E:398:THR:HB	1.92	0.68
1:G:414:LYS:HE2	1:G:425:TYR:CD2	2.29	0.68
1:G:100:THR:H	1:G:103:HIS:HD2	1.41	0.68
1:C:100:THR:N	1:C:103:HIS:HD2	1.89	0.68
1:G:397:PHE:O	1:G:398:THR:HG23	1.93	0.68
1:G:228:PRO:HD3	1:G:308:MET:HE1	1.75	0.68
1:A:405:PRO:HB3	1:A:408:LEU:HD11	1.76	0.68
1:F:227:PHE:HA	1:F:308:MET:HE3	1.74	0.68
1:H:380:GLU:HB2	1:H:393:LEU:HD11	1.76	0.68
1:C:249:LYS:HE2	1:C:253:GLU:OE1	1.93	0.67
1:H:431:LYS:O	1:H:433:ASN:N	2.27	0.67
1:H:431:LYS:HG3	1:H:432:ASP:N	2.04	0.67
1:D:380:GLU:HB2	1:D:393:LEU:HD11	1.77	0.67
1:D:306:VAL:HG13	1:D:308:MET:HE2	1.76	0.67
1:C:258:ILE:HG22	1:C:259:VAL:HG13	1.77	0.67
1:E:446:LYS:O	4:E:748:HOH:O	2.11	0.67
1:F:368:GLY:HA3	1:F:446:LYS:HE3	1.76	0.66
1:H:192:LEU:CD1	1:H:258:ILE:HD11	2.25	0.66
1:F:84:VAL:HG21	1:F:92:LEU:CD1	2.25	0.66
1:F:250:MET:HE1	1:F:258:ILE:HB	1.77	0.66
1:B:100:THR:H	1:B:103:HIS:CD2	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ARG:NH2	1:G:395:ARG:HH21	1.94	0.66
1:D:408:LEU:HD23	1:D:413:ILE:HG12	1.77	0.66
1:F:85:GLU:HG3	4:F:619:HOH:O	1.95	0.66
1:H:446:LYS:O	1:H:447:SER:HB2	1.95	0.66
1:C:362:ILE:HG22	1:C:413:ILE:HD11	1.77	0.65
1:D:399:TYR:CE2	1:D:401:ILE:HD11	2.30	0.65
1:C:369:ARG:NE	1:C:393:LEU:HD21	2.11	0.65
1:B:369:ARG:NH1	1:B:393:LEU:HD21	2.11	0.65
1:A:8:SER:O	1:A:12:GLU:HG3	1.96	0.65
1:A:378:LYS:HD2	1:A:378:LYS:N	2.11	0.65
1:E:276:TRP:HA	1:E:276:TRP:CE3	2.32	0.65
1:A:358:TYR:O	1:A:362:ILE:HG12	1.97	0.64
1:B:249:LYS:HB2	1:B:249:LYS:NZ	2.13	0.64
4:A:556:HOH:O	1:E:129:ASN:HB2	1.96	0.64
1:H:318:GLU:HG2	4:H:515:HOH:O	1.97	0.64
1:E:125:VAL:CG1	1:E:215:ILE:HD12	2.24	0.64
1:G:201:LYS:HD3	4:H:599:HOH:O	1.97	0.64
1:C:369:ARG:NE	1:C:393:LEU:CD2	2.61	0.64
1:D:433:ASN:HD22	1:G:434:LYS:CD	1.95	0.64
1:G:433:ASN:O	1:G:434:LYS:HG3	1.98	0.64
1:A:308:MET:HE2	1:A:308:MET:H	1.63	0.64
1:B:20:PRO:HG2	1:B:328:ASN:OD1	1.98	0.63
1:G:369:ARG:HB3	1:G:380:GLU:OE2	1.99	0.63
1:A:29:ASP:HA	1:A:320:LYS:HB3	1.80	0.63
1:B:308:MET:HE2	1:B:309:TYR:CD2	2.34	0.63
1:G:157:ARG:HD2	4:G:698:HOH:O	1.97	0.63
1:A:218:LYS:HG3	1:A:219:GLU:OE2	1.98	0.63
1:F:403:LEU:HD23	1:F:417:THR:HB	1.80	0.63
1:F:90:ILE:HG12	4:F:688:HOH:O	2.00	0.62
1:C:361:ARG:HH11	1:C:361:ARG:CB	2.07	0.62
1:F:435:VAL:HB	1:F:446:LYS:HB2	1.81	0.62
1:G:366:VAL:HG12	1:G:381:VAL:HG11	1.82	0.62
1:G:84:VAL:HG21	1:G:92:LEU:HD12	1.82	0.62
1:H:219:GLU:HB3	1:H:221:ARG:CD	2.30	0.62
1:E:378:LYS:HB3	1:E:393:LEU:HD12	1.81	0.62
1:G:228:PRO:HD3	1:G:308:MET:CE	2.28	0.62
1:H:339:MET:HE2	1:H:356:PHE:CZ	2.35	0.62
1:E:201:LYS:O	1:E:205:GLU:HG3	1.99	0.62
1:F:359:ARG:HG2	1:F:408:LEU:HD13	1.81	0.62
1:B:431:LYS:O	1:B:434:LYS:HG2	2.00	0.62
1:E:84:VAL:CG2	1:E:92:LEU:HD12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ARG:HH11	1:B:393:LEU:HD21	1.65	0.61
1:A:396:ALA:HB1	4:E:541:HOH:O	2.00	0.61
1:G:84:VAL:CG2	1:G:92:LEU:HD12	2.31	0.61
1:B:420:ASN:HA	1:H:359:ARG:NH2	2.14	0.61
1:H:306:VAL:O	1:H:308:MET:HE2	2.00	0.61
1:A:28:LYS:HE3	4:A:666:HOH:O	2.00	0.61
1:A:129:ASN:HB2	4:E:689:HOH:O	2.00	0.61
1:C:91:LYS:HG2	1:C:147:GLU:OE1	2.00	0.61
1:D:417:THR:HG22	1:D:424:MET:HB3	1.81	0.61
1:E:61:THR:HB	1:E:235:GLY:HA2	1.81	0.61
1:F:228:PRO:CD	1:F:308:MET:HE1	2.30	0.61
1:E:125:VAL:HG13	1:E:225:GLN:NE2	2.15	0.61
1:B:125:VAL:HG11	1:B:215:ILE:CD1	2.30	0.61
1:C:306:VAL:HG23	1:C:308:MET:CE	2.31	0.61
1:E:276:TRP:HA	1:E:276:TRP:HE3	1.64	0.61
1:H:369:ARG:O	1:H:447:SER:N	2.24	0.61
1:B:261:LYS:O	1:B:265:GLU:HG3	2.01	0.60
1:E:398:THR:HG23	1:E:398:THR:O	2.00	0.60
1:D:100:THR:H	1:D:103:HIS:CD2	2.19	0.60
1:E:434:LYS:HA	4:E:748:HOH:O	1.99	0.60
1:F:403:LEU:HB3	1:F:415:CYS:HB3	1.83	0.60
1:H:84:VAL:HG21	1:H:92:LEU:CD1	2.25	0.60
1:C:394:GLY:O	1:C:398:THR:HB	2.01	0.60
1:G:227:PHE:HA	1:G:308:MET:HE3	1.83	0.60
1:A:254:ARG:HG2	1:A:254:ARG:NH1	2.12	0.60
1:B:212:MET:HE2	1:B:213:GLY:N	2.12	0.60
1:G:362:ILE:HG22	1:G:413:ILE:HD11	1.82	0.60
1:D:125:VAL:HG12	1:D:125:VAL:O	2.01	0.60
1:F:201:LYS:O	1:F:205:GLU:HG2	2.01	0.60
1:A:348:LYS:HD3	1:A:353:GLU:OE1	2.02	0.60
1:D:129:ASN:HB2	4:F:623:HOH:O	2.02	0.60
1:D:378:LYS:HE2	1:D:393:LEU:CD2	2.32	0.60
1:D:386:ASP:OD2	1:F:418:LEU:HD12	2.02	0.60
1:E:397:PHE:O	1:E:398:THR:CB	2.48	0.60
1:A:53:THR:HG23	1:A:55:TYR:CE2	2.37	0.60
1:F:446:LYS:HB3	4:F:475:HOH:O	2.00	0.60
1:H:130:TRP:CD1	1:H:132:PRO:HD3	2.37	0.60
1:H:219:GLU:CB	1:H:221:ARG:HH11	2.15	0.60
1:H:392:ALA:HB3	1:H:398:THR:CB	2.26	0.60
1:H:403:LEU:HD23	1:H:417:THR:HB	1.82	0.59
1:C:141:ALA:HB1	4:D:535:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:VAL:HG22	1:D:306:VAL:O	2.02	0.59
1:F:215:ILE:CD1	1:F:308:MET:HB3	2.32	0.59
1:D:420:ASN:HA	1:F:359:ARG:NH2	2.17	0.59
1:F:408:LEU:HD23	1:F:413:ILE:HG12	1.84	0.59
1:G:18:LYS:HD3	1:G:216:LEU:CD1	2.29	0.59
1:A:179:SER:OG	1:A:182:GLU:HG2	2.03	0.59
1:B:3:VAL:HG23	1:B:4:GLY:N	2.17	0.59
1:G:380:GLU:CG	1:G:393:LEU:HD11	2.32	0.59
1:H:18:LYS:HD3	1:H:216:LEU:HD11	1.85	0.59
1:H:339:MET:HE2	1:H:356:PHE:HZ	1.66	0.59
1:A:355:PRO:HA	1:A:358:TYR:CE1	2.37	0.59
1:G:153:LYS:HD3	4:G:481:HOH:O	2.02	0.59
1:E:69:ILE:O	1:E:73:VAL:HG23	2.02	0.59
1:H:422:ARG:HG3	1:H:422:ARG:NH1	2.08	0.59
1:B:212:MET:HA	1:B:212:MET:HE3	1.85	0.58
1:C:74:GLU:HB2	1:C:263:TYR:CE2	2.38	0.58
1:C:373:TYR:O	1:C:376:THR:HG23	2.03	0.58
1:D:100:THR:H	1:D:103:HIS:HD2	1.49	0.58
1:E:183:TYR:CE1	1:E:187:LYS:HG3	2.38	0.58
1:E:369:ARG:HG2	1:E:369:ARG:HH11	1.68	0.58
1:F:398:THR:HG23	1:F:399:TYR:N	2.18	0.58
1:B:355:PRO:HB2	4:B:687:HOH:O	2.02	0.58
1:H:27:ILE:HD12	1:H:27:ILE:N	2.17	0.58
1:A:398:THR:HG22	1:E:218:LYS:NZ	2.18	0.58
1:H:416:TYR:HB2	1:H:423:LYS:HB2	1.86	0.58
1:A:306:VAL:O	1:A:308:MET:HE2	2.03	0.58
1:A:183:TYR:CZ	1:A:187:LYS:HG3	2.39	0.58
1:D:221:ARG:CZ	1:G:395:ARG:NH2	2.58	0.58
1:A:405:PRO:CB	1:A:408:LEU:HD11	2.33	0.58
1:A:391:ARG:HG3	1:A:400:THR:OG1	2.03	0.57
1:C:187:LYS:O	1:C:258:ILE:HD12	2.03	0.57
1:C:192:LEU:CD2	1:C:194:MET:HE1	2.32	0.57
1:D:93:ARG:NH1	1:D:98:PRO:HB3	2.18	0.57
1:F:153:LYS:O	1:F:156:GLU:HG2	2.04	0.57
1:E:369:ARG:HE	1:E:393:LEU:CD1	2.18	0.57
1:F:393:LEU:HG	1:F:394:GLY:H	1.70	0.57
1:G:366:VAL:HG13	1:G:428:PHE:CE1	2.38	0.57
1:B:212:MET:HE1	1:B:226:PRO:CA	2.34	0.57
1:D:221:ARG:HG3	4:D:542:HOH:O	2.04	0.57
1:D:378:LYS:CE	1:D:393:LEU:HD22	2.34	0.57
1:F:198:TYR:O	1:F:237:LEU:HD12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:LEU:HD13	1:F:422:ARG:O	2.04	0.57
1:H:97:GLU:HB3	1:H:154:PRO:HD2	1.85	0.57
1:C:129:ASN:ND2	1:G:376:THR:O	2.37	0.57
1:B:27:ILE:HD11	1:B:245:ALA:HA	1.87	0.57
1:G:418:LEU:HA	1:G:422:ARG:O	2.04	0.57
1:H:46:ARG:HD2	4:H:603:HOH:O	2.04	0.57
1:C:128:ASP:OD2	1:G:395:ARG:HG3	2.05	0.57
1:F:369:ARG:HG2	1:F:369:ARG:HH11	1.69	0.57
1:D:85:GLU:HG3	4:D:618:HOH:O	2.04	0.57
1:F:369:ARG:O	1:F:447:SER:N	2.37	0.57
1:A:398:THR:HG23	1:A:398:THR:O	2.05	0.57
1:E:183:TYR:CZ	1:E:187:LYS:HG3	2.40	0.57
1:E:369:ARG:HG2	1:E:369:ARG:NH1	2.20	0.57
1:G:157:ARG:HG3	1:G:158:PHE:N	2.20	0.57
1:G:219:GLU:HB2	1:G:221:ARG:HD3	1.87	0.57
1:H:308:MET:CE	1:H:308:MET:H	2.16	0.57
4:C:499:HOH:O	1:G:397:PHE:HZ	1.87	0.56
1:F:446:LYS:HD3	1:F:447:SER:N	2.19	0.56
1:H:362:ILE:HG22	1:H:413:ILE:HD11	1.85	0.56
1:H:391:ARG:HG3	1:H:400:THR:OG1	2.04	0.56
1:B:308:MET:HE2	1:B:309:TYR:HD2	1.69	0.56
1:D:433:ASN:HB2	4:G:621:HOH:O	2.04	0.56
1:G:208:LYS:NZ	1:G:208:LYS:HB2	2.20	0.56
1:A:188:ILE:O	1:A:192:LEU:HB2	2.05	0.56
1:B:180:TYR:O	1:B:184:ILE:HG12	2.05	0.56
1:G:417:THR:O	1:G:418:LEU:C	2.43	0.56
1:D:308:MET:CE	1:D:309:TYR:HD2	2.18	0.56
1:C:264:ILE:O	1:C:268:GLU:HG3	2.06	0.56
1:G:130:TRP:CD1	1:G:132:PRO:HD3	2.41	0.56
1:H:433:ASN:HB2	4:H:531:HOH:O	2.05	0.56
1:C:358:TYR:HB2	1:C:361:ARG:HH12	1.70	0.56
1:G:60:ILE:HD13	1:G:313:ILE:HG23	1.87	0.56
1:D:253:GLU:O	1:D:254:ARG:HB2	2.05	0.56
1:H:219:GLU:HB3	1:H:221:ARG:HD2	1.87	0.56
1:A:414:LYS:HE2	1:A:425:TYR:CD2	2.40	0.56
1:E:306:VAL:HG12	1:E:309:TYR:HB2	1.87	0.56
1:C:366:VAL:HG12	1:C:381:VAL:HG11	1.88	0.55
1:E:60:ILE:HD13	1:E:313:ILE:HG23	1.86	0.55
1:D:190:GLU:HB2	1:D:191:PRO:HD3	1.89	0.55
1:F:377:ILE:HD12	1:F:379:PHE:CE2	2.35	0.55
1:G:417:THR:O	1:G:418:LEU:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HD3	4:B:617:HOH:O	2.05	0.55
1:G:392:ALA:HB2	1:G:399:TYR:CE1	2.40	0.55
1:D:433:ASN:ND2	4:G:621:HOH:O	2.39	0.55
1:A:135:THR:HG21	4:A:661:HOH:O	2.06	0.55
1:A:370:TYR:CZ	1:A:446:LYS:HE3	2.42	0.55
1:D:201:LYS:O	1:D:205:GLU:HG3	2.07	0.55
1:A:366:VAL:HG12	1:A:381:VAL:HG11	1.88	0.54
1:B:273:LYS:HE3	4:B:713:HOH:O	2.06	0.54
1:D:362:ILE:HG22	1:D:413:ILE:HD11	1.88	0.54
1:A:53:THR:HG23	1:A:55:TYR:HE2	1.72	0.54
1:C:420:ASN:HA	1:G:359:ARG:NH2	2.22	0.54
1:D:228:PRO:CD	1:D:308:MET:HE1	2.37	0.54
4:D:523:HOH:O	1:F:217:ASP:HB2	2.07	0.54
1:F:306:VAL:HG13	1:F:308:MET:HE2	1.89	0.54
1:G:401:ILE:HG21	1:G:417:THR:HG21	1.89	0.54
1:C:359:ARG:NH1	4:C:524:HOH:O	2.40	0.54
1:D:359:ARG:HH11	1:D:359:ARG:HG2	1.71	0.54
1:A:398:THR:HG22	1:E:218:LYS:HZ1	1.72	0.54
1:B:422:ARG:HD2	1:H:277:GLU:O	2.06	0.54
1:F:361:ARG:NH2	1:F:410:GLU:OE2	2.33	0.54
1:B:226:PRO:HG2	1:C:46:ARG:NH2	2.22	0.54
1:D:128:ASP:OD1	1:F:395:ARG:HB2	2.08	0.54
1:F:306:VAL:HG22	1:F:306:VAL:O	2.08	0.54
1:G:1:MET:HE3	1:G:344:LEU:HB2	1.89	0.54
1:H:41:ARG:HD2	4:H:558:HOH:O	2.08	0.54
1:H:219:GLU:HB2	1:H:221:ARG:HH11	1.73	0.54
1:H:359:ARG:HG2	1:H:408:LEU:HD12	1.88	0.54
1:B:369:ARG:HD2	1:B:371:MET:CE	2.38	0.54
1:D:218:LYS:HG3	1:D:219:GLU:OE2	2.08	0.54
1:H:422:ARG:HH11	1:H:422:ARG:CG	2.07	0.54
1:C:107:HIS:HB2	1:C:158:PHE:CE1	2.43	0.53
1:A:419:SER:O	1:A:421:GLY:N	2.41	0.53
1:C:130:TRP:HZ2	1:D:20:PRO:HA	1.73	0.53
1:F:60:ILE:HD13	1:F:313:ILE:HG23	1.90	0.53
1:F:447:SER:HB2	4:F:565:HOH:O	2.08	0.53
1:A:60:ILE:HD13	1:A:313:ILE:HG23	1.90	0.53
1:D:431:LYS:HE3	4:D:514:HOH:O	2.09	0.53
1:G:1:MET:CE	1:G:344:LEU:HB2	2.38	0.53
1:G:153:LYS:HE2	4:G:533:HOH:O	2.08	0.53
1:H:308:MET:HE3	1:H:309:TYR:N	2.23	0.53
1:A:135:THR:HG22	1:A:138:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:HB3	1:A:129:ASN:OD1	2.08	0.53
1:B:373:TYR:O	1:B:376:THR:HG23	2.08	0.53
1:G:380:GLU:HB2	1:G:393:LEU:HD11	1.89	0.53
1:B:397:PHE:O	1:B:398:THR:HB	2.06	0.53
1:G:306:VAL:HG13	1:G:308:MET:HE2	1.90	0.53
1:H:359:ARG:HG2	1:H:408:LEU:CD1	2.38	0.53
1:F:219:GLU:CD	1:F:221:ARG:HH21	2.11	0.53
1:C:192:LEU:HD11	1:C:250:MET:HE3	1.90	0.53
1:F:19:VAL:HG22	1:F:331:GLY:HA3	1.90	0.53
1:B:306:VAL:O	1:B:308:MET:HE1	2.09	0.53
1:H:202:GLU:H	1:H:202:GLU:CD	2.12	0.53
1:D:228:PRO:HD2	1:D:308:MET:HE1	1.91	0.53
1:G:144:ARG:NE	4:G:587:HOH:O	2.40	0.53
1:H:366:VAL:HG13	1:H:428:PHE:CE1	2.44	0.53
1:B:308:MET:HE1	1:B:308:MET:H	1.74	0.52
1:C:308:MET:HE3	1:C:309:TYR:HD2	1.75	0.52
1:F:370:TYR:CZ	1:F:446:LYS:HG2	2.44	0.52
1:G:18:LYS:HE2	1:G:220:GLY:O	2.09	0.52
1:B:130:TRP:CD1	1:B:132:PRO:HD3	2.44	0.52
1:H:219:GLU:HB3	1:H:221:ARG:HD3	1.90	0.52
1:A:183:TYR:CE1	1:A:187:LYS:HG3	2.43	0.52
1:C:386:ASP:OD1	1:G:418:LEU:HD12	2.09	0.52
1:D:379:PHE:CE1	1:D:392:ALA:HB2	2.45	0.52
1:G:208:LYS:HB2	1:G:208:LYS:HZ3	1.75	0.52
1:G:422:ARG:HG2	1:G:422:ARG:HH11	1.74	0.52
1:A:198:TYR:O	1:A:237:LEU:HD12	2.09	0.52
1:B:423:LYS:HD3	1:B:425:TYR:OH	2.09	0.52
1:D:419:SER:CB	1:D:424:MET:HB2	2.40	0.52
1:E:192:LEU:CD1	1:E:258:ILE:HD11	2.39	0.52
1:D:217:ASP:OD1	1:D:219:GLU:N	2.40	0.52
1:G:107:HIS:HB2	1:G:158:PHE:CE1	2.45	0.52
1:G:125:VAL:HG23	1:G:225:GLN:HG3	1.92	0.52
1:H:124:MET:HE1	4:H:583:HOH:O	2.08	0.52
1:D:369:ARG:O	1:D:446:LYS:HA	2.10	0.52
1:B:125:VAL:O	1:B:125:VAL:CG1	2.56	0.52
1:G:187:LYS:O	1:G:258:ILE:HD12	2.08	0.52
1:B:3:VAL:HG23	1:B:4:GLY:H	1.74	0.52
1:C:217:ASP:OD1	1:C:221:ARG:HG2	2.10	0.52
1:E:369:ARG:HE	1:E:393:LEU:HD12	1.75	0.52
1:F:250:MET:CE	1:F:258:ILE:HD12	2.38	0.52
1:G:52:GLU:HG3	1:G:242:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:PRO:HG3	1:E:387:VAL:HG21	1.92	0.52
1:F:397:PHE:O	1:F:398:THR:HG22	2.10	0.52
1:H:178:VAL:HB	1:H:182:GLU:HG2	1.92	0.51
1:B:394:GLY:O	1:B:397:PHE:O	2.28	0.51
1:C:221:ARG:HB3	1:C:221:ARG:CZ	2.41	0.51
1:E:426:ALA:HB2	1:E:439:PHE:HD1	1.75	0.51
1:H:57:ILE:HG12	1:H:237:LEU:O	2.11	0.51
1:A:112:PRO:HG2	1:A:149:TRP:CD1	2.46	0.51
1:B:133:VAL:HG23	1:B:133:VAL:O	2.10	0.51
1:B:216:LEU:HD13	1:B:222:LEU:HD23	1.91	0.51
1:B:398:THR:O	1:B:398:THR:HG23	2.10	0.51
1:D:122:ASP:HB3	1:D:129:ASN:OD1	2.10	0.51
1:A:335:SER:O	1:A:339:MET:HG3	2.10	0.51
1:A:217:ASP:OD2	1:A:221:ARG:HB2	2.10	0.51
1:A:366:VAL:CG1	1:A:381:VAL:HG11	2.40	0.51
1:C:392:ALA:HB2	1:C:399:TYR:CE1	2.45	0.51
1:D:231:ILE:HG13	1:D:234:ASP:OD1	2.10	0.51
1:H:261:LYS:HE3	4:H:536:HOH:O	2.10	0.51
1:H:308:MET:HE2	1:H:308:MET:N	2.24	0.51
1:G:348:LYS:HD2	1:G:353:GLU:OE2	2.09	0.51
1:E:391:ARG:HG3	1:E:399:TYR:O	2.11	0.51
1:A:115:GLY:N	4:A:512:HOH:O	2.25	0.51
1:B:215:ILE:HA	4:B:578:HOH:O	2.09	0.51
1:B:277:GLU:HA	1:B:282:GLU:CG	2.41	0.51
1:D:308:MET:HE2	1:D:309:TYR:CD2	2.44	0.51
1:H:200:PHE:HB3	1:H:202:GLU:OE1	2.11	0.51
1:A:277:GLU:HG3	1:A:280:GLY:O	2.10	0.51
1:G:428:PHE:CE1	1:G:437:LEU:HD13	2.45	0.51
1:H:192:LEU:HD11	1:H:258:ILE:HD11	1.92	0.51
1:D:12:GLU:O	1:D:16:GLU:HB2	2.11	0.51
1:F:144:ARG:HD2	4:F:754:HOH:O	2.10	0.51
1:G:306:VAL:HG13	1:G:308:MET:CE	2.41	0.51
1:A:275:PRO:O	1:A:277:GLU:N	2.44	0.50
1:D:60:ILE:HD13	1:D:313:ILE:HG23	1.93	0.50
1:E:85:GLU:HG3	4:E:612:HOH:O	2.10	0.50
1:E:394:GLY:O	1:E:397:PHE:O	2.29	0.50
1:F:369:ARG:HG2	1:F:369:ARG:NH1	2.26	0.50
1:G:61:THR:HB	1:G:235:GLY:HA2	1.92	0.50
1:A:3:VAL:O	1:A:7:GLU:HG3	2.11	0.50
1:A:370:TYR:HB3	1:A:444:LEU:HB3	1.94	0.50
1:C:208:LYS:HB2	4:C:643:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:ARG:HD2	4:F:677:HOH:O	2.11	0.50
1:A:362:ILE:HD11	1:A:410:GLU:OE2	2.11	0.50
1:B:420:ASN:HA	1:H:359:ARG:HH21	1.75	0.50
1:C:144:ARG:HD3	4:C:498:HOH:O	2.11	0.50
1:F:73:VAL:HG11	4:F:700:HOH:O	2.10	0.50
1:C:414:LYS:HD2	1:C:425:TYR:CD2	2.47	0.50
1:E:432:ASP:N	4:E:699:HOH:O	2.44	0.50
1:F:84:VAL:CG2	1:F:92:LEU:HD12	2.40	0.50
1:F:188:ILE:HA	1:F:258:ILE:HD13	1.92	0.50
1:H:291:TYR:HB2	1:H:299:LEU:HB3	1.94	0.50
1:B:354:LEU:HD12	1:B:357:ILE:HD12	1.93	0.50
1:G:198:TYR:O	1:G:237:LEU:HD12	2.11	0.50
1:H:306:VAL:C	1:H:308:MET:HE2	2.32	0.50
1:B:264:ILE:O	1:B:268:GLU:HG3	2.11	0.50
1:B:277:GLU:O	1:H:422:ARG:NH2	2.44	0.50
1:D:306:VAL:HG22	1:D:308:MET:HE1	1.92	0.50
1:D:306:VAL:CG1	1:D:308:MET:HE2	2.41	0.50
1:F:446:LYS:O	1:F:447:SER:HB2	2.12	0.50
1:H:61:THR:HB	1:H:235:GLY:HA2	1.94	0.50
1:H:414:LYS:HZ3	1:H:414:LYS:HB3	1.76	0.50
1:D:74:GLU:HB2	1:D:263:TYR:CE2	2.47	0.50
1:D:227:PHE:HA	1:D:308:MET:HE3	1.94	0.50
1:C:395:ARG:HG3	1:G:128:ASP:OD1	2.11	0.50
1:H:371:MET:SD	1:H:378:LYS:HG2	2.52	0.50
1:D:27:ILE:N	1:D:27:ILE:HD12	2.27	0.49
1:D:414:LYS:HE2	1:D:425:TYR:CD2	2.47	0.49
1:F:61:THR:HB	1:F:235:GLY:HA2	1.94	0.49
1:F:125:VAL:O	1:F:125:VAL:HG22	2.12	0.49
1:H:320:LYS:HE3	4:H:673:HOH:O	2.12	0.49
1:B:4:GLY:HA2	4:B:514:HOH:O	2.10	0.49
1:D:34:TYR:OH	1:D:36:LYS:HD2	2.12	0.49
1:G:231:ILE:HG13	1:G:234:ASP:OD1	2.11	0.49
1:G:411:ASP:HA	1:G:430:ILE:HB	1.94	0.49
1:G:384:ASP:HB3	1:G:389:TYR:HE1	1.78	0.49
1:F:74:GLU:HB2	1:F:263:TYR:CE2	2.48	0.49
1:F:200:PHE:HB3	1:F:202:GLU:OE1	2.11	0.49
1:G:396:ALA:HB3	4:G:688:HOH:O	2.11	0.49
1:A:371:MET:CE	1:A:378:LYS:HG3	2.43	0.49
1:B:125:VAL:CG1	1:B:215:ILE:HD12	2.37	0.49
1:C:71:LYS:O	1:C:75:GLU:HG3	2.12	0.49
1:G:401:ILE:CG2	1:G:417:THR:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:VAL:HG11	1:D:215:ILE:HD12	1.93	0.49
1:D:353:GLU:O	1:D:355:PRO:HD3	2.13	0.49
1:E:133:VAL:O	1:E:133:VAL:HG23	2.12	0.49
1:G:217:ASP:C	1:G:217:ASP:OD1	2.50	0.49
1:H:294:PHE:HE1	1:H:339:MET:HE3	1.78	0.49
1:G:446:LYS:HB2	1:G:446:LYS:NZ	2.28	0.49
1:H:196:ARG:HH11	1:H:196:ARG:CG	2.23	0.49
1:G:380:GLU:CB	1:G:393:LEU:HD11	2.43	0.49
1:H:414:LYS:HE2	1:H:425:TYR:HE2	1.78	0.49
1:D:125:VAL:O	1:D:125:VAL:CG1	2.61	0.48
1:D:248:LEU:O	1:D:252:ILE:HG13	2.12	0.48
1:H:78:LEU:N	1:H:78:LEU:HD12	2.27	0.48
1:E:366:VAL:CG1	1:E:381:VAL:HG11	2.44	0.48
1:G:306:VAL:O	1:G:306:VAL:HG22	2.13	0.48
1:B:192:LEU:HD13	1:B:258:ILE:HD11	1.95	0.48
1:C:428:PHE:CE1	1:C:437:LEU:HD13	2.49	0.48
1:D:420:ASN:N	1:D:420:ASN:OD1	2.45	0.48
1:F:218:LYS:HD3	1:F:219:GLU:HG3	1.95	0.48
1:G:417:THR:O	1:G:417:THR:HG23	2.14	0.48
1:H:422:ARG:NH1	1:H:422:ARG:CG	2.71	0.48
1:A:192:LEU:HD13	1:A:258:ILE:HD11	1.95	0.48
1:A:373:TYR:CG	1:E:114:LEU:HD22	2.48	0.48
1:D:391:ARG:HH11	1:D:398:THR:CG2	2.27	0.48
1:E:198:TYR:O	1:E:237:LEU:HD12	2.13	0.48
1:G:394:GLY:C	1:G:396:ALA:N	2.65	0.48
1:H:97:GLU:HG2	4:H:633:HOH:O	2.12	0.48
1:G:394:GLY:C	1:G:396:ALA:H	2.17	0.48
1:B:2:ASP:OD2	1:B:5:LYS:HB2	2.13	0.48
1:B:276:TRP:O	1:B:282:GLU:HG3	2.14	0.48
1:B:434:LYS:NZ	1:B:434:LYS:CB	2.73	0.48
1:C:3:VAL:O	1:C:7:GLU:HG3	2.13	0.48
1:C:423:LYS:O	1:C:423:LYS:HG3	2.14	0.48
1:E:93:ARG:NH1	1:E:98:PRO:HB3	2.27	0.48
1:G:308:MET:CE	1:G:309:TYR:CD2	2.96	0.48
1:H:136:PRO:HG3	4:H:720:HOH:O	2.13	0.48
1:A:308:MET:CE	1:A:308:MET:H	2.27	0.48
1:E:203:GLU:OE1	4:E:518:HOH:O	2.20	0.48
1:G:83:PRO:HB3	1:G:98:PRO:HB2	1.96	0.48
1:H:414:LYS:HB3	1:H:414:LYS:NZ	2.29	0.48
1:G:367:GLU:OE2	1:G:382:LYS:HE2	2.14	0.48
1:A:295:LEU:HD12	1:A:295:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:MET:CE	1:B:308:MET:H	2.27	0.47
1:A:100:THR:N	1:A:103:HIS:HD2	2.09	0.47
1:A:276:TRP:HA	1:A:276:TRP:CE3	2.48	0.47
1:A:418:LEU:HD12	1:E:386:ASP:CB	2.43	0.47
1:G:113:SER:HA	1:G:161:LEU:HD12	1.97	0.47
1:A:135:THR:HG22	1:A:138:GLU:CG	2.44	0.47
1:D:407:VAL:HB	1:D:414:LYS:HB3	1.96	0.47
1:F:399:TYR:N	1:F:399:TYR:CD1	2.78	0.47
1:G:219:GLU:OE1	1:G:221:ARG:NH1	2.47	0.47
1:A:201:LYS:HG2	4:A:610:HOH:O	2.14	0.47
1:H:1:MET:HE3	1:H:344:LEU:HB2	1.96	0.47
1:H:25:SER:HB3	1:H:241:VAL:HB	1.97	0.47
1:C:362:ILE:HG13	1:C:408:LEU:HD21	1.96	0.47
1:D:420:ASN:HB3	4:D:594:HOH:O	2.14	0.47
1:E:18:LYS:HD3	1:E:216:LEU:HD11	1.97	0.47
1:E:107:HIS:HB2	1:E:158:PHE:CE1	2.50	0.47
1:F:432:ASP:N	4:F:762:HOH:O	2.47	0.47
1:A:107:HIS:HB2	1:A:158:PHE:CE1	2.49	0.47
1:A:354:LEU:HD12	1:A:357:ILE:HD12	1.97	0.47
1:B:125:VAL:HG13	1:B:225:GLN:CD	2.35	0.47
1:D:335:SER:O	1:D:339:MET:HG3	2.15	0.47
1:F:135:THR:HG22	1:F:137:GLU:N	2.30	0.47
1:F:446:LYS:O	4:F:475:HOH:O	2.20	0.47
1:G:122:ASP:O	1:G:125:VAL:HG12	2.14	0.47
1:G:228:PRO:HD2	1:G:308:MET:HE1	1.95	0.47
1:H:52:GLU:HG2	1:H:242:LEU:HD12	1.96	0.47
1:F:435:VAL:HB	1:F:446:LYS:CB	2.45	0.47
1:B:16:GLU:OE1	1:B:364:LYS:NZ	2.47	0.47
1:B:206:LYS:HB2	4:B:505:HOH:O	2.14	0.47
1:C:378:LYS:HE3	4:C:543:HOH:O	2.15	0.47
1:F:130:TRP:CD1	1:F:132:PRO:HD3	2.50	0.47
1:B:308:MET:CE	1:B:309:TYR:HD2	2.27	0.47
1:C:250:MET:HE2	1:C:258:ILE:CG1	2.44	0.47
1:C:308:MET:CE	1:C:309:TYR:HD2	2.28	0.47
1:G:85:GLU:HG2	1:G:90:ILE:O	2.15	0.47
1:G:295:LEU:N	1:G:295:LEU:HD12	2.30	0.47
1:G:430:ILE:N	1:G:430:ILE:HD12	2.30	0.47
1:H:122:ASP:OD2	1:H:129:ASN:OD1	2.33	0.47
1:D:61:THR:O	1:D:64:PHE:HB2	2.15	0.46
1:D:291:TYR:HB2	1:D:299:LEU:HB3	1.96	0.46
1:E:401:ILE:HD13	1:E:439:PHE:HZ	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:THR:HG22	1:F:137:GLU:H	1.79	0.46
1:H:107:HIS:HB2	1:H:158:PHE:CE1	2.50	0.46
1:A:5:LYS:HE2	4:A:646:HOH:O	2.13	0.46
1:C:130:TRP:CD1	1:D:18:LYS:HA	2.50	0.46
1:D:185:LYS:HA	1:D:189:LEU:HD12	1.97	0.46
1:D:306:VAL:CG2	1:D:308:MET:HE1	2.45	0.46
1:D:378:LYS:CG	1:D:393:LEU:HD22	2.45	0.46
1:E:217:ASP:OD2	1:E:221:ARG:HB2	2.14	0.46
1:H:18:LYS:O	1:H:222:LEU:HD21	2.15	0.46
1:A:41:ARG:HB2	1:A:211:ALA:HB2	1.97	0.46
1:B:356:PHE:N	4:B:687:HOH:O	2.49	0.46
1:E:169:GLY:O	1:E:173:GLU:HG3	2.16	0.46
1:E:217:ASP:OD1	1:E:219:GLU:N	2.47	0.46
1:E:377:ILE:HD12	1:E:379:PHE:HE2	1.80	0.46
1:F:218:LYS:CD	1:F:219:GLU:HG3	2.44	0.46
1:H:380:GLU:HB3	1:H:393:LEU:HD11	1.93	0.46
1:A:403:LEU:HD23	1:A:417:THR:HB	1.97	0.46
1:D:125:VAL:HG11	1:D:215:ILE:CD1	2.45	0.46
1:F:359:ARG:HH11	1:F:359:ARG:HB3	1.79	0.46
1:H:431:LYS:HD2	4:H:675:HOH:O	2.14	0.46
1:C:71:LYS:HE2	4:C:614:HOH:O	2.14	0.46
1:E:125:VAL:O	1:E:125:VAL:CG1	2.60	0.46
1:G:124:MET:HE1	4:G:597:HOH:O	2.15	0.46
1:D:25:SER:OG	1:D:324:ALA:HB3	2.16	0.46
1:F:401:ILE:HG23	1:F:417:THR:OG1	2.14	0.46
1:A:277:GLU:CG	1:A:280:GLY:O	2.64	0.46
1:B:437:LEU:HD12	1:B:438:ILE:N	2.31	0.46
1:C:129:ASN:ND2	1:G:378:LYS:NZ	2.64	0.46
1:E:84:VAL:HG13	1:E:99:VAL:O	2.15	0.46
1:G:258:ILE:HB	4:G:573:HOH:O	2.15	0.46
1:A:277:GLU:O	1:E:422:ARG:HG3	2.15	0.46
1:B:361:ARG:NH2	1:B:410:GLU:OE2	2.47	0.46
1:D:419:SER:HB3	1:D:424:MET:HB2	1.97	0.46
1:H:414:LYS:HE2	1:H:425:TYR:CE2	2.50	0.46
1:D:86:LYS:HE3	1:D:86:LYS:HB2	1.76	0.46
1:D:130:TRP:CD1	1:D:132:PRO:HD3	2.51	0.46
1:E:426:ALA:HB2	1:E:439:PHE:CD1	2.51	0.46
1:F:308:MET:CE	1:F:309:TYR:HD2	2.18	0.46
1:G:203:GLU:OE1	4:G:504:HOH:O	2.21	0.46
1:B:30:GLY:O	1:B:249:LYS:HE3	2.16	0.46
1:B:313:ILE:HG13	1:B:313:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:VAL:HG13	1:C:428:PHE:CE1	2.50	0.46
1:E:84:VAL:HG21	1:E:92:LEU:CD1	2.43	0.46
1:E:113:SER:HA	1:E:161:LEU:HD12	1.97	0.46
1:F:248:LEU:HD21	1:F:313:ILE:HB	1.98	0.46
1:F:267:MET:HA	1:F:286:TYR:HB2	1.98	0.46
1:G:412:PHE:C	1:G:413:ILE:HG13	2.36	0.46
1:H:1:MET:CE	1:H:6:LEU:HD22	2.46	0.45
1:B:52:GLU:HB3	1:B:196:ARG:NH1	2.31	0.45
1:E:348:LYS:HB3	1:E:353:GLU:OE2	2.17	0.45
1:G:329:SER:OG	1:G:330:SER:N	2.49	0.45
1:G:361:ARG:NH1	1:G:362:ILE:HD13	2.32	0.45
1:H:279:PHE:CZ	1:H:339:MET:CE	3.00	0.45
1:F:50:THR:HB	1:F:51:PRO:CD	2.47	0.45
1:F:201:LYS:HD3	4:G:690:HOH:O	2.16	0.45
1:F:306:VAL:HG13	1:F:308:MET:CE	2.46	0.45
1:B:10:ILE:O	1:B:14:MET:HG3	2.17	0.45
1:B:185:LYS:HD2	4:B:629:HOH:O	2.16	0.45
1:F:107:HIS:HB2	1:F:158:PHE:CE1	2.51	0.45
1:G:208:LYS:HA	4:G:485:HOH:O	2.15	0.45
1:G:419:SER:O	1:G:420:ASN:C	2.55	0.45
1:H:1:MET:HE1	1:H:6:LEU:HD22	1.98	0.45
1:A:318:GLU:HG3	4:A:623:HOH:O	2.17	0.45
1:B:122:ASP:OD2	1:B:129:ASN:HB2	2.16	0.45
1:C:254:ARG:NH2	1:C:317:PRO:HB3	2.32	0.45
1:F:288:LEU:HG	1:F:300:VAL:HG12	1.97	0.45
1:A:20:PRO:HA	1:D:130:TRP:HZ2	1.81	0.45
1:C:26:ILE:CG2	1:C:345:LEU:HD11	2.47	0.45
1:C:183:TYR:CE1	1:C:187:LYS:HG3	2.52	0.45
1:E:219:GLU:HB2	1:E:221:ARG:HE	1.81	0.45
1:F:120:PHE:O	1:F:124:MET:HG2	2.17	0.45
1:F:398:THR:HG22	4:F:648:HOH:O	2.15	0.45
1:C:306:VAL:HG23	1:C:308:MET:HE2	1.98	0.45
1:D:219:GLU:O	1:G:395:ARG:NH2	2.46	0.45
1:A:306:VAL:CG2	1:A:308:MET:HE1	2.47	0.45
1:E:78:LEU:C	1:E:78:LEU:HD22	2.38	0.45
1:E:130:TRP:CD1	1:E:132:PRO:HD3	2.52	0.45
1:F:188:ILE:HA	1:F:258:ILE:CD1	2.47	0.45
1:G:43:VAL:O	1:G:46:ARG:HD3	2.16	0.45
1:G:446:LYS:HG3	1:G:447:SER:N	2.31	0.45
1:A:418:LEU:HD12	1:E:386:ASP:HB3	1.99	0.45
1:B:199:PHE:CZ	1:B:237:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:VAL:CG1	1:G:308:MET:HE2	2.46	0.45
1:G:394:GLY:O	1:G:396:ALA:N	2.49	0.45
1:B:366:VAL:HG13	1:B:428:PHE:CE1	2.51	0.45
1:C:306:VAL:HB	1:C:308:MET:HE1	1.99	0.45
1:E:122:ASP:HB3	1:E:129:ASN:OD1	2.17	0.45
1:F:130:TRP:CD1	1:G:18:LYS:HA	2.52	0.45
1:H:185:LYS:O	1:H:190:GLU:HG3	2.17	0.45
1:B:369:ARG:HH11	1:B:369:ARG:CG	2.29	0.44
1:F:308:MET:CE	1:F:309:TYR:CD2	2.96	0.44
1:B:369:ARG:O	1:B:446:LYS:HG3	2.17	0.44
1:D:313:ILE:O	1:D:313:ILE:HG13	2.16	0.44
1:D:427:GLU:HG2	4:D:700:HOH:O	2.16	0.44
1:E:369:ARG:NE	1:E:393:LEU:CD1	2.80	0.44
1:F:218:LYS:HD2	1:F:219:GLU:N	2.32	0.44
1:G:354:LEU:HB2	1:G:357:ILE:HD12	1.98	0.44
1:A:57:ILE:HG12	1:A:237:LEU:O	2.16	0.44
1:A:61:THR:HB	1:A:235:GLY:HA2	1.98	0.44
1:F:362:ILE:CG2	1:F:413:ILE:HD11	2.41	0.44
1:B:249:LYS:HB2	1:B:249:LYS:HZ2	1.81	0.44
1:B:249:LYS:HB2	1:B:249:LYS:HZ3	1.82	0.44
1:D:306:VAL:CG1	1:D:309:TYR:HB2	2.48	0.44
1:F:188:ILE:O	1:F:191:PRO:HG2	2.18	0.44
1:F:215:ILE:HD11	1:F:308:MET:HB3	1.99	0.44
1:H:279:PHE:HZ	1:H:339:MET:CE	2.30	0.44
1:A:419:SER:C	1:A:421:GLY:H	2.21	0.44
1:C:216:LEU:HD13	1:C:222:LEU:HD23	2.00	0.44
1:D:79:SER:HB3	1:D:81:ASP:OD1	2.17	0.44
1:D:365:LYS:HD2	4:D:616:HOH:O	2.18	0.44
1:H:217:ASP:OD2	1:H:221:ARG:HD3	2.17	0.44
1:C:366:VAL:HG21	1:C:413:ILE:HD12	2.00	0.44
1:D:185:LYS:HD3	1:D:185:LYS:C	2.38	0.44
1:G:258:ILE:HG22	1:G:259:VAL:HG13	1.98	0.44
1:A:133:VAL:HG23	1:A:133:VAL:O	2.18	0.44
1:B:212:MET:HE2	1:B:225:GLN:O	2.18	0.44
1:B:382:LYS:HB3	1:B:382:LYS:HZ2	1.78	0.44
1:E:226:PRO:HG2	1:F:46:ARG:NH2	2.32	0.44
1:F:396:ALA:O	1:F:397:PHE:HB2	2.18	0.44
1:H:308:MET:HE3	1:H:309:TYR:CD2	2.53	0.44
1:C:358:TYR:O	1:C:362:ILE:HG12	2.18	0.44
1:C:399:TYR:HD1	1:C:399:TYR:H	1.64	0.44
1:C:423:LYS:HD3	1:C:425:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:PHE:CB	4:E:575:HOH:O	2.65	0.44
1:F:214:TYR:C	1:F:215:ILE:HD12	2.38	0.44
1:F:431:LYS:C	4:F:762:HOH:O	2.56	0.44
1:G:44:GLU:H	1:G:44:GLU:CD	2.21	0.44
1:A:369:ARG:NH1	1:A:371:MET:SD	2.91	0.44
1:A:378:LYS:HE3	1:E:129:ASN:HB3	2.00	0.44
1:C:161:LEU:HG	1:C:164:GLY:H	1.82	0.44
1:A:367:GLU:CG	1:A:383:VAL:HG23	2.48	0.43
1:F:249:LYS:O	1:F:253:GLU:HG2	2.17	0.43
1:G:188:ILE:O	1:G:192:LEU:HD13	2.17	0.43
1:G:218:LYS:HG3	1:G:219:GLU:CD	2.38	0.43
1:A:111:ILE:HA	1:A:150:ALA:HA	2.00	0.43
1:A:407:VAL:HB	1:A:414:LYS:HB3	2.00	0.43
1:B:187:LYS:O	1:B:258:ILE:HD12	2.17	0.43
1:B:306:VAL:CG2	1:B:308:MET:HE3	2.49	0.43
1:D:58:GLY:O	1:D:235:GLY:HA2	2.17	0.43
1:D:185:LYS:HD3	1:D:185:LYS:O	2.18	0.43
1:D:438:ILE:CD1	1:D:443:ARG:HG3	2.48	0.43
1:A:178:VAL:HB	1:A:182:GLU:CD	2.38	0.43
1:A:308:MET:HE3	1:A:309:TYR:CD2	2.53	0.43
1:D:386:ASP:N	4:D:677:HOH:O	2.47	0.43
1:G:231:ILE:HD11	4:G:620:HOH:O	2.17	0.43
1:G:380:GLU:HG2	1:G:393:LEU:HD21	1.99	0.43
1:G:418:LEU:HA	1:G:423:LYS:HA	1.99	0.43
1:H:14:MET:O	1:H:17:ARG:O	2.35	0.43
1:H:397:PHE:O	1:H:398:THR:OG1	2.30	0.43
1:C:306:VAL:CG2	1:C:308:MET:HE1	2.48	0.43
1:H:379:PHE:C	1:H:393:LEU:HD13	2.39	0.43
1:C:365:LYS:HE3	4:C:679:HOH:O	2.18	0.43
1:D:308:MET:CE	1:D:309:TYR:CD2	2.98	0.43
1:B:169:GLY:O	1:B:173:GLU:HG3	2.19	0.43
1:B:371:MET:SD	1:B:378:LYS:HG3	2.58	0.43
1:C:69:ILE:O	1:C:73:VAL:HG23	2.17	0.43
1:C:157:ARG:HD3	1:C:159:PHE:CZ	2.54	0.43
1:C:318:GLU:OE2	1:C:319:LYS:NZ	2.51	0.43
1:D:57:ILE:HG12	1:D:237:LEU:O	2.19	0.43
1:D:399:TYR:CD2	1:D:401:ILE:HD11	2.54	0.43
1:F:185:LYS:HG2	1:F:189:LEU:HD12	1.99	0.43
1:G:291:TYR:HB2	1:G:299:LEU:HB3	2.00	0.43
1:A:377:ILE:HD12	1:A:379:PHE:HE2	1.82	0.43
1:C:306:VAL:CG2	1:C:308:MET:CE	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:ILE:HG23	4:F:688:HOH:O	2.18	0.43
1:G:132:PRO:HA	4:G:597:HOH:O	2.19	0.43
1:H:368:GLY:HA3	1:H:446:LYS:HE2	2.01	0.43
1:B:58:GLY:O	1:B:235:GLY:HA2	2.19	0.43
1:B:201:LYS:O	1:B:205:GLU:HG3	2.19	0.43
1:E:73:VAL:HG22	1:E:78:LEU:HD22	2.01	0.43
1:E:333:PRO:HA	1:E:334:PRO:HD2	1.93	0.43
1:F:340:TYR:CD1	1:F:350:PRO:HB2	2.54	0.43
1:G:433:ASN:CB	4:G:477:HOH:O	2.66	0.43
1:G:446:LYS:O	4:G:796:HOH:O	2.21	0.43
1:C:27:ILE:HD11	1:C:245:ALA:HA	2.01	0.43
1:C:118:GLU:OE1	1:C:118:GLU:N	2.46	0.43
1:C:323:VAL:HG23	1:C:342:LEU:HD21	2.01	0.43
1:C:362:ILE:HA	1:C:365:LYS:HZ3	1.83	0.43
1:D:7:GLU:OE2	1:D:36:LYS:NZ	2.41	0.43
1:G:124:MET:CE	4:G:597:HOH:O	2.66	0.43
1:A:116:TYR:C	1:A:116:TYR:CD2	2.92	0.43
1:C:398:THR:HG23	1:C:398:THR:O	2.18	0.43
1:D:378:LYS:HG3	1:D:393:LEU:HD13	2.01	0.43
1:B:124:MET:HE2	1:B:124:MET:HA	2.01	0.42
1:C:107:HIS:HB3	1:C:159:PHE:O	2.19	0.42
1:C:250:MET:HE2	1:C:258:ILE:HB	2.01	0.42
1:E:411:ASP:HB3	1:E:430:ILE:O	2.19	0.42
1:F:219:GLU:OE2	1:F:221:ARG:NH2	2.52	0.42
1:G:93:ARG:NH1	1:G:98:PRO:HB3	2.34	0.42
1:B:403:LEU:HD23	1:B:417:THR:HB	2.01	0.42
1:D:221:ARG:NH1	1:G:395:ARG:NH2	2.66	0.42
1:F:18:LYS:CG	1:F:18:LYS:O	2.67	0.42
1:F:181:GLU:HG3	1:F:200:PHE:HZ	1.84	0.42
1:F:361:ARG:NH2	1:F:365:LYS:NZ	2.67	0.42
1:H:3:VAL:O	1:H:7:GLU:HG3	2.20	0.42
1:H:94:PRO:HD2	1:H:99:VAL:HG23	2.00	0.42
1:B:71:LYS:HG3	4:B:625:HOH:O	2.18	0.42
1:B:277:GLU:C	1:H:422:ARG:NH2	2.73	0.42
1:B:280:GLY:N	1:B:282:GLU:OE1	2.43	0.42
1:B:335:SER:O	1:B:339:MET:HG3	2.19	0.42
1:B:348:LYS:HB3	1:B:353:GLU:HG3	2.01	0.42
1:B:370:TYR:CE1	1:B:446:LYS:HB2	2.54	0.42
1:E:219:GLU:CB	1:E:221:ARG:HE	2.31	0.42
1:F:202:GLU:O	1:F:206:LYS:HG3	2.19	0.42
1:H:367:GLU:O	1:H:446:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:LYS:CG	1:H:432:ASP:H	2.04	0.42
1:A:72:LEU:O	1:A:77:GLY:N	2.53	0.42
1:C:365:LYS:CE	4:C:679:HOH:O	2.66	0.42
1:H:393:LEU:N	1:H:393:LEU:CD1	2.82	0.42
1:A:170:LYS:HE3	4:A:602:HOH:O	2.18	0.42
1:C:414:LYS:HG3	1:C:427:GLU:HG3	2.02	0.42
1:D:373:TYR:O	1:D:376:THR:HG23	2.19	0.42
1:D:394:GLY:O	1:D:395:ARG:HB3	2.19	0.42
1:F:97:GLU:HA	1:F:98:PRO:HD3	1.76	0.42
1:F:396:ALA:O	1:F:397:PHE:CB	2.68	0.42
1:G:24:ILE:O	1:G:35:ALA:HA	2.19	0.42
1:A:367:GLU:HG2	1:A:383:VAL:HG23	2.02	0.42
1:A:411:ASP:OD1	1:A:411:ASP:N	2.53	0.42
1:A:430:ILE:HD12	1:A:430:ILE:N	2.34	0.42
1:C:306:VAL:HG23	1:C:308:MET:HE1	2.00	0.42
1:E:192:LEU:HD11	1:E:258:ILE:HD11	2.02	0.42
1:B:1:MET:CE	1:B:3:VAL:HG12	2.50	0.42
1:C:327:GLU:OE1	1:C:332:TYR:O	2.38	0.42
1:D:250:MET:SD	1:D:258:ILE:HD12	2.60	0.42
1:D:340:TYR:O	1:D:344:LEU:HG	2.20	0.42
1:D:397:PHE:HB3	4:D:636:HOH:O	2.20	0.42
1:E:13:LYS:HA	1:E:13:LYS:HD3	1.84	0.42
1:E:181:GLU:H	1:E:181:GLU:CD	2.23	0.42
1:F:84:VAL:HG21	1:F:92:LEU:HD13	2.00	0.42
1:H:73:VAL:HG22	1:H:78:LEU:HD13	2.01	0.42
1:A:391:ARG:HG2	1:A:392:ALA:N	2.34	0.42
1:B:53:THR:CG2	1:B:211:ALA:HB2	2.50	0.42
1:D:2:ASP:OD2	1:D:5:LYS:HB2	2.20	0.42
1:D:401:ILE:HD12	1:D:401:ILE:N	2.35	0.42
1:D:419:SER:HB2	1:D:424:MET:HB2	2.02	0.42
1:E:93:ARG:NH1	4:E:674:HOH:O	2.52	0.42
1:F:181:GLU:HG3	1:F:200:PHE:CZ	2.54	0.42
1:H:393:LEU:N	1:H:393:LEU:HD12	2.34	0.42
1:A:277:GLU:OE1	1:A:280:GLY:O	2.37	0.42
1:B:306:VAL:C	1:B:308:MET:HE1	2.40	0.42
1:C:361:ARG:NH2	1:C:410:GLU:OE2	2.52	0.42
1:C:362:ILE:HD12	1:C:410:GLU:HA	2.01	0.42
1:E:401:ILE:HD13	1:E:439:PHE:CZ	2.54	0.42
1:E:432:ASP:N	1:E:432:ASP:OD1	2.52	0.42
1:F:26:ILE:HB	1:F:34:TYR:HB3	2.02	0.42
1:A:26:ILE:CG2	1:A:345:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLY:HA3	1:A:446:LYS:CD	2.49	0.42
1:A:386:ASP:OD2	1:E:419:SER:O	2.38	0.42
1:C:13:LYS:HE3	1:C:360:GLU:OE1	2.19	0.42
1:H:183:TYR:CZ	1:H:187:LYS:HG3	2.55	0.42
1:B:8:SER:O	1:B:12:GLU:HG3	2.20	0.41
1:B:125:VAL:HG13	1:B:225:GLN:NE2	2.34	0.41
1:E:125:VAL:HG13	1:E:225:GLN:CD	2.40	0.41
1:E:408:LEU:C	1:E:408:LEU:HD23	2.41	0.41
1:E:429:TYR:O	1:E:435:VAL:HA	2.20	0.41
1:H:413:ILE:HB	1:H:428:PHE:HB2	2.01	0.41
1:A:228:PRO:HD3	1:A:308:MET:SD	2.61	0.41
1:A:355:PRO:HA	1:A:358:TYR:CZ	2.55	0.41
1:D:359:ARG:HG2	1:D:359:ARG:NH1	2.34	0.41
1:G:84:VAL:HG22	1:G:92:LEU:HD12	2.02	0.41
4:G:534:HOH:O	1:H:18:LYS:HE3	2.19	0.41
1:H:392:ALA:O	1:H:398:THR:OG1	2.39	0.41
1:D:385:GLY:N	4:D:677:HOH:O	2.53	0.41
1:F:34:TYR:CZ	1:F:36:LYS:HG3	2.55	0.41
1:H:403:LEU:CD2	1:H:417:THR:HB	2.47	0.41
1:A:29:ASP:OD1	1:A:30:GLY:N	2.38	0.41
1:A:279:PHE:HB3	1:A:293:ASN:O	2.20	0.41
1:C:369:ARG:HG3	1:C:369:ARG:HH11	1.85	0.41
1:C:369:ARG:HG3	1:C:369:ARG:NH1	2.36	0.41
1:C:392:ALA:HB3	1:C:398:THR:HA	2.01	0.41
4:A:468:HOH:O	1:F:219:GLU:HG2	2.20	0.41
1:A:190:GLU:N	1:A:191:PRO:HD2	2.36	0.41
1:A:418:LEU:HD13	1:A:419:SER:N	2.36	0.41
1:A:419:SER:C	1:A:421:GLY:N	2.74	0.41
1:B:167:LEU:O	1:B:171:ILE:HG13	2.20	0.41
1:B:183:TYR:CZ	1:B:187:LYS:HG3	2.55	0.41
1:B:306:VAL:CG2	1:B:308:MET:CE	2.95	0.41
1:C:121:ILE:O	1:C:125:VAL:HG22	2.20	0.41
1:D:385:GLY:O	1:D:386:ASP:CB	2.68	0.41
1:G:252:ILE:HG22	1:G:320:LYS:HD2	2.02	0.41
1:A:306:VAL:HG23	1:A:308:MET:HE1	2.02	0.41
1:A:308:MET:HE2	1:A:308:MET:N	2.32	0.41
1:A:378:LYS:CB	1:A:393:LEU:HD22	2.51	0.41
1:B:277:GLU:HA	1:B:282:GLU:HG2	2.03	0.41
1:B:362:ILE:HG22	1:B:413:ILE:HD11	2.03	0.41
1:C:208:LYS:HD3	4:C:643:HOH:O	2.20	0.41
1:E:91:LYS:HE2	4:E:774:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ALA:HA	1:E:129:ASN:OD1	2.21	0.41
1:E:365:LYS:HE2	4:E:582:HOH:O	2.20	0.41
1:F:1:MET:HE2	1:F:3:VAL:HG12	2.02	0.41
1:A:28:LYS:O	1:A:29:ASP:CG	2.59	0.41
1:C:127:GLY:HA2	1:G:396:ALA:HB2	2.01	0.41
1:C:218:LYS:HA	4:C:653:HOH:O	2.20	0.41
1:E:391:ARG:HD2	1:E:398:THR:OG1	2.20	0.41
1:G:295:LEU:N	1:G:295:LEU:CD1	2.83	0.41
1:A:3:VAL:HG23	1:A:4:GLY:N	2.36	0.41
1:A:315:TYR:HA	1:A:322:GLY:HA2	2.02	0.41
1:A:369:ARG:O	1:A:446:LYS:HA	2.20	0.41
1:B:93:ARG:HA	1:B:97:GLU:O	2.20	0.41
1:B:242:LEU:O	1:B:245:ALA:HB3	2.21	0.41
1:C:189:LEU:HD23	1:C:194:MET:HE3	2.02	0.41
1:D:13:LYS:HD3	1:D:13:LYS:HA	1.91	0.41
1:E:291:TYR:HB2	1:E:299:LEU:HB3	2.02	0.41
1:E:431:LYS:O	1:E:432:ASP:HB2	2.21	0.41
1:F:102:HIS:CE1	3:F:451:DO3:H142	2.56	0.41
1:F:394:GLY:O	1:F:396:ALA:N	2.54	0.41
1:H:308:MET:CE	1:H:308:MET:N	2.81	0.41
1:B:212:MET:HE3	1:B:213:GLY:H	1.83	0.41
1:E:308:MET:HG2	1:E:309:TYR:CD2	2.56	0.41
1:F:100:THR:N	1:F:103:HIS:HD2	2.04	0.41
1:G:422:ARG:HG2	1:G:422:ARG:NH1	2.36	0.41
1:A:306:VAL:CG2	1:A:308:MET:CE	2.95	0.40
1:A:425:TYR:N	1:A:425:TYR:CD1	2.89	0.40
1:G:116:TYR:CG	1:G:117:ALA:N	2.88	0.40
1:A:332:TYR:HA	1:A:333:PRO:HD3	1.95	0.40
1:D:241:VAL:HG22	4:D:561:HOH:O	2.20	0.40
1:D:406:GLU:HG2	1:D:407:VAL:HG23	2.03	0.40
1:H:24:ILE:O	1:H:35:ALA:HA	2.21	0.40
1:A:135:THR:HG23	1:A:138:GLU:H	1.86	0.40
1:B:3:VAL:O	1:B:4:GLY:C	2.59	0.40
1:B:52:GLU:HG3	1:B:242:LEU:HD12	2.03	0.40
1:C:231:ILE:HG13	1:C:234:ASP:OD1	2.21	0.40
1:D:217:ASP:OD1	1:D:217:ASP:C	2.60	0.40
1:E:97:GLU:HA	1:E:98:PRO:HD2	1.93	0.40
1:E:306:VAL:HG11	1:E:309:TYR:HD2	1.86	0.40
1:G:84:VAL:HG13	1:G:99:VAL:O	2.20	0.40
4:G:534:HOH:O	1:H:18:LYS:CE	2.70	0.40
1:A:371:MET:HE1	1:A:378:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ILE:HB	1:B:34:TYR:HB3	2.02	0.40
1:B:170:LYS:HD2	1:B:170:LYS:HA	1.86	0.40
1:B:308:MET:HG2	1:B:309:TYR:CD2	2.56	0.40
1:B:382:LYS:NZ	1:B:382:LYS:CB	2.69	0.40
1:D:28:LYS:HD3	1:D:29:ASP:OD1	2.22	0.40
1:D:391:ARG:HH11	1:D:398:THR:HG23	1.87	0.40
1:F:133:VAL:O	1:F:133:VAL:HG23	2.22	0.40
1:H:319:LYS:O	1:H:321:ILE:HG23	2.22	0.40
1:H:401:ILE:HG23	1:H:417:THR:OG1	2.21	0.40
1:A:18:LYS:HA	1:D:130:TRP:CD1	2.57	0.40
1:A:306:VAL:C	1:A:308:MET:HE2	2.42	0.40
1:A:419:SER:O	1:A:419:SER:OG	2.38	0.40
1:C:199:PHE:CZ	1:C:237:LEU:HD13	2.57	0.40
1:D:277:GLU:HG2	1:D:280:GLY:HA2	2.04	0.40
1:E:434:LYS:CA	4:E:748:HOH:O	2.65	0.40
1:G:124:MET:CE	1:G:130:TRP:CZ3	3.05	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	445/447 (100%)	409 (92%)	32 (7%)	4 (1%)	17	16
1	B	445/447 (100%)	415 (93%)	26 (6%)	4 (1%)	17	16
1	C	444/447 (99%)	410 (92%)	33 (7%)	1 (0%)	47	55
1	D	444/447 (99%)	413 (93%)	27 (6%)	4 (1%)	17	16
1	E	444/447 (99%)	419 (94%)	23 (5%)	2 (0%)	29	31
1	F	445/447 (100%)	417 (94%)	23 (5%)	5 (1%)	14	12
1	G	445/447 (100%)	407 (92%)	33 (7%)	5 (1%)	14	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	445/447 (100%)	415 (93%)	26 (6%)	4 (1%)	17	16
All	All	3557/3576 (100%)	3305 (93%)	223 (6%)	29 (1%)	19	19

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	TRP
1	A	420	ASN
1	D	398	THR
1	E	398	THR
1	F	393	LEU
1	G	396	ALA
1	G	418	LEU
1	H	432	ASP
1	A	235	GLY
1	F	397	PHE
1	F	398	THR
1	B	235	GLY
1	C	235	GLY
1	D	385	GLY
1	E	235	GLY
1	F	235	GLY
1	G	235	GLY
1	G	395	ARG
1	G	420	ASN
1	A	329	SER
1	B	218	LYS
1	B	398	THR
1	B	432	ASP
1	D	235	GLY
1	F	395	ARG
1	H	235	GLY
1	D	329	SER
1	H	421	GLY
1	H	20	PRO

5.3.2 Protein sidechains (i)

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	378/381 (99%)	369 (98%)	9 (2%)	49	62
1	B	378/381 (99%)	371 (98%)	7 (2%)	57	71
1	C	375/381 (98%)	364 (97%)	11 (3%)	42	54
1	D	378/381 (99%)	366 (97%)	12 (3%)	39	50
1	E	377/381 (99%)	368 (98%)	9 (2%)	49	62
1	F	378/381 (99%)	362 (96%)	16 (4%)	30	38
1	G	380/381 (100%)	367 (97%)	13 (3%)	37	47
1	H	379/381 (100%)	369 (97%)	10 (3%)	46	58
All	All	3023/3048 (99%)	2936 (97%)	87 (3%)	42	54

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	TYR
1	A	192	LEU
1	A	255	ASP
1	A	288	LEU
1	A	306	VAL
1	A	308	MET
1	A	378	LYS
1	A	418	LEU
1	A	446	LYS
1	B	116	TYR
1	B	129	ASN
1	B	306	VAL
1	B	308	MET
1	B	386	ASP
1	B	434	LYS
1	B	436	ASP
1	C	16	GLU
1	C	116	TYR
1	C	186	LYS
1	C	192	LEU
1	C	208	LYS
1	C	218	LYS
1	C	288	LEU
1	C	298	LYS

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Mol	Chain	Res	Type
1	C	306	VAL
1	C	308	MET
1	C	386	ASP
1	D	116	TYR
1	D	192	LEU
1	D	208	LYS
1	D	288	LEU
1	D	308	MET
1	D	366	VAL
1	D	386	ASP
1	D	417	THR
1	D	418	LEU
1	D	420	ASN
1	D	427	GLU
1	D	436	ASP
1	E	78	LEU
1	E	105	LEU
1	E	116	TYR
1	E	128	ASP
1	E	219	GLU
1	E	276	TRP
1	E	288	LEU
1	E	360	GLU
1	E	432	ASP
1	F	17	ARG
1	F	78	LEU
1	F	116	TYR
1	F	128	ASP
1	F	185	LYS
1	F	192	LEU
1	F	218	LYS
1	F	288	LEU
1	F	308	MET
1	F	353	GLU
1	F	369	ARG
1	F	397	PHE
1	F	398	THR
1	F	399	TYR
1	F	418	LEU
1	F	432	ASP
1	G	52	GLU
1	G	105	LEU

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Mol	Chain	Res	Type
1	G	116	TYR
1	G	157	ARG
1	G	288	LEU
1	G	291	TYR
1	G	308	MET
1	G	378	LYS
1	G	398	THR
1	G	399	TYR
1	G	422	ARG
1	G	436	ASP
1	G	446	LYS
1	H	78	LEU
1	H	116	TYR
1	H	129	ASN
1	H	182	GLU
1	H	219	GLU
1	H	261	LYS
1	H	308	MET
1	H	386	ASP
1	H	432	ASP
1	H	436	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	420	ASN
1	B	103	HIS
1	C	103	HIS
1	C	129	ASN
1	D	103	HIS
1	D	433	ASN
1	E	103	HIS
1	E	293	ASN
1	F	103	HIS
1	F	129	ASN
1	G	103	HIS
1	H	103	HIS
1	H	293	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 17 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DO3	H	449	-	28,28,28	1.33	5 (17%)	36,36,36	1.28	4 (11%)
3	DO3	E	450	-	28,28,28	1.47	6 (21%)	36,36,36	1.44	7 (19%)
3	DO3	G	451	-	28,28,28	1.42	6 (21%)	36,36,36	1.40	5 (13%)
3	DO3	F	451	-	28,28,28	1.33	4 (14%)	36,36,36	1.29	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DO3	H	449	-	-	16/36/36/36	0/1/1/1
3	DO3	E	450	-	-	6/36/36/36	0/1/1/1
3	DO3	G	451	-	-	5/36/36/36	0/1/1/1
3	DO3	F	451	-	-	15/36/36/36	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	450	DO3	C2-N2	3.65	1.55	1.47
3	G	451	DO3	C2-N2	3.51	1.55	1.47
3	F	451	DO3	C2-N2	3.30	1.54	1.47
3	H	449	DO3	C2-N2	3.27	1.54	1.47
3	E	450	DO3	C4-N3	-3.04	1.40	1.47
3	G	451	DO3	C4-N3	-2.99	1.40	1.47
3	F	451	DO3	C4-N3	-2.77	1.41	1.47
3	H	449	DO3	C4-N3	-2.71	1.41	1.47
3	E	450	DO3	C16-N4	2.53	1.52	1.47
3	G	451	DO3	C16-N4	2.46	1.52	1.47
3	H	449	DO3	C17-C15	-2.21	1.42	1.51
3	F	451	DO3	C16-N4	2.20	1.51	1.47
3	E	450	DO3	C17-C15	-2.18	1.42	1.51
3	G	451	DO3	C12-N2	2.17	1.51	1.47
3	E	450	DO3	O7-C15	-2.13	1.34	1.43
3	F	451	DO3	C17-C15	-2.13	1.42	1.51
3	H	449	DO3	C16-N4	2.11	1.51	1.47
3	E	450	DO3	C12-N2	2.09	1.51	1.47
3	G	451	DO3	C17-C15	-2.08	1.42	1.51
3	H	449	DO3	O7-C15	-2.05	1.34	1.43
3	G	451	DO3	O7-C15	-2.05	1.34	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	449	DO3	C6-C5-N3	3.10	120.34	112.98
3	G	451	DO3	C6-C5-N3	2.81	119.65	112.98
3	E	450	DO3	C6-N4-C16	-2.81	105.34	111.89
3	F	451	DO3	C6-C5-N3	2.74	119.48	112.98
3	E	450	DO3	C8-N1-C1	-2.73	104.95	111.44
3	H	449	DO3	C7-N4-C6	-2.69	105.04	111.44
3	H	449	DO3	C8-N1-C1	-2.60	105.24	111.44
3	G	451	DO3	C8-N1-C1	-2.60	105.25	111.44
3	F	451	DO3	C8-N1-C1	-2.57	105.33	111.44
3	F	451	DO3	C7-N4-C6	-2.50	105.49	111.44
3	G	451	DO3	C6-N4-C16	-2.47	106.14	111.89
3	F	451	DO3	C6-N4-C16	-2.41	106.28	111.89
3	E	450	DO3	C3-N2-C2	-2.35	105.83	111.44
3	E	450	DO3	C7-N4-C6	-2.31	105.94	111.44
3	H	449	DO3	C6-N4-C16	-2.30	106.53	111.89
3	G	451	DO3	C7-N4-C6	-2.27	106.02	111.44
3	E	450	DO3	C6-C5-N3	2.21	118.22	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	450	DO3	C5-N3-C4	-2.19	106.21	111.44
3	E	450	DO3	C4-C3-N2	2.16	118.10	112.98
3	G	451	DO3	C5-N3-C4	-2.14	106.34	111.44

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	451	DO3	O3-C11-C12-N2
3	F	451	DO3	O5-C13-C14-N3
3	H	449	DO3	O5-C13-C14-N3
3	H	449	DO3	O6-C13-C14-N3
3	F	451	DO3	O4-C11-C12-N2
3	F	451	DO3	O6-C13-C14-N3
3	H	449	DO3	N1-C10-C9-O2
3	H	449	DO3	O3-C11-C12-N2
3	H	449	DO3	O4-C11-C12-N2
3	F	451	DO3	N3-C5-C6-N4
3	H	449	DO3	N3-C5-C6-N4
3	H	449	DO3	N1-C10-C9-O1
3	E	450	DO3	N2-C3-C4-N3
3	E	450	DO3	N3-C5-C6-N4
3	H	449	DO3	C6-C5-N3-C14
3	F	451	DO3	C6-C5-N3-C14
3	E	450	DO3	C6-C5-N3-C4
3	G	451	DO3	C6-C5-N3-C4
3	H	449	DO3	C5-C6-N4-C16
3	F	451	DO3	C5-C6-N4-C16
3	H	449	DO3	C13-C14-N3-C4
3	E	450	DO3	C6-C5-N3-C14
3	H	449	DO3	C7-C8-N1-C10
3	H	449	DO3	C13-C14-N3-C5
3	E	450	DO3	C3-C4-N3-C14
3	F	451	DO3	C9-C10-N1-C8
3	G	451	DO3	N2-C3-C4-N3
3	F	451	DO3	C9-C10-N1-C1
3	G	451	DO3	N3-C5-C6-N4
3	F	451	DO3	C1-C2-N2-C3
3	H	449	DO3	C6-C5-N3-C4
3	H	449	DO3	C15-C16-N4-C6
3	F	451	DO3	N1-C10-C9-O2
3	H	449	DO3	C5-C6-N4-C7

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Mol	Chain	Res	Type	Atoms
3	F	451	DO3	C6-C5-N3-C4
3	E	450	DO3	C15-C16-N4-C6
3	F	451	DO3	C15-C16-N4-C6
3	G	451	DO3	C15-C16-N4-C6
3	F	451	DO3	C5-C6-N4-C7
3	G	451	DO3	C6-C5-N3-C14
3	H	449	DO3	N4-C7-C8-N1
3	F	451	DO3	N1-C10-C9-O1

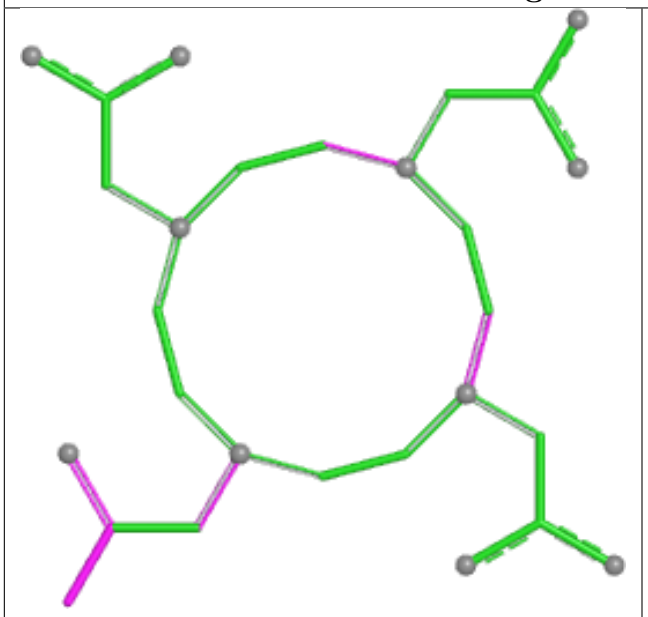
There are no ring outliers.

1 monomer is involved in 1 short contact:

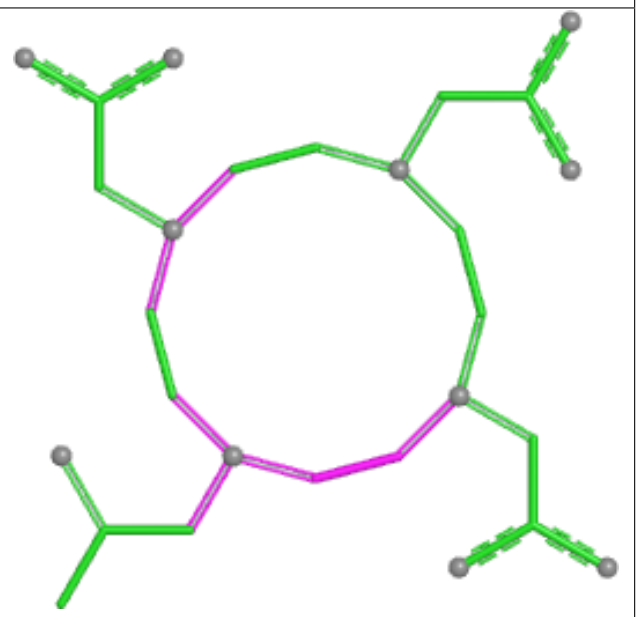
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	451	DO3	1	0

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 then 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.

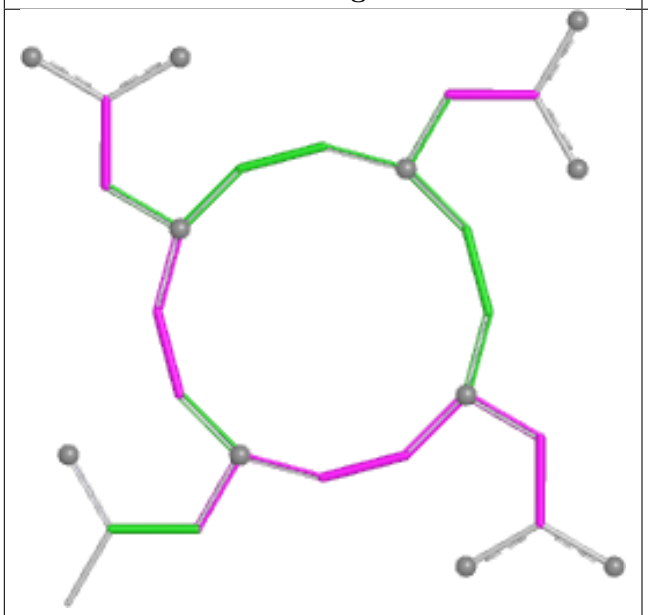
Ligand DO3 H 449



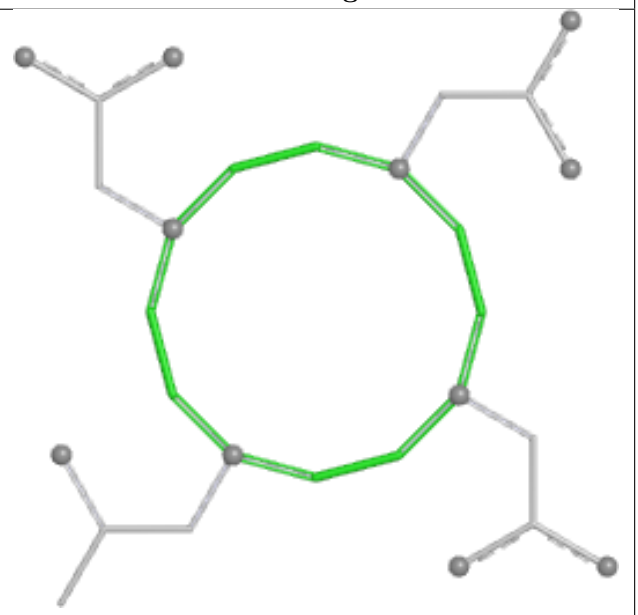
Bond lengths



Bond angles

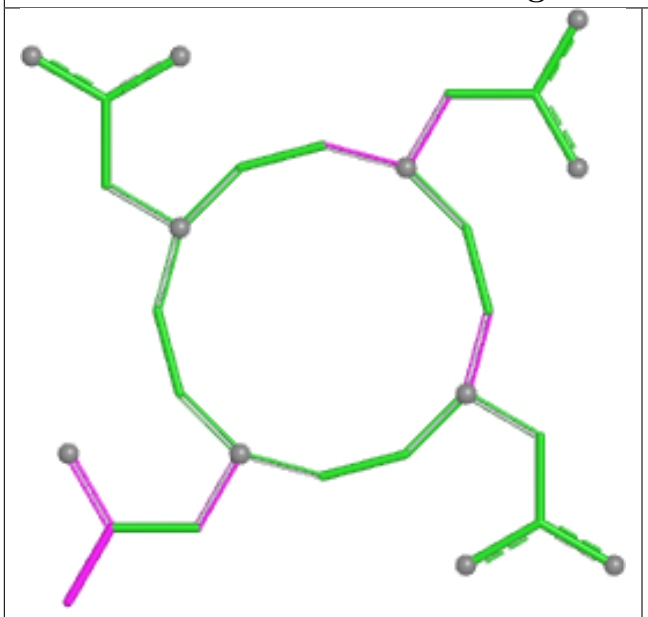


Torsions

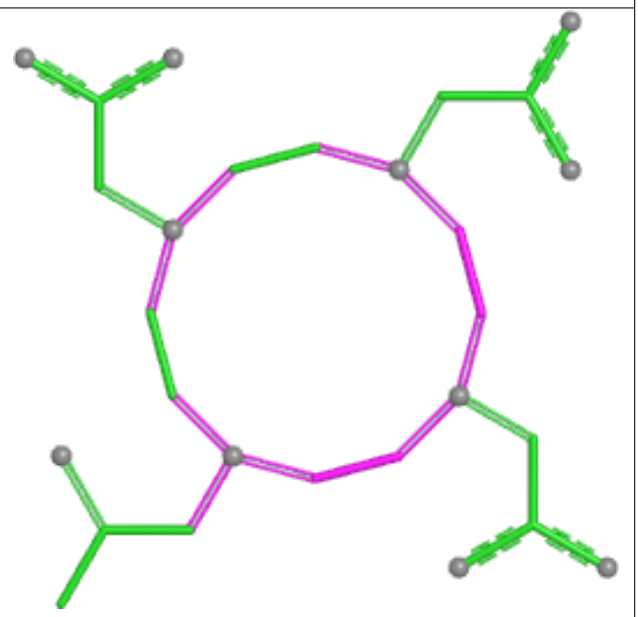


Rings

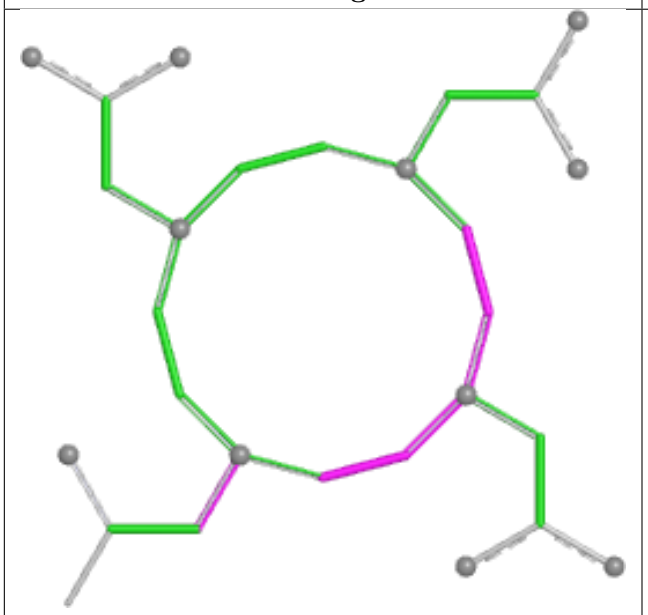
Ligand DO3 E 450



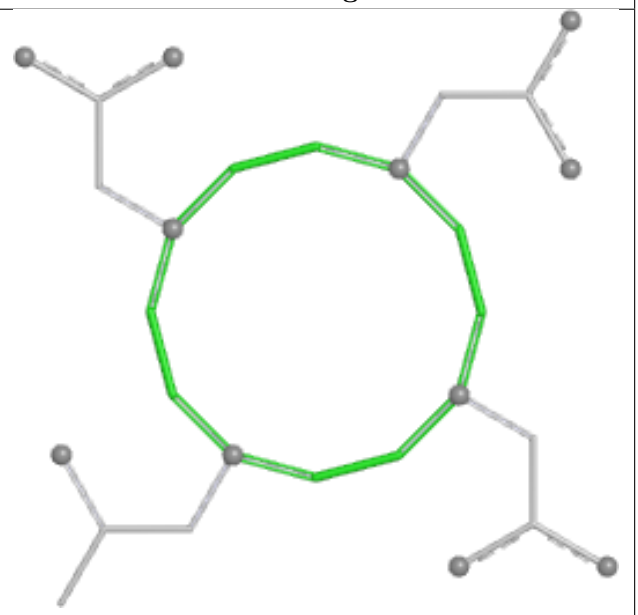
Bond lengths



Bond angles

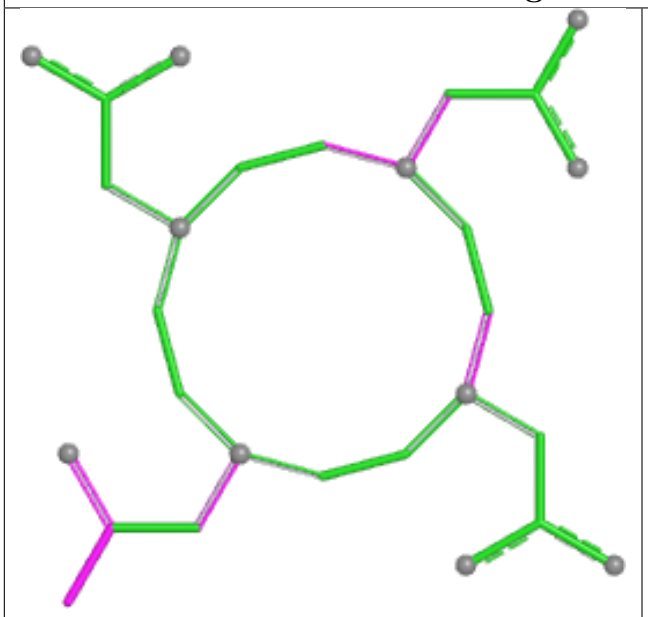


Torsions

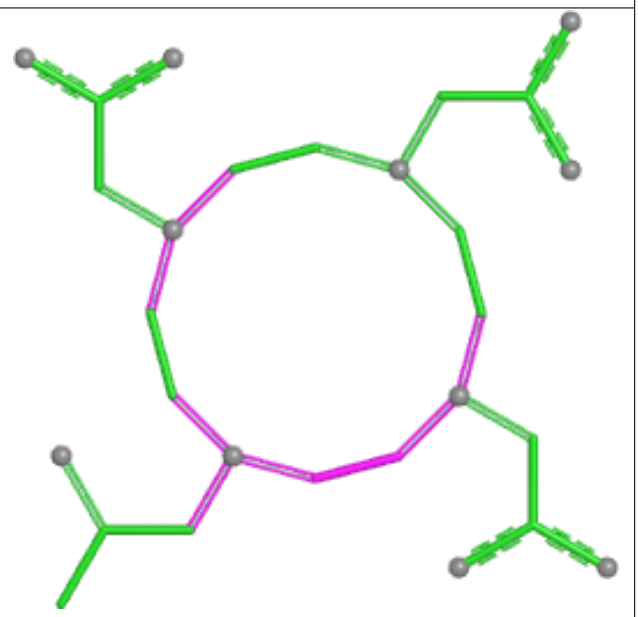


Rings

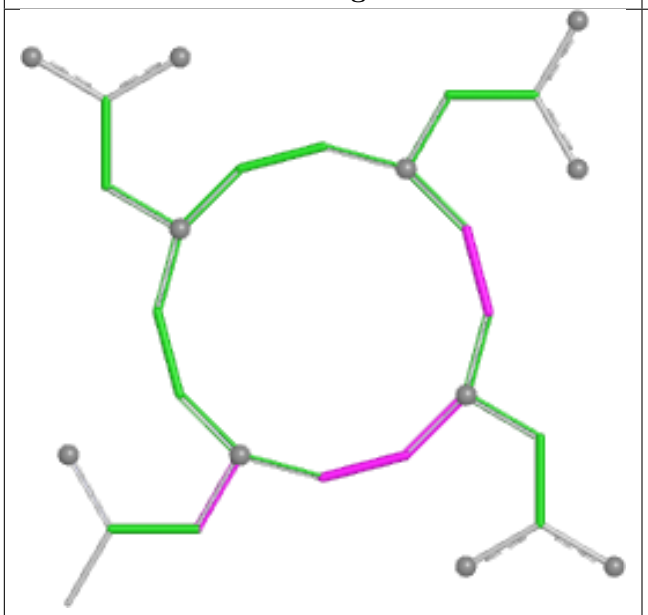
Ligand DO3 G 451



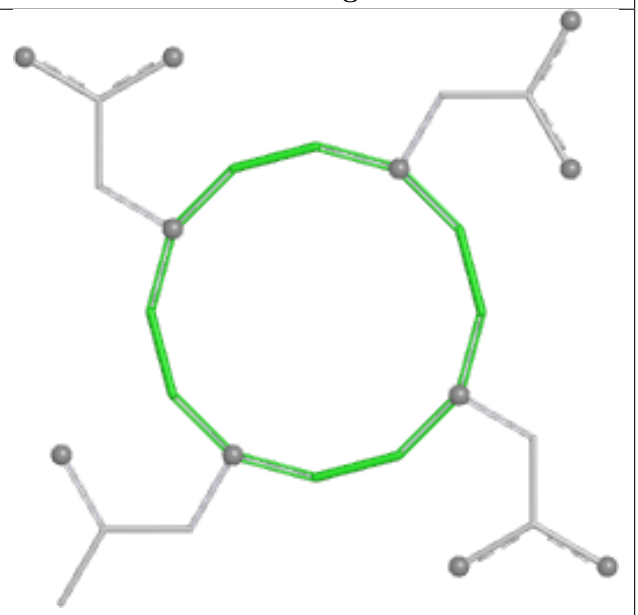
Bond lengths



Bond angles

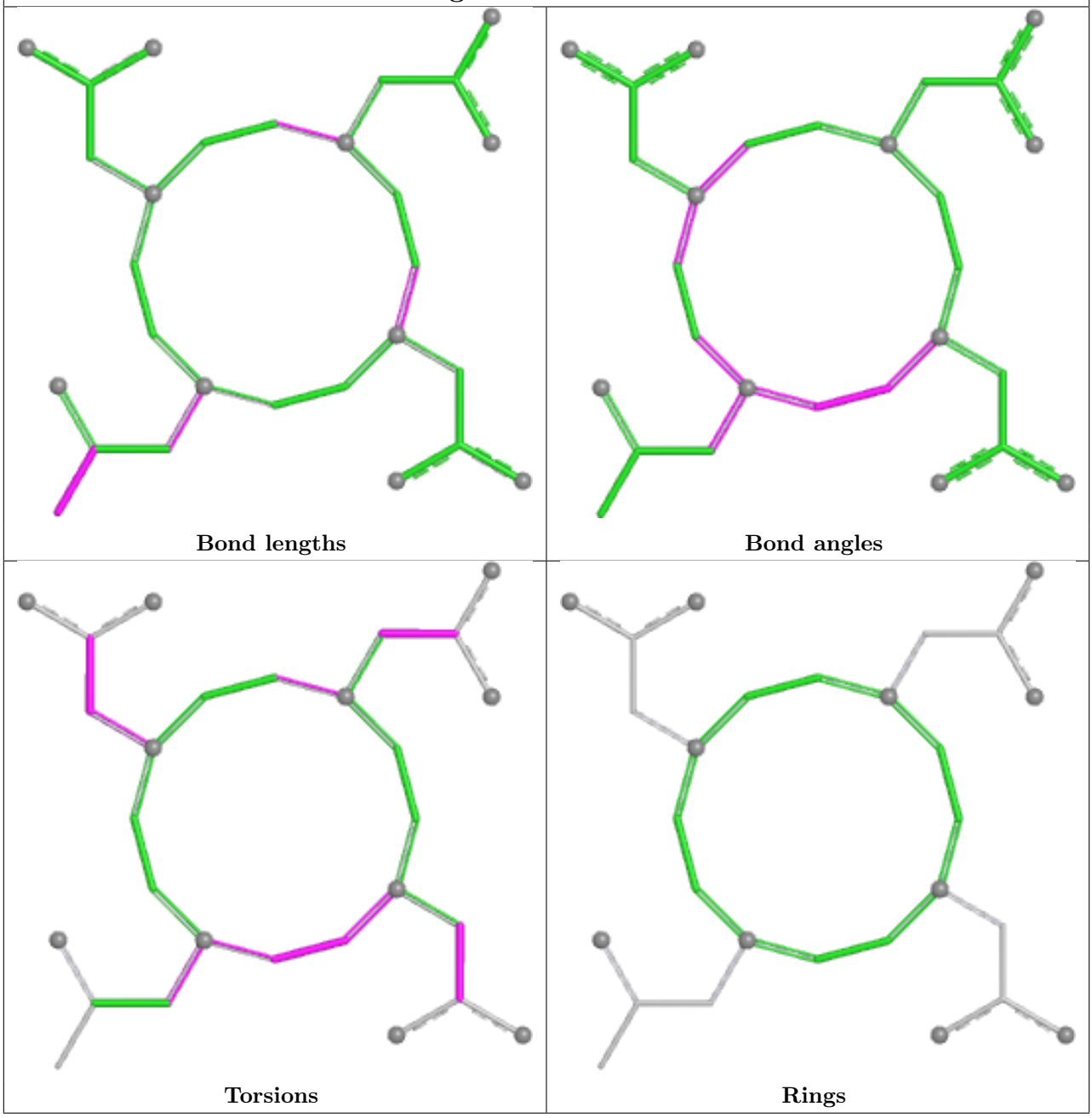


Torsions



Rings

Ligand DO3 F 451



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	447/447 (100%)	-0.30	7 (1%)	72	70	17, 24, 35, 40	0
1	B	447/447 (100%)	-0.34	8 (1%)	68	66	15, 23, 33, 40	0
1	C	446/447 (99%)	-0.30	7 (1%)	72	70	16, 25, 35, 39	0
1	D	446/447 (99%)	-0.35	5 (1%)	80	79	16, 25, 34, 41	0
1	E	446/447 (99%)	-0.38	10 (2%)	62	59	13, 21, 33, 39	0
1	F	447/447 (100%)	-0.38	11 (2%)	57	55	12, 21, 33, 40	0
1	G	447/447 (100%)	-0.29	10 (2%)	62	59	11, 22, 34, 40	0
1	H	447/447 (100%)	-0.40	12 (2%)	54	52	12, 21, 33, 40	0
All	All	3573/3576 (99%)	-0.34	70 (1%)	65	63	11, 23, 34, 41	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	398	THR	5.8
1	F	396	ALA	5.5
1	B	398	THR	5.4
1	H	398	THR	5.1
1	G	396	ALA	5.1
1	F	397	PHE	5.0
1	H	396	ALA	4.7
1	G	395	ARG	4.5
1	F	395	ARG	4.4
1	B	395	ARG	4.4
1	G	398	THR	4.4
1	B	396	ALA	4.4
1	E	398	THR	4.3
1	B	397	PHE	4.3
1	D	395	ARG	4.1
1	D	396	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	432	ASP	3.9
1	D	398	THR	3.9
1	F	394	GLY	3.9
1	E	395	ARG	3.8
1	A	397	PHE	3.8
1	F	393	LEU	3.7
1	H	397	PHE	3.7
1	F	432	ASP	3.7
1	H	432	ASP	3.7
1	H	394	GLY	3.7
1	C	396	ALA	3.7
1	G	397	PHE	3.6
1	E	276	TRP	3.6
1	A	398	THR	3.6
1	H	395	ARG	3.5
1	A	395	ARG	3.5
1	A	276	TRP	3.3
1	C	276	TRP	3.3
1	B	432	ASP	3.2
1	G	218	LYS	3.1
1	D	397	PHE	3.1
1	E	396	ALA	3.1
1	H	399	TYR	3.0
1	C	398	THR	3.0
1	H	276	TRP	3.0
1	G	432	ASP	2.9
1	A	432	ASP	2.9
1	E	397	PHE	2.9
1	H	393	LEU	2.8
1	G	394	GLY	2.8
1	B	276	TRP	2.7
1	A	30	GLY	2.7
1	B	394	GLY	2.6
1	C	395	ARG	2.6
1	E	431	LYS	2.6
1	H	431	LYS	2.6
1	C	432	ASP	2.5
1	F	421	GLY	2.4
1	G	276	TRP	2.4
1	A	218	LYS	2.3
1	C	399	TYR	2.3
1	E	421	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	208	LYS	2.3
1	D	276	TRP	2.2
1	E	399	TYR	2.2
1	H	447	SER	2.2
1	F	431	LYS	2.1
1	G	399	TYR	2.1
1	F	218	LYS	2.1
1	C	433	ASN	2.1
1	G	219	GLU	2.0
1	E	422	ARG	2.0
1	F	276	TRP	2.0
1	H	433	ASN	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 monosaccharides 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(Å^2)	Q<0.9
3	DO3	F	451	28/28	0.71	0.37	18,25,28,29	28
3	DO3	H	449	28/28	0.76	0.35	18,22,26,27	28
3	DO3	G	451	28/28	0.92	0.16	21,24,29,31	28
3	DO3	E	450	28/28	0.93	0.18	21,23,25,27	28
2	LU	A	449	1/1	0.96	0.07	30,30,30,30	1
2	LU	C	449	1/1	0.97	0.06	34,34,34,34	1
2	LU	D	448	1/1	0.97	0.15	33,33,33,33	1
2	LU	A	448	1/1	0.98	0.07	33,33,33,33	1
2	LU	D	449	1/1	0.98	0.04	32,32,32,32	1
2	LU	G	449	1/1	0.98	0.04	36,36,36,36	1
2	LU	G	450	1/1	0.98	0.07	26,26,26,26	1

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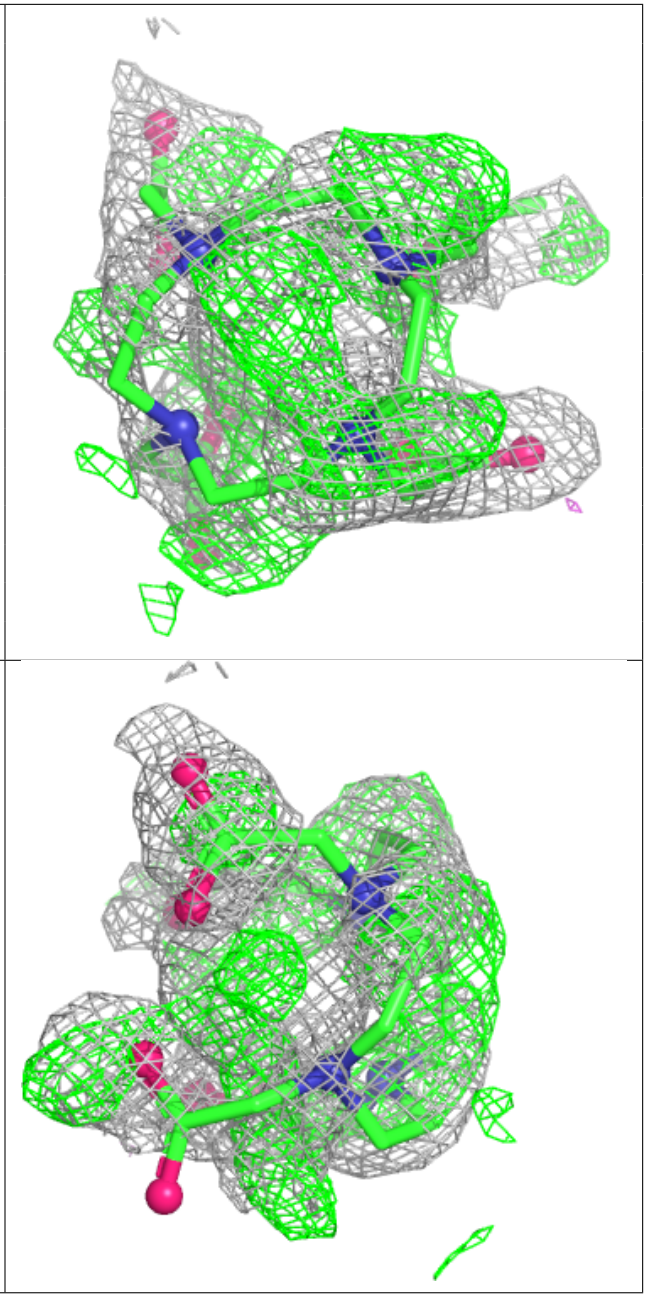
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LU	F	450	1/1	0.99	0.06	26,26,26,26	1
2	LU	B	448	1/1	0.99	0.06	27,27,27,27	1
2	LU	B	449	1/1	0.99	0.10	33,33,33,33	1
2	LU	H	448	1/1	0.99	0.09	32,32,32,32	1
2	LU	C	448	1/1	0.99	0.05	30,30,30,30	1
2	LU	E	448	1/1	0.99	0.04	25,25,25,25	1
2	LU	E	449	1/1	0.99	0.06	31,31,31,31	1
2	LU	F	448	1/1	0.99	0.05	24,24,24,24	1
2	LU	G	448	1/1	1.00	0.03	23,23,23,23	1
2	LU	F	449	1/1	1.00	0.01	24,24,24,24	1

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.

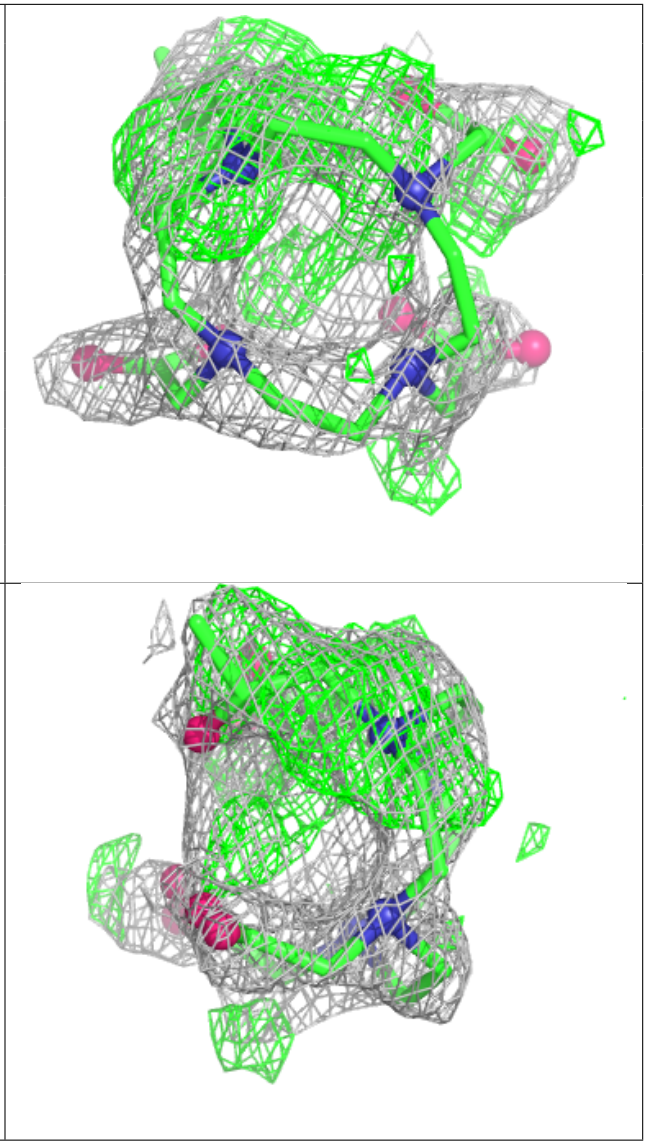
Electron density around DO3 F 451:

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



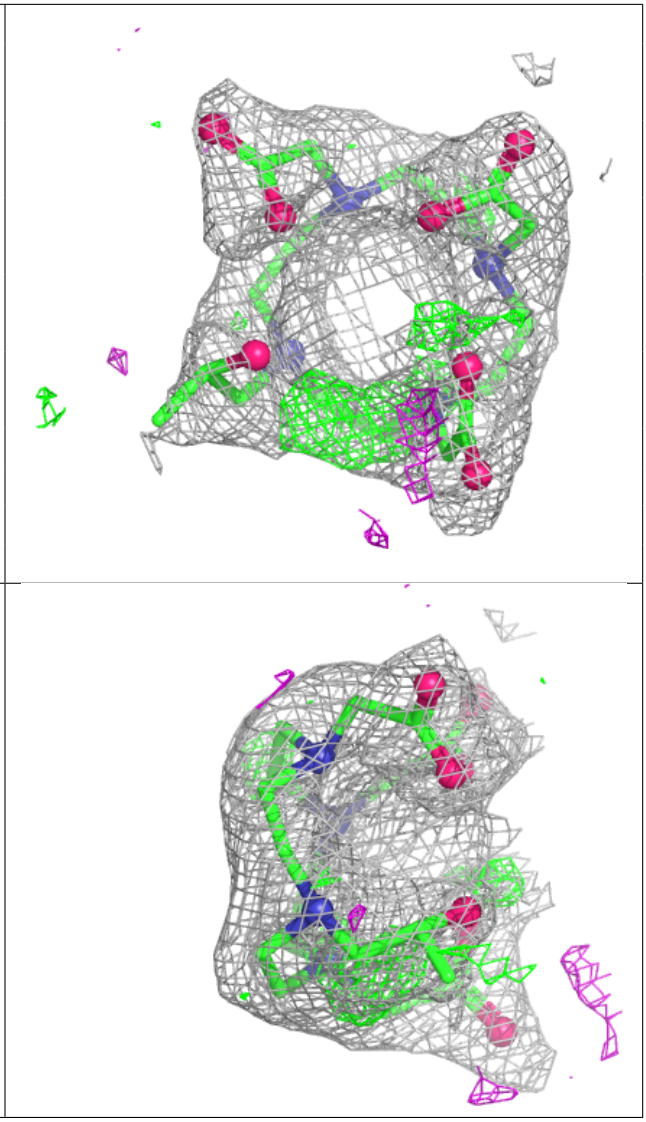
Electron density around DO3 H 449:

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



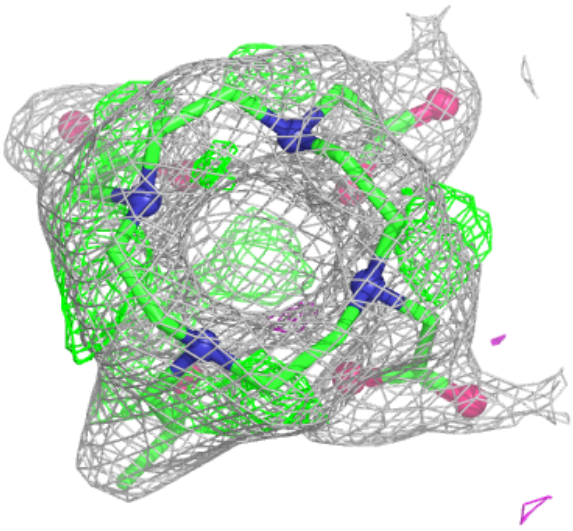
Electron density around DO3 G 451:

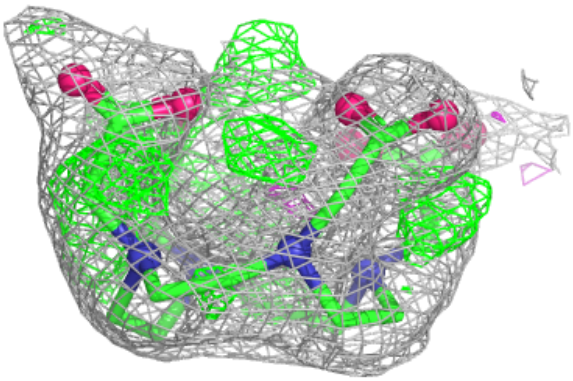
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

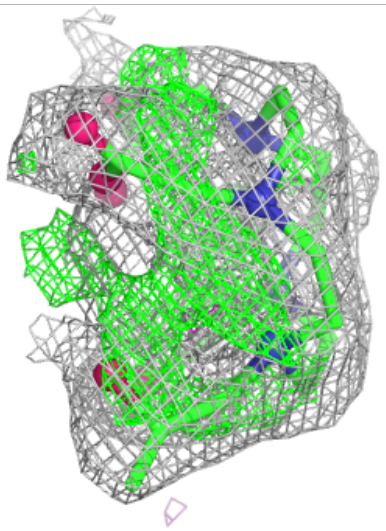


Electron density around DO3 E 450:

$2mF_o$-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.